

Supplementary Information

Li₂B₂₄: The simplest combination for a three-ring boron tube

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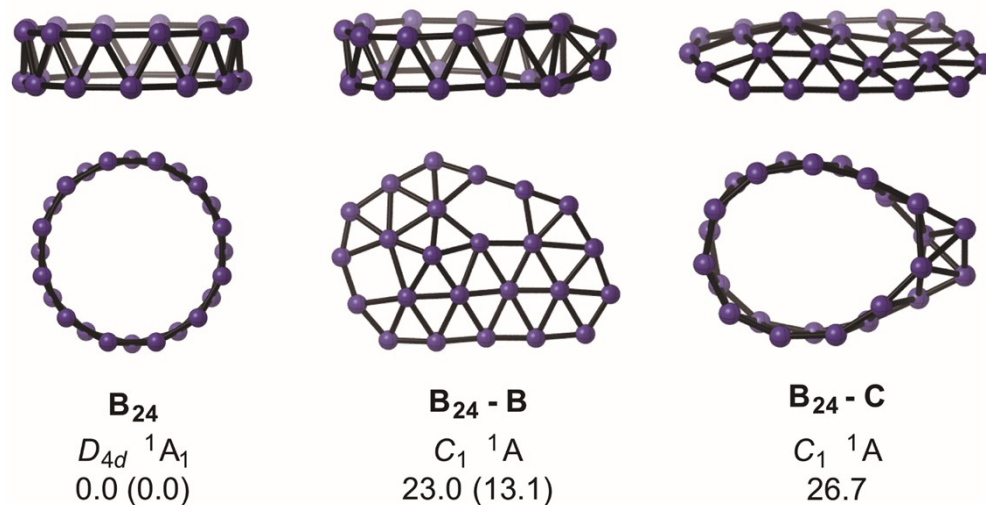


Figure S1. PBE0/6-311+G(d) structures for the lowest-lying energy isomers of B_{24} cluster. Values in parenthesis are computed at the CCSD(T)/6-311+G(d)//PBE0/6-311+G(d) level. All the relative energies are shown in kcal/mol.

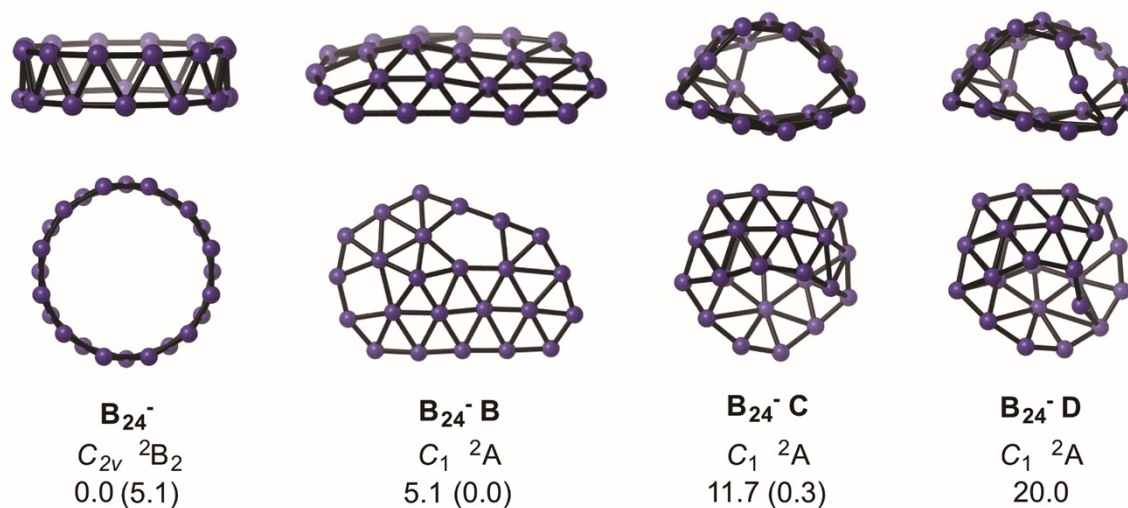


Figure S2. PBE0/6-311+G(d) structures for the lowest-lying energy isomers of B_{24}^- cluster. Values in parenthesis are computed at the CCSD(T)/6-311+G(d)//PBE0/6-311+G(d) level. All the relative energies are shown in kcal/mol.

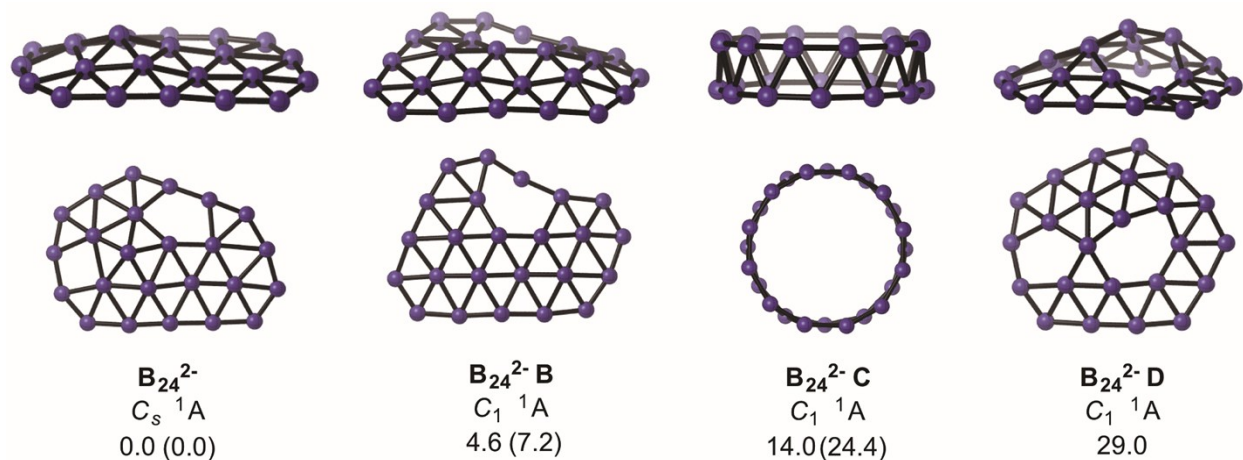


Figure S3. PBE0/6-311+G(d) structures for the lowest-lying energy isomers of the B_{24}^{2-} cluster. Values in parenthesis are computed at the CCSD(T)/6-311+G(d)//PBE0/6-311+G(d) level. All the relative energies are shown in kcal/mol.

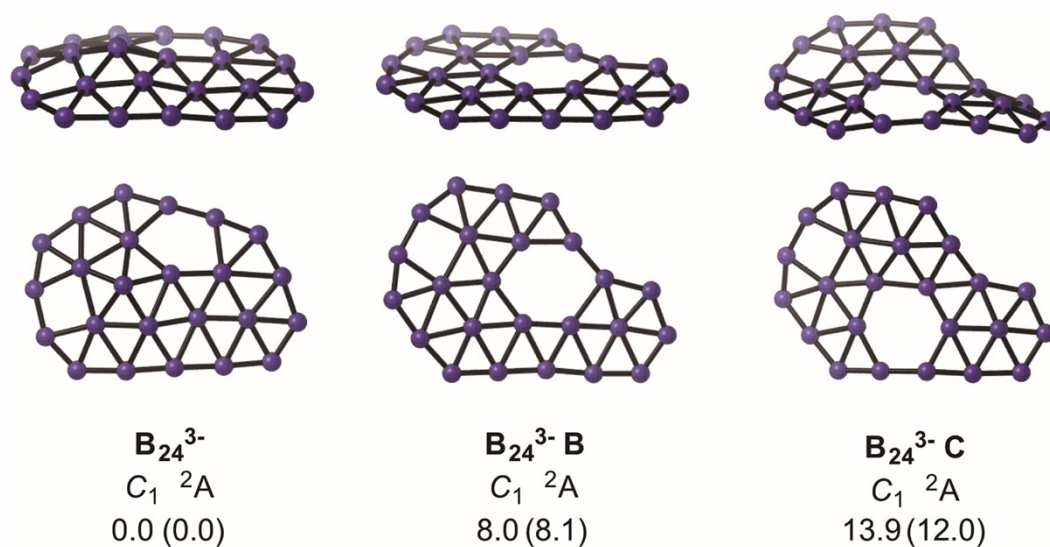


Figure S4. PBE0/6-311+G(d) structures for the lowest-lying energy isomers of the B_{24}^{3-} cluster. Values in parenthesis are computed at the CCSD(T)/6-311+G(d)//PBE0/6-311+G(d) level. All the relative energies are shown in kcal/mol.

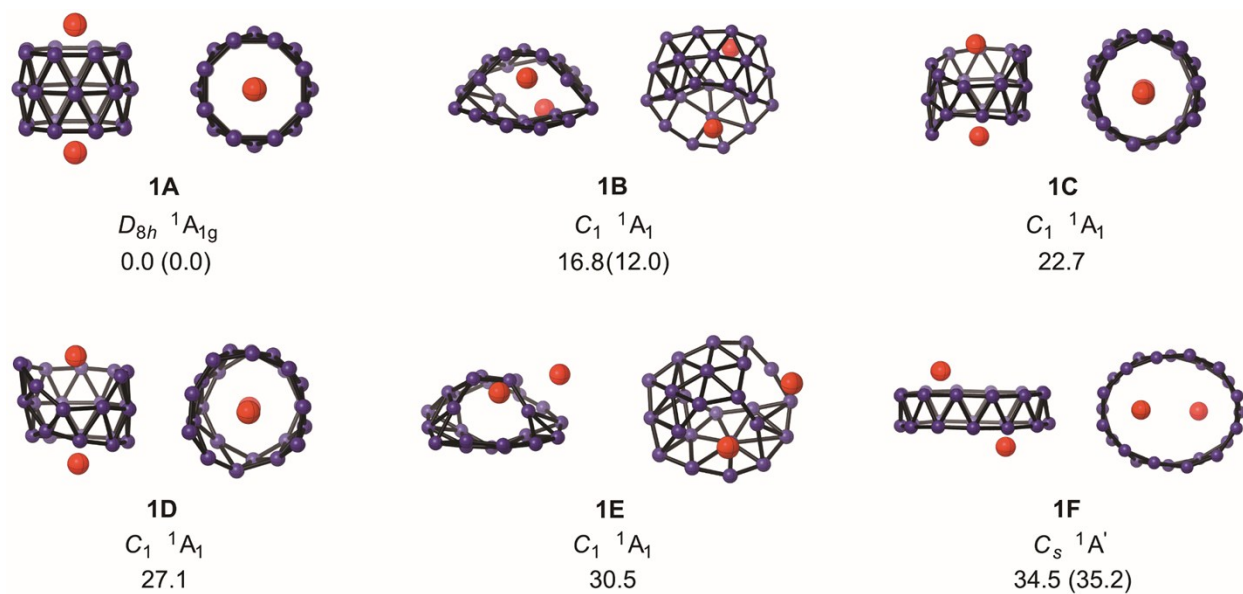


Figure S5. PBE0/6-311+G(d) structures for the lowest-lying energy isomers of the Li_2B_{24} cluster. Values in parenthesis are computed at the CCSD(T)/6-311+G(d)//PBE0/6-311+G(d) level. All the relative energies are shown in kcal/mol.

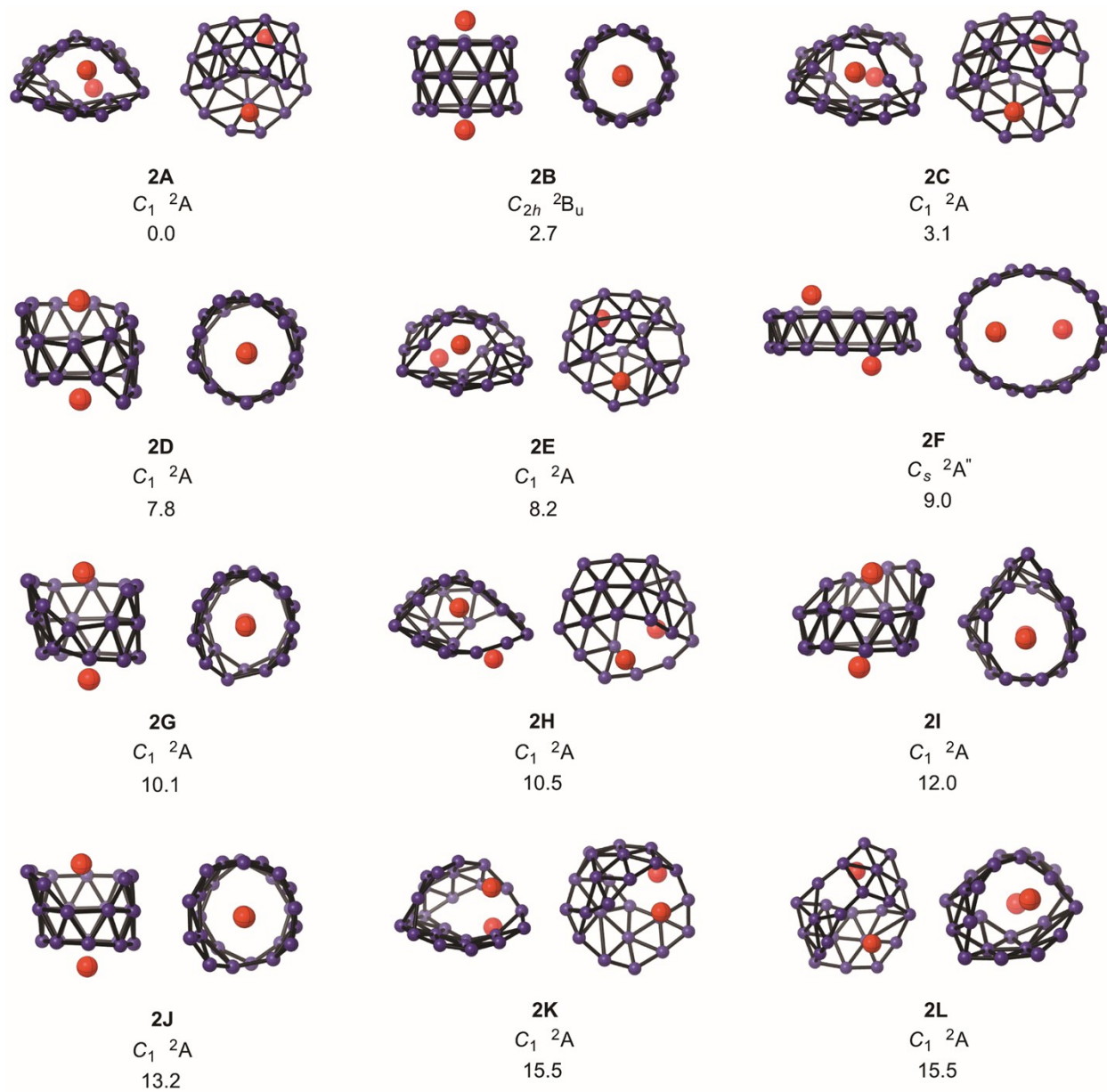


Figure S6. PBE0/6-311+G(d) structures for the lowest-lying energy isomers of the $\text{Li}_2\text{B}_{24}^-$ cluster. All the relative energies are shown in kcal/mol.

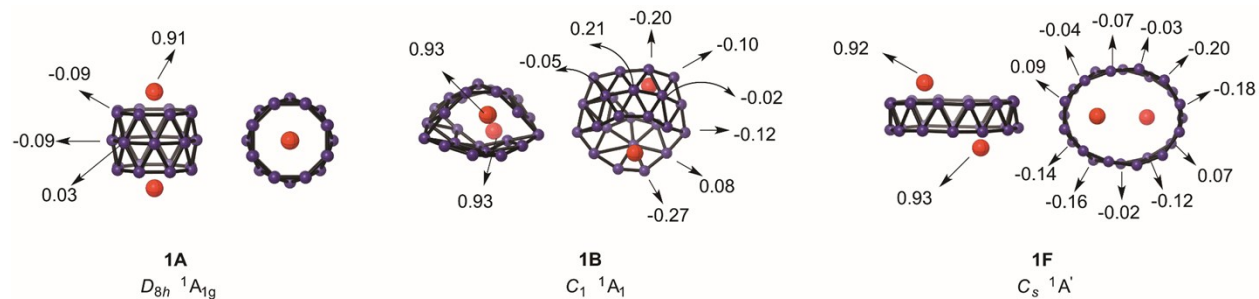


Figure S7. NPA charges of the **1A**, **1B** and **1F** isomers computed at the PBE0/6-311+G(d) level.

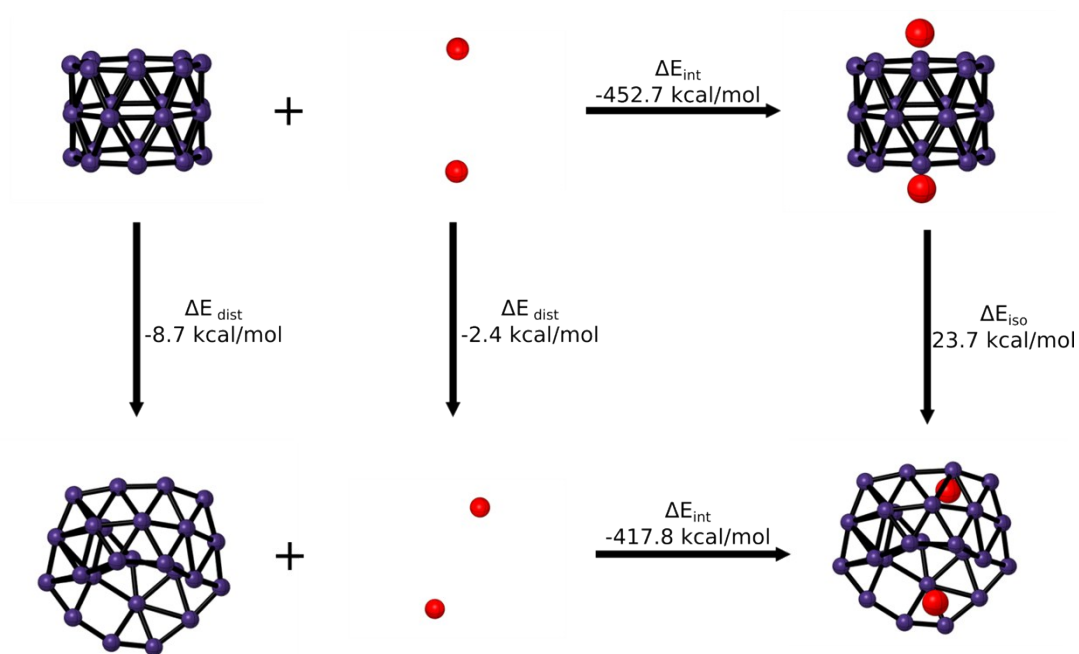


Figure S8. Energetic reaction cycle involving the isomerization of Li_2B_{24} between the **1B** and **1A** isomers.

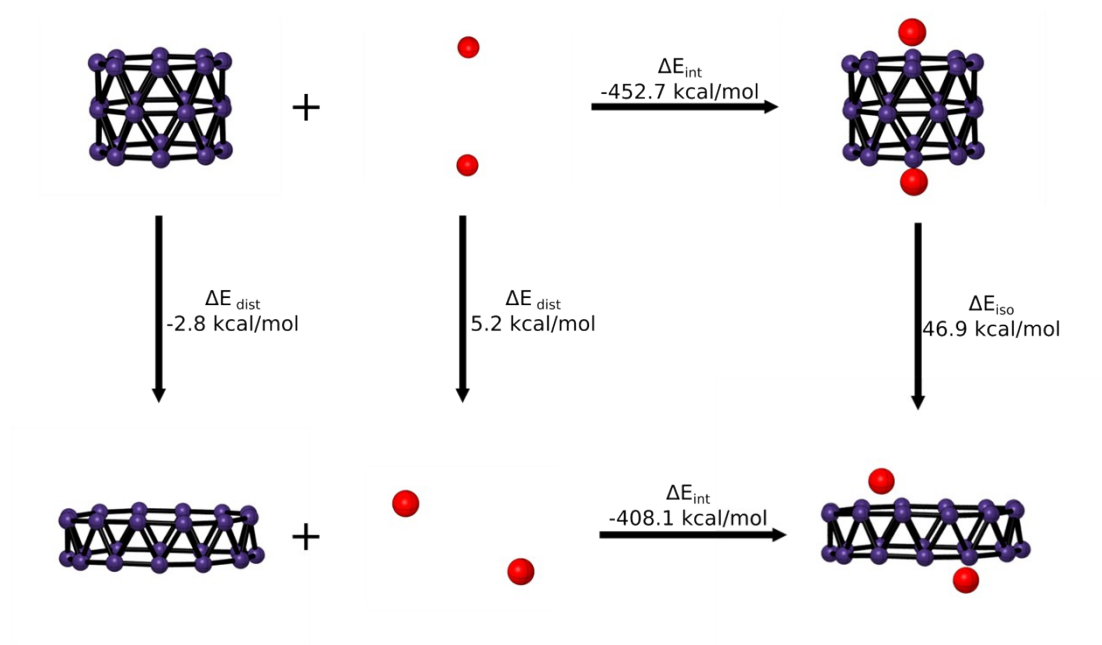


Figure S9. Energetic reaction cycle involving the isomerization of Li_2B_{24} between the **1F** and **1A** isomers.

Cartesian coordinates of the optimized geometries at the PBE0/6-311+G(d) level.

1A

Charge 0 Multiplicity = 1

$E_{\text{PBE0}} = -610.6355381$

$E_{\text{ZPE}} = 0.109477$

B	0.803351000	1.939462000	1.492628000
B	-0.803351000	1.939462000	1.492628000
B	-1.939462000	0.803351000	1.492628000
B	-1.939462000	-0.803351000	1.492628000
B	-0.803351000	-1.939462000	1.492628000
B	0.803351000	-1.939462000	1.492628000
B	1.939462000	-0.803351000	1.492628000
B	1.939462000	0.803351000	1.492628000
B	0.803351000	1.939462000	-1.492628000
B	1.939462000	0.803351000	-1.492628000
B	1.939462000	-0.803351000	-1.492628000
B	0.803351000	-1.939462000	-1.492628000
B	-0.803351000	-1.939462000	-1.492628000
B	-1.939462000	-0.803351000	-1.492628000
B	-1.939462000	0.803351000	-1.492628000
B	-0.803351000	1.939462000	-1.492628000
B	0.000000000	2.225635000	0.000000000
B	-1.573762000	1.573762000	0.000000000
B	-2.225635000	0.000000000	0.000000000
B	-1.573762000	-1.573762000	0.000000000
B	0.000000000	-2.225635000	0.000000000
B	1.573762000	-1.573762000	0.000000000
B	2.225635000	0.000000000	0.000000000
B	1.573762000	1.573762000	0.000000000
Li	0.000000000	0.000000000	2.554593000
Li	0.000000000	0.000000000	-2.554593000

1B

Charge 0 Multiplicity = 1

$E_{\text{PBE0}} = -610.6051359$

$E_{\text{ZPE}} = 0.105964$

B	-1.416563000	0.646403000	-0.978362000
B	0.781259000	-0.300636000	1.809625000
B	-0.190782000	-1.527946000	1.235215000

B	-0.859474000	-0.094860000	1.792492000
B	-1.902529000	0.665298000	0.882305000
B	-1.737290000	-1.114380000	0.837712000
Li	0.051253000	1.913319000	1.867468000
B	-1.161553000	-2.546057000	0.090416000
B	-2.869483000	-0.368738000	-0.447995000
B	-1.782018000	2.280281000	-0.259379000
B	-2.533185000	-1.929500000	-0.361817000
B	-0.430588000	3.133529000	-0.047169000
B	-2.943161000	1.230117000	-0.350476000
B	0.042360000	0.193449000	-1.514884000
B	0.993673000	-1.058089000	-1.083021000
B	1.503259000	0.612127000	-0.971036000
B	0.018153000	1.695321000	-0.801891000
B	1.453254000	-1.428571000	0.815850000
B	1.996896000	0.239640000	0.908421000
B	0.461810000	-2.580773000	-0.215192000
Li	-1.153195000	-1.538683000	-2.006058000
B	2.710879000	-0.940565000	-0.452354000
B	2.333188000	1.859938000	0.037490000
B	1.047518000	2.856485000	0.024528000
B	1.998391000	-2.360936000	-0.531907000
B	3.147153000	0.613685000	-0.335417000

1C

Charge 0 Multiplicity = 1

$E_{\text{PBE0}} = -610.5973448$

$E_{\text{ZPE}} = 0.107566$

B	-0.828291000	-2.081578000	-0.257812000
B	-1.993012000	-0.956591000	-0.601849000
Li	0.695090000	0.248402000	-2.124107000
B	-2.277419000	0.715558000	-0.454640000
B	-0.915248000	-1.406973000	-1.827201000
B	-1.622362000	0.074638000	-1.866479000
B	-1.242547000	1.584859000	-1.527270000
B	-1.440127000	2.100526000	0.252061000
B	-0.159225000	2.459286000	-0.786907000
B	0.462812000	-2.110924000	-1.459546000
B	1.901497000	-1.638453000	-0.977095000
B	2.693717000	-0.208504000	-0.967685000
B	2.557521000	1.319122000	-1.088130000
B	0.828293000	-2.081578000	0.257811000
B	1.993014000	-0.956592000	0.601849000

Li	-0.695091000	0.248398000	2.124105000
B	2.277417000	0.715559000	0.454640000
B	0.915249000	-1.406974000	1.827200000
B	1.622361000	0.074637000	1.866480000
B	1.242546000	1.584859000	1.527271000
B	1.440125000	2.100527000	-0.252060000
B	0.159223000	2.459285000	0.786910000
B	-0.462811000	-2.110926000	1.459543000
B	-1.901496000	-1.638455000	0.977093000
B	-2.693716000	-0.208507000	0.967685000
B	-2.557521000	1.319119000	1.088132000

1D

Charge 0 Multiplicity = 1

$E_{\text{PBE0}} = -610.5897714$

$E_{\text{ZPE}} = 0.106970$

B	2.283138000	0.423273000	-0.425775000
B	-1.769816000	1.617927000	-1.084648000
B	1.102812000	1.345400000	-1.329630000
B	-2.085698000	1.111191000	0.522560000
B	-0.842671000	2.298177000	0.373570000
B	-1.637481000	0.310193000	1.996436000
B	2.933322000	0.844182000	1.084190000
B	0.773052000	2.613898000	-0.159141000
B	2.087879000	1.959842000	0.425586000
B	-1.281223000	1.796079000	1.815892000
B	-0.311153000	2.265872000	-1.255092000
B	2.614609000	-0.665625000	0.965372000
Li	0.692460000	0.301936000	2.029843000
B	-2.126461000	-0.618402000	0.521026000
B	0.484347000	-2.266388000	-0.250835000
B	1.734209000	-1.188179000	-0.529310000
B	-1.154374000	-1.928608000	0.252065000
B	-1.263021000	-1.284582000	1.803010000
B	1.607975000	-1.940017000	0.990401000
B	-0.773965000	-2.193993000	-1.429457000
B	-2.526172000	0.242961000	-0.890970000
B	1.489535000	-0.132502000	-1.812738000
B	0.633625000	-1.515392000	-1.769024000
B	-2.042232000	-1.295327000	-1.062583000
B	0.100760000	-2.041254000	1.486094000
Li	-0.744122000	0.100189000	-2.424843000

1E

Charge 0 Multiplicity = 1

$E_{\text{PBE0}} = -610.5821803$

$E_{\text{ZPE}} = 0.104748$

B	0.786397000	0.240666000	1.526165000
B	0.343328000	-1.478441000	-0.845854000
B	1.469946000	-0.922225000	0.561960000
B	-1.323256000	-0.901966000	-1.004835000
B	-0.861449000	0.147253000	1.783240000
B	-1.860386000	-0.795811000	0.914921000
B	-1.496363000	-2.355882000	0.099133000
Li	0.031222000	-1.832037000	2.099538000
B	0.045454000	-2.912787000	0.093428000
B	2.690963000	-1.575804000	-0.492686000
B	1.529374000	-2.627675000	-0.122028000
B	-2.766348000	-1.577928000	-0.332438000
B	-0.068654000	-0.077798000	-1.638150000
B	1.487071000	-0.147397000	-1.098952000
B	-1.341847000	0.813003000	-1.180171000
B	-0.307576000	1.541741000	1.111653000
B	1.288855000	1.672815000	0.714225000
B	-1.881827000	0.928138000	0.757555000
B	-1.362695000	2.372436000	-0.307298000
B	0.174337000	2.811299000	0.098810000
B	2.503301000	1.392991000	-0.619832000
B	-2.895884000	0.040681000	-0.446947000
B	1.607374000	2.672243000	-0.585496000
B	3.101236000	-0.094893000	-0.615902000
B	-2.738467000	1.642903000	-0.545374000
Li	3.097305000	0.486096000	1.525249000

1F

Charge 0 Multiplicity = 1

$E_{\text{PBE0}} = 0.106003$

$E_{\text{ZPE}} = -610.5770168$

B	-0.732556000	-1.558971000	2.356520000
B	-0.648646000	-2.924673000	1.496385000

B	-0.605587000	-3.529259000	0.000000000
B	-0.648646000	-2.924673000	-1.496385000
B	-0.732556000	-1.558971000	-2.356520000
B	-0.745946000	0.006009000	-2.732811000
B	-0.724771000	1.611064000	-2.564707000
B	-0.815107000	2.854562000	-1.531416000
B	-0.848565000	3.376617000	0.000000000
B	-0.815107000	2.854562000	1.531416000
B	-0.724771000	1.611064000	2.564707000
B	-0.745946000	0.006009000	2.732811000
B	0.760873000	-2.303655000	2.157303000
B	0.836242000	-3.242594000	0.793537000
B	0.836242000	-3.242594000	-0.793537000
B	0.760873000	-2.303655000	-2.157303000
B	0.729349000	-0.835429000	-2.756872000
B	0.749736000	0.803536000	-2.581085000
B	0.700966000	2.274725000	-2.008540000
B	0.609567000	3.382843000	-0.795277000
B	0.609567000	3.382843000	0.795277000
B	0.700966000	2.274725000	2.008540000
B	0.749736000	0.803536000	2.581085000
B	0.729349000	-0.835429000	2.756872000
Li	-1.748675000	-1.535813000	0.000000000
Li	1.773245000	1.565492000	0.000000000

2A

Charge -1 Multiplicity = 2

$E_{\text{PBE0}} = -610.6868979$

$E_{\text{ZPE}} = 0.104315$

B	0.068110000	0.203771000	-1.553902000
B	-1.329026000	0.806732000	-1.004834000
B	1.546317000	0.431178000	-0.863027000
B	0.217625000	1.690435000	-0.805795000
B	0.885102000	-1.151768000	-1.213843000
B	-0.864971000	-0.033113000	1.774034000
B	1.268017000	-1.511327000	0.739700000
B	0.740861000	-0.359044000	1.788010000
B	-0.350297000	-1.580381000	1.304978000
B	-1.814481000	0.846928000	0.857479000
B	-1.854288000	-0.942026000	0.832574000
B	2.047185000	0.062044000	0.995918000
Li	0.249382000	1.825007000	1.781149000

B	0.197068000	-2.599157000	-0.224692000
Li	-1.318907000	-1.355147000	-1.917904000
B	-1.405489000	-2.440446000	0.102550000
B	-2.878808000	-0.107635000	-0.436278000
B	2.589200000	-1.168430000	-0.464324000
B	-1.554797000	2.424287000	-0.203506000
B	2.516746000	1.641691000	0.040229000
B	1.332627000	2.762839000	0.023301000
B	-0.123330000	3.155128000	-0.025260000
B	1.738583000	-2.517004000	-0.594467000
B	-2.741963000	-1.705808000	-0.312960000
B	-2.808402000	1.496860000	-0.396176000
B	3.220125000	0.312328000	-0.277653000

2B

Charge -1 Multiplicity = 2

$E_{\text{PBE0}} = -610.6846183$

$E_{\text{ZPE}} = 0.106392$

B	-0.860472000	-2.041704000	-0.016131000
B	0.861062000	-2.041499000	0.016294000
B	-2.090115000	-0.852768000	-0.090468000
B	2.090401000	-0.852189000	0.090511000
B	-0.079820000	2.092627000	1.489854000
B	-0.079217000	-2.092378000	1.490039000
B	2.024945000	0.000358000	1.583565000
B	-2.361018000	-0.000245000	1.390149000
B	-1.517994000	-1.399428000	1.436761000
B	1.428292000	-1.492569000	1.540299000
B	-1.518312000	1.399083000	1.436663000
Li	-0.087574000	0.000098000	2.483929000
B	1.427811000	1.493076000	1.540188000
B	0.860461000	2.041676000	0.016118000
B	-2.090397000	0.852191000	-0.090510000
B	-0.861071000	2.041528000	-0.016311000
B	2.090123000	0.852770000	0.090471000
B	1.518016000	1.399424000	-1.436767000
B	-1.427834000	-1.493078000	-1.540193000
B	-1.428315000	1.492570000	-1.540308000
B	1.518334000	-1.399082000	-1.436671000
B	0.079820000	-2.092584000	-1.489867000
B	-2.024974000	-0.000358000	-1.583573000
B	2.361076000	0.000246000	-1.390162000

Li	0.087541000	-0.000101000	-2.483764000
B	0.079218000	2.092335000	-1.490050000

2C

Charge -1 Multiplicity = 2

$E_{\text{PBE0}} = 0.104439$

$E_{\text{ZPE}} = -610.6820683$

B	0.043218000	0.162936000	-1.622858000
B	-1.369758000	0.752325000	-1.064008000
B	1.511496000	0.535805000	-1.015006000
B	1.002914000	-1.084704000	-1.210055000
B	-0.786356000	0.017897000	1.604925000
B	-1.692522000	-1.254202000	0.945577000
B	-1.353114000	1.245178000	0.693268000
B	0.129833000	1.618637000	-0.797103000
B	-0.086480000	-1.484728000	1.283341000
B	1.526133000	-1.260659000	0.700165000
B	0.859242000	-0.241294000	1.793969000
B	2.083626000	0.384158000	0.970648000
Li	0.400293000	1.874212000	1.996382000
B	0.666648000	-2.560489000	-0.263396000
Li	-1.247997000	-1.518006000	-1.775633000
B	-0.906870000	-2.640506000	0.252087000
B	2.756396000	-0.697257000	-0.501104000
B	-2.362082000	2.197993000	-0.326671000
B	1.896254000	1.956333000	0.000917000
B	-0.923927000	2.871499000	-0.052653000
B	2.192610000	-2.214342000	-0.565543000
B	3.057314000	0.904665000	-0.330267000
B	-2.999088000	-0.853023000	-0.217803000
B	-2.434315000	-2.283976000	-0.109924000
B	0.624554000	2.954967000	0.097240000
B	-2.927104000	0.759065000	-0.398198000

2D

Charge -1 Multiplicity = 2

$E_{\text{PBE0}} = -610.6758272$

$E_{\text{ZPE}} = 0.105646$

B	1.436989000	2.064353000	0.288712000
B	0.818412000	-2.064487000	-0.278879000

B	2.068469000	-0.994387000	-0.606928000
B	2.314255000	0.717081000	-0.432312000
B	1.268476000	1.577085000	-1.497037000
B	2.646852000	-0.222253000	0.992301000
B	0.875187000	-1.358926000	-1.813633000
B	1.981685000	-1.705275000	0.921519000
B	1.676689000	0.076050000	-1.851752000
B	0.176263000	2.471618000	-0.780504000
B	-0.486386000	-2.067446000	-1.441023000
B	2.604784000	1.325272000	1.099865000
Li	-0.647964000	0.303838000	-2.004051000
B	-1.437352000	2.064164000	-0.288782000
B	-0.818034000	-2.064534000	0.278938000
B	-2.068347000	-0.994713000	0.606975000
B	-2.314348000	0.716731000	0.432268000
B	-1.981337000	-1.705533000	-0.921501000
B	0.486763000	-2.067241000	1.441093000
B	-1.676698000	0.075859000	1.851729000
B	-0.176666000	2.471567000	0.780413000
B	-2.605013000	1.324857000	-1.099914000
B	-1.268799000	1.576970000	1.496995000
B	-2.646858000	-0.222669000	-0.992301000
B	-0.874934000	-1.358974000	1.813666000
Li	0.647878000	0.304214000	2.004201000

2E

Charge -1 Multiplicity = 2

$E_{\text{PBE0}} = -610.6735404$

$E_{\text{ZPE}} = 0.103956$

B	-0.765193000	-0.186852000	1.619882000
B	0.878734000	0.076221000	1.770268000
B	1.922894000	-0.784642000	0.849314000
B	0.355098000	-1.390157000	1.230643000
B	-1.884805000	0.773873000	0.949097000
B	-1.207773000	-1.636959000	0.850980000
B	1.773262000	0.980537000	0.806446000
Li	-0.133234000	1.970157000	1.888575000
B	0.010164000	-2.669262000	0.045418000
B	-0.073035000	0.087088000	-1.546663000
B	-0.242208000	1.574032000	-0.884176000
B	-0.817611000	-1.277854000	-1.004810000
B	1.297516000	0.799375000	-1.055300000

B	-1.534216000	0.380935000	-0.826137000
B	2.898718000	0.101805000	-0.451999000
Li	1.382270000	-1.389326000	-1.907531000
B	-2.540151000	-1.566547000	-0.362373000
B	1.620339000	-2.358792000	0.087080000
B	1.328672000	2.450745000	-0.252213000
B	-2.894513000	1.453118000	-0.230489000
B	-1.581677000	2.421091000	-0.014854000
B	-3.144804000	-0.050183000	-0.293393000
B	2.703931000	1.689009000	-0.454724000
B	2.861380000	-1.513296000	-0.293671000
B	-1.537396000	-2.753918000	-0.465387000
B	-0.176748000	3.052134000	-0.061567000

2F

Charge -1 Multiplicity = 2

$E_{\text{PBE0}} = -610.6732603$

$E_{\text{ZPE}} = 0.105039$

B	-0.742206000	-1.551652000	2.360441000
B	-0.664514000	-2.914595000	1.498124000
B	-0.606203000	-3.522879000	0.000000000
B	-0.664514000	-2.914595000	-1.498124000
B	-0.742206000	-1.551652000	-2.360441000
B	-0.752891000	0.007770000	-2.763054000
B	-0.728651000	1.613164000	-2.576657000
B	-0.806398000	2.871201000	-1.551907000
B	-0.846319000	3.341821000	0.000000000
B	-0.806398000	2.871201000	1.551907000
B	-0.728651000	1.613164000	2.576657000
B	-0.752891000	0.007770000	2.763054000
B	0.759658000	-2.313624000	2.163630000
B	0.838721000	-3.224127000	0.804612000
B	0.838721000	-3.224127000	-0.804612000
B	0.759658000	-2.313624000	-2.163630000
B	0.731350000	-0.825162000	-2.773328000
B	0.755844000	0.793063000	-2.612437000
B	0.711549000	2.272075000	-2.009776000
B	0.624150000	3.363824000	-0.804704000
B	0.624150000	3.363824000	0.804704000
B	0.711549000	2.272075000	2.009776000
B	0.755844000	0.793063000	2.612437000
B	0.731350000	-0.825162000	2.773328000

Li	-1.653854000	-1.518585000	0.000000000
Li	1.652682000	1.513891000	0.000000000

2G

Charge -1 Multiplicity = 2

$E_{\text{PBE0}} = -610.6722661$

$E_{\text{ZPE}} = 0.105762$

B	2.272725000	-0.133264000	-0.359433000
B	-1.317526000	2.102187000	-0.953891000
B	1.443987000	1.153048000	-1.221643000
B	-1.682573000	1.475524000	0.601324000
B	-0.265061000	2.439701000	0.483441000
B	-1.513306000	0.538994000	2.019562000
B	2.983174000	0.101350000	1.140030000
B	1.439126000	2.498820000	-0.133391000
B	2.457673000	1.392175000	0.418483000
B	-0.758230000	1.903110000	1.909086000
B	0.246306000	2.441259000	-1.153827000
B	2.349285000	-1.324531000	0.932588000
Li	0.688102000	-0.044821000	1.992999000
B	-2.236051000	-0.143630000	0.495842000
B	-0.089054000	-2.313275000	-0.360368000
B	1.393777000	-1.551470000	-0.588829000
B	-1.582253000	-1.637047000	0.152408000
B	-1.576779000	-1.080365000	1.747981000
B	1.088508000	-2.343446000	0.894825000
B	-1.282742000	-1.921524000	-1.546470000
B	-2.345962000	0.881051000	-0.867617000
B	1.392350000	-0.362857000	-1.789852000
B	0.243231000	-1.514622000	-1.841000000
B	-2.258740000	-0.711743000	-1.134904000
B	-0.439157000	-2.146247000	1.357934000
Li	-0.625947000	0.472825000	-2.330135000

2H

Charge -1 Multiplicity = 2

$E_{\text{PBE0}} = -610.6699226$

$E_{\text{ZPE}} = 0.104140$

B	-1.373603000	-1.260876000	0.647509000
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B	0.027240000	1.713320000	-0.897626000
B	-0.799979000	-0.196814000	1.734482000
B	-2.111130000	0.270909000	0.932402000
Li	-0.084318000	1.884551000	1.726578000
B	0.283063000	3.149343000	-0.076728000
B	-2.534661000	1.800134000	0.058110000
Li	-1.978704000	0.565342000	-1.808879000
B	-1.180306000	2.683511000	-0.137305000
B	-2.901636000	-0.930936000	-0.248911000
B	1.671089000	2.351047000	-0.184982000
B	-3.418664000	0.559906000	-0.096933000
B	0.072237000	0.179863000	-1.513747000
B	-0.532221000	-1.292526000	-1.175249000
B	1.480379000	0.744293000	-0.947470000
B	1.205904000	-0.952117000	-1.249670000
B	0.129000000	-1.555540000	1.355013000
B	0.852145000	-0.123657000	1.863912000
B	1.713299000	-1.137408000	0.904441000
B	1.964752000	0.630065000	1.029039000
B	1.001934000	-2.412124000	-0.208337000
B	-0.587740000	-2.719611000	-0.040398000
B	-1.943405000	-2.166922000	-0.706258000
B	2.852396000	-0.282986000	-0.335723000
B	2.462925000	-1.843441000	-0.468925000
B	2.904795000	1.322629000	-0.187267000

2I

Charge -1 Multiplicity = 2

$E_{\text{PBE0}} = -610.6681878$

$E_{\text{ZPE}} = 0.104672$

B	3.178252000	0.212120000	-0.381307000
B	1.157279000	-1.759776000	-0.356916000
Li	-0.443528000	1.010737000	-1.855334000
B	-0.133445000	-2.516603000	-1.035132000
B	1.717550000	-0.285577000	-1.217407000
B	0.403930000	-1.087744000	-1.702899000
B	-1.221330000	-1.280421000	-1.244555000
B	-2.464031000	1.225278000	-0.500146000
B	-2.522137000	-0.247667000	-1.144735000
B	2.370597000	1.406666000	-0.939526000
B	1.242495000	2.570384000	-1.031774000
B	-0.143699000	3.068836000	-0.713965000

B	-1.328405000	2.349724000	0.095254000
B	2.496503000	-1.026322000	0.419494000
B	1.817849000	0.759465000	0.625013000
Li	-0.976525000	-0.796059000	1.790994000
B	0.495618000	2.020052000	0.474180000
B	1.336434000	-0.491618000	1.691266000
B	0.664169000	0.965107000	1.796641000
B	-0.790629000	1.608017000	1.580442000
B	-2.799495000	-0.045143000	0.502075000
B	-2.294817000	1.382976000	1.125534000
B	1.479293000	-2.066010000	1.293251000
B	0.126573000	-2.737590000	0.698145000
B	-1.369637000	-2.604840000	0.078451000
B	-2.566884000	-1.548120000	-0.072779000

2J

Charge -1 Multiplicity = 2

$E_{\text{PBE0}} = -610.6666647$

$E_{\text{ZPE}} = 0.105187$

B	1.930746000	1.180352000	-0.668666000
B	1.257823000	-1.886922000	-0.201621000
B	-1.620861000	-1.146291000	0.589846000
B	-1.058524000	2.261827000	0.104893000
B	-2.032127000	0.615485000	0.474114000
B	-0.303764000	-2.285158000	0.359826000
B	0.642316000	2.332529000	-0.487373000
B	2.122011000	-0.499532000	-0.556266000
B	2.514628000	0.459467000	0.787515000
B	0.214660000	2.425085000	1.148599000
B	-1.376439000	-0.122287000	1.880704000
B	0.969645000	-2.136288000	1.493911000
B	1.031483000	1.778806000	-1.950227000
B	1.308047000	-1.315690000	-1.802312000
B	-1.544725000	-2.149397000	-0.838140000
B	-3.015087000	0.499250000	-0.952828000
B	-2.645142000	-1.045234000	-0.873010000
B	0.005376000	-2.133227000	-1.342527000
B	-0.448091000	-1.428057000	1.814599000
B	-2.359534000	1.844592000	-0.732141000
B	1.545585000	0.290953000	-2.063677000
B	-0.986542000	1.408865000	1.588969000
B	2.113800000	-1.076956000	1.074488000
B	1.690815000	1.838830000	0.882979000

Li	-0.761237000	0.132615000	-1.927532000
Li	0.834404000	0.349042000	2.374775000

2K

Charge -1 Multiplicity = 2

$E_{\text{PBE0}} = -610.6628148$

$E_{\text{ZPE}} = 0.104880$

B	0.578639000	-0.023400000	-1.446352000
B	1.804595000	0.889275000	-0.865966000
B	-1.842299000	1.078173000	0.788733000
B	-0.775286000	0.683563000	2.150250000
Li	1.386156000	1.057205000	1.605723000
B	-2.221818000	1.187149000	-0.936806000
B	-0.699360000	2.134496000	1.374939000
B	-1.319137000	2.367094000	-0.176896000
Li	-0.002837000	1.997452000	-1.886794000
B	0.215772000	2.782963000	0.180143000
B	1.768357000	2.496799000	-0.180602000
B	3.213836000	0.082543000	-0.137012000
B	3.058660000	1.663583000	-0.113197000
B	-0.005363000	-1.376634000	-0.794627000
B	-1.011497000	-0.175656000	-1.560608000
B	1.772312000	-0.920090000	-0.671263000
B	-1.671952000	-0.588570000	1.353958000
B	-0.513056000	-1.920750000	1.276250000
B	-0.361598000	-0.807165000	2.358701000
B	-2.603564000	-0.172177000	0.056991000
B	-2.000298000	-1.508862000	-0.961606000
B	-1.052728000	-2.656477000	-0.276460000
B	0.411849000	-2.887196000	0.123181000
B	-2.690095000	-0.213383000	-1.660122000
B	1.982442000	-2.465162000	0.181258000
B	3.131599000	-1.482910000	0.105754000

2L

Charge -1 Multiplicity = 2

$E_{\text{PBE0}} = -610.6626053$

$E_{\text{ZPE}} = 0.104674$

B	-0.890247000	1.446068000	-0.776780000
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B	-1.559174000	0.845969000	1.207447000
B	-1.222800000	-0.692715000	1.610003000
B	0.275580000	-1.109749000	2.012250000
Li	0.648382000	1.116746000	1.921269000
B	-2.497034000	-0.440375000	0.628224000
B	-1.823542000	-1.914343000	0.126821000
B	0.020379000	2.696798000	0.292269000
B	1.793703000	-0.863678000	2.045557000
B	-1.551322000	2.368233000	0.502727000
B	1.599014000	2.596599000	0.320849000
B	-2.554416000	1.330885000	-0.247509000
B	-3.511687000	0.087526000	-0.640345000
B	-3.228353000	-1.418463000	-0.510822000
B	0.098288000	0.499394000	-1.713295000
B	0.484075000	-1.017370000	-1.301852000
B	0.845614000	1.682072000	-0.814400000
B	1.669753000	0.288063000	-1.366892000
B	1.274349000	-1.670555000	0.691556000
B	-0.268930000	-2.299078000	-0.272656000
B	2.569147000	-0.449865000	0.754350000
B	2.258258000	-1.296352000	-0.818385000
Li	-1.800196000	-0.501544000	-1.958880000
B	2.530178000	1.402468000	-0.161621000
B	1.174907000	-2.487533000	-0.832230000
B	3.205347000	0.046878000	-0.712702000

B₂₄

Charge 0 Multiplicity = 1

E_{PBE0} = -595.4618672

E_{ZPE} = 0.102659

B	-0.806940000	3.011616000	0.728556000
B	0.806940000	3.011616000	0.728556000
B	2.204674000	2.204674000	0.728631000
B	3.011616000	0.806940000	0.728556000
B	3.011616000	-0.806940000	0.728556000
B	2.204674000	-2.204674000	0.728631000
B	0.806940000	-3.011616000	0.728556000
B	-0.806940000	-3.011616000	0.728556000
B	-2.204674000	-2.204674000	0.728631000
B	-3.011616000	-0.806940000	0.728556000
B	-3.011616000	0.806940000	0.728556000
B	-2.204674000	2.204674000	0.728631000

B	0.000000000	3.117880000	-0.728631000
B	1.558942000	2.700127000	-0.728556000
B	2.700127000	1.558942000	-0.728556000
B	3.117880000	0.000000000	-0.728631000
B	2.700127000	-1.558942000	-0.728556000
B	1.558942000	-2.700127000	-0.728556000
B	0.000000000	-3.117880000	-0.728631000
B	-1.558942000	-2.700127000	-0.728556000
B	-2.700127000	-1.558942000	-0.728556000
B	-3.117880000	0.000000000	-0.728631000
B	-2.700127000	1.558942000	-0.728556000
B	-1.558942000	2.700127000	-0.728556000

B₂₄ B

Charge 0 Multiplicity = 1

$E_{\text{PBE0}} = -595.4217631$

$E_{\text{ZPE}} = 0.099126$

B	-1.792515000	-1.457855000	0.417883000
B	-0.133694000	-1.099506000	0.320499000
B	-1.340363000	1.509201000	0.136422000
B	-0.251521000	2.816189000	-0.197652000
B	2.853212000	2.338202000	0.151864000
B	1.389432000	-0.699518000	-0.147551000
B	3.022160000	-0.422013000	-0.014071000
B	1.905401000	0.932779000	0.012084000
B	4.651319000	-0.267252000	-0.042715000
B	2.504449000	-2.078357000	-0.232212000
B	0.220478000	0.656888000	0.266692000
B	-2.702468000	0.294077000	0.250475000
B	-3.404589000	-1.977801000	-0.085410000
B	-0.659132000	-2.746112000	-0.139008000
B	-2.216046000	-2.959788000	-0.148738000
B	-1.169707000	0.027521000	0.830027000
B	-1.752492000	3.014095000	-0.424872000
B	1.343057000	2.584644000	0.042105000
B	3.881477000	1.114597000	0.098828000
B	4.062814000	-1.679514000	-0.216239000
B	0.907568000	-2.347198000	-0.240658000
B	-4.175633000	-0.557678000	-0.1111307000
B	-4.145391000	0.946721000	-0.211509000
B	-2.997817000	2.057676000	-0.314938000

B₂₄ C

Charge 0 Multiplicity = 1

$$E_{\text{PBE0}} = -595.4178454$$

$$E_{\text{ZPE}} = 0.101154$$

B	4.016100000	0.704852000	0.369582000
B	2.812200000	-0.382042000	0.887126000
B	1.690294000	-1.521249000	0.911599000
B	0.382360000	-2.385494000	0.803060000
B	-1.219861000	-2.464215000	0.745522000
B	-2.688346000	-1.842555000	0.705837000
B	-3.439434000	-0.424256000	0.727628000
B	-3.146301000	1.161320000	0.762108000
B	-1.948894000	2.228177000	0.759723000
B	-0.347714000	2.506205000	0.709036000
B	1.216818000	2.129182000	0.662561000
B	2.672307000	1.428395000	0.744366000
B	4.016554000	-0.703469000	-0.369642000
B	1.689478000	1.521527000	-0.911391000
B	2.811710000	0.382618000	-0.886952000
B	2.673232000	-1.427950000	-0.744245000
B	1.217867000	-2.128930000	-0.662437000
B	-0.346611000	-2.506236000	-0.709065000
B	-1.947824000	-2.228494000	-0.759804000
B	-3.145693000	-1.162158000	-0.762275000
B	-3.439542000	0.423271000	-0.727825000
B	-2.689211000	1.841989000	-0.705927000
B	-1.220876000	2.463974000	-0.745586000
B	0.381384000	2.385535000	-0.802994000

B₂₄⁻

Charge -1 Multiplicity = 2

$$E_{\text{PBE0}} = -595.5656756$$

$$E_{\text{ZPE}} = 0.100683$$

B	0.798773000	3.018317000	0.733711000
B	-0.798773000	-3.018317000	0.733711000
B	3.014137000	-0.817498000	0.733428000
B	-3.014137000	0.817498000	0.733428000
B	-3.014137000	-0.817498000	0.733428000
B	-2.214795000	-2.200688000	0.733449000
B	0.798773000	-3.018317000	0.733711000

B	2.214795000	-2.200688000	0.733449000
B	3.014137000	0.817498000	0.733428000
B	2.214795000	2.200688000	0.733449000
B	-0.798773000	3.018317000	0.733711000
B	-2.214795000	2.200688000	0.733449000
B	0.000000000	3.139627000	-0.730672000
B	0.000000000	-3.139627000	-0.730672000
B	3.098354000	0.000000000	-0.736208000
B	-3.098354000	0.000000000	-0.736208000
B	-2.718996000	-1.569638000	-0.730968000
B	-1.548593000	-2.682151000	-0.736180000
B	1.548593000	-2.682151000	-0.736180000
B	2.718996000	-1.569638000	-0.730968000
B	2.718996000	1.569638000	-0.730968000
B	1.548593000	2.682151000	-0.736180000
B	-1.548593000	2.682151000	-0.736180000
B	-2.718996000	1.569638000	-0.730968000

B₂₄⁻ B

Charge -1 Multiplicity = 2

E_{PBE0} = -595.5560821

E_{ZPE} = 0.099153

B	-1.885595000	-1.402785000	0.297474000
B	-0.195028000	-1.134829000	0.301497000
B	-1.279008000	1.538938000	0.152946000
B	-0.176871000	2.827562000	-0.181030000
B	2.931579000	2.287163000	0.099089000
B	1.369666000	-0.712687000	-0.090510000
B	3.004747000	-0.464346000	-0.044356000
B	1.918695000	0.897559000	0.107124000
B	4.644098000	-0.339309000	-0.066136000
B	2.447826000	-2.089242000	-0.247064000
B	0.251184000	0.633606000	0.329514000
B	-2.684442000	0.391824000	0.254982000
B	-3.487889000	-1.980536000	-0.093627000
B	-0.719819000	-2.738465000	-0.098475000
B	-2.305267000	-2.946523000	-0.125136000
B	-1.182232000	0.034693000	0.812029000
B	-1.677020000	3.051712000	-0.389821000
B	1.424179000	2.570025000	0.011751000
B	3.937422000	1.070315000	0.076025000
B	4.012945000	-1.736317000	-0.252825000
B	0.842952000	-2.376888000	-0.158035000

B	-4.141095000	-0.503043000	-0.150104000
B	-4.108371000	1.016137000	-0.244048000
B	-2.942659000	2.105437000	-0.301264000

B₂₄⁻ C

Charge -1 Multiplicity = 2

E_{PBE0} = -595.5459297

E_{ZPE} = 0.099653

B	-0.104757000	0.143838000	-1.539399000
B	-1.636170000	0.106738000	-0.959428000
B	1.160266000	1.019764000	-0.945263000
B	1.261349000	-0.689411000	-1.262205000
B	-0.733588000	-0.273727000	1.579148000
B	-1.234458000	-1.707280000	0.820704000
B	-1.591782000	0.888099000	0.777420000
B	-0.520881000	1.499954000	-0.662366000
B	0.357798000	-1.530323000	1.228628000
B	1.873758000	-0.844133000	0.705266000
B	0.909518000	-0.111376000	1.828049000
B	1.829659000	0.876666000	0.954751000
B	1.363877000	-2.253238000	-0.423914000
B	-0.095311000	-2.769196000	0.093405000
B	2.749416000	0.168424000	-0.515819000
B	-2.830527000	1.467896000	-0.273811000
B	1.302143000	2.438892000	0.242528000
B	-1.719123000	2.571193000	0.104316000
B	2.696060000	-1.452889000	-0.666314000
B	2.589393000	1.768043000	-0.316925000
B	-2.584043000	-1.491410000	-0.386360000
B	-1.599627000	-2.688684000	-0.469780000
B	-0.259960000	2.883682000	0.373004000
B	-3.183010000	-0.021521000	-0.285634000

B₂₄⁻ D

Charge -1 Multiplicity = 2

E_{PBE0} = -595.5323865

E_{ZPE} = 0.099289

B	0.001905000	0.305154000	-1.525601000
B	0.998145000	-0.932201000	-1.182628000
B	1.495728000	-1.415696000	0.748319000

B	-0.151850000	-1.606417000	1.109442000
B	-1.715205000	-1.306465000	0.716218000
B	0.571725000	-2.522207000	-0.440153000
B	-1.025926000	-2.607144000	-0.126394000
B	-2.822469000	-0.486775000	-0.501498000
B	2.662550000	-0.709273000	-0.462206000
B	2.087945000	-2.184840000	-0.661820000
B	-2.385510000	-2.010434000	-0.637496000
B	1.437543000	0.757972000	-0.936583000
B	-1.489609000	0.692592000	-1.029965000
B	-0.064918000	1.767697000	-0.643499000
B	-0.877215000	-0.227883000	1.734456000
B	0.754872000	-0.390175000	1.830399000
B	-2.045991000	0.476885000	0.908819000
B	1.942314000	0.292801000	0.975867000
B	-1.847716000	2.162292000	-0.098754000
B	2.173356000	1.981477000	0.257594000
B	0.861562000	2.913200000	0.336107000
B	-0.616103000	3.119948000	0.206111000
B	-2.998463000	1.094126000	-0.328733000
B	3.053332000	0.835365000	-0.248002000

B₂₄⁻²

Charge -2 Multiplicity = 1

E_{PBE0} = -595.5587897

E_{ZPE} = 0.099062

B	-1.965843000	-1.360858000	0.199130000
B	-0.236604000	-1.181888000	0.371534000
B	-1.226717000	1.551188000	0.154846000
B	-0.114679000	2.830621000	-0.154621000
B	2.995908000	2.244957000	0.080409000
B	1.348272000	-0.713292000	-0.067648000
B	2.987410000	-0.497788000	-0.050917000
B	1.926369000	0.869093000	0.118359000
B	4.638930000	-0.392643000	-0.115261000
B	2.400469000	-2.104938000	-0.217752000
B	0.266125000	0.621932000	0.321152000
B	-2.670163000	0.462700000	0.276216000
B	-3.547839000	-1.965303000	-0.125463000
B	-0.766779000	-2.734906000	-0.079450000
B	-2.376736000	-2.924986000	-0.133251000
B	-1.191756000	0.039049000	0.807007000

B	-1.614405000	3.079300000	-0.358047000
B	1.494036000	2.558962000	0.021474000
B	3.988979000	1.036893000	0.032082000
B	3.970615000	-1.783741000	-0.262983000
B	0.786019000	-2.397853000	-0.084546000
B	-4.110646000	-0.461864000	-0.182018000
B	-4.078008000	1.076951000	-0.256576000
B	-2.902956000	2.148414000	-0.293674000

B₂₄⁻² B

Charge -2 Multiplicity = 1

E_{PBE0} = -595.5369098

E_{ZPE} = 0.099478

B	-2.666227000	-0.746908000	1.544682000
B	-1.588194000	-0.726279000	2.751195000
B	-0.004572000	-0.747078000	3.083230000
B	1.569921000	-0.738468000	2.719737000
B	2.671106000	-0.746819000	1.537065000
B	3.175936000	-0.725888000	0.000000000
B	2.671106000	-0.746819000	-1.537065000
B	1.569921000	-0.738468000	-2.719737000
B	-0.004572000	-0.747078000	-3.083230000
B	-1.588194000	-0.726279000	-2.751195000
B	-2.666227000	-0.746908000	-1.544682000
B	-3.140595000	-0.737911000	0.000000000
B	-2.195107000	0.743799000	2.218174000
B	-0.822747000	0.743743000	3.010284000
B	0.835245000	0.734948000	3.035121000
B	2.209346000	0.735230000	2.240263000
B	3.017471000	0.744116000	0.792342000
B	3.017471000	0.744116000	-0.792342000
B	2.209346000	0.735230000	-2.240263000
B	0.835245000	0.734948000	-3.035121000
B	-0.822747000	0.743743000	-3.010284000
B	-2.195107000	0.743799000	-2.218174000
B	-3.043914000	0.735616000	-0.793652000
B	-3.043914000	0.735616000	0.793652000

B₂₄⁻² C

Charge -2 Multiplicity = 1

$$E_{\text{PBE0}} = -595.5133616$$

$$E_{\text{ZPE}} = 0.099886$$

B	-0.463415000	-0.748597000	1.335464000
B	0.745248000	-1.555343000	0.524741000
B	-2.003180000	-1.024021000	0.943851000
B	0.898179000	0.059790000	0.887983000
B	-0.799967000	-2.164010000	0.411605000
B	-2.268694000	0.359465000	-0.064707000
B	0.267662000	1.609949000	0.312808000
B	1.913616000	-2.494146000	-0.375052000
B	-1.295389000	1.651056000	-0.277631000
B	2.853359000	2.598506000	-0.222904000
B	2.221421000	-0.918888000	0.265549000
B	-0.400522000	3.097808000	-0.177003000
B	1.906560000	1.361748000	0.304825000
B	-3.366154000	-0.936497000	-0.054424000
B	0.343583000	-3.055081000	-0.553156000
B	-2.362928000	-2.203559000	-0.344101000
B	1.224413000	2.876685000	-0.171925000
B	-3.020000000	1.911070000	-0.362841000
B	3.356437000	-1.812868000	-0.535733000
B	-2.014847000	3.156207000	-0.304531000
B	3.758743000	-0.347512000	-0.277107000
B	-3.904398000	0.543852000	-0.329646000
B	3.588565000	1.267235000	-0.143397000
B	-1.178292000	-3.232850000	-0.792667000

B₂₄⁻³

Charge -3 Multiplicity = 2

$$E_{\text{PBE0}} = -595.4185777$$

$$E_{\text{ZPE}} = 0.097182$$

B	-1.947667000	-1.360188000	0.155918000
B	-0.214104000	-1.174735000	0.347831000
B	-1.225589000	1.547883000	0.118660000
B	-0.113307000	2.858620000	-0.157131000
B	2.974015000	2.289057000	0.072927000
B	1.350182000	-0.686634000	-0.136379000
B	2.989194000	-0.502494000	-0.024758000
B	1.955591000	0.884805000	0.152004000
B	4.627956000	-0.390001000	-0.071484000

B	2.415595000	-2.147684000	-0.242782000
B	0.280116000	0.610084000	0.247014000
B	-2.670115000	0.428020000	0.296615000
B	-3.545082000	-1.980787000	-0.102472000
B	-0.753397000	-2.737347000	-0.075738000
B	-2.364583000	-2.938389000	-0.103581000
B	-1.188527000	0.037158000	0.799897000
B	-1.635457000	3.072579000	-0.372148000
B	1.487331000	2.647311000	0.026483000
B	3.919183000	1.022661000	0.082359000
B	3.965509000	-1.798541000	-0.270911000
B	0.811218000	-2.416175000	-0.083306000
B	-4.119025000	-0.477842000	-0.144370000
B	-4.085047000	1.064751000	-0.221080000
B	-2.913989000	2.147890000	-0.293570000

B₂₄⁻³ B

Charge -3 Multiplicity = 2

E_{PBE0} = -595.4054623

E_{ZPE} = 0.096820

B	-0.605602000	1.618439000	-0.016592000
B	1.018992000	2.263880000	0.015305000
B	1.762805000	-2.041629000	-0.143219000
B	-2.314260000	1.184569000	-0.038983000
B	-0.180825000	3.226018000	-0.063578000
B	3.521731000	0.171915000	-0.101559000
B	-1.736895000	2.930992000	-0.092265000
B	3.295157000	-1.579571000	-0.148486000
B	-3.291560000	2.564121000	-0.091253000
B	-4.075511000	1.279903000	-0.037768000
B	-4.273487000	-0.310370000	0.022472000
B	4.762665000	-0.994340000	-0.111084000
B	5.121667000	0.531103000	0.018307000
B	0.454314000	-0.901564000	0.049315000
B	-1.041207000	0.023073000	0.034359000
B	1.975645000	-0.376615000	0.110154000
B	-1.067430000	-1.636041000	0.050636000
B	0.279458000	-2.704962000	-0.031310000
B	2.463679000	1.495299000	0.173533000
B	-2.550209000	-0.713052000	0.046405000
B	-1.146311000	-3.322546000	0.017936000
B	-2.557436000	-2.636920000	0.058710000

$$\mathbf{B}_{24}^{-3} \quad \mathbf{C}$$
$$E_{\text{PBE0}} = -595.3967751$$

B	0.697784000	-0.501422000	0.118132000
B	0.969680000	-2.205051000	-0.184488000
B	1.973237000	0.467019000	-0.140335000
B	0.309456000	2.735484000	-0.339386000
B	2.287134000	-1.291599000	0.313408000
B	1.814085000	2.110444000	-0.467819000
B	3.539987000	-0.133901000	-0.082412000
B	3.295541000	1.589040000	-0.344445000
B	3.868053000	-1.570542000	0.706899000
B	4.784637000	0.974066000	0.010128000
B	5.022927000	-0.531134000	0.439614000
B	-1.038541000	0.029267000	0.059119000
B	-1.048499000	1.662420000	-0.070494000
B	-0.595679000	-1.533406000	-0.283440000
B	-2.568544000	0.789519000	0.236367000
B	-1.088513000	3.321153000	-0.106245000
B	-2.280707000	-1.083875000	-0.034214000
B	-2.489116000	2.621575000	0.180205000
B	-0.227746000	-3.171223000	-0.390632000
B	-3.864768000	1.850215000	0.402670000
B	-4.282573000	0.402584000	0.326714000
B	-1.759891000	-2.911384000	-0.310416000
B	-3.271585000	-2.445178000	-0.142696000

Technical Bid on (cost-