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

D. Cory Lynch,[1] Yan Li,[2] Pieremanuele Canepa,[2,3,4] and N. A. W. Holzwarth[1]

[1] *Department of Physics, Wake Forest University, Winston-Salem, NC 27109, USA**

[2] *Department of Materials Science and Engineering, National University of Singapore, Singapore, 119077*

[3] *Department of Electrical and Computer Engineering, University of Houston, Houston, Texas 77204, USA*

[4] *Texas Center for Superconductivity at the University of Houston (TcSUH), Houston, Texas 77204, USA*

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Supplemental Materials Part I

Included in this document are three sections. For the lithium (thio)boracite materials considered in this study, Section I lists the primitive cell lattice parameters and fractional coordinates, Section II presents the electronic partial density of state, while Section III presents the phonon bands and the phonon partial density of states.

I. OPTIMIZED STRUCTURES FOR LITHIUM (THIO)BORACITE FAMILY OF MATERIALS

The following tables list the primitive cell lattice parameters (in Bohr units) and fractional coordinates, in the format of QUANTUM ESPRESSO [1], for the optimized structures calculated in this study. The space group nomenclatures follow the conventions of the International Tables of Crystallography [2].

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

TABLE I. Cartesian coordinates of primitive cell (in Bohr units) and fractional coordinates for the optimized structure of $Li_4B_7O_{12}Cl$ in the $R3c$ (No. 161) structure.

```
CELL_PARAMETERS (bohr)
   1.1450993E+01   1.1450993E+01  -1.7817383E-02
  -1.7817383E-02   1.1450993E+01   1.1450993E+01
   1.1450993E+01  -1.7817383E-02   1.1450993E+01

ATOMIC_POSITIONS (crystal)
Li       0.034657753  0.036146547  0.465200410
Li       0.465200410  0.034657753  0.036146547
Li       0.036146547  0.465200410  0.034657753
Li       0.965200410  0.536146947  0.534657553
Li       0.534657553  0.965200410  0.536146947
Li       0.536146947  0.534657553  0.965200410
Li       0.368767332  0.368767332  0.368767332
Li       0.868767332  0.868767332  0.868767332
B        0.250954251  0.260536544  0.753459028
B        0.753459028  0.250954251  0.260536544
B        0.260536544  0.753459028  0.250954251
B        0.253459028  0.760536544  0.750954251
B        0.750954251  0.253459028  0.760536544
B        0.760536544  0.750954251  0.253459028
B        0.601589598  0.601589598  0.601589598
B        0.101589598  0.101589598  0.101589598
B        0.609263229  0.608906508  0.197648790
B        0.197648790  0.609263229  0.608906508
B        0.608906508  0.197648790  0.609263229
B        0.697648790  0.108906508  0.109263229
B        0.109263229  0.697648790  0.108906508
B        0.108906508  0.109263229  0.697648790
O        0.438084097  0.613364257  0.756851211
O        0.756851211  0.438084097  0.613364257
O        0.613364257  0.756851211  0.438084097
O        0.256851211  0.113364257  0.938084097
O        0.938084097  0.256851211  0.113364257
O        0.113364257  0.938084097  0.256851211
O        0.446940185  0.765492979  0.197362316
O        0.197362316  0.446940185  0.765492979
O        0.765492979  0.197362316  0.446940185
O        0.697362316  0.265492979  0.946940185
O        0.946940185  0.697362316  0.265492979
O        0.265492979  0.946940185  0.697362316
O        0.187374502  0.771530364  0.614620997
O        0.614620997  0.187374502  0.771530364
O        0.771530364  0.614620997  0.187374502
O        0.114620997  0.271530364  0.687374502
O        0.687374502  0.114620997  0.271530364
O        0.271530364  0.687374502  0.114620997
O        0.712270603  0.942035598  0.106346125
O        0.106346125  0.712270603  0.942035598
O        0.942035598  0.106346125  0.712270603
O        0.606346125  0.442035598  0.212270603
O        0.212270603  0.606346125  0.442035598
O        0.442035598  0.212270603  0.606346125
Cl       0.250000000  0.250000000  0.250000000
Cl       0.750000000  0.750000000  0.750000000
```

TABLE II. Cartesian coordinates of primitive cell (in Bohr units) and fractional coordinates for the optimized structure of $Li_4Al_3B_4O_{12}Cl$ in the $R3c$ (No. 161) structure.

```
CELL_PARAMETERS (bohr)
   1.2180943E+01   1.2180943E+01  -2.3448974E-01
  -2.3448974E-01   1.2180943E+01   1.2180943E+01
   1.2180943E+01  -2.3448974E-01   1.2180943E+01

ATOMIC_POSITIONS (crystal)
Li       0.962522673  0.962643853  0.483087730
Li       0.483087730  0.962522673  0.962643853
Li       0.962643853  0.483087730  0.962522673
Li       0.983087730  0.462644253  0.462522472
Li       0.462522472  0.983087730  0.462644253
Li       0.462644253  0.462522472  0.983087730
Li       0.353676298  0.353676298  0.353676298
Li       0.853676298  0.853676298  0.853676298
Al       0.223294678  0.225877140  0.734609902
Al       0.734609902  0.223294678  0.225877140
Al       0.225877140  0.734609902  0.223294678
Al       0.234609902  0.725877140  0.723294678
Al       0.723294678  0.234609902  0.725877140
Al       0.725877140  0.723294678  0.234609902
B        0.585806041  0.585806041  0.585806041
B        0.085806041  0.085806041  0.085806041
B        0.580787541  0.580229894  0.161813817
B        0.161813817  0.580787541  0.580229894
B        0.580229894  0.161813817  0.580787541
B        0.661813817  0.080229894  0.080787541
B        0.080787541  0.661813817  0.080229894
B        0.080229894  0.080787541  0.661813817
O        0.443235184  0.571925923  0.738772045
O        0.738772045  0.443235184  0.571925923
O        0.571925923  0.738772045  0.443235184
O        0.238772045  0.071925923  0.943235184
O        0.943235184  0.238772045  0.071925923
O        0.071925923  0.943235184  0.238772045
O        0.441901301  0.735116102  0.158237503
O        0.158237503  0.441901301  0.735116102
O        0.735116102  0.158237503  0.441901301
O        0.658237503  0.235116102  0.941901301
O        0.941901301  0.658237503  0.235116102
O        0.235116102  0.941901301  0.658237503
O        0.162738185  0.736533798  0.567625863
O        0.567625863  0.162738185  0.736533798
O        0.736533798  0.567625863  0.162738185
O        0.067625863  0.236533798  0.662738185
O        0.662738185  0.067625863  0.236533798
O        0.236533798  0.662738185  0.067625863
O        0.677535452  0.929710511  0.062044746
O        0.062044746  0.677535452  0.929710511
O        0.929710511  0.062044746  0.677535452
O        0.562044746  0.429710511  0.177535452
O        0.177535452  0.562044746  0.429710511
O        0.429710511  0.177535452  0.562044746
Cl       0.250000000  0.250000000  0.250000000
Cl       0.750000000  0.750000000  0.750000000
```

TABLE III. Cartesian coordinates of primitive cell (in Bohr units) and fractional coordinates for the optimized structure of $Li_6B_7O_{13}Cl$ in the $R3c$ (No. 161) structure.

```
CELL_PARAMETERS (bohr)
   1.1545375E+01   1.1545375E+01   1.2547651E-01
   1.2547651E-01   1.1545375E+01   1.1545375E+01
   1.1545375E+01   1.2547651E-01   1.1545375E+01

ATOMIC_POSITIONS (crystal)
Li       0.643483192  0.633985098  0.105881042
Li       0.633985098  0.105881042  0.643483192
Li       0.105881042  0.643483192  0.633985098
Li       0.143483192  0.605881042  0.133985098
Li       0.133985098  0.143483192  0.605881042
Li       0.605881042  0.133985098  0.143483192
Li       0.538661284  0.533416368  0.942964155
Li       0.033416368  0.038661284  0.442964155
Li       0.942964155  0.538661284  0.533416368
Li       0.442964155  0.033416368  0.038661284
Li       0.533416368  0.942964155  0.538661284
Li       0.038661284  0.442964155  0.033416368
B        0.751676355  0.256833994  0.253576703
B        0.251676355  0.753576703  0.756833994
B        0.253576703  0.751676355  0.256833994
B        0.756833994  0.251676355  0.753576703
B        0.256833994  0.253576703  0.751676355
B        0.753576703  0.756833994  0.251676355
B        0.402808922  0.402808922  0.402808922
B        0.738996414  0.428802236  0.431043435
B        0.428802236  0.431043435  0.738996414
B        0.431043435  0.738996414  0.428802236
B        0.902808922  0.902808922  0.902808922
B        0.238996414  0.931043435  0.928802236
B        0.931043435  0.928802236  0.238996414
B        0.928802236  0.238996414  0.931043435
O        0.559642634  0.404024317  0.237013206
O        0.786520815  0.251642519  0.406144993
O        0.390356399  0.566469244  0.816355156
O        0.246763956  0.800615243  0.569343379
O        0.237013206  0.559642634  0.404024317
O        0.816355156  0.390356399  0.566469244
O        0.569343379  0.246763956  0.800615243
O        0.406144993  0.786520815  0.251642519
O        0.404024317  0.237013206  0.559642634
O        0.800615243  0.569343379  0.246763956
O        0.251642519  0.406144993  0.786520815
O        0.566469244  0.816355156  0.390356399
O        0.059642634  0.737013206  0.904024317
O        0.286520815  0.906144993  0.751642519
O        0.746763956  0.069343379  0.300615243
O        0.890356399  0.316355156  0.066469244
O        0.737013206  0.904024317  0.059642634
O        0.316355156  0.066469244  0.890356399
O        0.906144993  0.751642519  0.286520815
O        0.069343379  0.300615243  0.746763956
O        0.904024317  0.059642634  0.737013206
O        0.300615243  0.746763956  0.069343379
O        0.066469244  0.890356399  0.316355156
O        0.751642519  0.286520815  0.906144993
O        0.515966113  0.515966113  0.515966113
O        0.015966113  0.015966113  0.015966113
Cl       0.250000000  0.250000000  0.250000000
Cl       0.750000000  0.750000000  0.750000000
```

TABLE IV. Cartesian coordinates of primitive cell (in Bohr units) and fractional coordinates for the optimized structure of $Li_6Al_3B_4O_{12}Cl$ in the $R3c$ (No. 161) structure.

```
CELL_PARAMETERS (bohr)
   1.2475298E+01   1.2475298E+01   3.6771834E-01
   3.6771834E-01   1.2475298E+01   1.2475298E+01
   1.2475298E+01   3.6771834E-01   1.2475298E+01

ATOMIC_POSITIONS (crystal)
Li       0.656993455  0.624049124  0.120647353
Li       0.624049124  0.120647353  0.656993455
Li       0.120647353  0.656993455  0.624049124
Li       0.156993455  0.620647353  0.124049124
Li       0.124049124  0.156993455  0.620647353
Li       0.620647353  0.124049124  0.156993455
Li       0.531974611  0.545911946  0.944300076
Li       0.045911946  0.031974611  0.444300076
Li       0.944300076  0.531974611  0.545911946
Li       0.444300076  0.045911946  0.031974611
Li       0.545911946  0.944300076  0.531974611
Li       0.031974611  0.444300076  0.045911946
Al       0.761103801  0.422240968  0.440168873
Al       0.422240968  0.440168873  0.761103801
Al       0.440168873  0.761103801  0.422240968
Al       0.261103801  0.940168873  0.922240968
Al       0.940168873  0.922240968  0.261103801
Al       0.922240968  0.261103801  0.940168873
B        0.750222892  0.259053411  0.280635728
B        0.250222892  0.780635728  0.759053411
B        0.280635728  0.750222892  0.259053411
B        0.759053411  0.250222892  0.780635728
B        0.259053411  0.280635728  0.750222892
B        0.780635728  0.759053411  0.250222892
B        0.421361896  0.421361896  0.421361896
B        0.921361896  0.921361896  0.921361896
O        0.575317777  0.411873610  0.272465662
O        0.803295981  0.222082781  0.424577787
O        0.378442360  0.603802024  0.830695285
O        0.232052112  0.813118490  0.594466315
O        0.272465662  0.575317777  0.411873610
O        0.830695285  0.378442360  0.603802024
O        0.594466315  0.232052112  0.813118490
O        0.424577787  0.803295981  0.222082781
O        0.411873610  0.272465662  0.575317777
O        0.813118490  0.594466315  0.232052112
O        0.222082781  0.424577787  0.803295981
O        0.603802024  0.830695285  0.378442360
O        0.075317777  0.772465662  0.911873610
O        0.303295981  0.924577787  0.722082781
O        0.732052112  0.094466315  0.313118490
O        0.878442360  0.330695285  0.103802024
O        0.772465662  0.911873610  0.075317777
O        0.330695285  0.103802024  0.878442360
O        0.924577787  0.722082781  0.303295981
O        0.094466315  0.313118490  0.732052112
O        0.911873610  0.075317777  0.772465662
O        0.313118490  0.732052112  0.094466315
O        0.103802024  0.878442360  0.330695285
O        0.722082781  0.303295981  0.924577787
O        0.523380949  0.523380949  0.523380949
O        0.023380949  0.023380949  0.023380949
Cl       0.250000000  0.250000000  0.250000000
Cl       0.750000000  0.750000000  0.750000000
```

TABLE V. Cartesian coordinates of primitive cell (in Bohr units) and fractional coordinates for the optimized structure of $Li_4B_7S_{12}Cl$ in the $R3c$ (No. 161) structure.

```
CELL_PARAMETERS (bohr)
   1.4125317E+01   1.4125317E+01   4.4366577E-02
   4.4366577E-02   1.4125317E+01   1.4125317E+01
   1.4125317E+01   4.4366577E-02   1.4125317E+01

ATOMIC_POSITIONS (crystal)
Li       0.911737829  0.910632126  0.563559085
Li       0.563559085  0.911737829  0.910632126
Li       0.910632126  0.563559085  0.911737829
Li       0.063559085  0.410632126  0.411737829
Li       0.411737829  0.063559085  0.410632126
Li       0.410632126  0.411737829  0.063559085
Li       0.629869578  0.629869578  0.629869578
Li       0.129869578  0.129869578  0.129869578
B        0.727544302  0.741131296  0.231319373
B        0.231319373  0.727544302  0.741131296
B        0.741131296  0.231319373  0.727544302
B        0.731319373  0.241131296  0.227544302
B        0.227544302  0.731319373  0.241131296
B        0.241131296  0.227544302  0.731319373
B        0.387603814  0.387603814  0.387603814
B        0.887603814  0.887603814  0.887603814
B        0.391089944  0.375650572  0.778930144
B        0.778930144  0.391089944  0.375650572
B        0.375650572  0.778930144  0.391089944
B        0.278930144  0.875650572  0.891089944
B        0.891089944  0.278930144  0.875650572
B        0.875650572  0.891089944  0.278930144
S        0.545161454  0.412245541  0.204559657
S        0.204559657  0.545161454  0.412245541
S        0.412245541  0.204559657  0.545161454
S        0.704559657  0.912245541  0.045161454
S        0.045161454  0.704559657  0.912245541
S        0.912245541  0.045161454  0.704559657
S        0.558209062  0.203253145  0.766613229
S        0.766613229  0.558209062  0.203253145
S        0.203253145  0.766613229  0.558209062
S        0.266613229  0.703253145  0.058209062
S        0.058209062  0.266613229  0.703253145
S        0.703253145  0.058209062  0.266613229
S        0.786135615  0.209848714  0.391287696
S        0.391287696  0.786135615  0.209848714
S        0.209848714  0.391287696  0.786135615
S        0.891287696  0.709848714  0.286135615
S        0.286135615  0.891287696  0.709848714
S        0.709848714  0.286135615  0.891287696
S        0.288852547  0.038494241  0.899752038
S        0.899752038  0.288852547  0.038494241
S        0.038494241  0.899752038  0.288852547
S        0.399752038  0.538494241  0.788852547
S        0.788852547  0.399752038  0.538494241
S        0.538494241  0.788852547  0.399752038
Cl       0.750000000  0.750000000  0.750000000
Cl       0.250000000  0.250000000  0.250000000
```

TABLE VI. Cartesian coordinates of primitive cell (in Bohr units) and fractional coordinates for the optimized structure of $Li_4Al_3B_4S_{12}Cl$ in the $R3c$ (No. 161) structure.

```
CELL_PARAMETERS (bohr)
   1.5218014E+01   1.5218014E+01   1.0441647E-01
   1.0441647E-01   1.5218014E+01   1.5218014E+01
   1.5218014E+01   1.0441647E-01   1.5218014E+01

ATOMIC_POSITIONS (crystal)
Li       0.892359242  0.893498524  0.506682462
Li       0.506682462  0.892359242  0.893498524
Li       0.893498524  0.506682462  0.892359242
Li       0.006682462  0.393498524  0.392359242
Li       0.392359242  0.006682462  0.393498524
Li       0.393498524  0.392359242  0.006682462
Li       0.331703457  0.331703457  0.331703457
Li       0.831703457  0.831703457  0.831703457
Al       0.190532269  0.194515067  0.705666885
Al       0.705666885  0.190532269  0.194515067
Al       0.194515067  0.705666885  0.190532269
Al       0.205666885  0.694515067  0.690532269
Al       0.690532269  0.205666885  0.694515067
Al       0.694515067  0.690532269  0.205666885
B        0.549812763  0.549812763  0.549812763
B        0.049812763  0.049812763  0.049812763
B        0.548997970  0.548022969  0.143869041
B        0.143869041  0.548997970  0.548022969
B        0.548022969  0.143869041  0.548997970
B        0.643869041  0.048022969  0.048997970
B        0.048997970  0.643869041  0.048022969
B        0.048022969  0.048997970  0.643869041
S        0.409665829  0.513247396  0.723772823
S        0.723772823  0.409665829  0.513247396
S        0.513247396  0.723772823  0.409665829
S        0.223772823  0.013247396  0.909665829
S        0.909665829  0.223772823  0.013247396
S        0.013247396  0.909665829  0.223772823
S        0.406931482  0.720069701  0.144507664
S        0.144507664  0.406931482  0.720069701
S        0.720069701  0.144507664  0.406931482
S        0.644507664  0.220069701  0.906931482
S        0.906931482  0.644507664  0.220069701
S        0.220069701  0.906931482  0.644507664
S        0.146296878  0.721714229  0.513209092
S        0.513209092  0.146296878  0.721714229
S        0.721714229  0.513209092  0.146296878
S        0.013209092  0.221714229  0.646296878
S        0.646296878  0.013209092  0.221714229
S        0.221714229  0.646296878  0.013209092
S        0.633497850  0.905071993  0.027869929
S        0.027869929  0.633497850  0.905071993
S        0.905071993  0.027869929  0.633497850
S        0.527869929  0.405071993  0.133497850
S        0.133497850  0.527869929  0.405071993
S        0.405071993  0.133497850  0.527869929
Cl       0.250000000  0.250000000  0.250000000
Cl       0.750000000  0.750000000  0.750000000
```

TABLE VII. Cartesian coordinates of primitive cell (in Bohr units) and fractional coordinates for the optimized structure of $Li_6B_7S_{13}Cl$ in the $R3c$ (No. 161) structure.

```
CELL_PARAMETERS (bohr)
   1.4378936E+01   1.4378936E+01   2.0067467E-01
   2.0067467E-01   1.4378936E+01   1.4378936E+01
   1.4378936E+01   2.0067467E-01   1.4378936E+01

ATOMIC_POSITIONS (crystal)
Li       0.672321725  0.653819822  0.105780147
Li       0.653819822  0.105780147  0.672321725
Li       0.105780147  0.672321725  0.653819822
Li       0.172321725  0.605780147  0.153819822
Li       0.153819822  0.172321725  0.605780147
Li       0.605780147  0.153819822  0.172321725
Li       0.585143836  0.589506203  0.914010330
Li       0.089506203  0.085143836  0.414010330
Li       0.914010330  0.585143836  0.589506203
Li       0.414010330  0.089506203  0.085143836
Li       0.589506203  0.914010330  0.585143836
Li       0.085143836  0.414010330  0.089506203
B        0.768734158  0.267757112  0.273997739
B        0.268734158  0.773997739  0.767757112
B        0.273997739  0.768734158  0.267757112
B        0.767757112  0.268734158  0.773997739
B        0.267757112  0.273997739  0.768734158
B        0.773997739  0.767757112  0.268734158
B        0.442917684  0.442917684  0.442917684
B        0.750968548  0.440892189  0.445962993
B        0.440892189  0.445962993  0.750968548
B        0.445962993  0.750968548  0.440892189
B        0.942917684  0.942917684  0.942917684
B        0.250968548  0.945962993  0.940892189
B        0.945962993  0.940892189  0.250968548
B        0.940892189  0.250968548  0.945962993
S        0.582649053  0.431871419  0.246967832
S        0.816656281  0.244457383  0.435792314
S        0.427049732  0.583734844  0.818375755
S        0.248447854  0.827847540  0.576414927
S        0.246967832  0.582649053  0.431871419
S        0.818375755  0.427049732  0.583734844
S        0.576414927  0.248447854  0.827847540
S        0.435792314  0.816656281  0.244457383
S        0.431871419  0.246967832  0.582649053
S        0.827847540  0.576414927  0.248447854
S        0.244457383  0.435792314  0.816656281
S        0.583734844  0.818375755  0.427049732
S        0.082649053  0.746967832  0.931871419
S        0.316656281  0.935792314  0.744457383
S        0.748447854  0.076414927  0.327847540
S        0.927049732  0.318375755  0.083734844
S        0.746967832  0.931871419  0.082649053
S        0.318375755  0.083734844  0.927049732
S        0.935792314  0.744457383  0.316656281
S        0.076414927  0.327847540  0.748447854
S        0.931871419  0.082649053  0.746967832
S        0.327847540  0.748447854  0.076414927
S        0.083734844  0.927049732  0.318375755
S        0.744457383  0.316656281  0.935792314
S        0.519871877  0.519871877  0.519871877
S        0.019871877  0.019871877  0.019871877
Cl       0.250000000  0.250000000  0.250000000
Cl       0.750000000  0.750000000  0.750000000
```

TABLE VIII. Cartesian coordinates of primitive cell (in Bohr units) and fractional coordinates for the optimized structure of $Li_6Al_3B_4S_{12}Cl$ in the $R3c$ (No. 161) structure.

```
CELL_PARAMETERS (bohr)
   1.5484091E+01   1.5484091E+01   5.7151820E-01
   5.7151820E-01   1.5484091E+01   1.5484091E+01
   1.5484091E+01   5.7151820E-01   1.5484091E+01

ATOMIC_POSITIONS (crystal)
Li       0.702479886  0.633405499  0.160226804
Li       0.633405499  0.160226804  0.702479886
Li       0.160226804  0.702479886  0.633405499
Li       0.202479886  0.660226804  0.133405499
Li       0.133405499  0.202479886  0.660226804
Li       0.660226804  0.133405499  0.202479886
Li       0.596408590  0.610033487  0.918884539
Li       0.110033487  0.096408590  0.418884539
Li       0.918884539  0.596408590  0.610033487
Li       0.418884539  0.110033487  0.096408590
Li       0.610033487  0.918884539  0.596408590
Li       0.096408590  0.418884539  0.110033487
Al       0.785807764  0.440844787  0.471402620
Al       0.440844787  0.471402620  0.785807764
Al       0.471402620  0.785807764  0.440844787
Al       0.285807764  0.971402620  0.940844787
Al       0.971402620  0.940844787  0.285807764
Al       0.940844787  0.285807764  0.971402620
B        0.781670512  0.268433632  0.323018235
B        0.281670512  0.823018235  0.768433632
B        0.323018235  0.781670512  0.268433632
B        0.768433632  0.281670512  0.823018235
B        0.268433632  0.323018235  0.781670512
B        0.823018235  0.768433632  0.281670512
B        0.463669666  0.463669666  0.463669666
B        0.963669666  0.963669666  0.963669666
S        0.612122808  0.435111216  0.289462473
S        0.836148552  0.221471883  0.479130335
S        0.436421143  0.644404795  0.819363600
S        0.250155991  0.870045382  0.595653138
S        0.289462473  0.612122808  0.435111216
S        0.819363600  0.436421143  0.644404795
S        0.595653138  0.250155991  0.870045382
S        0.479130335  0.836148552  0.221471883
S        0.435111216  0.289462473  0.612122808
S        0.870045382  0.595653138  0.250155991
S        0.221471883  0.479130335  0.836148552
S        0.644404795  0.819363600  0.436421143
S        0.112122808  0.789462473  0.935111216
S        0.336148552  0.979130335  0.721471883
S        0.750155991  0.095653138  0.370045382
S        0.936421143  0.319363600  0.144404795
S        0.789462473  0.935111216  0.112122808
S        0.319363600  0.144404795  0.936421143
S        0.979130335  0.721471883  0.336148552
S        0.095653138  0.370045382  0.750155991
S        0.935111216  0.112122808  0.789462473
S        0.370045382  0.750155991  0.095653138
S        0.144404795  0.936421143  0.319363600
S        0.721471883  0.336148552  0.979130335
S        0.534219817  0.534219817  0.534219817
S        0.034219817  0.034219817  0.034219817
Cl       0.250000000  0.250000000  0.250000000
Cl       0.750000000  0.750000000  0.750000000
```

TABLE IX. Cartesian coordinates of primitive cell (in Bohr units) and fractional coordinates for the optimized structure of $Li_4B_7O_{12}Cl$ in the ordered $F\bar{4}3c$ (No. 219) structure.

```
CELL_PARAMETERS (bohr)
 -11.490210368   0.000000000  11.490210368
   0.000000000  11.490210368  11.490210368
 -11.490210368  11.490210368   0.000000000

ATOMIC_POSITIONS (crystal)
Li           -0.3639937079       -0.3639937079       -0.3639937079
Li           -0.8639937079       -0.8639937079       -0.8639937079
Li           -0.3639937079       -0.3639937079        0.0919811238
Li           -0.8639937079       -0.8639937079        0.5919811238
Li           -0.3639937079        0.0919811238       -0.3639937079
Li           -0.8639937079        0.5919811238       -0.8639937079
Li            0.0919811238       -0.3639937079       -0.3639937079
Li            0.5919811238       -0.8639937079       -0.8639937079
B             0.2500000000        0.2500000000       -0.2500000000
B             0.2500000000       -0.2500000000        0.2500000000
B            -0.2500000000        0.2500000000        0.2500000000
B             0.2500000000       -0.2500000000       -0.2500000000
B            -0.2500000000        0.2500000000       -0.2500000000
B            -0.2500000000       -0.2500000000        0.2500000000
B            -0.6001674381       -0.6001674381       -0.6001674381
B            -0.1001674381       -0.1001674381       -0.1001674381
B            -0.6001674381       -0.6001674381        0.8005023143
B            -0.1001674381       -0.1001674381        0.3005023143
B            -0.6001674381        0.8005023143       -0.6001674381
B            -0.1001674381        0.3005023143       -0.1001674381
B             0.8005023143       -0.6001674381       -0.6001674381
B             0.3005023143       -0.1001674381       -0.1001674381
O             0.5633443562        0.7964728978        0.3971560451
O             0.3971560451        0.7964728978        0.2430267010
O             0.2430267010        0.7964728978        0.5633443562
O             0.7964728978        0.5633443562        0.2430267010
O             0.2430267010        0.5633443562        0.3971560451
O             0.3971560451        0.5633443562        0.7964728978
O             0.3971560451        0.2430267010        0.5633443562
O             0.5633443562        0.2430267010        0.7964728978
O             0.7964728978        0.2430267010        0.3971560451
O             0.2430267010        0.3971560451        0.7964728978
O             0.7964728978        0.3971560451        0.5633443562
O             0.5633443562        0.3971560451        0.2430267010
O             0.0633443562        0.2964728978        0.7430267010
O             0.8971560451        0.2964728978        0.0633443562
O             0.7430267010        0.2964728978        0.8971560451
O             0.2964728978        0.0633443562        0.8971560451
O             0.7430267010        0.0633443562        0.2964728978
O             0.8971560451        0.0633443562        0.7430267010
O             0.8971560451        0.7430267010        0.2964728978
O             0.0633443562        0.7430267010        0.8971560451
O             0.2964728978        0.7430267010        0.0633443562
O             0.7430267010        0.8971560451        0.0633443562
O             0.2964728978        0.8971560451        0.7430267010
O             0.0633443562        0.8971560451        0.2964728978
Cl            0.2500000000        0.2500000000        0.2500000000
Cl            0.7500000000        0.7500000000        0.7500000000
```

TABLE X. Cartesian coordinates of primitive cell (in Bohr units) and fractional coordinates for the optimized structure of $Li_4Al_3B_4O_{12}Cl$ in the ordered $F\bar{4}3c$ (No. 219) structure.

```
CELL_PARAMETERS (bohr)
 -12.244447727   0.000000000  12.244447727
  -0.000000000  12.244447727  12.244447727
 -12.244447727  12.244447727  -0.000000000

ATOMIC_POSITIONS (crystal)
Li           -0.3642386573       -0.3642386573       -0.3642386573
Li           -0.8642386573       -0.8642386573       -0.8642386573
Li           -0.3642386573       -0.3642386573        0.0927159718
Li           -0.8642386573       -0.8642386573        0.5927159718
Li           -0.3642386573        0.0927159718       -0.3642386573
Li           -0.8642386573        0.5927159718       -0.8642386573
Li            0.0927159718       -0.3642386573       -0.3642386573
Li            0.5927159718       -0.8642386573       -0.8642386573
Al            0.2500000000        0.2500000000       -0.2500000000
Al            0.2500000000       -0.2500000000        0.2500000000
Al           -0.2500000000        0.2500000000        0.2500000000
Al            0.2500000000       -0.2500000000       -0.2500000000
Al           -0.2500000000        0.2500000000       -0.2500000000
Al           -0.2500000000       -0.2500000000        0.2500000000
B            -0.5984176312       -0.5984176312       -0.5984176312
B            -0.0984176312       -0.0984176312       -0.0984176312
B            -0.5984176312       -0.5984176312        0.7952528935
B            -0.0984176312       -0.0984176312        0.2952528935
B            -0.5984176312        0.7952528935       -0.5984176312
B            -0.0984176312        0.2952528935       -0.0984176312
B             0.7952528935       -0.5984176312       -0.5984176312
B             0.2952528935       -0.0984176312       -0.0984176312
O             0.5424181920        0.7926035181        0.4220828299
O             0.4220828299        0.7926035181        0.2428954600
O             0.2428954600        0.7926035181        0.5424181920
O             0.7926035181        0.5424181920        0.2428954600
O             0.2428954600        0.5424181920        0.4220828299
O             0.4220828299        0.5424181920        0.7926035181
O             0.4220828299        0.2428954600        0.5424181920
O             0.5424181920        0.2428954600        0.7926035181
O             0.7926035181        0.2428954600        0.4220828299
O             0.2428954600        0.4220828299        0.7926035181
O             0.7926035181        0.4220828299        0.5424181920
O             0.5424181920        0.4220828299        0.2428954600
O             0.0424181920        0.2926035181        0.7428954600
O             0.9220828299        0.2926035181        0.0424181920
O             0.7428954600        0.2926035181        0.9220828299
O             0.2926035181        0.0424181920        0.9220828299
O             0.7428954600        0.0424181920        0.2926035181
O             0.9220828299        0.0424181920        0.7428954600
O             0.9220828299        0.7428954600        0.2926035181
O             0.0424181920        0.7428954600        0.9220828299
O             0.2926035181        0.7428954600        0.0424181920
O             0.7428954600        0.9220828299        0.0424181920
O             0.2926035181        0.9220828299        0.7428954600
O             0.0424181920        0.9220828299        0.2926035181
Cl            0.2500000000        0.2500000000        0.2500000000
Cl            0.7500000000        0.7500000000        0.7500000000
```

TABLE XI. Cartesian coordinates of primitive cell (in Bohr units) and fractional coordinates for the optimized structure of $Li_4B_7S_{12}Cl$ in the ordered $F\bar{4}3c$ (No. 219) structure.

```
CELL_PARAMETERS (bohr)
 -14.091280057   0.000000000  14.091280057
   0.000000000  14.091280057  14.091280057
 -14.091280057  14.091280057   0.000000000

ATOMIC_POSITIONS (crystal)
Li           -0.3483832301       -0.3483832301       -0.3483832301
Li           -0.8483832301       -0.8483832301       -0.8483832301
Li           -0.3483832301       -0.3483832301        0.0451496902
Li           -0.8483832301       -0.8483832301        0.5451496902
Li           -0.3483832301        0.0451496902       -0.3483832301
Li           -0.8483832301        0.5451496902       -0.8483832301
Li            0.0451496902       -0.3483832301       -0.3483832301
Li            0.5451496902       -0.8483832301       -0.8483832301
B             0.2500000000        0.2500000000       -0.2500000000
B             0.2500000000       -0.2500000000        0.2500000000
B            -0.2500000000        0.2500000000        0.2500000000
B             0.2500000000       -0.2500000000       -0.2500000000
B            -0.2500000000        0.2500000000       -0.2500000000
B            -0.2500000000       -0.2500000000        0.2500000000
B            -0.5974846614       -0.5974846614       -0.5974846614
B            -0.0974846614       -0.0974846614       -0.0974846614
B            -0.5974846614       -0.5974846614        0.7924539843
B            -0.0974846614       -0.0974846614        0.2924539843
B            -0.5974846614        0.7924539843       -0.5974846614
B            -0.0974846614        0.2924539843       -0.0974846614
B             0.7924539843       -0.5974846614       -0.5974846614
B             0.2924539843       -0.0974846614       -0.0974846614
S             0.5625710937        0.8008849482        0.4154978587
S             0.4154978587        0.8008849482        0.2210460994
S             0.2210460994        0.8008849482        0.5625710937
S             0.8008849482        0.5625710937        0.2210460994
S             0.2210460994        0.5625710937        0.4154978587
S             0.4154978587        0.5625710937        0.8008849482
S             0.4154978587        0.2210460994        0.5625710937
S             0.5625710937        0.2210460994        0.8008849482
S             0.8008849482        0.2210460994        0.4154978587
S             0.2210460994        0.4154978587        0.8008849482
S             0.8008849482        0.4154978587        0.5625710937
S             0.5625710937        0.4154978587        0.2210460994
S             0.0625710937        0.3008849482        0.7210460994
S             0.9154978587        0.3008849482        0.0625710937
S             0.7210460994        0.3008849482        0.9154978587
S             0.3008849482        0.0625710937        0.9154978587
S             0.7210460994        0.0625710937        0.3008849482
S             0.9154978587        0.0625710937        0.7210460994
S             0.9154978587        0.7210460994        0.3008849482
S             0.0625710937        0.7210460994        0.9154978587
S             0.3008849482        0.7210460994        0.0625710937
S             0.7210460994        0.9154978587        0.0625710937
S             0.3008849482        0.9154978587        0.7210460994
S             0.0625710937        0.9154978587        0.3008849482
Cl            0.2500000000        0.2500000000        0.2500000000
Cl            0.7500000000        0.7500000000        0.7500000000
```

TABLE XII. Cartesian coordinates of primitive cell (in Bohr units) and fractional coordinates for the optimized structure of $Li_4Al_3B_4S_{12}Cl$ in the ordered $F\bar{4}3c$ (No. 219) structure.

```
CELL_PARAMETERS (bohr)
 -14.887641376   0.000000000  14.887641376
   0.000000000  14.887641376  14.887641376
 -14.887641376  14.887641376   0.000000000

ATOMIC_POSITIONS (crystal)
Li           -0.3502228656       -0.3502228656       -0.3502228656
Li           -0.8502228656       -0.8502228656       -0.8502228656
Li           -0.3502228656       -0.3502228656        0.0506685967
Li           -0.8502228656       -0.8502228656        0.5506685967
Li           -0.3502228656        0.0506685967       -0.3502228656
Li           -0.8502228656        0.5506685967       -0.8502228656
Li            0.0506685967       -0.3502228656       -0.3502228656
Li            0.5506685967       -0.8502228656       -0.8502228656
Al            0.2500000000        0.2500000000       -0.2500000000
Al            0.2500000000       -0.2500000000        0.2500000000
Al           -0.2500000000        0.2500000000        0.2500000000
Al            0.2500000000       -0.2500000000       -0.2500000000
Al           -0.2500000000        0.2500000000       -0.2500000000
Al           -0.2500000000       -0.2500000000        0.2500000000
B            -0.5985646056       -0.5985646056       -0.5985646056
B            -0.0985646056       -0.0985646056       -0.0985646056
B            -0.5985646056       -0.5985646056        0.7956938169
B            -0.0985646056       -0.0985646056        0.2956938169
B            -0.5985646056        0.7956938169       -0.5985646056
B            -0.0985646056        0.2956938169       -0.0985646056
B             0.7956938169       -0.5985646056       -0.5985646056
B             0.2956938169       -0.0985646056       -0.0985646056
S             0.5397227688        0.8067197158        0.4330404256
S             0.4330404256        0.8067197158        0.2205170898
S             0.2205170898        0.8067197158        0.5397227688
S             0.8067197158        0.5397227688        0.2205170898
S             0.2205170898        0.5397227688        0.4330404256
S             0.4330404256        0.5397227688        0.8067197158
S             0.4330404256        0.2205170898        0.5397227688
S             0.5397227688        0.2205170898        0.8067197158
S             0.8067197158        0.2205170898        0.4330404256
S             0.2205170898        0.4330404256        0.8067197158
S             0.8067197158        0.4330404256        0.5397227688
S             0.5397227688        0.4330404256        0.2205170898
S             0.0397227688        0.3067197158        0.7205170898
S             0.9330404256        0.3067197158        0.0397227688
S             0.7205170898        0.3067197158        0.9330404256
S             0.3067197158        0.0397227688        0.9330404256
S             0.7205170898        0.0397227688        0.3067197158
S             0.9330404256        0.0397227688        0.7205170898
S             0.9330404256        0.7205170898        0.3067197158
S             0.0397227688        0.7205170898        0.9330404256
S             0.3067197158        0.7205170898        0.0397227688
S             0.7205170898        0.9330404256        0.0397227688
S             0.3067197158        0.9330404256        0.7205170898
S             0.0397227688        0.9330404256        0.3067197158
Cl            0.2500000000        0.2500000000        0.2500000000
Cl            0.7500000000        0.7500000000        0.7500000000
```

TABLE XIII. Cartesian coordinates of primitive cell (in Bohr units) and fractional coordinates for the optimized structure of $Li_6B_7O_{13}Cl$ in the Cc (No. 9) structure.

```
CELL_PARAMETERS (bohr)
   1.4133187E+01   8.1031139E+00   0.0000000E+00
  -1.4133187E+01   8.1031139E+00   0.0000000E+00
  -9.2261456E+00   0.0000000E+00   1.3308154E+01

ATOMIC_POSITIONS (crystal)
Li       0.743915002  0.440190739  0.370076152
Li       0.559809261  0.256084998  0.870076152
Li       0.629753588  0.927833529  0.270188355
Li       0.072166471  0.370246412  0.770188355
Li       0.616319610  0.867883442  0.904076679
Li       0.132116558  0.383680390  0.404076679
Li       0.105690481  0.836293193  0.391722161
Li       0.163706807  0.894309519  0.891722161
Li       0.489885160  0.472393493  0.996365297
Li       0.527606507  0.510114840  0.496365297
Li       0.997643877  0.998270836  0.509299597
Li       0.001729164  0.002356123  0.009299597
B        0.747742787  0.246414890  0.251008527
B        0.753585110  0.252257213  0.751008527
B        0.250234718  0.744416806  0.754149393
B        0.255583194  0.749765282  0.254149393
B        0.253961577  0.252922073  0.260031501
B        0.747077927  0.746038423  0.760031501
B        0.422122673  0.082133052  0.273119046
B        0.917866948  0.577877327  0.773119046
B        0.731637600  0.077417488  0.580152697
B        0.922582512  0.268362400  0.080152697
B        0.404813554  0.701187008  0.599758787
B        0.298812992  0.595186446  0.099758787
B        0.425850134  0.084812848  0.579809945
B        0.915187152  0.574149866  0.079809945
O        0.564599602  0.260341218  0.204152130
O        0.739658782  0.435400398  0.704152130
O        0.789692040  0.095729259  0.437110223
O        0.904270741  0.210307960  0.937110223
O        0.392649245  0.685642478  0.763777146
O        0.314357522  0.607350755  0.263777146
O        0.246928656  0.930498941  0.607277905
O        0.069501059  0.753071344  0.107277905
O        0.240118151  0.098310046  0.218358358
O        0.901689954  0.759881849  0.718358358
O        0.780813977  0.931398659  0.760527442
O        0.068601341  0.219186023  0.260527442
O        0.562052133  0.687681984  0.609683704
O        0.312318016  0.437947867  0.109683704
O        0.395724617  0.262205932  0.446041812
O        0.737794068  0.604275383  0.946041812
O        0.395494703  0.937171604  0.213306474
O        0.062828396  0.604505297  0.713306474
O        0.808405887  0.258650033  0.610390773
O        0.741349967  0.191594113  0.110390773
O        0.240376375  0.683519370  0.444190828
O        0.316480630  0.759623625  0.944190828
O        0.567772796  0.104519174  0.760378566
O        0.895480826  0.432227204  0.260378566
O        0.506944613  0.024487405  0.496320507
O        0.975512595  0.493055387  0.996320507
Cl       0.238421461  0.233459719  0.754065993
Cl       0.766540281  0.761578539  0.254065993
```

TABLE XIV. Cartesian coordinates of primitive cell (in Bohr units) and fractional coordinates for the optimized structure of $Li_6Al_3B_4O_{13}Cl$ in the Cc (No. 9) structure.

```
CELL_PARAMETERS (bohr)
   1.5091092E+01   8.3630495E+00   0.0000000E+00
  -1.5091092E+01   8.3630495E+00   0.0000000E+00
  -1.1075558E+01   0.0000000E+00   1.4637820E+01

ATOMIC_POSITIONS (crystal)
Li       0.640497659  0.398591211  0.365204581
Li       0.601408789  0.359502341  0.865204581
Li       0.511789548  0.959197568  0.099860212
Li       0.040802432  0.488210452  0.599860212
Li       0.687148211  0.900672698  0.893511551
Li       0.099327302  0.312851789  0.393511551
Li       0.119340086  0.893882983  0.387868542
Li       0.106117017  0.880659914  0.887868542
Li       0.466714113  0.468836098  0.996484274
Li       0.531163902  0.533285887  0.496484274
Li       0.901072442  0.909000493  0.500567045
Li       0.090999507  0.098927558  0.000567045
Al       0.277291843  0.774882979  0.781401550
Al       0.225117021  0.722708157  0.281401550
Al       0.762974445  0.088666970  0.572276739
Al       0.911333030  0.237025555  0.072276739
Al       0.436491322  0.750156894  0.610095621
Al       0.249843106  0.563508678  0.110095621
B        0.753325224  0.241956789  0.247690944
B        0.758043211  0.246674776  0.747690944
B        0.281745939  0.246737095  0.265263259
B        0.753262905  0.718254061  0.765263259
B        0.441098870  0.068209511  0.288690410
B        0.931790489  0.558901130  0.788690410
B        0.416373245  0.115786601  0.585902234
B        0.884213399  0.583626755  0.085902234
O        0.587443554  0.244544900  0.238128546
O        0.755455100  0.412556446  0.738128546
O        0.845991290  0.126917893  0.423526915
O        0.873082107  0.154008710  0.923526915
O        0.446924001  0.712900967  0.811574633
O        0.287099033  0.553075999  0.311574633
O        0.252002686  0.971705287  0.592228322
O        0.028294713  0.747997314  0.092228322
O        0.271163331  0.096204068  0.238628672
O        0.903795932  0.728836669  0.738628672
O        0.800057023  0.900703608  0.763097153
O        0.099296392  0.199942977  0.263097153
O        0.576428956  0.653015497  0.637778583
O        0.346984503  0.423571044  0.137778583
O        0.425540190  0.267969273  0.438383293
O        0.732030727  0.574459810  0.938383293
O        0.396219000  0.935439709  0.224235593
O        0.064560291  0.603781000  0.724235593
O        0.812049837  0.282458488  0.610239243
O        0.717541512  0.187950163  0.110239243
O        0.206124731  0.683902491  0.470138857
O        0.316097509  0.793875269  0.970138857
O        0.567189651  0.107978461  0.735450896
O        0.892021539  0.432810349  0.235450896
O        0.516952516  0.991875149  0.486721805
O        0.008124851  0.483047484  0.986721805
Cl       0.252083884  0.236060115  0.800390528
Cl       0.763939885  0.747916116  0.300390528
```

TABLE XV. Cartesian coordinates of primitive cell (in Bohr units) and fractional coordinates for the optimized structure of $Li_6B_7S_{13}Cl$ in the Cc (No. 9) structure.

```
CELL_PARAMETERS (bohr)
   1.7506379E+01   9.9077117E+00   0.0000000E+00
  -1.7506379E+01   9.9077117E+00   0.0000000E+00
  -1.1555429E+01   0.0000000E+00   1.6724750E+01

ATOMIC_POSITIONS (crystal)
Li       0.682061700  0.430250400  0.368013000
Li       0.569749600  0.317938300  0.868013000
Li       0.637083800  0.883091200  0.330081400
Li       0.116908800  0.362916200  0.830081400
Li       0.622485200  0.866831600  0.910693400
Li       0.133168400  0.377514800  0.410693400
Li       0.070310100  0.817589900  0.382464000
Li       0.182410100  0.929689900  0.882464000
Li       0.453847700  0.446391300  0.965134000
Li       0.553608700  0.546152300  0.465134000
Li       0.961735300  0.953471300  0.472877800
Li       0.046528700  0.038264700  0.972877800
B        0.751360500  0.247988300  0.253374600
B        0.752011700  0.248639500  0.753374600
B        0.252627800  0.748430500  0.750875600
B        0.251569500  0.747372200  0.250875600
B        0.251475600  0.247594500  0.253307000
B        0.752405500  0.748524400  0.753307000
B        0.420866900  0.071475900  0.275910200
B        0.928524100  0.579133100  0.775910200
B        0.735062700  0.076530900  0.582802100
B        0.923469100  0.264937300  0.082802100
B        0.424787200  0.764881600  0.573959000
B        0.235118400  0.575212800  0.073959000
B        0.425477400  0.081756700  0.574112700
B        0.918243300  0.574522600  0.074112700
S        0.564716000  0.269698400  0.210828500
S        0.730301600  0.435284000  0.710828500
S        0.807465700  0.092932200  0.443884100
S        0.907067800  0.192534300  0.943884100
S        0.409926000  0.696007800  0.767367300
S        0.303992200  0.590074000  0.267367300
S        0.228286600  0.935548300  0.589690700
S        0.064451700  0.771713400  0.089690700
S        0.222953100  0.073111800  0.220091100
S        0.926888200  0.777046900  0.720091100
S        0.796348500  0.935649200  0.776738400
S        0.064350800  0.203651500  0.276738400
S        0.570919000  0.705731700  0.585052300
S        0.294268300  0.429081000  0.085052300
S        0.419555800  0.279016500  0.434431700
S        0.720983500  0.580444200  0.934431700
S        0.408362000  0.941275500  0.197447900
S        0.058724500  0.591638000  0.697447900
S        0.813672700  0.273051100  0.600635600
S        0.726948900  0.186327300  0.100635600
S        0.228988400  0.683823200  0.441823700
S        0.316176800  0.771011600  0.941823700
S        0.555478100  0.093818700  0.768525500
S        0.906181300  0.444521900  0.268525500
S        0.502261100  0.998267200  0.502734800
S        0.001732800  0.497738900  0.002734800
Cl       0.254770700  0.234890100  0.832483600
Cl       0.765109900  0.745229300  0.332483600
```

TABLE XVI. Cartesian coordinates of primitive cell (in Bohr units) and fractional coordinates for the optimized structure of $Li_6Al_3B_4S_{13}Cl$ in the Cc (No. 9) structure.

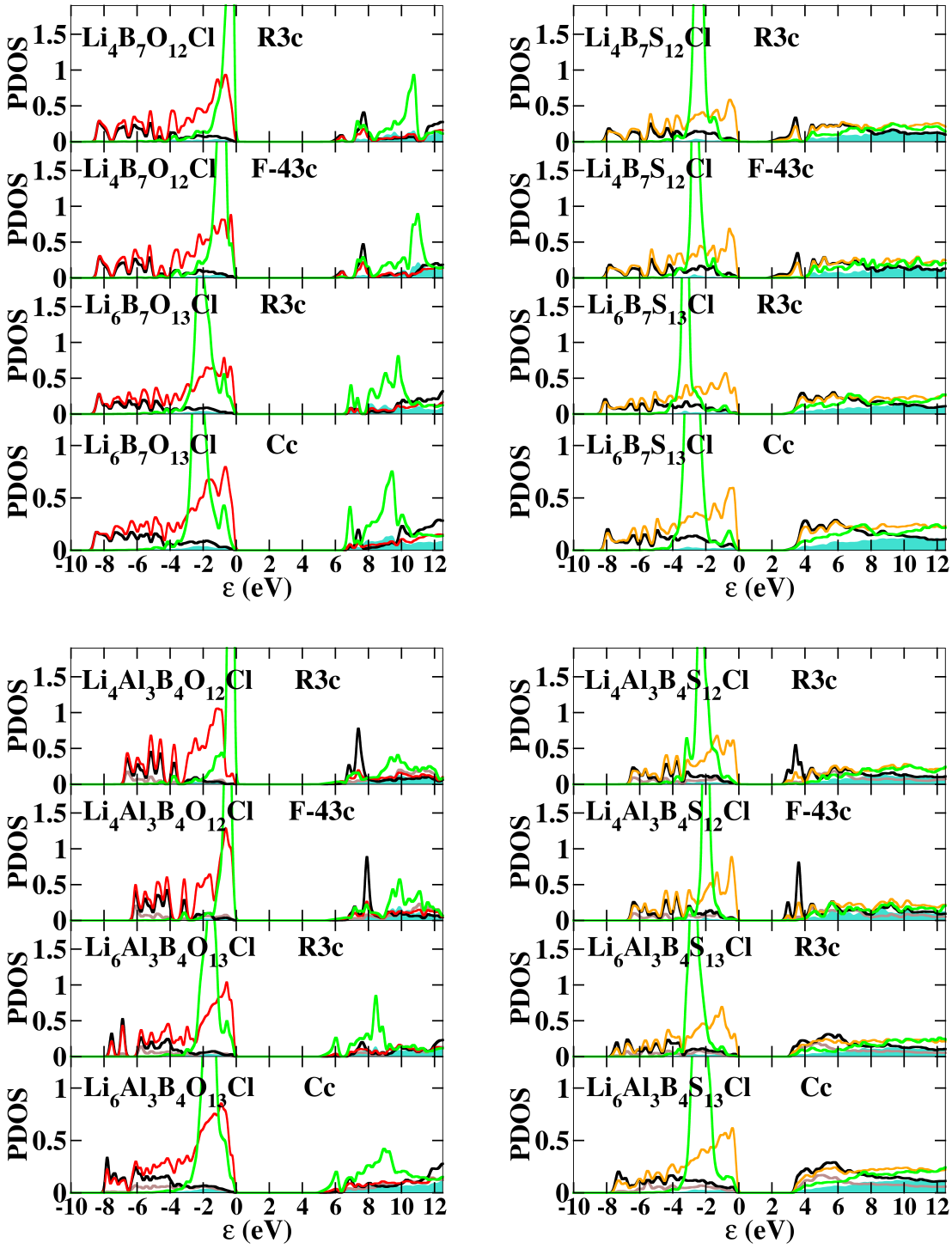
```
CELL_PARAMETERS (bohr)
   1.8693301E+01   1.0161255E+01   0.0000000E+00
  -1.8693301E+01   1.0161255E+01   0.0000000E+00
  -1.3183861E+01   0.0000000E+00   1.8054032E+01

ATOMIC_POSITIONS (crystal)
Li       0.660269004  0.403534009  0.364936506
Li       0.596465991  0.339730996  0.864936506
Li       0.632933505  0.883710418  0.348152081
Li       0.116289582  0.367066495  0.848152081
Li       0.662563928  0.914658650  0.869861236
Li       0.085341350  0.337436072  0.369861236
Li       0.107809624  0.847550340  0.394227045
Li       0.152449660  0.892190376  0.894227045
Li       0.445018245  0.424233940  0.980495885
Li       0.575766060  0.554981755  0.480495885
Li       0.954907199  0.939534828  0.474073719
Li       0.060465172  0.045092801  0.974073719
Al       0.280557044  0.772648734  0.777064446
Al       0.227351266  0.719442956  0.277064446
Al       0.754124777  0.097649659  0.571433154
Al       0.902350341  0.245875223  0.071433154
Al       0.416310217  0.747138969  0.593555990
Al       0.252861031  0.583689783  0.093555990
B        0.736363516  0.244965596  0.230846747
B        0.755034404  0.263636484  0.730846747
B        0.254764336  0.239328155  0.249837097
B        0.760671845  0.745235664  0.749837097
B        0.421907823  0.073567200  0.279023518
B        0.926432800  0.578092177  0.779023518
B        0.427565103  0.100035641  0.550391660
B        0.899964359  0.572434897  0.050391660
S        0.568211144  0.265403504  0.216488013
S        0.734596496  0.431788856  0.716488013
S        0.820225380  0.112812611  0.413743765
S        0.887187389  0.179774620  0.913743765
S        0.448096071  0.693881137  0.814889833
S        0.306118863  0.551903929  0.314889833
S        0.237574968  0.960664160  0.574436236
S        0.039335840  0.762425032  0.074436236
S        0.228769011  0.071807668  0.221381645
S        0.928192332  0.771230989  0.721381645
S        0.822650987  0.929556136  0.778174997
S        0.070443864  0.177349013  0.278174997
S        0.588578637  0.709125680  0.587744817
S        0.290874320  0.411421363  0.087744817
S        0.424293881  0.285727774  0.411426969
S        0.714272226  0.575706119  0.911426969
S        0.411685898  0.939798046  0.223751699
S        0.060201954  0.588314102  0.723751699
S        0.829954238  0.316804851  0.590877954
S        0.683195149  0.170045762  0.090877954
S        0.179731285  0.646211784  0.469666756
S        0.353788216  0.820268715  0.969666756
S        0.560209943  0.109933706  0.730159192
S        0.890066294  0.439790057  0.230159192
S        0.491744139  0.010776993  0.489731519
S        0.989223007  0.508255861  0.989731519
Cl       0.242688046  0.244667959  0.858967520
Cl       0.755332041  0.757311954  0.358967520
```

II. ELECTRONIC PARTIAL DENSITY OF STATES OF THE LITHIUM (THIO)BORACITE FAMILY OF MATERIALS

Here we present the electronic partial density of states for the 16 Li (thio)boracites listed in Table I of the manuscript. Note that in this section, the label "PDOS" refers to the electronic partial density of states. The partial density of states PDOS were calculated using Eqs. (2-4) of Ref. 3. In practice, by using the projector augmented wave formalism, [4] the PDOS plots are able to represent the approximate average number of valence electrons within the augmentation sphere about each atom type per Rydberg. For the PAW datasets used in this work, the augmentation sphere radii in Bohr units are 1.6 for Li, 1.4 for B, 1.2 for O, 1.6 for Al, 1.7 for S, and 1.7 for Cl. The PDOS plots were calculated using a simple Gaussian smoothing of width 0.01 Ryd. The color scheme for the plots is Li (shaded turquoise), B (black line), O (red line), Al (brown line) , S (orange line), and Cl (green line). Plots of the PDOS for each composition are grouped together for comparison and plotted as a function of the band energy ε in eV units, with $\varepsilon = 0$ representing the energy of the highest occupied band for each material.

FIG. 1. Electronic partial densitites of states for 16 Li (thio)boracites listed in Table I of the manusript. The color scheme for the curves in each plot is given by Li (shaded turquoise), B (black line), O (red line), Al (brown line) , S (orange line), and Cl (green line).



III. PHONON BAND DISPERSIONS AND PHONON DENSITY OF STATES OF THE LITHIUM (THIO)BORACITE FAMILY OF MATERIALS.

Here we present the phonon band diagrams calculated for the 13 Li (thio)boracites listed in Table III of the manuscript, including those also given in the manuscript. As explained in the manuscript, these results were generated using the PHONOPY code [5, 6] with QUANTUM ESPRESSO [1] to evaluate the forces in the supercell and also to evaluate the long-range dipolar electric field couplings [7–9] using DFPT at $\mathbf{q} = 0$.

The band plots use the standard Brilliouin path given in Ref. [10], reproduced in Appendix D, Fig. 19 of the manuscript. The phonon frequencies are given in units of cm^{-1}. The side panel presents the phonon density of states $g(\omega)$ in units of (states per unit cell)/cm^{-1} as indicated with the full curve. The width of the shaded curve segment indicates the contribution of each partial density of states component $g_a(\omega)$. The curve segments are presented in the following order: Li (light blue), Al (grey, if present), B (black), O (red) or S (orange), and Cl (green). Note that within this section, the label "PDOS" refers to the phonon partial density of states.

FIG. 2. Phonon bands and density of states for $Li_4B_7O_{12}Cl$ in the $R3c$ structure.

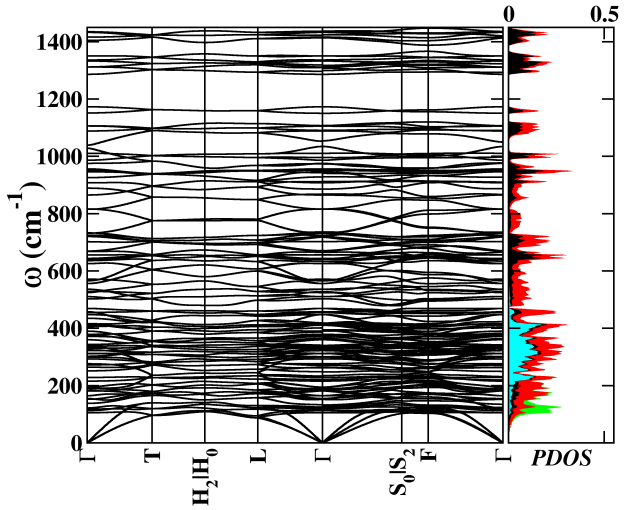


FIG. 3. Phonon bands and density of states for $Li_4Al_3B_4O_{12}Cl$ in the $R3c$ structure.

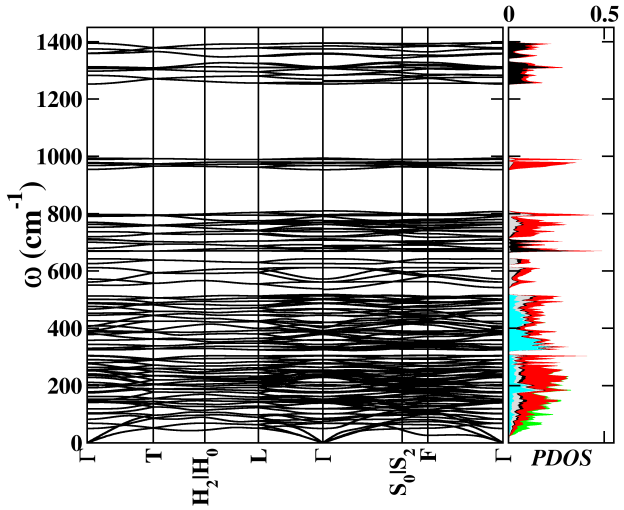


FIG. 4. Phonon bands and density of states for $Li_4B_7S_{12}Cl$ in the $F\bar{4}3c$ (left) and $R3c$ (right) structures.

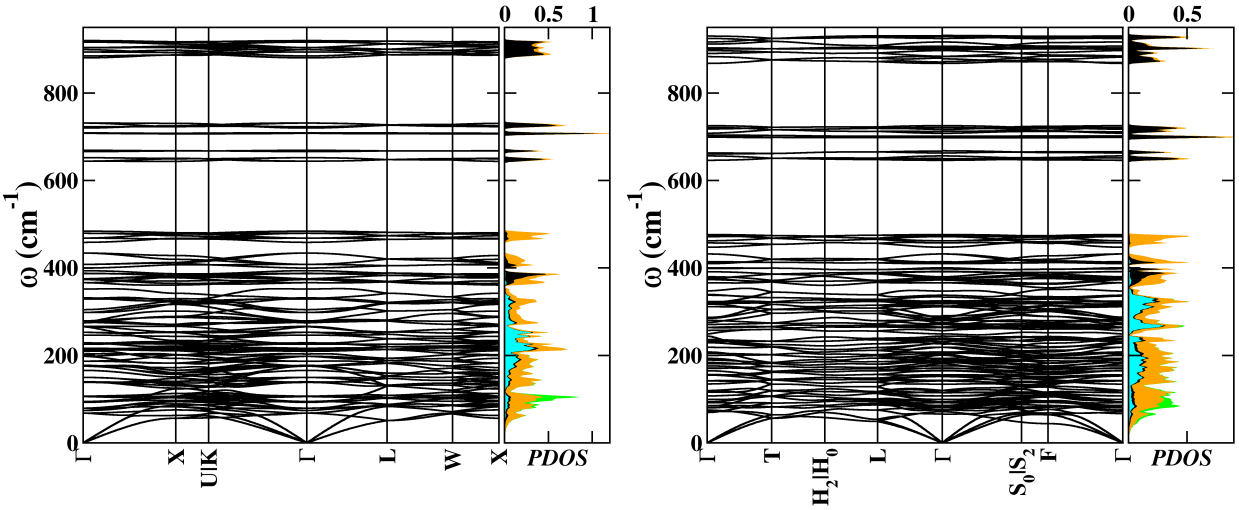


FIG. 5. Phonon bands and density of states for $Li_4Al_3B_4S_{12}Cl$ in the $R3c$ structure.

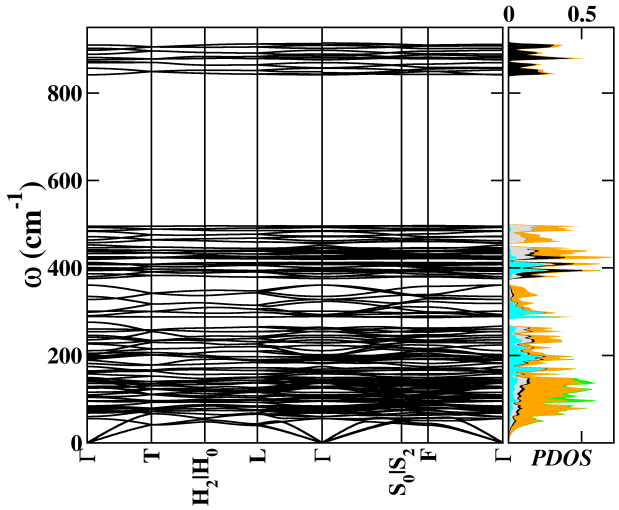


FIG. 6. Phonon bands and density of states for $Li_6B_7O_{13}Cl$ in the $R3c$ (left) and Cc (right) structures.

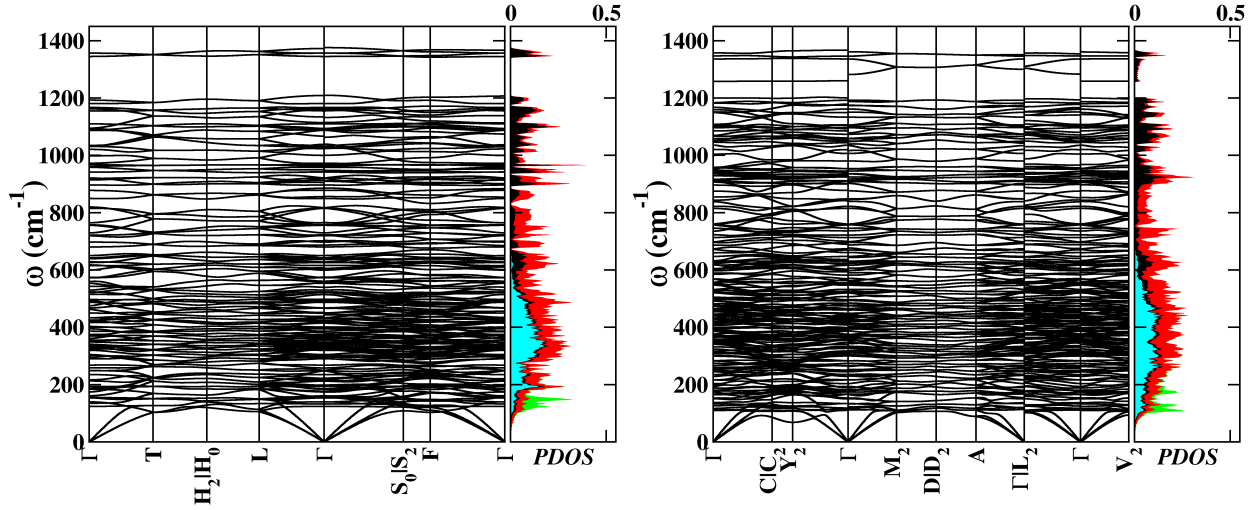


FIG. 7. Phonon bands and density of states for $Li_6Al_3B_4O_{13}Cl$ in the Cc (left) and $R3c$ (right) structures.

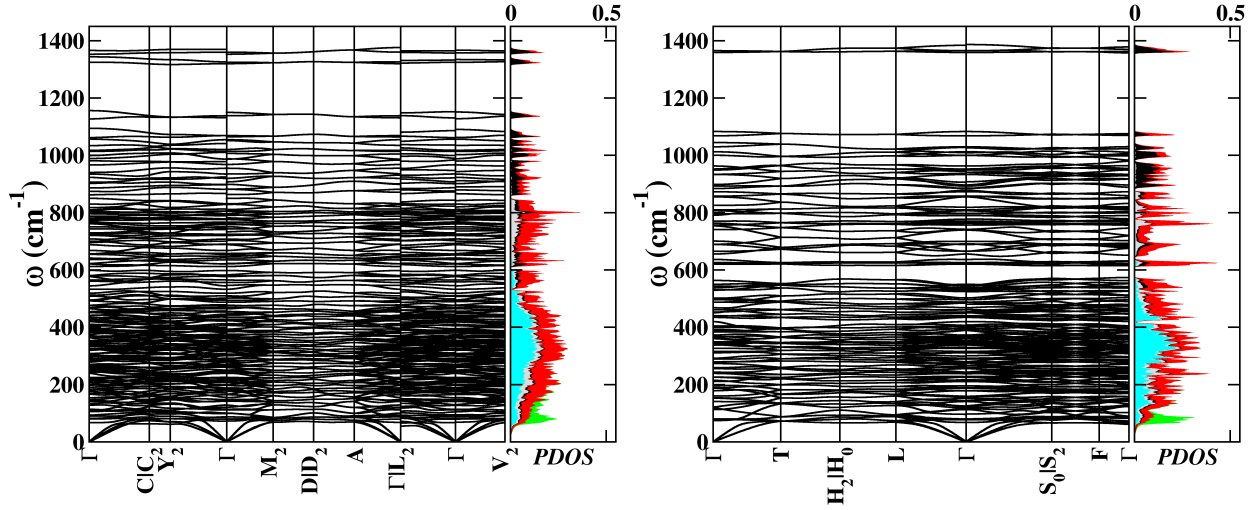


FIG. 8. Phonon bands and density of states for $Li_6B_7S_{13}Cl$ in the Cc (left) and $R3c$ (right) structures.

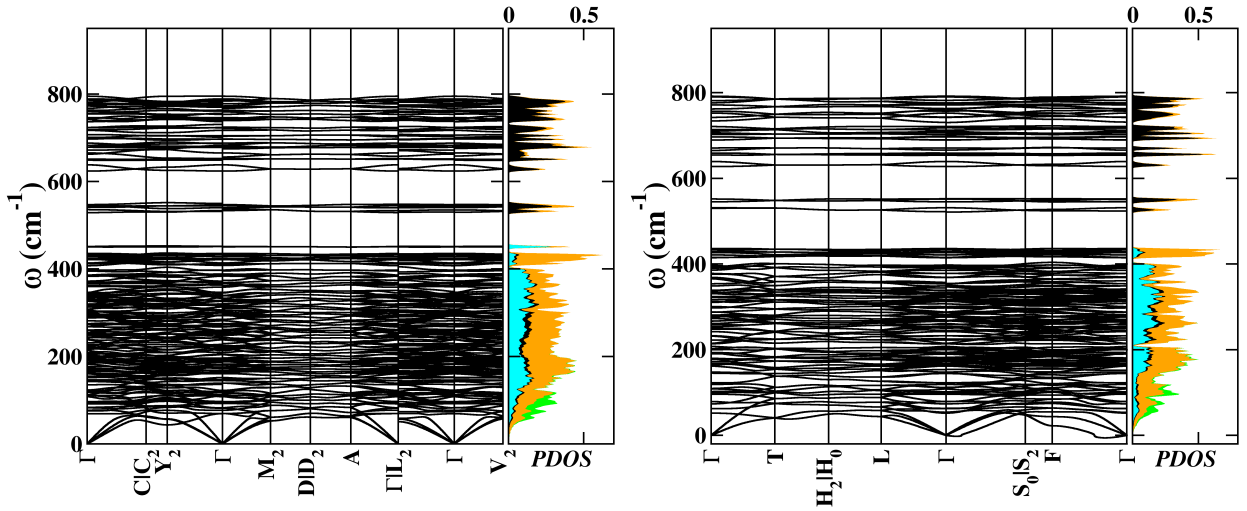
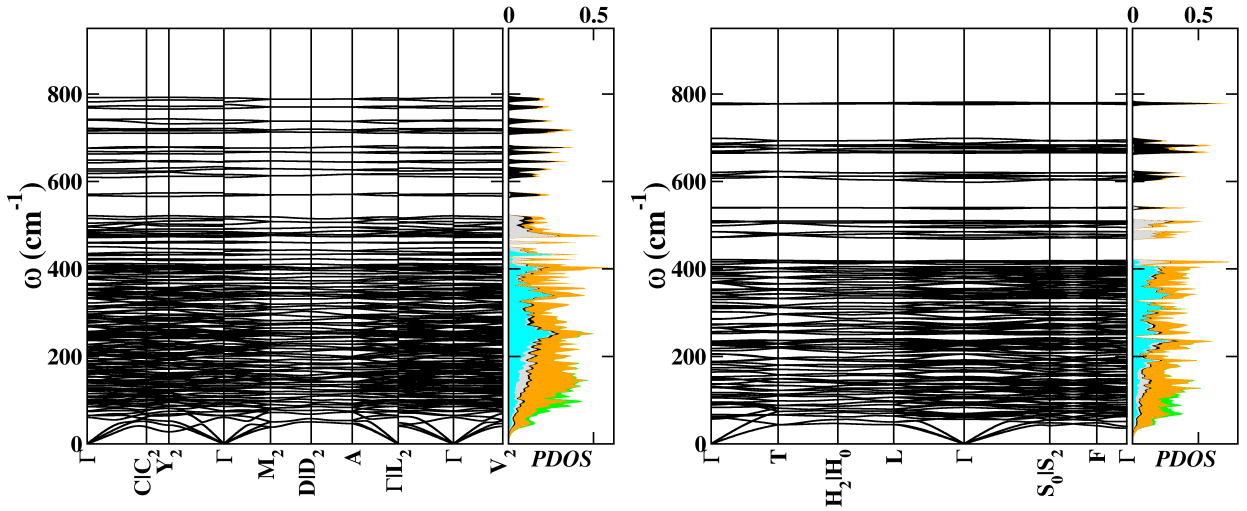


FIG. 9. Phonon bands and density of states for $Li_6Al_3B_4S_{13}Cl$ in the Cc (left) and $R3c$ (right) structures.



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