Computational investigation of the structural and electrolyte properties of the extended family of lithium (thio)boracite materials – $Li_4B_7O_{12}Cl$ and beyond

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Supplemental Materials Part II

Included in this document is the detailed structural information about the materials listed in Appendix B, Table VIII of the manuscript. Materials 1-66 are listed below, while the structural information for materials 67-82 is given in the Supplemental Materials Part 1 document.

* D. Cory Lynch and Yan Li contributed equivalently to this work.

Structural Data for Material # 1

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of Li in the $Im\bar{3}m$ (No. 229) structure.

```
CELL_PARAMETERS (bohr)
   6.496158177   0.000000000   0.000000000
   0.000000000   6.496158177   0.000000000
   0.000000000   0.000000000   6.496158177

ATOMIC_POSITIONS (crystal)
Li            0.0000000000        0.0000000000        0.0000000000
Li            0.5000000000        0.5000000000        0.5000000000
```

Structural Data for Material # 2

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of Al in the $F3m3$ (No. 225) structure.

```
CELL_PARAMETERS (bohr)
  -3.792318850   0.000000000   3.792318850
   0.000000000   3.792318850   3.792318850
  -3.792318850   3.792318850   0.000000000

ATOMIC_POSITIONS (crystal)
Al            0.0000000000        0.0000000000        0.0000000000
```

Structural Data for Material # 3

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of B in the $R\bar{3}m$ (No. 166) structure.

```
CELL_PARAMETERS (bohr)
   8.887454787   2.373173784   2.373173784
   2.373173784   8.887454787   2.373173784
   2.373173784   2.373173784   8.887454787

ATOMIC_POSITIONS (crystal)
B             0.5106130995        0.1538000193        0.5106130995
B             0.4893869005        0.8461999807        0.4893869005
B             0.5106130995        0.5106130995        0.1538000193
B             0.4893869005        0.4893869005        0.8461999807
B             0.1538000193        0.5106130995        0.5106130995
B             0.8461999807        0.4893869005        0.4893869005
B             0.7216649545        0.1296900229        0.7216649545
B             0.2783350455        0.8703099921        0.2783350455
B             0.7216649545        0.7216649545        0.1296900229
B             0.2783350455        0.2783350455        0.8703099921
B             0.1296900229        0.7216649545        0.7216649545
B             0.8703099921        0.2783350455        0.2783350455
```

Structural Data for Material # 4

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of S in the $P2/c$ (No. 13) structure.

```
CELL_PARAMETERS (bohr)
 -13.195905109   0.000000000  -8.543264946
  13.367467775   0.000000000  -9.418518763
   0.000000000 -24.983705309   0.000000000

ATOMIC_POSITIONS (crystal)
S             0.1760280949        0.8225327143        0.3470683992
S             0.3239719051        0.6774672857        0.3470683992
S             0.8239719051        0.1774672857        0.6529316008
S             0.6760280949        0.3225327143        0.6529316008
S             0.0342931693        0.8449531152        0.5803504224
S             0.4657068307        0.6550468848        0.5803504224
S             0.9657068307        0.1550468848        0.4196495776
S             0.5342931693        0.3449531152        0.4196495776
S             0.9711378564        0.7201013619        0.4448591870
S             0.5288621436        0.7798986381        0.4448591870
S             0.0288621436        0.2798986381        0.5551408130
S             0.4711378564        0.2201013619        0.5551408130
S             0.1168120061        0.7063672675        0.6797267643
S             0.3831879939        0.7936327325        0.6797267643
S             0.8831879939        0.2936327325        0.3202732357
S             0.6168120061        0.2063672675        0.3202732357
S             0.2832318260        0.3771779315        0.7812379246
S             0.2167681740        0.1228220685        0.7812379246
S             0.7167681740        0.6228220685        0.2187620754
S             0.7832318260        0.8771779315        0.2187620754
S             0.2395374707        0.5046309675        0.0147454444
S             0.2604625293        0.9953690325        0.0147454444
S             0.7604625293        0.4953690325        0.9852545556
S             0.7395374707        0.0046309675        0.9852545556
S             0.1167987327        0.4309960822        0.8777758888
S             0.3832012673        0.0690039178        0.8777758888
S             0.8832012673        0.5690039178        0.1222241112
S             0.6167987327        0.9309960822        0.1222241112
S             0.1596880400        0.3051464679        0.1124933893
S             0.3403119600        0.1948535321        0.1124933893
S             0.8403119600        0.6948535321        0.8875066107
S             0.6596880400        0.8051464679        0.8875066107
```

Structural Data for Material # 5

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of O_2 in the $C2/m$ (No. 12) structure.

```
CELL_PARAMETERS (bohr)
   0.205723680  -0.000000000   8.036878955
  -7.164339044   5.706682403   3.619870037
  -7.164339044  -5.706682403   3.619870037

ATOMIC_POSITIONS (crystal)
O             0.8633441065        0.8505411761        0.8505411761
O             0.1366558935        0.1494588239        0.1494588239
O             0.8210586302        0.2093454294        0.2093454294
O             0.1789413698        0.7906545706        0.7906545706
O             0.8423048622        0.2756492331        0.7843373763
O             0.8423048622        0.7843373763        0.2756492331
O             0.1576951378        0.7243507669        0.2156626237
O             0.1576951378        0.2156626237        0.7243507669
```

Structural Data for Material # 6

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of Cl_2 in the $Cmce$ (No. 64) structure.

```
CELL_PARAMETERS (bohr)
   6.570923082   3.678696544   0.000000000
  -6.570923082   3.678696544   0.000000000
   0.000000000   0.000000000  15.195615739

ATOMIC_POSITIONS (crystal)
Cl            0.3747686487        0.3747686487        0.6106987485
Cl            0.6252313513        0.6252313513        0.3893012515
Cl            0.1252313513        0.1252313513        0.1106987485
Cl            0.8747686487        0.8747686487        0.8893012515
```

Structural Data for Material # 7

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of Li_9Al_4 in the $C2/m$ (No. 12) structure.

```
CELL_PARAMETERS (bohr)
  -0.000000000   8.564190407  -0.000000000
   0.073874203  -0.000000000  10.091507767
  16.184494760  -4.282095154  -4.485062538

ATOMIC_POSITIONS (crystal)
Li            0.1481366894        0.2550947723        0.2962733787
Li            0.8518633106        0.7449052277        0.7037266213
Li            0.6143233001        0.9167507583        0.2286466001
Li            0.3856766999        0.0832492417        0.7713533999
Li            0.0000000000        0.0000000000        0.0000000000
```

```
Li            0.0722341879        0.6166504045        0.1444683756
Li            0.9277658121        0.3833495955        0.8555316244
Li            0.7691127521        0.1407925014        0.5382255042
Li            0.2308872479        0.8592074986        0.4617744958
Al            0.6997000826        0.5480948180        0.3994001654
Al            0.3002999174        0.4519051820        0.6005998346
Al            0.5425302543        0.3119844358        0.0850605085
Al            0.4574697457        0.6880155642        0.9149394915
```

Structural Data for Material # 8

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of LiAl in the $I4_1/amd$ (No. 141) structure.

```
CELL_PARAMETERS (bohr)
   8.418033360  -0.000000000  -0.000000000
  -0.000000000   8.418033360  -0.000000000
  -4.209016730  -4.209016730   6.007549384

ATOMIC_POSITIONS (crystal)
Li            0.7500000000        0.2500000000        0.5000000000
Li            0.5000000000        0.5000000000        1.0000000000
Al            0.2500000000        0.7500000000        0.5000000000
Al            0.0000000000        0.0000000000        0.0000000000
```

Structural Data for Material # 9

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of $LiAl_3$ in the $Pm\bar{3}m$ (No. 221) structure.

```
CELL_PARAMETERS (bohr)
   7.559846596   0.000000000   0.000000000
   0.000000000   7.559846596   0.000000000
   0.000000000   0.000000000   7.559846596

ATOMIC_POSITIONS (crystal)
Li            0.0000000000       -0.0000000000       -0.0000000000
Al            0.5000000000        0.5000000000        0.0000000000
Al            0.5000000000       -0.0000000000        0.5000000000
Al            0.0000000000        0.5000000000        0.5000000000
```

Structural Data for Material # 10

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of Li_2Al in the $Cmcm$ (No. 63) structure.

```
CELL_PARAMETERS (bohr)
   0.000000000  -0.000000000   8.425653826
   8.677616633  -0.000000000  -0.000000000
  -4.338808316   8.939560110   0.000000000

ATOMIC_POSITIONS (crystal)
Li            0.2500000000        0.0899354533        0.1798709067
Li            0.7500000000        0.9100645467        0.8201290933
Li            0.7500000000        0.2572698124        0.5145396249
Li            0.2500000000        0.7427301876        0.4854603751
Al            0.2500000000        0.4229261550        0.8458523101
Al            0.7500000000        0.5770738450        0.1541476899
```

Structural Data for Material # 11

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of Li_3Al_2 in the $R\bar{3}m$ (No. 166) structure.

```
CELL_PARAMETERS (bohr)
  -4.198592093  -7.272175771  -0.000000007
  -8.397184186  -0.000000000  -0.000000000
  -4.198592093  -2.424059191  -8.398291071

ATOMIC_POSITIONS (crystal)
Li            0.1959584809        0.1959584811        0.4121245569
Li            0.8040415191        0.8040415189        0.5878754431
Li            0.0000000000       -0.0000000000        0.0000000000
Al            0.6049884781        0.6049884757        0.1850345704
Al            0.3950115219        0.3950115243        0.8149654296
```

Structural Data for Material # 12

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of LiB_3 in the $P4/mbm$ (No. 127) structure.

```
CELL_PARAMETERS (bohr)
   0.000000000   0.000000000   7.821589131
  11.247220521   0.000000000   0.000000000
   0.000000000  11.247220521   0.000000000

ATOMIC_POSITIONS (crystal)
Li            0.5000000000        0.1800689492        0.6800689492
Li            0.5000000000        0.8199310508        0.3199310508
```

```
Li            0.5000000000        0.3199310508        0.1800689492
Li            0.5000000000        0.6800689492        0.8199310508
B             0.7058445147        0.5000000000        0.5000000000
B             0.7058445147        0.0000000000        0.0000000000
B             0.2941554853        0.5000000000        0.5000000000
B             0.2941554853        0.0000000000        0.0000000000
B             0.0000000000        0.6643472166        0.6322584945
B             1.0000000000        0.3356527834        0.3677415055
B            -0.0000000000        0.8356527834        0.1322584945
B             1.0000000000        0.1643472166        0.8677415055
B             1.0000000000        0.6322584945        0.3356527834
B             1.0000000000        0.3677415055        0.6643472166
B             1.0000000000        0.1322584945        0.1643472166
B             1.0000000000        0.8677415055        0.8356527834
```

Structural Data for Material # 13

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of Li_5B_4 in the Cm (No. 8) structure.

```
CELL_PARAMETERS (bohr)
   9.591124019   5.537438096   4.321297919
   6.818558705  -1.706368742  -4.241998330
   1.931520881   6.758229636  -4.241998338

ATOMIC_POSITIONS (crystal)
Li            0.7249505092        0.7338776843        0.7338776941
Li            0.2090385608        0.8337920450        0.2789414482
Li            0.2090385656        0.2789414553        0.8337920428
Li           -0.0486980311        0.9237982063        0.9237982127
Li            0.4980122673        0.2165404642        0.2165404609
B             0.6194428391        0.3254970394        0.6406458532
B             0.6194428373        0.6406458486        0.3254970422
B             0.8602445761        0.2916749988        0.2916749910
B             0.3835178757        0.6802422582        0.6802422550
```

Structural Data for Material # 14

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of LiB in the $P6_3/mmc$ (No. 194) structure.

```
CELL_PARAMETERS (bohr)
  -0.000000000  -0.000000000  -5.869459764
  -3.770954350  -6.531484075  -0.000000000
  -3.770954350   6.531484075   0.000000000

ATOMIC_POSITIONS (crystal)
Li            0.7500000000        0.6666666670        0.3333333330
Li            0.2500000000        0.3333333330        0.6666666670
B             0.7500000000       -0.0000000000        0.0000000000
B             0.2500000000       -0.0000000000       -0.0000000000
```

Structural Data for Material # 15

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of Li_2S in the $Fm\bar{3}m$ (No. 225) structure.

```
CELL_PARAMETERS (bohr)
  -5.349536508  -0.000000000   5.349536508
   0.000000000   5.349536508   5.349536508
  -5.349536508   5.349536508  -0.000000000

ATOMIC_POSITIONS (crystal)
Li            0.2500000000        0.2500000000        0.2500000000
Li            0.7500000000        0.7500000000        0.7500000000
S             0.0000000000        0.0000000000        0.0000000000
```

Structural Data for Material # 16

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of Li_2O in the $Fm\bar{3}m$ (No. 225) structure.

```
CELL_PARAMETERS (bohr)
  -4.335534096   0.000000000   4.335534096
   0.000000000   4.335534096   4.335534096
  -4.335534096   4.335534096   0.000000000

ATOMIC_POSITIONS (crystal)
Li            0.2500000000        0.2500000000        0.2500000000
Li            0.7500000000        0.7500000000        0.7500000000
O             0.0000000000        0.0000000000        0.0000000000
```

Structural Data for Material # 17

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of Li_2O_2 in the $P6_3/mmc$ (No. 194) structure.

```
CELL_PARAMETERS (bohr)
  -2.954798406  -5.117861257  -0.000000000
  -2.954798406   5.117861257  -0.000000000
  -0.000000000   0.000000000 -14.299615027

ATOMIC_POSITIONS (crystal)
Li            0.6666666670        0.3333333330        0.7500000000
Li            0.3333333330        0.6666666670        0.2500000000
Li           -0.0000000000       -0.0000000000        0.5000000000
Li           -0.0000000000       -0.0000000000       -0.0000000000
O             0.6666666670        0.3333333330        0.1490506017
O             0.3333333330        0.6666666670        0.8509493983
O             0.3333333330        0.6666666670        0.6490506017
O             0.6666666670        0.3333333330        0.3509493983
```

Structural Data for Material # 18

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of LiCl in the $Fm\bar{3}m$ (No. 225) structure.

```
CELL_PARAMETERS (bohr)
  -4.787518518  -4.787518518  -0.000000000
  -4.787518518   0.000000000  -4.787518518
   0.000000000  -4.787518518  -4.787518518

ATOMIC_POSITIONS (crystal)
Li             0.5000000000        0.5000000000        0.5000000000
Cl             0.0000000000        0.0000000000       -0.0000000000
```

Structural Data for Material # 19

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of AlB_2 in the $P6/mmm$ (No. 191) structure.

```
CELL_PARAMETERS (bohr)
  -2.834592864  -4.909659553  -0.000000000
  -2.834592864   4.909659553  -0.000000000
   0.000000000   0.000000000  -6.138936275

ATOMIC_POSITIONS (crystal)
Al             0.0000000000        0.0000000000        0.0000000000
B              0.3333333330        0.6666666670        0.5000000000
B              0.6666666670        0.3333333330        0.5000000000
```

Structural Data for Material # 20

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of AlB_{12} in the $P4_12_12$ (No. 92) structure.

```
CELL_PARAMETERS (bohr)
  19.170128847   0.000000000   0.000000000
   0.000000000  19.170128847   0.000000000
   0.000000000   0.000000000  29.227316687

ATOMIC_POSITIONS (crystal)
Al             0.5307483046        0.2783435236        0.5738269015
Al             0.4692516954        0.7216564764        0.0738269015
Al             0.7783435236       -0.0307483046        0.3238269015
Al             0.2216564764        0.0307483046        0.8238269015
Al             0.7216564764        0.4692516954        0.9261730985
```

Al	0.2783435236	0.5307483046	0.4261730985
Al	-0.0307483046	0.7783435236	0.6761730985
Al	0.0307483046	0.2216564764	0.1761730985
Al	0.4304592733	0.7544113205	0.7210328072
Al	0.5695407267	0.2455886795	0.2210328072
Al	0.2544113205	0.0695407267	0.4710328072
Al	0.7455886795	-0.0695407267	0.9710328072
Al	0.2455886795	0.5695407267	0.7789671928
Al	0.7544113205	0.4304592733	0.2789671928
Al	0.0695407267	0.2544113205	0.5289671928
Al	-0.0695407267	0.7455886795	0.0289671928
B	0.7488852630	0.3604219671	0.6156235951
B	0.2511147370	0.6395780329	0.1156235951
B	0.8604219671	0.7511147370	0.3656235951
B	0.1395780329	0.2488852630	0.8656235951
B	0.6395780329	0.2511147370	0.8843764049
B	0.3604219671	0.7488852630	0.3843764049
B	0.7511147370	0.8604219671	0.6343764049
B	0.2488852630	0.1395780329	0.1343764049
B	0.1083470307	0.6870021580	0.4943139018
B	0.8916529693	0.3129978420	-0.0056860982
B	0.1870021580	0.3916529693	0.2443139018
B	0.8129978420	0.6083470307	0.7443139018
B	0.3129978420	0.8916529693	1.0056860982
B	0.6870021580	0.1083470307	0.5056860982
B	0.3916529693	0.1870021580	0.7556860982
B	0.6083470307	0.8129978420	0.2556860982
B	0.8478622959	0.5887001687	0.6312681883
B	0.1521377041	0.4112998313	0.1312681883
B	0.0887001687	0.6521377041	0.3812681883
B	0.9112998313	0.3478622959	0.8812681883
B	0.4112998313	0.1521377041	0.8687318117
B	0.5887001687	0.8478622959	0.3687318117
B	0.6521377041	0.0887001687	0.6187318117
B	0.3478622959	0.9112998313	0.1187318117
B	0.7427875895	0.7456259858	0.7931071272
B	0.2572124105	0.2543740142	0.2931071272
B	0.2456259858	0.7572124105	0.5431071272
B	0.7543740142	0.2427875895	1.0431071272
B	0.2543740142	0.2572124105	0.7068928728
B	0.7456259858	0.7427875895	0.2068928728
B	0.7572124105	0.2456259858	0.4568928728
B	0.2427875895	0.7543740142	-0.0431071272
B	0.9298835466	0.4336366096	0.6139161942
B	0.0701164534	0.5663633904	0.1139161942
B	0.9336366096	0.5701164534	0.3639161942
B	0.0663633904	0.4298835466	0.8639161942
B	0.5663633904	0.0701164534	0.8860838058
B	0.4336366096	0.9298835466	0.3860838058
B	0.5701164534	0.9336366096	0.6360838058
B	0.4298835466	0.0663633904	0.1360838058
B	0.6914400238	0.3981215292	0.5120245427
B	0.3085599762	0.6018784708	0.0120245427
B	0.8981215292	0.8085599762	0.2620245427
B	0.1018784708	0.1914400238	0.7620245427
B	0.6018784708	0.3085599762	0.9879754573
B	0.3981215292	0.6914400238	0.4879754573
B	0.8085599762	0.8981215292	0.7379754573
B	0.1914400238	0.1018784708	0.2379754573

B	0.5426915260	0.6375624737	0.5349244037
B	0.4573084740	0.3624375263	0.0349244037
B	0.1375624737	0.9573084740	0.2849244037
B	0.8624375263	0.0426915260	0.7849244037
B	0.3624375263	0.4573084740	0.9650755963
B	0.6375624737	0.5426915260	0.4650755963
B	0.9573084740	0.1375624737	0.7150755963
B	0.0426915260	0.8624375263	0.2150755963
B	0.6934796860	0.5769933719	0.5712637391
B	0.3065203140	0.4230066281	0.0712637391
B	0.0769933719	0.8065203140	0.3212637391
B	0.9230066281	0.1934796860	0.8212637391
B	0.4230066281	0.3065203140	0.9287362609
B	0.5769933719	0.6934796860	0.4287362609
B	0.8065203140	0.0769933719	0.6787362609
B	0.1934796860	0.9230066281	0.1787362609
B	0.6998343507	0.5183624428	0.6786584254
B	0.3001656493	0.4816375572	0.1786584254
B	0.0183624428	0.8001656493	0.4286584254
B	0.9816375572	0.1998343507	0.9286584254
B	0.4816375572	0.3001656493	0.8213415746
B	0.5183624428	0.6998343507	0.3213415746
B	0.8001656493	0.0183624428	0.5713415746
B	0.1998343507	0.9816375572	0.0713415746
B	0.7294760592	0.3675310780	0.7227957616
B	0.2705239408	0.6324689220	0.2227957616
B	0.8675310780	0.7705239408	0.4727957616
B	0.1324689220	0.2294760592	0.9727957616
B	0.6324689220	0.2705239408	0.7772042384
B	0.3675310780	0.7294760592	0.2772042384
B	0.7705239408	0.8675310780	0.5272042384
B	0.2294760592	0.1324689220	0.0272042384
B	0.6917247715	0.2173602547	0.6799020497
B	0.3082752285	0.7826397453	0.1799020497
B	0.7173602547	0.8082752285	0.4299020497
B	0.2826397453	0.1917247715	0.9299020497
B	0.7826397453	0.3082752285	0.8200979503
B	0.2173602547	0.6917247715	0.3200979503
B	0.8082752285	0.7173602547	0.5700979503
B	0.1917247715	0.2826397453	0.0700979503
B	0.5489437147	0.5815123902	0.6476599691
B	0.4510562853	0.4184876098	0.1476599691
B	1.0815123902	0.9510562853	0.3976599691
B	-0.0815123902	0.0489437147	0.8976599691
B	0.4184876098	0.4510562853	0.8523400309
B	0.5815123902	0.5489437147	0.3523400309
B	0.9510562853	1.0815123902	0.6023400309
B	0.0489437147	-0.0815123902	0.1023400309
B	0.4278829573	0.4457257352	0.6498000221
B	0.5721170427	0.5542742648	0.1498000221
B	0.9457257352	0.0721170427	0.3998000221
B	0.0542742648	0.9278829573	0.8998000221
B	0.5542742648	0.5721170427	0.8501999779
B	0.4457257352	0.4278829573	0.3501999779
B	0.0721170427	0.9457257352	0.6001999779
B	0.9278829573	0.0542742648	0.1001999779
B	0.3632132460	0.4108109666	0.5509544068
B	0.6367867540	0.5891890334	0.0509544068
B	0.9108109666	0.1367867540	0.3009544068

```
B          0.0891890334      0.8632132460      0.8009544068
B          0.5891890334      0.6367867540      0.9490455932
B          0.4108109666      0.3632132460      0.4490455932
B          0.1367867540      0.9108109666      0.6990455932
B          0.8632132460      0.0891890334      0.1990455932
B          0.2659037233      0.6748269133      0.6442316500
B          0.7340962767      0.3251730867      0.1442316500
B          0.1748269133      0.2340962767      0.3942316500
B          0.8251730867      0.7659037233      0.8942316500
B          0.3251730867      0.7340962767      0.8557683500
B          0.6748269133      0.2659037233      0.3557683500
B          0.2340962767      0.1748269133      0.6057683500
B          0.7659037233      0.8251730867      0.1057683500
B         -0.0124312721      0.5866645654      0.7433738985
B          1.0124312721      0.4133354346      0.2433738985
B          0.0866645654      0.5124312721      0.4933738985
B          0.9133354346      0.4875687279     -0.0066261015
B          0.4133354346      1.0124312721      0.7566261015
B          0.5866645654     -0.0124312721      0.2566261015
B          0.5124312721      0.0866645654      0.5066261015
B          0.4875687279      0.9133354346      1.0066261015
B          0.1555973372      0.3564808891      0.7714714578
B          0.8444026628      0.6435191109      0.2714714578
B          0.8564808891      0.3444026628      0.5214714578
B          0.1435191109      0.6555973372      1.0214714578
B          0.6435191109      0.8444026628      0.7285285422
B          0.3564808891      0.1555973372      0.2285285422
B          0.3444026628      0.8564808891      0.4785285422
B          0.6555973372      0.1435191109     -0.0214714578
B          0.3929511807      0.5864060347      0.5864363998
B          0.6070488193      0.4135939653      0.0864363998
B          0.0864060347      0.1070488193      0.3364363998
B          0.9135939653      0.8929511807      0.8364363998
B          0.4135939653      0.6070488193      0.9135636002
B          0.5864060347      0.3929511807      0.4135636002
B          0.1070488193      0.0864060347      0.6635636002
B          0.8929511807      0.9135939653      0.1635636002
B          0.0200970459      0.5970099907      0.5752450739
B          0.9799029541      0.4029900093      0.0752450739
B          1.0970099907      0.4799029541      0.3252450739
B         -0.0970099907      0.5200970459      0.8252450739
B          0.4029900093      0.9799029541      0.9247549261
B          0.5970099907      0.0200970459      0.4247549261
B          0.4799029541      1.0970099907      0.6747549261
B          0.5200970459     -0.0970099907      0.1747549261
B          0.1057748197      0.4504364085      0.6018653688
B          0.8942251803      0.5495635915      0.1018653688
B          0.9504364085      0.3942251803      0.3518653688
B          0.0495635915      0.6057748197      0.8518653688
B          0.5495635915      0.8942251803      0.8981346312
B          0.4504364085      0.1057748197      0.3981346312
B          0.3942251803      0.9504364085      0.6481346312
B          0.6057748197      0.0495635915      0.1481346312
B          0.1145943921      0.5947350698      0.6680366808
B          0.8854056079      0.4052649302      0.1680366808
B          0.0947350698      0.3854056079      0.4180366808
B          0.9052649302      0.6145943921      0.9180366808
B          0.4052649302      0.8854056079      0.8319633192
B          0.5947350698      0.1145943921      0.3319633192
```

```
B             0.3854056079        0.0947350698        0.5819633192
B             0.6145943921        0.9052649302        0.0819633192
B             0.3549241374        0.3896579990        0.7494871708
B             0.6450758626        0.6103420010        0.2494871708
B             0.8896579990        0.1450758626        0.4994871708
B             0.1103420010        0.8549241374       -0.0005128292
B             0.6103420010        0.6450758626        0.7505128292
B             0.3896579990        0.3549241374        0.2505128292
B             0.1450758626        0.8896579990        0.5005128292
B             0.8549241374        0.1103420010        1.0005128292
B             0.2340130823        0.3406757100        0.6003542197
B             0.7659869177        0.6593242900        0.1003542197
B             0.8406757100        0.2659869177        0.3503542197
B             0.1593242900        0.7340130823        0.8503542197
B             0.6593242900        0.7659869177        0.8996457803
B             0.3406757100        0.2340130823        0.3996457803
B             0.2659869177        0.8406757100        0.6496457803
B             0.7340130823        0.1593242900        0.1496457803
B             0.0493172621        0.4411250100        0.7049272769
B             0.9506827379        0.5588749900        0.2049272769
B             0.9411250100        0.4506827379        0.4549272769
B             0.0588749900        0.5493172621        0.9549272769
B             0.5588749900        0.9506827379        0.7950727231
B             0.4411250100        0.0493172621        0.2950727231
B             0.4506827379        0.9411250100        0.5450727231
B             0.5493172621        0.0588749900        0.0450727231
```

Structural Data for Material # 21

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of Al_2S_3 in the $I4_1/amd$ (No. 141) structure.

```
CELL_PARAMETERS (bohr)
  13.260253399   0.000000000   0.000000000
   0.000000000  13.260253399   0.000000000
  -6.630126649  -6.630126649  28.252385139

ATOMIC_POSITIONS (crystal)
Al            0.5000000000        1.0000000000        0.5000000000
Al            1.0000000000        0.5000000000        1.0000000000
Al            0.0000000000       -0.0000000000        0.0000000000
Al           -0.0000000000       -0.0000000000        0.5000000000
Al            0.1474157856        0.6681736882        0.8363473764
Al            0.6681736882        0.1474157856        0.3363473764
Al            0.6681736882        0.6889315909        0.3363473764
Al            0.6889315909        0.6681736882        0.8363473764
Al            0.8525842144        0.3318263118        0.1636526236
Al            0.3318263118        0.8525842144        0.6636526236
Al            0.3318263118        0.3110684091        0.6636526236
Al            0.3110684091        0.3318263118        0.1636526236
Al            0.5453763141        0.7953763141        0.0907526281
Al            0.7953763141        0.5453763141        0.5907526281
Al            0.4546236859        0.2046236859        0.9092473719
```

```
Al            0.2046236859        0.4546236859        0.4092473719
S             0.2416967205        0.7493690994        0.9987381988
S             0.7493690994        0.2416967205        0.4987381988
S             0.7493690994        0.7570414783        0.4987381988
S             0.7570414783        0.7493690994        0.9987381988
S             0.7583032795        0.2506309006        0.0012618012
S             0.2506309006        0.7583032795        0.5012618012
S             0.2506309006        0.2429585217        0.5012618012
S             0.2429585217        0.2506309006        0.0012618012
S             0.4317866745        0.9216732624        0.3433465249
S             0.9216732624        0.4317866745        0.8433465249
S             0.9216732624        0.9115598503        0.8433465249
S             0.9115598503        0.9216732624        0.3433465249
S             0.5682133255        0.0783267376        0.6566534751
S             0.0783267376        0.5682133255        0.1566534751
S             0.0783267376        0.0884401497        0.1566534751
S             0.0884401497        0.0783267376        0.6566534751
S             0.1075720104        0.5869707572        0.6739415143
S             0.5869707572        0.1075720104        0.1739415143
S             0.5869707572        0.5663695039        0.1739415143
S             0.5663695039        0.5869707572        0.6739415143
S             0.8924279896        0.4130292428        0.3260584857
S             0.4130292428        0.8924279896        0.8260584857
S             0.4130292428        0.4336304961        0.8260584857
S             0.4336304961        0.4130292428        0.3260584857
```

Structural Data for Material # 22

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of Al_2O_3 in the $R\bar{3}c$ (No. 167) structure.

```
CELL_PARAMETERS (bohr)
  -4.513893079  -7.818291884   0.000000002
  -9.027786159  -0.000000000   0.000000000
  -4.513893079  -2.606097961  -8.201729689

ATOMIC_POSITIONS (crystal)
Al            0.3520389133        0.3520389133        0.9438832601
Al            0.8520389133        0.8520389133        0.4438832601
Al            0.6479610867        0.6479610867        0.0561167399
Al            0.1479610867        0.1479610867        0.5561167399
O             0.2500000000        0.9442175997        0.2500000000
O             0.5557824002        0.2500000000        0.2500000000
O             0.9442175998        0.5557824003        0.2500000000
O             0.4442175998        0.7500000000        0.7500000000
O             0.0557824002        0.4442175997        0.7500000000
O             0.7500000000        0.0557824003        0.7500000000
```

Structural Data for Material # 23

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of $AlCl_3$ in the $C2/m$ (No. 12) structure.

```
CELL_PARAMETERS (bohr)
  -5.332703436  -9.719787872   1.748638813
  -5.332703436   9.719787872   1.748638813
  -0.318973506  -0.000000000 -12.575949325

ATOMIC_POSITIONS (crystal)
Al             0.8333892574        0.1666107426       -0.0000000000
Al             0.1666107426        0.8333892574       -0.0000000000
Cl             0.2076704837        0.2076704837        0.2084325770
Cl             0.7923295163        0.7923295163        0.7915674230
Cl             0.0734841300        0.4328940915        0.7916602949
Cl             0.4328940915        0.0734841300        0.7916602949
Cl             0.9265158700        0.5671059085        0.2083397051
Cl             0.5671059085        0.9265158700        0.2083397051
```

Structural Data for Material # 24

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of BS in the $R\bar{3}m$ (No. 166) structure.

```
CELL_PARAMETERS (bohr)
  -2.866185146  -4.964377660  -0.000000000
  -5.732370291  -0.000000000   0.000000000
  -2.866185146  -1.654793212 -13.560635002

ATOMIC_POSITIONS (crystal)
B              0.9605745780        0.9605745699        0.1182762822
B              0.0394254220        0.0394254301        0.8817237178
S              0.2550479087        0.2550478961        0.2348562991
S              0.7449520913        0.7449521039        0.7651437009
```

Structural Data for Material # 25

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of BS_2 in the $P2_1/c$ (No. 14) structure.

```
CELL_PARAMETERS (bohr)
   0.000000000   7.805061945   0.000000000
  21.896676109   0.000000000  -6.923349774
 -21.941019134   0.000000000 -34.538636786

ATOMIC_POSITIONS (crystal)
B              0.8518665150        0.2770171571        0.3639507863
```

B	0.3518665150	0.2229828429	0.1360492137
B	0.1481334850	0.7229828429	0.6360492137
B	0.6481334850	0.7770171571	0.8639507863
B	0.6834772753	0.1874166206	0.4632772809
B	0.1834772753	0.3125833794	0.0367227191
B	0.3165227247	0.8125833794	0.5367227191
B	0.8165227247	0.6874166206	0.9632772809
B	0.6049984701	0.7188035606	0.4063973951
B	0.1049984701	0.7811964394	0.0936026049
B	0.3950015299	0.2811964394	0.5936026049
B	0.8950015299	0.2188035606	0.9063973951
B	0.8224004026	0.5091040277	0.3394671795
B	0.3224004026	0.9908959723	0.1605328205
B	0.1775995974	0.4908959723	0.6605328205
B	0.6775995974	0.0091040277	0.8394671795
S	0.9641327648	0.1304622291	0.3319807075
S	0.4641327648	0.3695377709	0.1680192925
S	0.0358672352	0.8695377709	0.6680192925
S	0.5358672352	0.6304622291	0.8319807075
S	0.8342181917	0.0627168962	0.4066344990
S	0.3342181917	0.4372831038	0.0933655010
S	0.1657818083	0.9372831038	0.5933655010
S	0.6657818083	0.5627168962	0.9066344990
S	0.7378729663	0.7497560661	0.3334695246
S	0.2378729663	0.7502439339	0.1665304754
S	0.2621270337	0.2502439339	0.6665304754
S	0.7621270337	0.2497560661	0.8334695246
S	0.9041961533	0.5919498881	0.2833402091
S	0.4041961533	0.9080501119	0.2166597909
S	0.0958038467	0.4080501119	0.7166597909
S	0.5958038467	0.0919498881	0.7833402091
S	0.6783229173	0.3226487182	0.4429730414
S	0.1783229173	0.1773512818	0.0570269586
S	0.3216770827	0.6773512818	0.5570269586
S	0.8216770827	0.8226487182	0.9429730414
S	0.5603499991	0.1565274708	0.5375484978
S	0.0603499991	0.3434725292	0.9624515022
S	0.4396500009	0.8434725292	0.4624515022
S	0.9396500009	0.6565274708	0.0375484978
S	0.6441521005	0.5761118802	0.4160608712
S	0.1441521005	0.9238881198	0.0839391288
S	0.3558478995	0.4238881198	0.5839391288
S	0.8558478995	0.0761118802	0.9160608712
S	0.9376019195	0.3613000360	0.3077786094
S	0.4376019195	0.1386999640	0.1922213906
S	0.0623980805	0.6386999640	0.6922213906
S	0.5623980805	0.8613000360	0.8077786094

Structural Data for Material # 26

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of B_2S_3 in the $P2_1/c$ (No. 14) structure.

```
CELL_PARAMETERS (bohr)
   7.717006515   0.000000000  -0.855228406
   0.000000000  20.375154731   0.000000000
  -0.080107886   0.000000000  35.605958210

ATOMIC_POSITIONS (crystal)
B             0.5724964540        0.0294264261        0.6814378055
B             0.4275035460        0.5294264261        0.8185621945
B             0.4275035460        0.9705735739        0.3185621945
B             0.5724964540        0.4705735739        0.1814378055
B             0.5375653962        0.7770871013        0.7413103685
B             0.4624346038        0.2770871013        0.7586896315
B             0.4624346038        0.2229128987        0.2586896315
B             0.5375653962        0.7229128987        0.2413103685
B             0.7380077200        0.8100670968        0.5978683425
B             0.2619922800        0.3100670968        0.9021316575
B             0.2619922800        0.1899329032        0.4021316575
B             0.7380077200        0.6899329032        0.0978683425
B             0.0561937284        0.0983837673        0.9907255581
B             0.9438062716        0.5983837673        0.5092744419
B             0.9438062716        0.9016162327        0.0092744419
B             0.0561937284        0.4016162327        0.4907255581
S             0.5595497915        0.1982923377        0.6780865515
S             0.4404502085        0.6982923377        0.8219134485
S             0.4404502085        0.8017076623        0.3219134485
S             0.5595497915        0.3017076623        0.1780865515
S             0.4790514256        0.9412940709        0.7571865023
S             0.5209485744        0.4412940709        0.7428134977
S             0.5209485744        0.0587059291        0.2428134977
S             0.4790514256        0.5587059291        0.2571865023
S             0.6736460781        0.6977264586        0.6658814265
S             0.3263539219        0.1977264586        0.8341185735
S             0.3263539219        0.3022735414        0.3341185735
S             0.6736460781        0.8022735414        0.1658814265
S             0.6941615086        0.9764643121        0.5971777211
S             0.3058384914        0.4764643121        0.9028222789
S             0.3058384914        0.0235356879        0.4028222789
S             0.6941615086        0.5235356879        0.0971777211
S             0.1227753452        0.2631068968        0.9868368809
S             0.8772246548        0.7631068968        0.5131631191
S             0.8772246548        0.7368931032        0.0131631191
S             0.1227753452        0.2368931032        0.4868368809
S             0.1014799752        0.9690653766        0.9303295822
S             0.8985200248        0.4690653766        0.5696704178
S             0.8985200248        0.0309346234        0.0696704178
S             0.1014799752        0.5309346234        0.4303295822
```

Structural Data for Material # 27

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of B_6O in the $R\bar{3}m$ (No. 166) structure.

```
CELL_PARAMETERS (bohr)
```

```
   5.070247288   2.927308281   7.717567453
  -5.070247288   2.927308281   7.717567453
   0.000000000  -5.854616661   7.717567454

ATOMIC_POSITIONS (crystal)
B             0.8244042605        0.2983320692        0.2983320711
B             0.2983320712        0.2983320712        0.8244042585
B             0.2983320692        0.8244042605        0.2983320711
B             0.1755957395        0.7016679308        0.7016679289
B             0.7016679288        0.7016679288        0.1755957415
B             0.7016679308        0.1755957395        0.7016679289
B             0.8332268257        0.5021237480        0.5021237487
B             0.5021237487        0.5021237487        0.8332268250
B             0.5021237480        0.8332268257        0.5021237487
B             0.1667731743        0.4978762520        0.4978762513
B             0.4978762513        0.4978762513        0.1667731750
B             0.4978762520        0.1667731743        0.4978762513
O             0.8782835029        0.8782835029        0.8782835028
O             0.1217164971        0.1217164971        0.1217164972
```

Structural Data for Material # 28

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of B_2O_3 in the $Cmc2_1$ (No. 36) structure.

```
CELL_PARAMETERS (bohr)
  8.73609960E+00  0.00000000E+00  2.78953787E-07
  0.00000000E+00  1.47913113E+01  0.00000000E+00
  2.52801869E-07  0.00000000E+00  7.81239743E+00

ATOMIC_POSITIONS (crystal)
B             0.1589768697        0.1651314387        0.4323330705
B             0.8410231391        0.8348685455        0.9323331786
B             0.8410231391        0.1651314545        0.9323331786
B             0.1589768697        0.8348685613        0.4323330705
B             0.6589768721        0.6651314361        0.4323330678
B             0.3410231368        0.3348685480        0.9323331759
B             0.3410231368        0.6651314520        0.9323331759
B             0.6589768721        0.3348685639        0.4323330678
O             0.2450244357        0.0000000000        0.5000305444
O             0.7549757237        0.0000000000        0.0000314010
O             0.7450244421        0.5000000000        0.5000305498
O             0.2549757177        0.5000000000        0.0000314064
O             0.3697084500        0.2906404211        0.5813514167
O             0.6302914549        0.7093596180        0.0813513362
O             0.6302914549        0.2906403520        0.0813513362
O             0.3697084500        0.7093595489        0.5813514167
O             0.8697084504        0.7906404563        0.5813514181
O             0.1302914544        0.2093596589        0.0813513375
O             0.1302914544        0.7906403871        0.0813513375
O             0.8697084504        0.2093595897        0.5813514181
```

Structural Data for Material # 29

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of BCl_2 in the *Pbca* (No. 61) structure.

```
CELL_PARAMETERS (bohr)
   0.000000000  12.312956176   0.000000000
   0.000000000   0.000000000  14.315934713
  24.153449082   0.000000000   0.000000000

ATOMIC_POSITIONS (crystal)
B             0.8938668991        0.4408024874        0.4829012814
B             0.6061331009        0.5591975126        0.9829012814
B             0.3938668991        0.0591975126        0.5170987186
B             0.1061331009        0.9408024874        0.0170987186
B             0.1061331009        0.5591975126        0.5170987186
B             0.3938668991        0.4408024874        0.0170987186
B             0.6061331009        0.9408024874        0.4829012814
B             0.8938668991        0.0591975126        0.9829012814
Cl            0.7684918622        0.3105018542        0.5770022152
Cl            0.7315081378        0.6894981458        0.0770022152
Cl            0.2684918622        0.1894981458        0.4229977848
Cl            0.2315081378        0.8105018542        0.9229977848
Cl            0.2315081378        0.6894981458        0.4229977848
Cl            0.2684918622        0.3105018542        0.9229977848
Cl            0.7315081378        0.8105018542        0.5770022152
Cl            0.7684918622        0.1894981458        0.0770022152
Cl            0.7952436964        0.4469945938        0.3564647743
Cl            0.7047563036        0.5530054062        0.8564647743
Cl            0.2952436964        0.0530054062        0.6435352257
Cl            0.2047563036        0.9469945938        0.1435352257
Cl            0.2047563036        0.5530054062        0.6435352257
Cl            0.2952436964        0.4469945938        0.1435352257
Cl            0.7047563036        0.9469945938        0.3564647743
Cl            0.7952436964        0.0530054062        0.8564647743
```

Structural Data for Material # 30

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of BCl in the $Pa\bar{3}$ (No. 205) structure.

```
CELL_PARAMETERS (bohr)
  23.758627451   0.000000000   0.000000000
   0.000000000  23.758627451   0.000000000
   0.000000000   0.000000000  23.758627451

ATOMIC_POSITIONS (crystal)
B             0.4046954244        0.0770124592        0.4394874176
B             0.5953045756        0.5770124592        0.0605125824
B             0.0953045756        0.9229875408        0.9394874176
B             0.9046954244        0.4229875408        0.5605125824
```

```
B       0.4394874176    0.4046954244    0.0770124592
B       0.0605125824    0.5953045756    0.5770124592
B       0.9394874176    0.0953045756    0.9229875408
B       0.5605125824    0.9046954244    0.4229875408
B       0.0770124592    0.4394874176    0.4046954244
B       0.5770124592    0.0605125824    0.5953045756
B       0.9229875408    0.9394874176    0.0953045756
B       0.4229875408    0.5605125824    0.9046954244
B       0.5953045756    0.9229875408    0.5605125824
B       0.4046954244    0.4229875408    0.9394874176
B       0.9046954244    0.0770124592    0.0605125824
B       0.0953045756    0.5770124592    0.4394874176
B       0.5605125824    0.5953045756    0.9229875408
B       0.9394874176    0.4046954244    0.4229875408
B       0.0605125824    0.9046954244    0.0770124592
B       0.4394874176    0.0953045756    0.5770124592
B       0.9229875408    0.5605125824    0.5953045756
B       0.4229875408    0.9394874176    0.4046954244
B       0.0770124592    0.0605125824    0.9046954244
B       0.5770124592    0.4394874176    0.0953045756
B       0.0349716369    0.3697654084    0.5245128106
B       0.9650283631    0.8697654084    0.9754871894
B       0.4650283631    0.6302345916    0.0245128106
B       0.5349716369    0.1302345916    0.4754871894
B       0.5245128106    0.0349716369    0.3697654084
B       0.9754871894    0.9650283631    0.8697654084
B       0.0245128106    0.4650283631    0.6302345916
B       0.4754871894    0.5349716369    0.1302345916
B       0.3697654084    0.5245128106    0.0349716369
B       0.8697654084    0.9754871894    0.9650283631
B       0.6302345916    0.0245128106    0.4650283631
B       0.1302345916    0.4754871894    0.5349716369
B       0.9650283631    0.6302345916    0.4754871894
B       0.0349716369    0.1302345916    0.0245128106
B       0.5349716369    0.3697654084    0.9754871894
B       0.4650283631    0.8697654084    0.5245128106
B       0.4754871894    0.9650283631    0.6302345916
B       0.0245128106    0.0349716369    0.1302345916
B       0.9754871894    0.5349716369    0.3697654084
B       0.5245128106    0.4650283631    0.8697654084
B       0.6302345916    0.4754871894    0.9650283631
B       0.1302345916    0.0245128106    0.0349716369
B       0.3697654084    0.9754871894    0.5349716369
B       0.8697654084    0.5245128106    0.4650283631
Cl      0.3077864499    0.1553181034    0.3772885618
Cl      0.6922135501    0.6553181034    0.1227114382
Cl      0.1922135501    0.8446818966    0.8772885618
Cl      0.8077864499    0.3446818966    0.6227114382
Cl      0.3772885618    0.3077864499    0.1553181034
Cl      0.1227114382    0.6922135501    0.6553181034
Cl      0.8772885618    0.1922135501    0.8446818966
Cl      0.6227114382    0.8077864499    0.3446818966
Cl      0.1553181034    0.3772885618    0.3077864499
Cl      0.6553181034    0.1227114382    0.6922135501
Cl      0.8446818966    0.8772885618    0.1922135501
Cl      0.3446818966    0.6227114382    0.8077864499
Cl      0.6922135501    0.8446818966    0.6227114382
Cl      0.3077864499    0.3446818966    0.8772885618
Cl      0.8077864499    0.1553181034    0.1227114382
```

```
Cl          0.1922135501        0.6553181034        0.3772885618
Cl          0.6227114382        0.6922135501        0.8446818966
Cl          0.8772885618        0.3077864499        0.3446818966
Cl          0.1227114382        0.8077864499        0.1553181034
Cl          0.3772885618        0.1922135501        0.6553181034
Cl          0.8446818966        0.6227114382        0.6922135501
Cl          0.3446818966        0.8772885618        0.3077864499
Cl          0.1553181034        0.1227114382        0.8077864499
Cl          0.6553181034        0.3772885618        0.1922135501
Cl          0.0697797822        0.2367917025        0.5485197206
Cl          0.9302202178        0.7367917025        0.9514802794
Cl          0.4302202178        0.7632082975        0.0485197206
Cl          0.5697797822        0.2632082975        0.4514802794
Cl          0.5485197206        0.0697797822        0.2367917025
Cl          0.9514802794        0.9302202178        0.7367917025
Cl          0.0485197206        0.4302202178        0.7632082975
Cl          0.4514802794        0.5697797822        0.2632082975
Cl          0.2367917025        0.5485197206        0.0697797822
Cl          0.7367917025        0.9514802794        0.9302202178
Cl          0.7632082975        0.0485197206        0.4302202178
Cl          0.2632082975        0.4514802794        0.5697797822
Cl          0.9302202178        0.7632082975        0.4514802794
Cl          0.0697797822        0.2632082975        0.0485197206
Cl          0.5697797822        0.2367917025        0.9514802794
Cl          0.4302202178        0.7367917025        0.5485197206
Cl          0.4514802794        0.9302202178        0.7632082975
Cl          0.0485197206        0.0697797822        0.2632082975
Cl          0.9514802794        0.5697797822        0.2367917025
Cl          0.5485197206        0.4302202178        0.7367917025
Cl          0.7632082975        0.4514802794        0.9302202178
Cl          0.2632082975        0.0485197206        0.0697797822
Cl          0.2367917025        0.9514802794        0.5697797822
Cl          0.7367917025        0.5485197206        0.4302202178
```

Structural Data for Material # 31

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of BCl_3 in the $P6_3/m$ (No. 176) structure.

```
CELL_PARAMETERS (bohr)
  1.20921447E+01   0.00000000E+00   0.00000000E+00
 -6.04607237E+00   1.47210453E+01  -0.00000000E+00
 -0.00000000E+00   0.00000000E+00   1.30604768E+01

ATOMIC_POSITIONS (crystal)
B           0.3333330000        0.6666670000        0.2500000000
B           0.6666670000        0.3333330000        0.7500000000
Cl          0.0773700163        0.3811023955        0.2500000000
Cl          0.9226299837        0.6188976045        0.7500000000
Cl          0.6188976045        0.6962676208        0.2500000000
Cl          0.3811023955        0.3037323792        0.7500000000
Cl          0.3037323792        0.9226299837        0.2500000000
Cl          0.6962676208        0.0773700163        0.7500000000
```

Structural Data for Material # 32

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of SCl_2 in the $P2_12_12_1$ (No. 19) structure.

```
CELL_PARAMETERS (bohr)
   8.181511123   0.000000000   0.000000000
   0.000000000  17.138239025   0.000000000
   0.000000000   0.000000000  30.924594299

ATOMIC_POSITIONS (crystal)
S              0.7482766669        0.8065951966        0.1978081848
S              0.7517233331        0.1934048034        0.6978081848
S              0.2482766669        0.6934048034        0.8021918152
S              0.2517233331        0.3065951966        0.3021918152
S              0.3751577418        0.7939876116        0.3477400326
S              0.1248422582        0.2060123884        0.8477400326
S              0.8751577418        0.7060123884        0.6522599674
S              0.6248422582        0.2939876116        0.1522599674
Cl             0.9691362878        0.7937372032        0.0849739466
Cl             0.5308637122        0.2062627968        0.5849739466
Cl             0.4691362878        0.7062627968        0.9150260534
Cl             0.0308637122        0.2937372032        0.4150260534
Cl             0.9272781448        0.9983900470        0.2421484446
Cl             0.5727218552        0.0016099530        0.7421484446
Cl             0.4272781448        0.5016099530        0.7578515554
Cl             0.0727218552        0.4983900470        0.2578515554
Cl             0.4930244332        0.9759387485        0.4120212907
Cl             1.0069755668        0.0240612515        0.9120212907
Cl            -0.0069755668        0.5240612515        0.5879787093
Cl             0.5069755668        0.4759387485        0.0879787093
Cl             0.5784327034        0.6315805231        0.4125857081
Cl             0.9215672966        0.3684194769        0.9125857081
Cl             0.0784327034        0.8684194769        0.5874142919
Cl             0.4215672966        0.1315805231        0.0874142919
```

Structural Data for Material # 33

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of SCl in the $Fdd2$ (No. 43) structure.

```
CELL_PARAMETERS (bohr)
  -0.000000000  -0.000000000   8.163587795
  27.591938843  -0.000000000   4.081793898
  -0.000000000  15.909037670   4.081793898

ATOMIC_POSITIONS (crystal)
S              0.6055653389        0.6614140550        0.4215851094
S              0.6885645033        0.3385859450        0.5784148906
S              1.0169793939        0.8385859450       -0.0784148906
S              0.7771504483        0.1614140550        1.0784148906
```

```
S             0.2882964749        0.9281471778        0.8219310151
S             0.0383746678        0.0718528222        0.1780689849
S            -0.0335563473        0.5718528222        0.3219310151
S             0.8602274901        0.4281471778        0.6780689849
Cl           -0.0260561292        0.7481109869        0.7484742246
Cl            0.4705290823        0.2518890131        0.2515257754
Cl            0.4720548578        0.7518890131        0.2484742246
Cl            0.4724180954        0.2481109869        0.7515257754
Cl            0.0070236210        0.0405030208        0.7451757991
Cl            0.7927024409        0.9594969792        0.2548242009
Cl            0.7975266418        0.4594969792        0.2451757991
Cl            0.5021994201        0.5405030208        0.7548242009
```

Structural Data for Material # 34

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of Cl_2O in the $I4_1/amd$ (No. 141) structure.

```
CELL_PARAMETERS (bohr)
   7.046954710   7.046954710   8.502294720
   7.046954710  -7.046954710  -8.502294720
  -7.046954710   7.046954710  -8.502294720

ATOMIC_POSITIONS (crystal)
Cl            0.0564458936        0.2556476394        0.6992017458
Cl            0.5564458936        0.1992017458        0.7556476394
Cl            0.9435541064        0.1992017458        0.1427558522
Cl            0.4435541064        0.6427558522        0.6992017458
Cl            0.9435541064        0.7443523606        0.3007982542
Cl            0.4435541064        0.8007982542        0.2443523606
Cl            0.0564458936        0.8007982542        0.8572441478
Cl            0.5564458936        0.3572441478        0.3007982542
O             0.2500000000        0.3432121031        0.5932121031
O             0.7500000000        0.0932121031        0.8432121031
O             0.7500000000        0.6567878969        0.4067878969
O             0.2500000000        0.9067878969        0.1567878969
```

Structural Data for Material # 35

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of ClO_3 in the Cc (No. 9) structure.

```
CELL_PARAMETERS (bohr)
  -5.220427243  -8.405069702   1.166122011
  -5.220427243   8.405069702   1.166122011
   0.644816494   0.000000000 -18.997050311
```

```
ATOMIC_POSITIONS (crystal)
Cl            0.4344075596        0.3199406431        0.1826220271
Cl            0.3199406431        0.4344075596        0.6826220271
Cl            0.9414547923        0.8127185996        0.4505804075
Cl            0.8127185996        0.9414547923        0.9505804075
O             0.4788606240        0.1177899866        0.2533551693
O             0.1177899866        0.4788606240        0.7533551693
O             0.2509067909        0.4354205440        0.2290756823
O             0.4354205440        0.2509067909        0.7290756823
O             0.8873492052        0.7499860472        0.2995988165
O             0.7499860472        0.8873492052        0.7995988165
O             0.2049289923        0.8084097355        0.5078382080
O             0.8084097355        0.2049289923        0.0078382080
O             0.9718181682        0.1081701394        0.4933902745
O             0.1081701394        0.9718181682        0.9933902745
O             0.6992788122        0.6107593598        0.4939394148
O             0.6107593598        0.6992788122        0.9939394148
```

Structural Data for Material # 36

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of Cl_2O_7 in the $C2/c$ (No. 15) structure.

```
CELL_PARAMETERS (bohr)
   0.000000000  -9.056772209   0.000000000
 -12.330345782   4.528386105   4.970493849
  -0.049362241   0.000000000 -17.065883895

ATOMIC_POSITIONS (crystal)
Cl            0.0130417767        0.2199572954        0.2722524532
Cl            0.7930844813        0.7800427046        0.2277475468
Cl            0.9869582233        0.7800427046        0.7277475468
Cl            0.2069155187        0.2199572954        0.7722524532
O             0.0912806794       -0.0000000000        0.2500000000
O             0.9087193206        1.0000000000        0.7500000000
O             0.8579549217        0.2547093114        0.4081462813
O             0.6032456103        0.7452906886        0.0918537187
O             0.1420450783        0.7452906886        0.5918537187
O             0.3967543897        0.2547093114        0.9081462813
O             0.8436626225        0.1733474413        0.1257505007
O             0.6703151812        0.8266525587        0.3742494993
O             0.1563373775        0.8266525587        0.8742494993
O             0.3296848188        0.1733474413        0.6257505007
O             0.9577382334        0.6459060939        0.2044576836
O             0.3118321394        0.3540939061        0.2955423164
O             0.0422617666        0.3540939061        0.7955423164
O             0.6881678606        0.6459060939        0.7044576836
```

Structural Data for Material # 37

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of ClO_2 in the *Pbca* (No. 61) structure.

```
CELL_PARAMETERS (bohr)
 -11.283192697   0.000000000   0.000000000
   0.000000000   0.000000000 -12.231186970
   0.000000000 -20.099900378   0.000000000

ATOMIC_POSITIONS (crystal)
Cl             0.3653250006        0.5262785410        0.6179802112
Cl             0.8653250006        0.4737214590        0.8820197888
Cl             0.6346749994        0.9737214590        0.1179802112
Cl             0.1346749994        0.0262785410        0.3820197888
Cl             0.6346749994        0.4737214590        0.3820197888
Cl             0.1346749994        0.5262785410        0.1179802112
Cl             0.3653250006        0.0262785410        0.8820197888
Cl             0.8653250006        0.9737214590        0.6179802112
O              0.4830297057        0.6549539317        0.7126428784
O              0.9830297057        0.3450460683        0.7873571216
O              0.5169702943        0.8450460683        0.2126428784
O              0.0169702943        0.1549539317        0.2873571216
O              0.5169702943        0.3450460683        0.2873571216
O              0.0169702943        0.6549539317        0.2126428784
O              0.4830297057        0.1549539317        0.7873571216
O              0.9830297057        0.8450460683        0.7126428784
O              0.1746667582        0.6279203151        0.9934860168
O              0.6746667582        0.3720796849        0.5065139832
O              0.8253332418        0.8720796849        0.4934860168
O              0.3253332418        0.1279203151        0.0065139832
O              0.8253332418        0.3720796849        0.0065139832
O              0.3253332418        0.6279203151        0.4934860168
O              0.1746667582        0.1279203151        0.5065139832
O              0.6746667582        0.8720796849        0.9934860168
```

Structural Data for Material # 38

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of $LiAlB_{14}$ in the *C*2 (No. 5) structure.

```
CELL_PARAMETERS (bohr)
  11.664250268   0.000000000   0.000000004
   5.832125085   6.921594097   9.339396666
   5.832125084  -7.933300138  10.122686504

ATOMIC_POSITIONS (crystal)
Li             0.0411234506        0.5323606305        0.9274235067
Li             0.5009075880        0.4676393696        0.0725764934
Al             0.0472730023        0.7003696696        0.5389813728
Al             0.2866240445        0.2996303299        0.4610186267
B              0.6909079014        0.1297586666        0.0282939738
B              0.8489605416        0.8702413335        0.9717060264
B              0.8188799651        0.4577896182        0.3767496870
```

```
B             0.6534192704        0.5422103818        0.6232503129
B             0.3177025731        0.8641536528        0.9750790226
B             0.1569352486        0.1358463472        0.0249209773
B             0.3103391754        0.8572789186        0.3648367163
B             0.5324548088        0.1427210819        0.6351632842
B             0.8086195059        0.8919649107        0.2218388506
B             0.9224232672        0.1080350895        0.7781611495
B             0.7479993106        0.2621698503        0.6076169606
B             0.6177861213        0.7378301499        0.3923830395
B             0.2127613927        0.1011109323        0.7846946325
B             0.0985669573        0.8988890677        0.2153053675
B             0.4373441733        0.4003801590        0.7398430300
B             0.5775673626        0.5996198411        0.2601569700
B             0.9074493388        0.2899373530        0.9067335755
B             0.1041202671        0.7100626470        0.0932664245
B             0.3371541164        0.7085661080        0.6264400505
B             0.6721602748        0.2914338921        0.3735599496
B             0.8354351403        0.1539579997        0.1819199831
B             0.1713131230        0.8460420004        0.8180800169
B             0.3685622428        0.2689120755       -0.0034930354
B             0.6339812832        0.7310879245        1.0034930354
B             0.7832456123        0.5724727319        0.7735390425
B             0.1292573865        0.4275272678        0.2264609573
B             0.6476148917        0.8642280153        0.7692677565
B             0.2811106624        0.1357719845        0.2307322433
```

Structural Data for Material # 39

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of Li_5AlS_4 in the $P2_1/m$ (No. 11) structure.

```
CELL_PARAMETERS (bohr)
  -0.025137306   0.000000000  11.597390671
  12.893471679   0.000000000  -0.101344711
   0.000000000  14.657434655   0.000000000

ATOMIC_POSITIONS (crystal)
Li            0.3532664535        0.3345376954        0.4854072563
Li            0.6467335465        0.6654623046        0.9854072563
Li            0.6467335465        0.6654623046        0.5145927437
Li            0.3532664535        0.3345376954        0.0145927437
Li            0.6559320763        0.1653766058        0.2500000000
Li            0.3440679237        0.8346233942        0.7500000000
Li            0.0147553814        0.4722493979        0.7500000000
Li            0.9852446186        0.5277506021        0.2500000000
Li           -0.0000000000        1.0000000000        0.5000000000
Li            0.0000000000        0.0000000000        0.0000000000
Al            0.6333113681        0.1730896195        0.7500000000
Al            0.3666886319        0.8269103805        0.2500000000
S             0.7561486193        0.8641775671        0.7500000000
S             0.2438513807        0.1358224329        0.2500000000
S             0.2641762037        0.1750320126        0.7500000000
S             0.7358237963        0.8249679874        0.2500000000
```

```
S             0.7601409839        0.3302544689        0.9864526314
S             0.2398590161        0.6697455311        0.4864526314
S             0.2398590161        0.6697455311        0.0135473686
S             0.7601409839        0.3302544689        0.5135473686
```

Structural Data for Material # 40

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of Li_5AlO_4 in the *Pbca* (No. 61) structure.

```
CELL_PARAMETERS (bohr)
 -16.888167054   0.000000000   0.000000000
   0.000000000   0.000000000 -17.117384718
   0.000000000 -17.188502938   0.000000000

ATOMIC_POSITIONS (crystal)
Li            0.3612522793        0.6139584291        0.6018920273
Li            0.8612522793        0.3860415709        0.8981079727
Li            0.6387477207        0.8860415709        0.1018920273
Li            0.1387477207        0.1139584291        0.3981079727
Li            0.6387477207        0.3860415709        0.3981079727
Li            0.1387477207        0.6139584291        0.1018920273
Li            0.3612522793        0.1139584291        0.8981079727
Li            0.8612522793        0.8860415709        0.6018920273
Li            0.1028694796        0.6185358813        0.8406013941
Li            0.6028694796        0.3814641187        0.6593986059
Li            0.8971305204        0.8814641187        0.3406013941
Li            0.3971305204        0.1185358813        0.1593986059
Li            0.8971305204        0.3814641187        0.1593986059
Li            0.3971305204        0.6185358813        0.3406013941
Li            0.1028694796        0.1185358813        0.6593986059
Li            0.6028694796        0.8814641187        0.8406013941
Li            0.4011637749        0.8730106397        0.6446207259
Li            0.9011637749        0.1269893603        0.8553792741
Li            0.5988362251        0.6269893603        0.1446207259
Li            0.0988362251        0.3730106397        0.3553792741
Li            0.5988362251        0.1269893603        0.3553792741
Li            0.0988362251        0.8730106397        0.1446207259
Li            0.4011637749        0.3730106397        0.8553792741
Li            0.9011637749        0.6269893603        0.6446207259
Li            0.1672836551        0.8940380516        0.8804289039
Li            0.6672836551        0.1059619484        0.6195710961
Li            0.8327163449        0.6059619484        0.3804289039
Li            0.3327163449        0.3940380516        0.1195710961
Li            0.8327163449        0.1059619484        0.1195710961
Li            0.3327163449        0.8940380516        0.3804289039
Li            0.1672836551        0.3940380516        0.6195710961
Li            0.6672836551        0.6059619484        0.8804289039
Li            0.1315581445        0.8530739934        0.6207435586
Li            0.6315581445        0.1469260066        0.8792564414
Li            0.8684418555        0.6469260066        0.1207435586
Li            0.3684418555        0.3530739934        0.3792564414
Li            0.8684418555        0.1469260066        0.3792564414
```

```
Li          0.3684418555        0.8530739934        0.1207435586
Li          0.1315581445        0.3530739934        0.8792564414
Li          0.6315581445        0.6469260066        0.6207435586
Al          0.3840933969        0.6443318144        0.8772649287
Al          0.8840933969        0.3556681856        0.6227350713
Al          0.6159066031        0.8556681856        0.3772649287
Al          0.1159066031        0.1443318144        0.1227350713
Al          0.6159066031        0.3556681856        0.1227350713
Al          0.1159066031        0.6443318144        0.3772649287
Al          0.3840933969        0.1443318144        0.6227350713
Al          0.8840933969        0.8556681856        0.8772649287
O           0.0068905320        0.7520991859        0.9898110323
O           0.5068905320        0.2479008141        0.5101889677
O           0.9931094680        0.7479008141        0.4898110323
O           0.4931094680        0.2520991859        0.0101889677
O           0.9931094680        0.2479008141        0.0101889677
O           0.4931094680        0.7520991859        0.4898110323
O           0.0068905320        0.2520991859        0.5101889677
O           0.5068905320        0.7479008141        0.9898110323
O           0.4999100042        0.5369268187        0.7572656839
O           0.9999100042        0.4630731813        0.7427343161
O           0.5000899958        0.9630731813        0.2572656839
O           0.0000899958        0.0369268187        0.2427343161
O           0.5000899958        0.4630731813        0.2427343161
O           0.0000899958        0.5369268187        0.2572656839
O           0.4999100042        0.0369268187        0.7427343161
O           0.9999100042        0.9630731813        0.7572656839
O           0.2611377178        0.5140616043        0.9617982506
O           0.7611377178        0.4859383957        0.5382017494
O           0.7388622822        0.9859383957        0.4617982506
O           0.2388622822        0.0140616043        0.0382017494
O           0.7388622822        0.4859383957        0.0382017494
O           0.2388622822        0.5140616043        0.4617982506
O           0.2611377178        0.0140616043        0.5382017494
O           0.7611377178        0.9859383957        0.9617982506
O           0.2676710406        0.7481370577        0.7566607680
O           0.7676710406        0.2518629423        0.7433392320
O           0.7323289594        0.7518629423        0.2566607680
O           0.2323289594        0.2481370577        0.2433392320
O           0.7323289594        0.2518629423        0.2433392320
O           0.2323289594        0.7481370577        0.2566607680
O           0.2676710406        0.2481370577        0.7433392320
O           0.7676710406        0.7518629423        0.7566607680
```

Structural Data for Material # 41

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of $LiAlO_2$ in the $R\bar{3}m$ (No. 166) structure.

```
CELL_PARAMETERS (bohr)
  -2.649891646  -4.589747134  -0.000000000
  -5.299783392  -0.000000000  -0.000000000
  -2.649891646  -1.529915678  -8.938524090
```

```
ATOMIC_POSITIONS (crystal)
Li            0.5000000000        0.5000000000        0.5000000000
Al            0.0000000000       -0.0000000000       -0.0000000000
O             0.7388520511        0.7388520508        0.7834438482
O             0.2611479489        0.2611479492        0.2165561518
```

Structural Data for Material # 42

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of $LiAl_5O_8$ in the $P4_332$ (No. 212) structure.

```
CELL_PARAMETERS (bohr)
  14.986768282   0.000000000   0.000000000
   0.000000000  14.986768282   0.000000000
   0.000000000   0.000000000  14.986768282

ATOMIC_POSITIONS (crystal)
Li            0.8750000000        0.3750000000        0.1250000000
Li            0.1250000000        0.8750000000        0.3750000000
Li            0.3750000000        0.1250000000        0.8750000000
Li            0.6250000000        0.6250000000        0.6250000000
Al            0.2477078817        0.7477078817        0.7522921183
Al            0.7522921183        0.2477078817        0.7477078817
Al            0.7477078817        0.7522921183        0.2477078817
Al            0.2522921183        0.2522921183        0.2522921183
Al            0.5022921183        0.0022921183        0.4977078817
Al            0.0022921183        0.4977078817        0.5022921183
Al            0.4977078817        0.5022921183        0.0022921183
Al            0.9977078817        0.9977078817        0.9977078817
Al            0.3750000000        0.6311808731        0.3811808731
Al            0.6250000000        0.1311808731        0.1188191269
Al            0.1311808731        0.1188191269        0.6250000000
Al            0.8688191269        0.6188191269        0.8750000000
Al            0.6188191269        0.8750000000        0.8688191269
Al            0.3811808731        0.3750000000        0.6311808731
Al            0.8750000000        0.8688191269        0.6188191269
Al            0.1250000000        0.3688191269        0.8811808731
Al            0.6311808731        0.3811808731        0.3750000000
Al            0.3688191269        0.8811808731        0.1250000000
Al            0.1188191269        0.6250000000        0.1311808731
Al            0.8811808731        0.1250000000        0.3688191269
O             0.6347872312        0.8821795441        0.6349368952
O             0.3652127688        0.3821795441        0.8650631048
O             0.3821795441        0.8650631048        0.3652127688
O             0.6178204559        0.3650631048        0.1347872312
O             0.3650631048        0.1347872312        0.6178204559
O             0.6349368952        0.6347872312        0.8821795441
O             0.1347872312        0.6178204559        0.3650631048
O             0.8652127688        0.1178204559        0.1349368952
O             0.8821795441        0.6349368952        0.6347872312
O             0.1178204559        0.1349368952        0.8652127688
O             0.8650631048        0.3652127688        0.3821795441
```

```
O             0.1349368952        0.8652127688        0.1178204559
O             0.3678204559        0.6152127688        0.6150631048
O             0.8678204559        0.8847872312        0.3849368952
O             0.6321795441        0.1152127688        0.8849368952
O             0.1321795441        0.3847872312        0.1150631048
O             0.8847872312        0.3849368952        0.8678204559
O             0.1152127688        0.8849368952        0.6321795441
O             0.6152127688        0.6150631048        0.3678204559
O             0.3847872312        0.1150631048        0.1321795441
O             0.3849368952        0.8678204559        0.8847872312
O             0.8849368952        0.6321795441        0.1152127688
O             0.6150631048        0.3678204559        0.6152127688
O             0.1150631048        0.1321795441        0.3847872312
O             0.6354849354        0.1354849354        0.3645150646
O             0.3645150646        0.6354849354        0.1354849354
O             0.1354849354        0.3645150646        0.6354849354
O             0.8645150646        0.8645150646        0.8645150646
O             0.1145150646        0.6145150646        0.8854849354
O             0.6145150646        0.8854849354        0.1145150646
O             0.8854849354        0.1145150646        0.6145150646
O             0.3854849354        0.3854849354        0.3854849354
```

Structural Data for Material # 43

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of $LiAlCl_4$ in the $P2_1/c$ (No. 14) structure.

```
CELL_PARAMETERS (bohr)
   0.000000000 -13.589043681   0.000000000
 -13.105924901   0.000000000   0.898726149
   0.310609070   0.000000000 -23.531601243

ATOMIC_POSITIONS (crystal)
Li            0.5807884372        0.8520427274        0.1221686231
Li            0.0807884372        0.1479572726        0.3778313769
Li            0.4192115628        0.1479572726        0.8778313769
Li            0.9192115628        0.8520427274        0.6221686231
Al            0.9108142361        0.6960878580        0.3700742878
Al            0.4108142361        0.3039121420        0.1299257122
Al            0.0891857639        0.3039121420        0.6299257122
Al            0.5891857639        0.6960878580        0.8700742878
Cl            0.7953032015        0.6791480554       -0.0072586673
Cl            0.2953032015        0.3208519446        0.5072586673
Cl            0.2046967985        0.3208519446        1.0072586673
Cl            0.7046967985        0.6791480554        0.4927413327
Cl            0.1545174532        0.8136686401        0.4548463979
Cl            0.6545174532        0.1863313599        0.0451536021
Cl            0.8454825468        0.1863313599        0.5451536021
Cl            0.3454825468        0.8136686401        0.9548463979
Cl            0.8454303203        0.9182554671        0.2632905512
Cl            0.3454303203        0.0817445329        0.2367094488
Cl            0.1545696797        0.0817445329        0.7367094488
Cl            0.6545696797        0.9182554671        0.7632905512
```

```
Cl            0.9618225994        0.4248447255        0.2807095545
Cl            0.4618225994        0.5751552745        0.2192904455
Cl            0.0381774006        0.5751552745        0.7192904455
Cl            0.5381774006        0.4248447255        0.7807095545
```

Structural Data for Material # 44

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of $Li_2B_2S_5$ in the $Cmcm$ (No. 63) structure.

```
CELL_PARAMETERS (bohr)
  -0.000000000  10.920700175   0.000000000
   0.000000000   0.000000000   9.429180592
  19.246796428  -5.460350088  -0.000000000

ATOMIC_POSITIONS (crystal)
Li            0.1927223949        0.7500000000        0.8122663392
Li            0.6195439444        0.2500000000        0.8122663392
Li            0.8072776051        0.2500000000        0.1877336608
Li            0.3804560556        0.7500000000        0.1877336608
B             0.7491662270        0.0000000000        0.4983324540
B             0.7491662270        0.5000000000        0.4983324540
B             0.2508337730       -0.0000000000        0.5016675460
B             0.2508337730        0.5000000000        0.5016675460
S             0.0763915188        0.7500000000        1.0000000000
S             0.9236084812        0.2500000000        0.0000000000
S             0.7163346946        0.7500000000        0.1012221746
S             0.3848874800        0.2500000000        0.1012221746
S             0.2836653054        0.2500000000        0.8987778254
S             0.6151125200        0.7500000000        0.8987778254
S             0.0347213548        0.7500000000        0.5744512843
S             0.5397299295        0.2500000000        0.5744512843
S             0.9652786452        0.2500000000        0.4255487157
S             0.4602700705        0.7500000000        0.4255487157
```

Structural Data for Material # 45

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of $Li_5B_7S_{13}$ in the Cc (No. 9) structure.

```
CELL_PARAMETERS (bohr)
  20.746701568  -0.109950489 -10.023691549
  -5.099242180  20.275412865 -10.123845570
   0.042094011  -0.029886502  26.244920592

ATOMIC_POSITIONS (crystal)
Li            0.7926790978        0.5253359330        0.7413304158
```

Li	0.4458317614	0.1657742238	0.7044761790
Li	0.2413226572	0.4612619170	0.2955901800
Li	0.5513135403	0.7839901024	0.2586086164
Li	0.6926689803	0.6161908624	0.4286144764
Li	0.1923673251	0.8228520434	0.4401566851
Li	0.2523759281	0.3826624500	0.5598869457
Li	0.7642074798	0.1875596862	0.5713913517
Li	0.6959832658	0.2712793813	0.2216978552
Li	0.0286916894	0.9396766860	0.2257052494
Li	0.3029990113	0.7140746042	0.7742807117
Li	0.9742848922	0.0495416474	0.7782017443
Li	0.1149824322	0.7297373093	0.9354341585
Li	0.3294160634	0.2343886973	0.9429353631
Li	0.8864701997	0.2915597502	0.0570742829
Li	0.6794930928	0.7942899748	0.0645032717
Li	0.5374149705	0.4967953745	0.9704498951
Li	0.0671753927	0.5264754604	0.0297406799
Li	0.9667654588	0.5477080024	0.4853078454
Li	0.9815093678	0.0624330595	0.5147026886
B	0.4742947837	0.2297312961	0.4533167260
B	0.5209510609	0.7764367839	0.5466718430
B	0.4350622506	0.2945542327	0.2493139281
B	0.3162690405	0.9557384264	0.2513738622
B	0.5648873316	0.7043641119	0.7486094398
B	0.6857597118	0.0452495363	0.7506938327
B	0.2040772208	0.1815241280	0.2499170992
B	0.5493130604	0.0714891952	0.2577592381
B	0.7915444730	0.8137244947	0.7422275545
B	0.4541664990	0.9316208895	0.7500811450
B	0.2785688383	0.0259983802	0.0509666042
B	0.7276176813	0.9750275960	0.9490265839
B	0.6992836032	0.3336458208	0.4510308021
B	0.2501678935	0.1190619414	0.4474630718
B	0.3026886833	0.6716160238	0.5525314535
B	0.7482295233	0.8826283512	0.5489584030
B	0.1733587930	0.2482486851	0.0542197241
B	0.3851381509	0.8086751031	0.0571657860
B	0.8279630107	0.7514880772	0.9428107198
B	0.6191619260	0.1940299485	0.9457929180
B	0.7413537944	0.4840280796	0.1517353132
B	0.9053106677	0.6621283842	0.1443177147
B	0.2610225254	0.5178123665	0.8556701304
B	0.0896585374	0.3323161152	0.8482922076
B	0.0155286922	0.5879115687	0.3400774975
B	0.8364618155	0.7566944200	0.3452638798
B	0.9912222306	0.4114203682	0.6547373179
B	0.1754784213	0.2478308041	0.6599363082
S	0.3693672489	0.2962422544	0.3535911389
S	0.4850153530	0.0626060617	0.3595012053
S	0.6254937475	0.7031143105	0.6404786742
S	0.5157740109	0.9426747146	0.6464124137
S	0.4469529918	0.1316314429	0.1490794786
S	0.2048937969	0.0149123755	0.1457608045
S	0.5591394311	0.8691547072	0.8542292409
S	0.7978868736	0.9825487643	0.8509164139
S	0.6375109435	0.3344608420	0.5563309516
S	0.4106267971	0.2353085288	0.5556801445
S	0.3549158601	0.6796479295	0.4443109715
S	0.5811337618	0.7781817786	0.4436544289

```
S             0.6015366380        0.3980724011        0.3465589736
S             0.2508770612        0.9499546897        0.3511096491
S             0.3997520943        0.5988624680        0.6488879872
S             0.7549780467        0.0515271490        0.6534438643
S             0.3366087868        0.3645461334        0.1529599681
S             0.3167426538        0.7895296740        0.1522033377
S             0.6645260793        0.6373121986        0.8477673433
S             0.6836718451        0.2115994137        0.8470572239
S             0.8958174159        0.7484200824        0.8406293171
S             0.4490659901        0.0953429481        0.8482864053
S             0.1007645375        0.2470481481        0.1517160180
S             0.5551748863        0.9077908413        0.1593452616
S             0.1331454889        0.1781796382        0.3464494819
S             0.7175391154        0.1711825036        0.3577190747
S             0.8597844724        0.8134442159        0.6422466064
S             0.2866943129        0.8317541392        0.6535524550
S             0.2774455109        0.8633952311        0.9484917933
S             0.1812060889        0.0878889128        0.9482906511
S             0.7329481624        0.1395947940        0.0517114624
S             0.8289580194        0.9148828918        0.0514911974
S             0.0574980842        0.6266159719        0.2384689773
S             0.6922338513        0.6186106881        0.2512964100
S             0.9409817135        0.3673332559        0.7487254473
S             0.3190661956        0.3881364190        0.7615418696
S             0.7691290206        0.5164308460        0.0410074396
S             0.2281737335        0.4754397338        0.9589990966
S             0.8803753204        0.4396856867        0.2488268301
S             0.8677407295        0.8059868468        0.2432677790
S             0.1244992194        0.5627053963        0.7567065411
S             0.1315815464        0.1908690219        0.7512015069
S             0.9846680469        0.7290985930        0.4491233771
S             0.0355656406        0.2799618299        0.5508820026
S             0.8551438071        0.4603273493        0.5573551504
S             0.2048978193        0.0975448848        0.5560192683
S             0.1488605145        0.5415491909        0.4439985849
S             0.7977853359        0.9029947764        0.4426501287
S             0.5940584602        0.3455291113        0.0516798448
S             0.9548154699        0.7014069421        0.0463480356
S             0.4084822543        0.6550775387        0.9536371920
S             0.0424023867        0.2939014370        0.9483508793
```

Structural Data for Material # 46

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of Li_3BS_3 in the *Pnma* (No. 62) structure.

```
CELL_PARAMETERS (bohr)
   0.000000000   0.000000000  11.569937198
  15.263125419   0.000000000   0.000000000
   0.000000000  18.855286337   0.000000000

ATOMIC_POSITIONS (crystal)
Li            0.9486128717        0.5079473063        0.2500000000
```

```
Li            0.5513871283        0.0079473063        0.2500000000
Li            0.0513871283        0.4920526937        0.7500000000
Li            0.4486128717        0.9920526937        0.7500000000
Li            0.9033530400        0.8270918340        0.0077999273
Li            0.5966469600        0.3270918340        0.4922000727
Li            0.0966469600        0.1729081660        0.5077999273
Li            0.4033530400        0.6729081660        0.9922000727
Li            0.0966469600        0.1729081660        0.9922000727
Li            0.4033530400        0.6729081660        0.5077999273
Li            0.9033530400        0.8270918340        0.4922000727
Li            0.5966469600        0.3270918340        0.0077999273
B             0.1200634585        0.8843345693        0.2500000000
B             0.3799365415        0.3843345693        0.2500000000
B             0.8799365415        0.1156654307        0.7500000000
B             0.6200634585        0.6156654307        0.7500000000
S             0.8424448436        0.8001872755        0.2500000000
S             0.6575551564        0.3001872755        0.2500000000
S             0.1575551564        0.1998127245        0.7500000000
S             0.3424448436        0.6998127245        0.7500000000
S             0.2618228651        0.9263357993        0.0922348896
S             0.2381771349        0.4263357993        0.4077651104
S             0.7381771349        0.0736642007        0.5922348896
S             0.7618228651        0.5736642007        0.9077651104
S             0.7381771349        0.0736642007        0.9077651104
S             0.7618228651        0.5736642007        0.5922348896
S             0.2618228651        0.9263357993        0.4077651104
S             0.2381771349        0.4263357993        0.0922348896
```

Structural Data for Material # 47

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of $Li_2B_4O_7$ in the $I4_1cd$ (No. 110) structure.

```
CELL_PARAMETERS (bohr)
  1.78884418E+01  -3.47176689E-06   0.00000000E+00
 -3.47176689E-06   1.78884416E+01   0.00000000E+00
  0.00000000E+00   0.00000000E+00   1.97696237E+01

ATOMIC_POSITIONS (crystal)
Li            0.1726786580        0.1565214888        0.1592520832
Li            0.3273213837        0.3434785601        0.6592522716
Li            0.8434784300        0.6726786391        0.4092522003
Li            0.6565213736        0.8273214173        0.9092520977
Li            0.1726787097        0.8434785376        0.6592522329
Li            0.3273212490        0.6565213817        0.1592521444
Li            0.8434784916        0.3273212352        0.9092522160
Li            0.6565213435        0.1726786144        0.4092521385
Li            0.6726786163        0.6565214399        0.6592522716
Li            0.8273213420        0.8434785112        0.1592520832
Li            0.3434786264        0.1726785827        0.9092520977
Li            0.1565215700        0.3273213609        0.4092522003
Li            0.6726787510        0.3434786183        0.1592521444
Li            0.8273212903        0.1565214624        0.6592522329
```

Li	0.3434786565	0.8273213856	0.4092521385
Li	0.1565215084	0.6726787648	0.9092522160
B	0.0850747889	0.1682614107	0.8009406184
B	0.4149258668	0.3317393622	0.3009410363
B	0.8317393202	0.5850744583	0.0509409694
B	0.6682606646	0.9149253848	0.5509410789
B	0.0850744931	0.8317391723	0.3009409074
B	0.4149257614	0.6682605049	0.8009411163
B	0.8317383439	0.4149254596	0.5509404483
B	0.6682600004	0.0850742639	0.0509414000
B	0.5850741332	0.6682606378	0.3009410363
B	0.9149252111	0.8317385893	0.8009406184
B	0.3317393354	0.0850746152	0.5509410789
B	0.1682606798	0.4149255417	0.0509409694
B	0.5850742386	0.3317394951	0.8009411163
B	0.9149255069	0.1682608277	0.3009409074
B	0.3317399996	0.9149257361	0.0509414000
B	0.1682616561	0.5850745404	0.5509404483
B	0.1126368507	0.9481325800	0.9192642630
B	0.3873634238	0.5518674541	0.4192641777
B	0.0518674066	0.6126367122	0.1692642065
B	0.4481326283	0.8873632584	0.6692641672
B	0.1126367962	0.0518674599	0.4192641486
B	0.3873633658	0.4481325720	0.9192642115
B	0.0518675565	0.3873632766	0.6692642002
B	0.4481326742	0.1126367237	0.1692642094
B	0.6126365762	0.4481325459	0.4192641777
B	0.8873631493	0.0518674200	0.9192642630
B	0.5518673717	0.1126367416	0.6692641672
B	0.9481325934	0.3873632878	0.1692642065
B	0.6126366342	0.5518674280	0.9192642115
B	0.8873632038	0.9481325401	0.4192641486
B	0.5518673258	0.8873632763	0.1692642094
B	0.9481324435	0.6126367234	0.6692642002
O	0.1361353782	0.2809976401	0.7350543279
O	0.3638643262	0.2190019131	0.2350540395
O	0.7190019911	0.6361355842	0.9850540010
O	0.7809981872	0.8638644224	0.4850540893
O	0.1361354257	0.7190020397	0.2350540810
O	0.3638643417	0.7809982636	0.7350539399
O	0.7190026712	0.3638645661	0.4850544974
O	0.7809985826	0.1361355045	0.9850536913
O	0.6361356738	0.7809980869	0.2350540395
O	0.8638646218	0.7190023599	0.7350543279
O	0.2190018128	0.1361355776	0.4850540893
O	0.2809980089	0.3638644158	0.9850540010
O	0.6361356583	0.2190017364	0.7350539399
O	0.8638645743	0.2809979603	0.2350540810
O	0.2190014174	0.8638644955	0.9850536913
O	0.2809973288	0.6361354339	0.4850544974
O	0.1778623804	0.0688655371	0.8468931454
O	0.3221375791	0.4311342754	0.3468930803
O	0.9311342675	0.6778623573	0.0968929583
O	0.5688657907	0.8221377374	0.5968931430
O	0.1778622790	0.9311343046	0.3468930599
O	0.3221376537	0.5688657951	0.8468930765
O	0.9311344990	0.3221375493	0.5968931297
O	0.5688659167	0.1778622583	0.0968930224
O	0.6778624209	0.5688657246	0.3468930803

```
O             0.8221376196        0.9311344629        0.8468931454
O             0.4311342093        0.1778622626        0.5968931430
O             0.0688657325        0.3221376427        0.0968929583
O             0.6778623463        0.4311342049        0.8468930765
O             0.8221377210        0.0688656954        0.3468930599
O             0.4311340833        0.8221377417        0.0968930224
O             0.0688655010        0.6778624507        0.5968931297
O             0.9415616606        0.1558499497        0.8209116307
O             0.5584378301        0.3441498976        0.3209113719
O             0.8441499604        0.4415619359        0.0709114727
O             0.6558500363        0.0584381623        0.5709115534
O             0.9415617696        0.8441499755        0.3209114805
O             0.5584379953        0.6558501001        0.8209114930
O             0.8441499507        0.5584381575        0.5709114931
O             0.6558500416        0.9415619455        0.0709114122
O             0.4415621699        0.6558501024        0.3209113719
O             0.0584383394        0.8441500503        0.8209116307
O             0.3441499637        0.9415618377        0.5709115534
O             0.1558500396        0.5584380641        0.0709114727
O             0.4415620047        0.3441498999        0.8209114930
O             0.0584382304        0.1558500245        0.3209114805
O             0.3441499584        0.0584380545        0.0709114122
O             0.1558500493        0.4415618425        0.5709114931
O             0.0000000000        0.0000000000       -0.0006319634
O             0.5000000000        0.5000000000        0.4993681007
O             0.0000000000        0.5000000000        0.2493680342
O             0.5000000000        0.0000000000        0.7493681405
O             0.0000000000        0.0000000000        0.4993680422
O             0.5000000000        0.5000000000       -0.0006319013
O             0.0000000000        0.5000000000        0.7493679604
O             0.5000000000        0.0000000000        0.2493681187
```

Structural Data for Material # 48

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of $Li_3B_{11}O_{18}$ in the $P2_1/c$ (No. 14) structure.

```
CELL_PARAMETERS (bohr)
   0.000000000  14.732129015   0.000000000
   0.115634832   0.000000000  18.319834711
  33.166679238   0.000000000  -6.155657795

ATOMIC_POSITIONS (crystal)
Li            0.1850541786        0.5030943636        0.0411536643
Li            0.6850541786        0.9969056364        0.9588463357
Li            0.8149458214        0.4969056364        0.9588463357
Li            0.3149458214        0.0030943636        0.0411536643
Li            0.4124228716        0.7165433969        0.2457600858
Li            0.9124228716        0.7834566031        0.7542399142
Li            0.5875771284        0.2834566031        0.7542399142
Li            0.0875771284        0.2165433969        0.2457600858
Li            0.0518983617        0.8591144968        0.4202950436
Li            0.5518983617        0.6408855032        0.5797049564
```

```
Li          0.9481016383        0.1408855032        0.5797049564
Li          0.4481016383        0.3591144968        0.4202950436
B           0.6222311831        0.7517958362        0.0057908593
B           0.1222311831        0.7482041638        0.9942091407
B           0.3777688169        0.2482041638        0.9942091407
B           0.8777688169        0.2517958362        0.0057908593
B           0.9247819821        0.0961617184        0.0952817863
B           0.4247819821        0.4038382816        0.9047182137
B           0.0752180179        0.9038382816        0.9047182137
B           0.5752180179        0.5961617184        0.0952817863
B           0.3767106419        0.9881241440        0.1939048201
B           0.8767106419        0.5118758560        0.8060951799
B           0.6232893581        0.0118758560        0.8060951799
B           0.1232893581        0.4881241440        0.1939048201
B           0.8953830341        0.5021654113        0.2839737612
B           0.3953830341        0.9978345887        0.7160262388
B           0.1046169659        0.4978345887        0.7160262388
B           0.6046169659        0.0021654113        0.2839737612
B           0.1642028204        0.6633886456        0.6286726671
B           0.6642028204        0.8366113544        0.3713273329
B           0.8357971796        0.3366113544        0.3713273329
B           0.3357971796        0.1633886456        0.6286726671
B           0.2151834972        0.7526129509        0.5142586787
B           0.7151834972        0.7473870491        0.4857413213
B           0.7848165028        0.2473870491        0.4857413213
B           0.2848165028        0.2526129509        0.5142586787
B           0.0573139628        0.9612380724        0.3082897303
B           0.5573139628        0.5387619276        0.6917102697
B           0.9426860372        0.0387619276        0.6917102697
B           0.4426860372        0.4612380724        0.3082897303
B           0.9394983218        0.9239527332        0.1827500428
B           0.4394983218        0.5760472668        0.8172499572
B           0.0605016782        0.0760472668        0.8172499572
B           0.5605016782        0.4239527332        0.1827500428
B           0.3670077904        0.7806541309        0.0877691117
B           0.8670077904        0.7193458691        0.9122308883
B           0.6329922096        0.2193458691        0.9122308883
B           0.1329922096        0.2806541309        0.0877691117
B           0.4442572529        0.6820635086        0.4130971430
B           0.9442572529        0.8179364914        0.5869028570
B           0.5557427471        0.3179364914        0.5869028570
B           0.0557427471        0.1820635086        0.4130971430
B           0.9960746548        0.7182305677        0.2428309382
B           0.4960746548        0.7817694323        0.7571690618
B           0.0039253452        0.2817694323        0.7571690618
B           0.5039253452        0.2182305677        0.2428309382
O           0.2277903742        0.7004811023        0.0444581905
O           0.7277903742        0.7995188977        0.9555418095
O           0.7722096258        0.2995188977        0.9555418095
O           0.2722096258        0.2004811023        0.0444581905
O           0.4882297227        0.8339647639        0.0349134407
O           0.9882297227        0.6660352361        0.9650865593
O           0.5117702773        0.1660352361        0.9650865593
O           0.0117702773        0.3339647639        0.0349134407
O           0.4544738933        0.6862352516        0.1304675467
O           0.9544738933        0.8137647484        0.8695324533
O           0.5455261067        0.3137647484        0.8695324533
O           0.0455261067        0.1862352516        0.1304675467
O           0.6521726738        0.6217644169        0.0280024337
```

```
0    0.1521726738    0.8782355831    0.9719975663
0    0.3478273262    0.3782355831    0.9719975663
0    0.8478273262    0.1217644169    0.0280024337
0    0.2949829709    0.9071478659    0.1335804735
0    0.7949829709    0.5928521341    0.8664195265
0    0.7050170291    0.0928521341    0.8664195265
0    0.2050170291    0.4071478659    0.1335804735
0    0.4770686822    0.9214015318    0.2417644799
0    0.9770686822    0.5785984682    0.7582355201
0    0.5229313178    0.0785984682    0.7582355201
0    0.0229313178    0.4214015318    0.2417644799
0    0.2069136688    0.5577056120    0.6676505974
0    0.7069136688    0.9422943880    0.3323494026
0    0.7930863312    0.4422943880    0.3323494026
0    0.2930863312    0.0577056120    0.6676505974
0    0.0155689980    0.7364931385    0.6420745981
0    0.5155689980    0.7635068615    0.3579254019
0    0.9844310020    0.2635068615    0.3579254019
0    0.4844310020    0.2364931385    0.6420745981
0    0.4866664620    0.5164286521    0.2435488500
0    0.9866664620    0.9835713479    0.7564511500
0    0.5133335380    0.4835713479    0.7564511500
0    0.0133335380    0.0164286521    0.2435488500
0    0.2751071686    0.6777834415    0.5689785341
0    0.7751071686    0.8222165585    0.4310214659
0    0.7248928314    0.3222165585    0.4310214659
0    0.2248928314    0.1777834415    0.5689785341
0    0.0665547951    0.8277300512    0.5257907070
0    0.5665547951    0.6722699488    0.4742092930
0    0.9334452049    0.1722699488    0.4742092930
0    0.4334452049    0.3277300512    0.5257907070
0    0.2896086877    0.7536621885    0.4459151701
0    0.7896086877    0.7463378115    0.5540848299
0    0.7103913123    0.2463378115    0.5540848299
0    0.2103913123    0.2536621885    0.4459151701
0    0.4008744656    0.5397727653    0.3762202878
0    0.9008744656    0.9602272347    0.6237797122
0    0.5991255344    0.4602272347    0.6237797122
0    0.0991255344    0.0397727653    0.3762202878
0    0.0690976233    0.8200850066    0.3052592252
0    0.5690976233    0.6799149934    0.6947407748
0    0.9309023767    0.1799149934    0.6947407748
0    0.4309023767    0.3200850066    0.3052592252
0    0.8679709247    0.6357156586    0.2758419208
0    0.3679709247    0.8642843414    0.7241580792
0    0.1320290753    0.3642843414    0.7241580792
0    0.6320290753    0.1357156586    0.2758419208
0    0.1381252106    0.6292603612    0.2065385299
0    0.6381252106    0.8707396388    0.7934614701
0    0.8618747894    0.3707396388    0.7934614701
0    0.3618747894    0.1292603612    0.2065385299
0    0.9160347239    0.7877044157    0.1851069356
0    0.4160347239    0.7122955843    0.8148930644
0    0.0839652761    0.2122955843    0.8148930644
0    0.5839652761    0.2877044157    0.1851069356
0    0.8782555499    0.9766071696    0.1203020498
0    0.3782555499    0.5233928304    0.8796979502
0    0.1217444501    0.0233928304    0.8796979502
0    0.6217444501    0.4766071696    0.1203020498
```

Structural Data for Material # 49

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of LiB_3O_5 in the $Pna2_1$ (No. 33) structure.

```
CELL_PARAMETERS (bohr)
   0.000000000   0.000000000  -9.860337042
   0.000000000 -13.890337013   0.000000000
 -15.833326620   0.000000000   0.000000000

ATOMIC_POSITIONS (crystal)
Li             0.4465854800        0.5684238597        0.4181209601
Li             0.9465854800        0.4315761403        0.5818790399
Li             0.9465854800        0.0684238597        0.0818790399
Li             0.4465854800        0.9315761403        0.9181209601
B              0.8122848592        0.6645104735        0.0086175993
B              0.3122848592        0.3354895265        0.9913824007
B              0.3122848592        0.1645104735        0.4913824007
B              0.8122848592        0.8354895265        0.5086175993
B              0.5073446429        0.9413541150        0.3054375049
B              0.0073446429        0.0586458850        0.6945624951
B              0.0073446429        0.4413541150        0.1945624951
B              0.5073446429        0.5586458850        0.8054375049
B              0.6887575170        0.2476538789        0.3426812743
B              0.1887575170        0.7523461211        0.6573187257
B              0.1887575170        0.7476538789        0.1573187257
B              0.6887575170        0.2523461211        0.8426812743
O              0.8086597860        0.5019003686        0.0837519237
O              0.3086597860        0.4980996314        0.9162480763
O              0.3086597860        0.0019003686        0.4162480763
O              0.8086597860        0.9980996314        0.5837519237
O              0.6546124352        0.7929966250        0.3833671764
O              0.1546124352        0.2070033750        0.6166328236
O              0.1546124352        0.2929966250        0.1166328236
O              0.6546124352        0.7070033750        0.8833671764
O              0.9860915119        0.7985933188        0.0580247701
O              0.4860915119        0.2014066812        0.9419752299
O              0.4860915119        0.2985933188        0.4419752299
O              0.9860915119        0.7014066812        0.5580247701
O              0.6875461625        0.0889318783        0.2590480989
O              0.1875461625        0.9110681217        0.7409519011
O              0.1875461625        0.5889318783        0.2409519011
O              0.6875461625        0.4110681217        0.7590480989
O              0.3832176054        0.8731133530        0.1604887661
O              0.8832176054        0.1268866470        0.8395112339
O              0.8832176054        0.3731133530        0.3395112339
O              0.3832176054        0.6268866470        0.6604887661
```

Structural Data for Material # 50

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of Li_3BO_3 in the $P2_1/c$ (No. 14) structure.

```
CELL_PARAMETERS (bohr)
  -6.019008570   0.000000000   1.169741302
  -0.021798331   0.000000000 -15.656204301
   0.000000000 -17.331245457   0.000000000

ATOMIC_POSITIONS (crystal)
Li             0.5061281707        0.4810377406        0.7666127713
Li             0.4938718293        0.0189622594        0.2666127713
Li             0.4938718293        0.5189622594        0.2333872287
Li             0.5061281707        0.9810377406        0.7333872287
Li             0.7238373459        0.3871881587        0.5228043615
Li             0.2761626541        0.1128118413        0.0228043615
Li             0.2761626541        0.6128118413        0.4771956385
Li             0.7238373459        0.8871881587        0.9771956385
Li             0.9082776111        0.3676569362        0.0737942838
Li             0.0917223889        0.1323430638        0.5737942838
Li             0.0917223889        0.6323430638        0.9262057162
Li             0.9082776111        0.8676569362        0.4262057162
B              0.8016228526        0.2453458099        0.8142178549
B              0.1983771474        0.2546541901        0.3142178549
B              0.1983771474        0.7546541901        0.1857821451
B              0.8016228526        0.7453458099        0.6857821451
O              0.9724137458        0.4011551614        0.8631051648
O              0.0275862542        0.0988448386        0.3631051648
O              0.0275862542        0.5988448386        0.1368948352
O              0.9724137458        0.9011551614        0.6368948352
O              0.7727511923        0.1109040886        0.9065858904
O              0.2272488077        0.3890959114        0.4065858904
O              0.2272488077        0.8890959114        0.0934141096
O              0.7727511923        0.6109040886        0.5934141096
O              0.6341659396        0.2213955051        0.6739400675
O              0.3658340604        0.2786044949        0.1739400675
O              0.3658340604        0.7786044949        0.3260599325
O              0.6341659396        0.7213955051        0.8260599325
```

Structural Data for Material # 51

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of $Li_3B_7O_{12}$ in the $P\bar{1}$ (No. 2) structure.

```
CELL_PARAMETERS (bohr)
  11.877730829   0.009774097  -3.148006747
  -2.647544310  14.618710277  -0.496079088
   0.006613556   0.057787968  16.138409435

ATOMIC_POSITIONS (crystal)
Li             0.5138182904        0.8059067268        0.6844201312
Li             0.4861817096        0.1940932732        0.3155798688
Li             0.9856262015        0.4239538151        0.6938530656
Li             0.0143737985        0.5760461849        0.3061469344
Li             0.2814649352        0.6987636457        0.9689214599
Li             0.7185350648        0.3012363543        0.0310785401
B              0.2339357273        0.9967860281        0.7288276440
```

```
B             0.7660642727        0.0032139719        0.2711723560
B             0.4065314994        0.4637598683        0.7984870694
B             0.5934685006        0.5362401317        0.2015129306
B             0.8864495138        0.0737804886        0.7126426430
B             0.1135504862        0.9262195114        0.2873573570
B             0.4556663823        0.7899847332        0.3116369716
B             0.5443336177        0.2100152668        0.6883630284
B             0.9410348289        0.7744431716        0.7739144259
B             0.0589651711        0.2255568284        0.2260855741
B             0.7144052828        0.6374257950        0.4929441309
B             0.2855947172        0.3625742050        0.5070558691
B             0.7484847775        0.6316879740        0.9618228368
B             0.2515152225        0.3683120260        0.0381771632
O             0.9074527964        0.8880154571        0.3115081540
O             0.0925472036        0.1119845429        0.6884918460
O             0.1716901949        0.8403240789        0.7856437106
O             0.8283098051        0.1596759211        0.2143562894
O             0.9392017636        0.6977793088        0.9283173242
O             0.0607982364        0.3022206912        0.0716826758
O             0.8152822052        0.9136789495        0.7541105154
O             0.1847177948        0.0863210505        0.2458894846
O             0.2384296734        0.4435214587        0.8930668872
O             0.7615703266        0.5564785413        0.1069331128
O             0.5589326432        0.7390601174        0.4728414024
O             0.4410673568        0.2609398826        0.5271585976
O             0.7255408248        0.5284527973        0.3677829713
O             0.2744591752        0.4715472027        0.6322170287
O             0.7723751190        0.2056564557        0.6918027473
O             0.2276248810        0.7943435443        0.3081972527
O             0.5494580315        0.6365847729        0.8535476964
O             0.4505419685        0.3634152271        0.1464523036
O             0.5369909245        0.3301544751        0.8187051314
O             0.4630090755        0.6698455249        0.1812948686
O             0.5624650512        0.9667446214        0.2890916413
O             0.4375349488        0.0332553786        0.7109083587
O             0.8605571357        0.6362819917        0.6408029401
O             0.1394428643        0.3637180083        0.3591970599
```

Structural Data for Material # 52

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of $Li_6B_4O_9$ in the $P2_1/c$ (No. 14) structure.

```
CELL_PARAMETERS (bohr)
   5.967825389   0.000000000  -1.886951076
  -5.991522293   0.000000000 -16.265515885
   0.000000000  44.199160722   0.000000000

ATOMIC_POSITIONS (crystal)
Li            0.3090075139        0.1806802141        0.8798336693
Li            0.1909924861        0.3193197859        0.3798336693
Li            0.6909924861        0.8193197859        0.1201663307
Li            0.8090075139        0.6806802141        0.6201663307
```

Li	0.8203279983	0.4583351540	0.9427276909
Li	0.6796720017	0.0416648460	0.4427276909
Li	0.1796720017	0.5416648460	0.0572723091
Li	0.3203279983	0.9583351540	0.5572723091
Li	0.7422246809	0.4895130950	0.4580845624
Li	0.7577753191	0.0104869050	0.9580845624
Li	0.2577753191	0.5104869050	0.5419154376
Li	0.2422246809	0.9895130950	0.0419154376
Li	0.1799678448	0.0238776334	0.3571077997
Li	0.3200321552	0.4761223666	0.8571077997
Li	0.8200321552	0.9761223666	0.6428922003
Li	0.6799678448	0.5238776334	0.1428922003
Li	0.1685430096	0.3528197883	0.2037143707
Li	0.3314569904	0.1471802117	0.7037143707
Li	0.8314569904	0.6471802117	0.7962856293
Li	0.6685430096	0.8528197883	0.2962856293
Li	0.6843107965	0.3038338650	0.2932161177
Li	0.8156892035	0.1961661350	0.7932161177
Li	0.3156892035	0.6961661350	0.7067838823
Li	0.1843107965	0.8038338650	0.2067838823
B	0.2436236467	0.2378169217	0.4764681545
B	0.2563763533	0.2621830783	0.9764681545
B	0.7563763533	0.7621830783	0.5235318455
B	0.7436236467	0.7378169217	0.0235318455
B	0.3260288528	0.2019750896	0.5860568640
B	0.1739711472	0.2980249104	0.0860568640
B	0.6739711472	0.7980249104	0.4139431360
B	0.8260288528	0.7019750896	0.9139431360
B	0.1951237292	0.0653996673	0.1480923405
B	0.3048762708	0.4346003327	0.6480923405
B	0.8048762708	0.9346003327	0.8519076595
B	0.6951237292	0.5653996673	0.3519076595
B	0.1730026378	0.0845846344	0.2572290141
B	0.3269973622	0.4154153656	0.7572290141
B	0.8269973622	0.9154153656	0.7427709859
B	0.6730026378	0.5845846344	0.2427709859
O	0.2758409619	0.1164604102	0.9735966327
O	0.2241590381	0.3835395898	0.4735966327
O	0.7241590381	0.8835395898	0.0264033673
O	0.7758409619	0.6164604102	0.5264033673
O	0.1901447139	0.1461758722	0.4304061420
O	0.3098552861	0.3538241278	0.9304061420
O	0.8098552861	0.8538241278	0.5695938580
O	0.6901447139	0.6461758722	0.0695938580
O	0.1607666091	0.3381897384	0.0281417556
O	0.3392333909	0.1618102616	0.5281417556
O	0.8392333909	0.6618102616	0.9718582444
O	0.6607666091	0.8381897384	0.4718582444
O	0.1622445550	0.4071661075	0.1241928125
O	0.3377554450	0.0928338925	0.6241928125
O	0.8377554450	0.5928338925	0.8758071875
O	0.6622445550	0.9071661075	0.3758071875
O	0.2054301429	0.1509295085	0.0979490514
O	0.2945698571	0.3490704915	0.5979490514
O	0.7945698571	0.8490704915	0.9020509486
O	0.7054301429	0.6509295085	0.4020509486
O	0.1685401559	0.1398348859	0.1996784777
O	0.3314598441	0.3601651141	0.6996784777
O	0.8314598441	0.8601651141	0.8003215223

```
O             0.6685401559        0.6398348859        0.3003215223
O             0.7093941501        0.4214723877        0.3593498799
O             0.7906058499        0.0785276123        0.8593498799
O             0.2906058499        0.5785276123        0.6406501201
O             0.2093941501        0.9214723877        0.1406501201
O             0.3315011054        0.3105411902        0.7986457236
O             0.1684988946        0.1894588098        0.2986457236
O             0.6684988946        0.6894588098        0.2013542764
O             0.8315011054        0.8105411902        0.7013542764
O             0.6814381673        0.4400685469        0.2312769377
O             0.8185618327        0.0599314531        0.7312769377
O             0.3185618327        0.5599314531        0.7687230623
O             0.1814381673        0.9400685469        0.2687230623
```

Structural Data for Material # 53

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of $LiBO_2$ in the $I\bar{4}2d$ (No. 122) structure.

```
CELL_PARAMETERS (bohr)
   7.91972942E+00   0.00000000E+00   0.00000000E+00
   0.00000000E+00   7.91972942E+00   0.00000000E+00
   0.00000000E+00   0.00000000E+00   1.23304990E+00

ATOMIC_POSITIONS (crystal)
Li            0.0000000000        0.0000000000        0.5000000000
Li            0.5000000000       -0.0000000000        0.2499915347
Li            0.5000000000        0.5000000000        0.0000000000
Li            0.0000000000        0.5000000000        0.7500084653
B             0.0000000000        0.0000000000        0.0000000000
B             0.5000000000       -0.0000000000        0.7499997106
B             0.5000000000        0.5000000000        0.5000000000
B             0.0000000000        0.5000000000        0.2500002894
O             0.1584554863        0.2500008096        0.1249991615
O             0.8415445137        0.7499991904        0.1249991615
O             0.2500008096        0.8415445137        0.8750008385
O             0.7499991904        0.1584554863        0.8750008385
O             0.3415451072        0.2500002947        0.6250005842
O             0.6584548928        0.7499997053        0.6250005842
O             0.7499997053        0.3415451072        0.3749994158
O             0.2500002947        0.6584548928        0.3749994158
```

Structural Data for Material # 54

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of $LiClO_2$ in the $P4_2/ncm$ (No. 138) structure.

```
CELL_PARAMETERS (bohr)
   8.977441828   0.000000000   0.000000000
   0.000000000   8.977441828   0.000000000
   0.000000000   0.000000000  19.146643255

ATOMIC_POSITIONS (crystal)
Li             0.7500000000        0.2500000000        0.2500000000
Li             0.7500000000        0.2500000000        0.7500000000
Li             0.2500000000        0.7500000000        0.2500000000
Li             0.2500000000        0.7500000000        0.7500000000
Cl             0.7500000000        0.7500000000        0.9330818187
Cl             0.7500000000        0.7500000000        0.4330818187
Cl             0.2500000000        0.2500000000        0.0669181813
Cl             0.2500000000        0.2500000000        0.5669181813
O              0.5567407727        0.5567407727        0.8431466624
O              0.5567407727        0.9432592273        0.3431466624
O              0.9432592273        0.5567407727        0.3431466624
O              0.9432592273        0.9432592273        0.8431466624
O              0.4432592273        0.4432592273        0.1568533376
O              0.4432592273        0.0567407727        0.6568533376
O              0.0567407727        0.4432592273        0.6568533376
O              0.0567407727        0.0567407727        0.1568533376
```

Structural Data for Material # 55

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of Li_5Cl_3O in the $Fmm2$ (No. 42) structure.

```
CELL_PARAMETERS (bohr)
  12.900286669  -4.239070095  -0.000000000
  -4.239070095  12.900286669   0.000000000
  -4.330608287  -4.330608287  13.145432617

ATOMIC_POSITIONS (crystal)
Li             0.3160640255        0.3160640255        0.6321280510
Li             0.8160640255        0.8160640255        0.6321280510
Li             0.0865863596        0.5865863596       -0.2260136381
Li             0.6874000023        0.1874000023        0.7739863619
Li             0.3697772940        0.0480845440       -0.0821381620
Li             0.5480845440        0.8697772940       -0.0821381620
Li             0.5810849194        0.5810849194        1.1621698389
Li             0.0810849194        0.0810849194        0.1621698389
Li             0.4801096600        0.9801096600        0.4579765566
Li            -0.0221331034        0.4778668966        0.4579765566
Cl             0.7171455220        0.6802190608        0.8973645829
Cl             1.1802190608        0.2171455220        0.8973645829
Cl             0.3048006647       -0.1951993353        0.1091654347
Cl             0.8043647700        0.3043647700        0.1091654347
Cl             0.4023824221        0.4957471105        0.3981295326
Cl            -0.0042528895        0.9023824221        0.3981295326
O              0.7970781647        0.2970781647        0.5941563295
O              0.3541396387        0.8541396387        0.7082792773
```

Structural Data for Material # 56

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of $LiClO_4$ in the *Pnma* (No. 62) structure.

```
CELL_PARAMETERS (bohr)
   0.000000000   0.000000000  -9.164428312
   0.000000000 -12.898601245   0.000000000
 -16.354625212   0.000000000   0.000000000

ATOMIC_POSITIONS (crystal)
Li            0.5000000000        0.0000000000        0.5000000000
Li            0.0000000000        0.5000000000        1.0000000000
Li            0.5000000000        0.5000000000        0.5000000000
Li           -0.0000000000       -0.0000000000        0.0000000000
Cl            0.5356783522        0.7500000000        0.1822172238
Cl            0.9643216478        0.7500000000        0.6822172238
Cl            0.4643216478        0.2500000000        0.8177827762
Cl            0.0356783522        0.2500000000        0.3177827762
O             0.5434067782        0.7500000000        0.3519918239
O             0.9565932218        0.7500000000        0.8519918239
O             0.4565932218        0.2500000000        0.6480081761
O             0.0434067782        0.2500000000        0.1480081761
O             0.6732544482        0.9255721006        0.1280935099
O             0.8267455518        0.5744278994        0.6280935099
O             0.3267455518        0.4255721006        0.8719064901
O             0.1732544482        0.0744278994        0.3719064901
O             0.3267455518        0.0744278994        0.8719064901
O             0.1732544482        0.4255721006        0.3719064901
O             0.6732544482        0.5744278994        0.1280935099
O             0.8267455518        0.9255721006        0.6280935099
O             0.2509934404        0.7500000000        0.1288619780
O             0.2490065596        0.7500000000        0.6288619780
O             0.7490065596        0.2500000000        0.8711380220
O             0.7509934404        0.2500000000        0.3711380220
```

Structural Data for Material # 57

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of Al_5BO_9 in the $Cmc2_1$ (No. 36) structure.

```
CELL_PARAMETERS (bohr)
  -0.000000000  -0.000000000  10.796772950
  14.580644957  -0.000000000  -0.000000000
  -0.000000000  14.189703411  -5.398386425

ATOMIC_POSITIONS (crystal)
Al            0.8638564397        0.0006985625        0.2312167426
Al            0.3673603029        0.0006985625        0.2312167426
Al            0.1361435603        0.5006985625        0.7687832574
Al            0.6326396971        0.5006985625        0.7687832574
```

```
Al            0.2556735529        0.1823140207        0.5113471059
Al            0.7443264471        0.6823140207        0.4886528941
Al            0.4432957174        0.1878170637        0.8865914348
Al            0.5567042826        0.6878170637        0.1134085652
Al            0.7025183183        0.3330487241        0.4050366366
Al            0.2974816817        0.8330487241        0.5949633634
B             0.9850399435        0.2238721079        0.9700798871
B             0.0149600565        0.7238721079        0.0299201129
O             0.1621819701        0.2884415200        0.9054373188
O             0.7432553486        0.2884415200        0.9054373187
O             0.8378180299        0.7884415200        0.0945626812
O             0.2567446514        0.7884415200        0.0945626813
O             0.9331834652        0.1995410351        0.3809100173
O             0.4477265521        0.1995410351        0.3809100173
O             0.0668165348        0.6995410351        0.6190899827
O             0.5522734479        0.6995410351        0.6190899827
O             0.3530246379        0.0365034491        0.7060492758
O             0.6469753621        0.5365034491        0.2939507242
O             0.8084901433        0.4365122845        0.6169802866
O             0.1915098567        0.9365122845        0.3830197134
O             0.3319765338        0.3661895490        0.6639530676
O             0.6680234662        0.8661895490        0.3360469324
O             0.5455937619        0.0748234221        0.0911875238
O             0.4544062381        0.5748234221        0.9088124762
O             0.0466494723        0.0945571437        0.0932989446
O             0.9533505277        0.5945571437        0.9067010554
```

Structural Data for Material # 58

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of $Al_4B_6O_{15}$ in the $R3$ (No. 146) structure.

```
CELL_PARAMETERS (bohr)
  -0.000000003  -0.000000002  12.283600531
  10.841838792  -6.259539101  -4.094532844
   0.000000005  12.519076304  -4.094532844

ATOMIC_POSITIONS (crystal)
Al           -0.0025839045        0.0000000003        0.0000000003
Al            0.1966396867        0.4892292262        0.2811305200
Al            0.7074104606        0.7919012943        0.5107707750
Al            0.9155091668        0.7188694804        0.2080987058
B             0.4760449319        0.3315004625        0.0758076221
B             0.1445444693        0.7443071592        0.6684995357
B             0.4002373095        0.9241923773        0.2556928413
B             0.7264871693        0.2263218845        0.9013440481
B             0.5001652838        0.6750221651        0.7736781169
B             0.8251431186        0.0986559495        0.3249778341
O             0.9227677818        0.4479752405        0.0273095667
O             0.4747925411        0.5793343268        0.5520247605
O             0.8954582145        0.9726904329        0.4206656729
O             0.4998613195        0.1878887936        0.8943229833
O             0.3119725257        0.7064341888        0.8121112063
```

```
O             0.6055383370        0.1056770170        0.2935658098
O             0.7592669748        0.0387813255        0.7874676032
O             0.7204856492        0.7486862779        0.9612186758
O             0.9717993717        0.2125323970        0.2513137215
O             0.2563267622        0.2724691765        0.0811725360
O             0.9838575853        0.8087033591        0.7275308246
O             0.1751542266        0.9188274641        0.1912966391
O             0.1242431201        0.7020113675        0.4558969755
O             0.4222317530        0.7538856079        0.2979886329
O             0.6683461454        0.5441030256        0.2461143926
```

Structural Data for Material # 59

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of $AlSCl_7$ in the Pc (No. 7) structure.

```
CELL_PARAMETERS (bohr)
   0.000000000 -11.880072120   0.000000000
 -12.586381282   0.000000000   2.720121509
   0.816425043   0.000000000 -23.948623219

ATOMIC_POSITIONS (crystal)
Al            0.5079054307        0.4560404225        0.3527362612
Al            0.4920945693        0.4560404225        0.8527362612
S             0.0849100984        0.1201051601        0.6963682540
S             0.9150899016        0.1201051601        0.1963682540
Cl            0.3051561237        0.9394195886        0.6028999032
Cl            0.6948438763        0.9394195886        0.1028999032
Cl            0.9163449593        0.9113106149        0.7508692500
Cl            0.0836550407        0.9113106149        0.2508692500
Cl            0.8919576098        0.1746458425        0.5790264392
Cl            0.1080423902        0.1746458425        0.0790264392
Cl            0.1670241356        0.4749408911        0.3507049537
Cl            0.8329758644        0.4749408911        0.8507049537
Cl            0.6357898309        0.6976298031        0.4778292808
Cl            0.3642101691        0.6976298031        0.9778292808
Cl            0.6374793940        0.4657920569        0.1963513483
Cl            0.3625206060        0.4657920569        0.6963513483
Cl            0.6067737021        0.1684156203        0.3811143096
Cl            0.3932262979        0.1684156203        0.8811143096
```

Structural Data for Material # 60

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of AlClO in the $Pmmn$ (No. 59) structure.

```
CELL_PARAMETERS (bohr)
  -6.880831189   0.000000000   0.000000000
   0.000000000   0.000000000  -5.938732853
   0.000000000 -15.347479105   0.000000000

ATOMIC_POSITIONS (crystal)
Al             0.5000000000        1.0000000000        0.1014916183
Al             1.0000000000        0.5000000000        0.8985083817
Cl             0.5000000000        0.5000000000        0.3079012940
Cl             0.0000000000        1.0000000000        0.6920987060
O              0.5000000000        0.5000000000        0.9522317170
O              0.0000000000        1.0000000000        0.0477682830
```

Structural Data for Material # 61

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of Li_2AlBO_4 in the $P2_1/c$ (No. 14) structure.

```
CELL_PARAMETERS (bohr)
   0.000000000  -9.581313985   0.000000000
 -11.811732600   0.000000000   1.189432948
  -0.040222887   0.000000000 -19.449135562

ATOMIC_POSITIONS (crystal)
Li             0.6716070676        0.2742277790        0.4276046234
Li             0.1716070676        0.7257722210        0.0723953766
Li             0.3283929324        0.7257722210        0.5723953766
Li             0.8283929324        0.2742277790        0.9276046234
Li             0.8612866163        0.3948112575        0.2105984783
Li             0.3612866163        0.6051887425        0.2894015217
Li             0.1387133837        0.6051887425        0.7894015217
Li             0.6387133837        0.3948112575        0.7105984783
Al             0.6473460791        0.9975980247        0.1576707344
Al             0.1473460791        0.0024019753        0.3423292656
Al             0.3526539209        0.0024019753        0.8423292656
Al             0.8526539209        0.9975980247        0.6576707344
B              0.8223557220        0.7010999581        0.4409199959
B              0.3223557220        0.2989000419        0.0590800041
B              0.1776442780        0.2989000419        0.5590800041
B              0.6776442780        0.7010999581        0.9409199959
O              0.3539423748        0.8980264983        0.2158177180
O              0.8539423748        0.1019735017        0.2841822820
O              0.6460576252        0.1019735017        0.7841822820
O              0.1460576252        0.8980264983        0.7158177180
O              0.7020390000        0.5511350809        0.3590584382
O              0.2020390000        0.4488649191        0.1409415618
O              0.2979610000        0.4488649191        0.6409415618
O              0.7979610000        0.5511350809        0.8590584382
O              0.8065693531        0.8007417964        0.0499103667
O              0.3065693531        0.1992582036        0.4500896333
O              0.1934306469        0.1992582036        0.9500896333
O              0.6934306469        0.8007417964        0.5499103667
O              0.0869389798        0.7640186079        0.4215657678
```

```
O             0.5869389798        0.2359813921        0.0784342322
O             0.9130610202        0.2359813921        0.5784342322
O             0.4130610202        0.7640186079        0.9215657678
```

Structural Data for Material # 62

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of $Li_2AlB_5O_{10}$ in the $P2_1/c$ (No. 14) structure.

```
CELL_PARAMETERS (bohr)
 -13.367884394   0.000000000   0.173218809
   0.009381294   0.000000000 -13.378095068
   0.000000000 -28.288870456   0.000000000

ATOMIC_POSITIONS (crystal)
Li            0.8981082607        0.0019287829        0.8281081917
Li            0.1018917393        0.4980712171        0.3281081917
Li            0.1018917393        0.9980712171        0.1718918083
Li            0.8981082607        0.5019287829        0.6718918083
Li            0.6988642921        0.4131901134        0.0711294613
Li            0.3011357079        0.0868098866        0.5711294613
Li            0.3011357079        0.5868098866        0.9288705387
Li            0.6988642921        0.9131901134        0.4288705387
Al            0.8508018843        0.4626881514        0.8758833588
Al            0.1491981157        0.0373118486        0.3758833588
Al            0.1491981157        0.5373118486        0.1241166412
Al            0.8508018843        0.9626881514        0.6241166412
B             0.7890567829        0.4805439166        0.2207103046
B             0.2109432171        0.0194560834        0.7207103046
B             0.2109432171        0.5194560834        0.7792896954
B             0.7890567829        0.9805439166        0.2792896954
B             0.7996511907        0.0976081106        0.9717321879
B             0.2003488093        0.4023918894        0.4717321879
B             0.2003488093        0.9023918894        0.0282678121
B             0.7996511907        0.5976081106        0.5282678121
B             0.7593257954        0.2641898804        0.4994799896
B             0.2406742046        0.2358101196       -0.0005200104
B             0.2406742046        0.7358101196        0.5005200104
B             0.7593257954        0.7641898804        1.0005200104
B             0.5445112900        0.5002439366        0.7462998377
B             0.4554887100       -0.0002439366        0.2462998377
B             0.4554887100        0.4997560634        0.2537001623
B             0.5445112900        1.0002439366        0.7537001623
B             0.6809188343        0.9931772669        0.1202718982
B             0.3190811657        0.5068227331        0.6202718982
B             0.3190811657        0.0068227331        0.8797281018
B             0.6809188343        0.4931772669        0.3797281018
O             0.9188378228        0.4681211750        0.1543081455
O             0.0811621772        0.0318788250        0.6543081455
O             0.0811621772        0.5318788250        0.8456918545
O             0.9188378228        0.9681211750        0.3456918545
O             0.7266538152        0.4876357609        0.7750055247
O             0.2733461848        0.0123642391        0.2750055247
```

```
O             0.2733461848        0.5123642391        0.2249944753
O             0.7266538152        0.9876357609        0.7249944753
O             0.8505165982        0.2249831810        0.9082406743
O             0.1494834018        0.2750168190        0.4082406743
O             0.1494834018        0.7750168190        0.0917593257
O             0.8505165982        0.7249831810        0.5917593257
O             0.7604360381        0.0824085766        0.5305371792
O             0.2395639619        0.4175914234        0.0305371792
O             0.2395639619        0.9175914234        0.4694628208
O             0.7604360381        0.5824085766        0.9694628208
O             0.7195758436        0.1412271877        0.0517890812
O             0.2804241564        0.3587728123        0.5517890812
O             0.2804241564        0.8587728123        0.9482109188
O             0.7195758436        0.6412271877        0.4482109188
O             0.8368991760        0.4094465659        0.5516394997
O             0.1631008240        0.0905534341        0.0516394997
O             0.1631008240        0.5905534341        0.4483605003
O             0.8368991760        0.9094465659        0.9483605003
O             0.5033730089        0.4739241244        0.6589080461
O             0.4966269911        0.0260758756        0.1589080461
O             0.4966269911        0.5260758756        0.3410919539
O             0.5033730089        0.9739241244        0.8410919539
O             0.1679369397        0.4923852874        0.6912578541
O             0.8320630603        0.0076147126        0.1912578541
O             0.8320630603        0.5076147126        0.3087421459
O             0.1679369397        0.9923852874        0.8087421459
O             0.3995201423        0.0393864939        0.6930732006
O             0.6004798577        0.4606135061        0.1930732006
O             0.6004798577        0.9606135061        0.3069267994
O             0.3995201423        0.5393864939        0.8069267994
O             0.3162412146        0.1954544512        0.9189807526
O             0.6837587854        0.3045455488        0.4189807526
O             0.6837587854        0.8045455488        0.0810192474
O             0.3162412146        0.6954544512        0.5810192474
```

Structural Data for Material # 63

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of $LiAlB_2O_5$ in the $C2/c$ (No. 15) structure.

```
CELL_PARAMETERS (bohr)
  -9.227148960  -9.187658351   4.992549084
  -9.227148960   9.187658351   4.992549084
   1.882847544   0.000000000 -15.312938208

ATOMIC_POSITIONS (crystal)
Li            0.3342622554        0.6065975992        0.4195098872
Li            0.3934024008        0.6657377446        0.0804901128
Li            0.6657377446        0.3934024008        0.5804901128
Li            0.6065975992        0.3342622554        0.9195098872
Al            0.0200893882        0.7340897058        0.8406617335
Al            0.2659102942        0.9799106118        0.6593382665
Al            0.9799106118        0.2659102942        0.1593382665
```

```
Al            0.7340897058        0.0200893882        0.3406617335
B             0.7121426705        0.7396747357        0.4691672504
B             0.2603252643        0.2878573295        0.0308327496
B             0.2878573295        0.2603252643        0.5308327496
B             0.7396747357        0.7121426705        0.9691672504
B             0.0791640934        0.9208359066        0.2500000000
B             0.9208359066        0.0791640934        0.7500000000
B             0.6231559922        0.3768440078        0.2500000000
B             0.3768440078        0.6231559922        0.7500000000
O             0.1443457449        0.8466473959        0.3964161420
O             0.1533526041        0.8556542551        0.1035838580
O             0.8556542551        0.1533526041        0.6035838580
O             0.8466473959        0.1443457449        0.8964161420
O             0.7924606169        0.4001382831        0.2182850250
O             0.5998617169        0.2075393831        0.2817149750
O             0.2075393831        0.5998617169        0.7817149750
O             0.4001382831        0.7924606169        0.7182850250
O             0.8380910008        0.8888353798        0.1494988606
O             0.1111646202        0.1619089992        0.3505011394
O             0.1619089992        0.1111646202        0.8505011394
O             0.8888353798        0.8380910008        0.6494988606
O             0.1801226212        0.3794210034        0.1652185108
O             0.6205789966        0.8198773788        0.3347814892
O             0.8198773788        0.6205789966        0.8347814892
O             0.3794210034        0.1801226212        0.6652185108
O             0.6290691613        0.5641779150        0.4362958507
O             0.4358220850        0.3709308387        0.0637041493
O             0.3709308387        0.4358220850        0.5637041493
O             0.5641779150        0.6290691613        0.9362958507
```

Structural Data for Material # 64

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of $Li_3AlB_2O_6$ in the $P\bar{1}$ (No. 2) structure.

```
CELL_PARAMETERS (bohr)
   9.246271740   0.009875789  -0.063400499
   0.055267054  11.126443924  -3.265457428
  -0.096152416   0.362865236  14.862878296

ATOMIC_POSITIONS (crystal)
Li            0.8191034217        0.6038585103        0.4275341646
Li            0.1808965783        0.3961414897        0.5724658354
Li            0.6773836188        0.4692862575        0.7610169951
Li            0.3226163812        0.5307137425        0.2389830049
Li            0.6663645961        0.7616944563        0.1088868601
Li            0.3336354039        0.2383055437        0.8911131399
Al            0.8525978099        0.9484748827        0.7706919921
Al            0.1474021901        0.0515251173        0.2293080079
B             0.3363569513        0.8278767255        0.5901183881
B             0.6636430487        0.1721232745        0.4098816119
B             0.1589655604        0.6787518925        0.9303470846
B             0.8410344396        0.3212481075        0.0696529154
```

```
O             0.7274755615        0.2079414177        0.9064202427
O             0.2725244385        0.7920585823        0.0935797573
O             0.6211532118        0.8368328970        0.6008439299
O             0.3788467882        0.1631671030        0.3991560701
O             0.7943399779        0.3347779218        0.5317839598
O             0.2056600221        0.6652220782        0.4682160402
O             0.2935650028        0.5115280726        0.8187114012
O             0.7064349972        0.4884719274        0.1812885988
O             0.8884555622        0.7414187918        0.8956474534
O             0.1115444378        0.2585812082        0.1043525466
O             0.8071854114        1.0116498843        0.2828616453
O             0.1928145886       -0.0116498843        0.7171383547
```

Structural Data for Material # 65

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of $Li_{7.5}B_{10}S_{18}Cl_{1.5}$ in the $C2/c$ (No. 15) structure.

```
CELL_PARAMETERS (bohr)
   1.9805745E+01  2.0464245E+01  1.8916384E-02
  -1.9805745E+01  2.0464245E+01 -1.8916384E-02
  -1.8973438E+01 -0.0000000E+00  2.3593867E+01

ATOMIC_POSITIONS (crystal)
Li            0.3034596592        0.2311606593        0.5624078776
Li            0.2311606593        0.3034596592       -0.0624078776
Li            0.6965403408        0.7688393407        0.4375921224
Li            0.7688393407        0.6965403408        1.0624078776
Li            0.1696754402        0.1696754402        0.2500000000
Li            0.8303245598        0.8303245598        0.7500000000
Li            0.9371825932        0.9371825932        0.2500000000
Li            0.0628174068        0.0628174068        0.7500000000
Li            0.1118886835        0.7803184734        0.9525498385
Li            0.8881113165        0.2196815266        0.0474501615
Li            0.7803184734        0.1118886835        0.5474501615
Li            0.2196815266        0.8881113165        0.4525498385
Li            0.5703503650        0.7164210719        0.2235516993
Li            0.4296496350        0.2835789281        0.7764483007
Li            0.7164210719        0.5703503650        0.2764483007
Li            0.2835789281        0.4296496350        0.7235516993
Li            0.3965116239        0.6463896990        0.0867691625
Li            0.6034883761        0.3536103010        0.9132308375
Li            0.6463896990        0.3965116239        0.4132308375
Li            0.3536103010        0.6034883761        0.5867691625
Li            0.6887608565        0.0598102022        0.2826886311
Li            0.3112391435        0.9401897978        0.7173113689
Li            0.0598102022        0.6887608565        0.2173113689
Li            0.9401897978        0.3112391435        0.7826886311
Li            0.5000000000       -0.0000000000        0.5000000000
Li           -0.0000000000        0.5000000000        0.0000000000
Li            0.6157506194        0.9018212697        0.0554807973
Li            0.3842493806        0.0981787303        0.9445192027
Li            0.9018212697        0.6157506194        0.4445192027
```

Li	0.0981787303	0.3842493806	0.5554807973
B	0.2086450872	0.1138403214	0.4687061968
B	0.7913549128	0.8861596786	0.5312938032
B	0.1138403214	0.2086450872	0.0312938032
B	0.8861596786	0.7913549128	0.9687061968
B	0.2160109262	0.0472899197	0.0132458773
B	0.7839890738	0.9527100803	0.9867541227
B	0.0472899197	0.2160109262	0.4867541227
B	0.9527100803	0.7839890738	0.5132458773
B	0.1570783688	0.9851155320	0.1896728762
B	0.8429216312	0.0148844680	0.8103271238
B	0.9851155320	0.1570783688	0.3103271238
B	0.0148844680	0.8429216312	0.6896728762
B	0.3331345422	0.0943854386	0.2001009138
B	0.6668654578	0.9056145614	0.7998990862
B	0.0943854386	0.3331345422	0.2998990862
B	0.9056145614	0.6668654578	0.7001009138
B	0.3237605768	0.8816756163	0.0034683304
B	0.6762394232	0.1183243837	0.9965316696
B	0.8816756163	0.3237605768	0.4965316696
B	0.1183243837	0.6762394232	0.5034683304
B	0.2682020875	0.8191306188	0.1791214163
B	0.7317979125	0.1808693812	0.8208785837
B	0.8191306188	0.2682020875	0.3208785837
B	0.1808693812	0.7317979125	0.6791214163
B	0.4428875859	0.9255817263	0.1882185946
B	0.5571124141	0.0744182737	0.8117814054
B	0.9255817263	0.4428875859	0.3117814054
B	0.0744182737	0.5571124141	0.6882185946
B	0.3877441724	0.8620538704	0.3657534614
B	0.6122558276	0.1379461296	0.6342465386
B	0.8620538704	0.3877441724	0.1342465386
B	0.1379461296	0.6122558276	0.8657534614
B	0.7611622032	0.2125508366	0.1490838151
B	0.2388377968	0.7874491634	0.8509161849
B	0.2125508366	0.7611622032	0.3509161849
B	0.7874491634	0.2388377968	0.6490838151
B	0.5495544507	0.9705381964	0.3667641985
B	0.4504455493	0.0294618036	0.6332358015
B	0.9705381964	0.5495544507	0.1332358015
B	0.0294618036	0.4504455493	0.8667641985
S	0.2398077371	0.2259464035	0.1202056760
S	0.7601922629	0.7740535965	0.8797943240
S	0.2259464035	0.2398077371	0.3797943240
S	0.7740535965	0.7601922629	0.6202056760
S	0.1149829316	0.0635162717	0.3854869028
S	0.8850170684	0.9364837283	0.6145130972
S	0.0635162717	0.1149829316	0.1145130972
S	0.9364837283	0.8850170684	0.8854869028
S	0.1786102348	0.1231159766	0.5698603275
S	0.8213897652	0.8768840234	0.4301396725
S	0.1231159766	0.1786102348	0.9301396725
S	0.8768840234	0.8213897652	0.0698603275
S	0.1639788597	0.9478886544	0.0909764003
S	0.8360211403	0.0521113456	0.9090235997
S	0.9478886544	0.1639788597	0.4090235997
S	0.0521113456	0.8360211403	0.5909764003
S	0.3469795449	0.0581945704	0.1032850804
S	0.6530204551	0.9418054296	0.8967149196

```
S       0.0581945704    0.3469795449    0.3967149196
S       0.9418054296    0.6530204551    0.6032850804
S       0.2868830450    0.9935611169    0.2846159239
S       0.7131169550    0.0064388831    0.7153840761
S       0.9935611169    0.2868830450    0.2153840761
S       0.0064388831    0.7131169550    0.7846159239
S       0.3290916049    0.0026928012    0.5489371335
S       0.6709083951    0.9973071988    0.4510628665
S       0.0026928012    0.3290916049    0.9510628665
S       0.9973071988    0.6709083951    0.0489371335
S       0.4578152510    0.1034619708    0.2915293825
S       0.5421847490    0.8965380292    0.7084706175
S       0.1034619708    0.4578152510    0.2084706175
S       0.8965380292    0.5421847490    0.7915293825
S       0.6479787354    0.1697050002    0.0746559248
S       0.3520212646    0.8302949998    0.9253440752
S       0.1697050002    0.6479787354    0.4253440752
S       0.8302949998    0.3520212646    0.5746559248
S       0.7151561920    0.2302033949    0.2357707791
S       0.2848438080    0.7697966051    0.7642292209
S       0.2302033949    0.7151561920    0.2642292209
S       0.7697966051    0.2848438080    0.7357707791
S       0.2795857598    0.7800425534    0.0860625165
S       0.7204142402    0.2199574466    0.9139374835
S       0.7800425534    0.2795857598    0.4139374835
S       0.2199574466    0.7204142402    0.5860625165
S       0.4581906114    0.8904126013    0.0933057282
S       0.5418093886    0.1095873987    0.9066942718
S       0.8904126013    0.4581906114    0.4066942718
S       0.1095873987    0.5418093886    0.5933057282
S       0.4027054787    0.8191450775    0.2740324198
S       0.5972945213    0.1808549225    0.7259675802
S       0.8191450775    0.4027054787    0.2259675802
S       0.1808549225    0.5972945213    0.7740324198
S       0.3396770051    0.7691834232    0.4500808591
S       0.6603229949    0.2308165768    0.5499191409
S       0.7691834232    0.3396770051    0.0499191409
S       0.2308165768    0.6603229949    0.9500808591
S       0.5730118951    0.9322844489    0.2758102332
S       0.4269881049    0.0677155511    0.7241897668
S       0.9322844489    0.5730118951    0.2241897668
S       0.0677155511    0.4269881049    0.7758102332
S       0.5165596768    0.8632147942    0.4601054785
S       0.4834403232    0.1367852058    0.5398945215
S       0.8632147942    0.5165596768    0.0398945215
S       0.1367852058    0.4834403232    0.9601054785
S       0.8895062617    0.1096714037    0.2270643570
S       0.1104937383    0.8903285963    0.7729356430
S       0.1096714037    0.8895062617    0.2729356430
S       0.8903285963    0.1104937383    0.7270643570
S       0.7673602056    0.9816870834    0.0847633801
S       0.2326397944    0.0183129166    0.9152366199
S       0.9816870834    0.7673602056    0.4152366199
S       0.0183129166    0.2326397944    0.5847633801
Cl      0.3461689866    0.2760748585    0.8829385539
Cl      0.6538310134    0.7239251415    0.1170614461
Cl      0.2760748585    0.3461689866    0.6170614461
Cl      0.7239251415    0.6538310134    0.3829385539
Cl      0.5498859650    0.5498859650    0.2500000000
```

```
Cl            0.4501140350        0.4501140350        0.7500000000
```

Structural Data for Material # 66

Cartesian coordinates (in Bohr units) and fractional coordinates for the optimized structure of $Li_5B_7O_{12.5}Cl$ in the $F23$ (No. 196) structure.

```
CELL_PARAMETERS (bohr)
  -1.1431241E+01   0.00000000000   1.1431241E+01
  -0.00000000000   1.1431241E+01   1.1431241E+01
  -1.1431241E+01   1.1431241E+01   0.00000000000

ATOMIC_POSITIONS (crystal)
Li           -0.0432719715        0.5432719715       -0.0432719715
Li           -0.4567280285        0.9567280285        0.5432719715
Li           -0.0432719715        0.5432719715       -0.4567280285
Li            0.5432719715        0.9567280285       -0.0432719715
Li           -0.4567280285        0.5432719715       -0.0432719715
Li           -0.0432719715        0.9567280285       -0.4567280285
Li           -0.8647462244        0.5942386731       -0.8647462244
Li            0.5942386731       -0.8647462244       -0.8647462244
Li           -0.8647462244       -0.8647462244        0.5942386731
Li           -0.8647462244       -0.8647462244       -0.8647462244
B            -0.2505957545        0.2505957545       -0.2505957545
B             0.2505957545       -0.2505957545        0.2505957545
B            -0.2505957545        0.2505957545        0.2505957545
B             0.2505957545       -0.2505957545       -0.2505957545
B             0.2505957545        0.2505957545       -0.2505957545
B            -0.2505957545       -0.2505957545        0.2505957545
B            -0.0806239706        0.2418719117       -0.0806239706
B             0.2418719117       -0.0806239706       -0.0806239706
B            -0.0806239706       -0.0806239706        0.2418719117
B            -0.0806239706       -0.0806239706       -0.0806239706
B            -0.6008866049        0.8026598146       -0.6008866049
B             0.8026598146       -0.6008866049       -0.6008866049
B            -0.6008866049       -0.6008866049        0.8026598146
B            -0.6008866049       -0.6008866049       -0.6008866049
O             0.0637474144        0.2959286459       -0.1001409310
O             0.2959286459        0.0637474144       -0.2595351292
O            -0.2595351292       -0.1001409310        0.2959286459
O            -0.1001409310       -0.2595351292        0.0637474144
O            -0.1001409310        0.2959286459       -0.2595351292
O            -0.2595351292        0.0637474144       -0.1001409310
O             0.2959286459       -0.1001409310        0.0637474144
O             0.0637474144       -0.2595351292        0.2959286459
O            -0.2595351292        0.2959286459        0.0637474144
O            -0.1001409310        0.0637474144        0.2959286459
O             0.0637474144       -0.1001409310       -0.2595351292
O             0.2959286459       -0.2595351292       -0.1001409310
O             0.3954154647        0.8037119001       -0.4386084470
O             0.8037119001        0.3954154647       -0.7605189178
O            -0.7605189178       -0.4386084470        0.8037119001
O            -0.4386084470       -0.7605189178        0.3954154647
```

```
O          -0.4386084470       0.8037119001      -0.7605189178
O          -0.7605189178       0.3954154647      -0.4386084470
O           0.8037119001      -0.4386084470       0.3954154647
O           0.3954154647      -0.7605189178       0.8037119001
O          -0.7605189178       0.8037119001       0.3954154647
O          -0.4386084470       0.3954154647       0.8037119001
O           0.3954154647      -0.4386084470      -0.7605189178
O           0.8037119001      -0.7605189178      -0.4386084470
O          -0.0000000000       0.0000000000      -0.0000000000
Cl         -0.2500000000       0.7500000000      -0.2500000000
Cl         -0.7500000000       0.2500000000      -0.7500000000
```