Supplementary Materials: High-throughput first principles search for new ferroelectrics

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(Dated: January 5, 2018)

Supplementary materials for "High-throughput first principles search for new ferroelectrics" Includes structural data on all compounds.

I. STRUCTURAL DATA

This section contains structural data for the high and low symmetry structures of proposed ferroelectrics.

A. $SrNb_6O_{16}$

Non-polar
ICSD 60783[4]

```
Space Group = 38
Full Formula (Sr1 Nb6 O16)
Reduced Formula: SrNb6O16
abc   :   9.017667   9.017667   3.859704
angles:  90.000000  90.000000 110.009663
Sites (23)
0 Sr     0.398500     0.601500     0.500000
1 Nb     0.993902     0.006098     0.000000
2 Nb     0.207569     0.792431     0.000000
3 Nb     0.378259     0.257859     1.000000
4 Nb     0.742141     0.621741     1.000000
5 Nb     0.627663     0.999301     0.000000
6 Nb     0.000699     0.372337     1.000000
7 O     0.002828     0.997172     0.500000
8 O     0.224374     0.775626     0.500000
9 O     0.366568     0.291867     0.500000
10 O     0.708133     0.633432     0.500000
11 O     0.626481     0.001655     0.500000
12 O     0.998345     0.373519     0.500000
13 O     0.235588     0.013890     1.000000
14 O     0.986110     0.764412     1.000000
15 O     0.442310     0.812625     0.000000
16 O     0.187375     0.557690     0.000000
17 O     0.761732     0.854220     0.000000
18 O     0.145780     0.238268     1.000000
19 O     0.534385     0.166952     0.000000
20 O     0.833048     0.465615     1.000000
21 O     0.856734     0.143266     0.000000
22 O     0.511475     0.488525     1.000000
```

Polar

```
Space Group = 8
Full Formula (Sr1 Nb6 O16)
Reduced Formula: SrNb6O16
abc   :   8.975020   8.975020   3.930378
```

```
angles:  89.705769  90.294231 110.229607
Sites (23)
0 Sr     0.398472     0.601528     0.494185
1 Nb     0.995626     0.004374     0.063034
2 Nb     0.209298     0.790702     0.964611
3 Nb     0.377699     0.257918     0.977629
4 Nb     0.742082     0.622301     0.977629
5 Nb     0.629262     0.001380     0.954623
6 Nb     0.998620     0.370738     0.954623
7 O     0.999641     0.000359     0.518978
8 O     0.221829     0.778171     0.498754
9 O     0.370179     0.289742     0.508752
10 O     0.710258     0.629821     0.508752
11 O     0.626485     0.995866     0.495997
12 O     0.004134     0.373515     0.495997
13 O     0.234536     0.014254     0.012973
14 O     0.985746     0.765464     0.012973
15 O     0.440806     0.813838     0.005906
16 O     0.186162     0.559194     0.005906
17 O     0.760372     0.852610     0.012941
18 O     0.147390     0.239628     0.012941
19 O     0.536121     0.166427     0.000061
20 O     0.833573     0.463879     0.000061
21 O     0.856484     0.143516     0.014057
22 O     0.509695     0.490305     0.008604
```

Alternate-low energy structure

```
Space Group = 1
Full Formula (Sr1 Nb6 O16)
Reduced Formula: SrNb6O16
abc   :   3.930916   8.973540   8.976735
angles:  69.746063  89.807687  89.537025
Sites (23)
0 Sr     0.493476     0.602413     0.600452
1 Nb     0.054725     0.003845     0.004849
2 Nb     0.959485     0.790935     0.790526
3 Nb     0.973461     0.622521     0.257708
4 Nb     0.976748     0.258121     0.623174
5 Nb     0.060381     0.371746     0.001485
6 Nb     0.950575     0.002063     0.370913
7 O     0.511439     0.999451     0.001012
8 O     0.494622     0.778721     0.777402
9 O     0.505055     0.630026     0.289431
10 O     0.507712     0.290348     0.630540
11 O     0.519292     0.373819     0.996552
12 O     0.492069     0.996711     0.373555
13 O     0.006399     0.765323     0.014331
14 O     0.006428     0.014192     0.766224
15 O     0.005008     0.559606     0.813706
16 O     0.001622     0.814048     0.559305
17 O     0.015492     0.239788     0.852780
18 O     0.007397     0.852205     0.240241
19 O     0.003497     0.463695     0.166866
20 O     0.998404     0.166160     0.465007
21 O     0.010220     0.143622     0.143558
22 O     0.006487     0.490641     0.490379
```

B. $NaNb_6O_{16}F$

Non-polar
ICSD 24109[5]

```
Space Group = 38
Full Formula (Na1 Nb6 O15 F1)
Reduced Formula: NaNb6O15F
abc   :   8.996016   8.996016   3.887490
angles:  90.000000  90.000000 109.954098
Sites (23)
0 Na     0.403993     0.596007     0.500000
1 Nb     0.998950     0.001050     1.000000
2 Nb     0.217437     0.782563     1.000000
3 Nb     0.376935     0.262472     0.000000
4 Nb     0.737528     0.623065     1.000000
5 Nb     0.627975     0.005242     0.000000
6 Nb     0.994758     0.372025     1.000000
7 O     0.220751     0.779249     0.500000
8 O     0.362981     0.283193     0.500000
9 O     0.716807     0.637019     0.500000
10 O     0.640783     0.007997     0.500000
11 O     0.992003     0.359217     0.500000
12 O     0.227551     0.010583     0.000000
13 O     0.989417     0.772449     1.000000
14 O     0.445298     0.819325     1.000000
15 O     0.180675     0.554702     1.000000
16 O     0.768521     0.857079     0.000000
17 O     0.142921     0.231479     0.000000
18 O     0.531765     0.165200     0.000000
19 O     0.834800     0.468235     0.000000
20 O     0.862695     0.137305     1.000000
21 O     0.514101     0.485899     1.000000
22 F     0.999353     0.000647     0.500000
```

Polar

```
Space Group = 8
Full Formula (Na1 Nb6 O15 F1)
Reduced Formula: NaNb6O15F
abc   :   8.946903   8.946903   3.970948
angles:  89.533486  90.466514 109.968577
Sites (23)
0 Na     0.595246     0.404754     0.525670
1 Nb     0.000740     0.999260     0.994077
2 Nb     0.781360     0.218640     0.055607
3 Nb     0.262328     0.377633     0.035943
4 Nb     0.622367     0.737672     0.035943
5 Nb     0.005187     0.628468     0.932469
6 Nb     0.371532     0.994813     0.932469
7 O     0.780687     0.219313     0.510310
8 O     0.280287     0.365461     0.493855
9 O     0.634539     0.719713     0.493855
10 O     0.005350     0.636949     0.480625
11 O     0.363051     0.994650     0.480625
12 O     0.010809     0.227044     0.004016
```

```
13 O     0.772956     0.989191     0.004016
14 O     0.819556     0.444254     0.993307
15 O     0.555746     0.180444     0.993307
16 O     0.856232     0.766434     0.987046
17 O     0.233566     0.143768     0.987046
18 O     0.166859     0.534718     0.994023
19 O     0.465282     0.833141     0.994023
20 O     0.138727     0.861273     0.993159
21 O     0.487212     0.512788     0.994208
22 F     0.002384     0.997616     0.494401
```

Alternate low energy

```
Space Group = 1
Full Formula (Na1 Nb6 O15 F1)
Reduced Formula: NaNb6O15F
abc   :   3.968460   8.956992   8.946166
angles:  69.962292  89.481844  89.753396
Sites (23)
0 Na     0.526026     0.407124     0.401169
1 Nb     0.982931     0.999062     0.999624
2 Nb     0.047429     0.218250     0.218725
3 Nb     0.032559     0.738182     0.378131
4 Nb     0.031107     0.377320     0.737380
5 Nb     0.924874     0.994482     0.628890
6 Nb     0.049917     0.628588     0.994395
7 O     0.502900     0.219540     0.218806
8 O     0.491089     0.720758     0.365989
9 O     0.489050     0.364924     0.719251
10 O     0.472830     0.994509     0.637295
11 O     0.502303     0.636648     0.994833
12 O     0.993990     0.988928     0.227642
13 O     0.996576     0.226713     0.989234
14 O     0.985543     0.179969     0.444252
15 O     0.991565     0.444221     0.180530
16 O     0.980071     0.143384     0.766688
17 O     0.990499     0.766313     0.144104
18 O     0.989431     0.833160     0.535447
19 O     0.998067     0.534354     0.833151
20 O     0.986667     0.861233     0.861700
21 O     0.989647     0.513167     0.512709
22 F     0.484933     0.997175     0.998055
```

C. $RbCa_2Nb_3O_{10}$

Non-polar
ICSD 260289[6]

```
Space Group = 123
Full Formula (Rb1 Ca2 Nb3 O10)
Reduced Formula: RbCa2Nb3O10
abc   :   3.900514   3.900514  14.996799
angles:  90.000000  90.000000  90.000000
Sites (16)
0 Rb     0.500000     0.500000     0.500000
1 Ca     0.500000     0.500000     0.850282
```

```
2 Ca     0.500000     0.500000     0.149718
3 Nb     0.000000     0.000000     0.000000
4 Nb     0.000000     0.000000     0.718679
5 Nb     0.000000     0.000000     0.281321
6 O     0.000000     0.500000     0.000000
7 O     0.500000     0.000000     0.000000
8 O     0.000000     0.000000     0.870367
9 O     0.000000     0.000000     0.129633
10 O     0.000000     0.500000     0.746924
11 O     0.500000     0.000000     0.746924
12 O     0.000000     0.500000     0.253076
13 O     0.500000     0.000000     0.253076
14 O     0.000000     0.000000     0.600394
15 O     0.000000     0.000000     0.399606
```

Polar

```
Space Group = 7
Full Formula (Rb2 Ca4 Nb6 O20)
Reduced Formula: RbCa2Nb3O10
abc   :   5.460413   5.426493  14.970151
angles:  90.000000  90.526522  90.000000
Sites (32)
0 Rb     0.481742     0.239793     0.510061
1 Rb     0.981742     0.760207     0.510061
2 Ca     0.473565     0.260809     0.149634
3 Ca     0.461092     0.252237     0.856661
4 Ca     0.973565     0.739191     0.149634
5 Ca     0.961092     0.747763     0.856661
6 Nb     0.987605     0.240946     0.997906
7 Nb     0.995831     0.242838     0.284453
8 Nb     0.996791     0.250594     0.717021
9 Nb     0.487605     0.759054     0.997906
10 Nb     0.495831     0.757162     0.284453
11 Nb     0.496791     0.749406     0.717021
12 O     0.829237     0.929853     0.018033
13 O     0.706454     0.441685     0.974002
14 O     0.011177     0.319822     0.123643
15 O     0.036032     0.169426     0.872257
16 O     0.734191     0.014948     0.239938
17 O     0.772194     0.520955     0.268832
18 O     0.802155     0.953276     0.725587
19 O     0.728614     0.467469     0.759900
20 O     0.995050     0.195536     0.400615
21 O     0.987958     0.300328     0.600111
22 O     0.206454     0.558315     0.974002
23 O     0.329237     0.070147     0.018033
24 O     0.511177     0.680178     0.123643
25 O     0.536032     0.830574     0.872257
26 O     0.272194     0.479045     0.268832
27 O     0.234191     0.985052     0.239938
28 O     0.228614     0.532531     0.759900
29 O     0.302155     0.046724     0.725587
30 O     0.495050     0.804464     0.400615
31 O     0.487958     0.699672     0.600111
```

D. $BaBi_2Ta_2O_9$

Non-polar
ICSD 92058, 93752

```
Space Group = 139
Full Formula (Ba1 Ta2 Bi2 O9)
Reduced Formula: BaTa2Bi2O9
abc   :  12.626511  12.626511  12.626511
angles: 162.076460 162.076460  25.453271
Sites (14)
0 Ba     0.000000     0.000000     0.000000
1 Ta     0.588742     0.588742     0.000000
2 Ta     0.411258     0.411258     0.000000
3 Bi     0.799023     0.799023     0.000000
4 Bi     0.200977     0.200977     0.000000
5 O     0.500000     0.500000     0.000000
6 O     0.664841     0.664841     0.000000
7 O     0.335159     0.335159     0.000000
8 O     0.750000     0.250000     0.500000
9 O     0.250000     0.750000     0.500000
10 O     0.581338     0.081338     0.500000
11 O     0.081338     0.581338     0.500000
12 O     0.418662     0.918662     0.500000
13 O     0.918662     0.418662     0.500000
```

Polar

```
Space Group = 36
Full Formula (Ba2 Ta4 Bi4 O18)
Reduced Formula: BaTa2Bi2O9
abc   :  12.884322  12.884322   5.609108
angles:  90.000000  90.000000 154.929890
Sites (28)
0 Ba     0.751948     0.751948     0.980406
1 Ba     0.248052     0.248052     0.480406
2 Ta     0.166813     0.338151     0.984262
3 Ta     0.833187     0.661849     0.484262
4 Ta     0.338151     0.166813     0.984262
5 Ta     0.661849     0.833187     0.484262
6 Bi     0.519791     0.921429     0.080586
7 Bi     0.480209     0.078571     0.580586
8 Bi     0.921429     0.519791     0.080586
9 Bi     0.078571     0.480209     0.580586
10 O     0.460894     0.141567     0.965749
11 O     0.539106     0.858433     0.465749
12 O     0.141567     0.460894     0.965749
13 O     0.858433     0.539106     0.465749
14 O     0.574050     0.424740     0.227022
15 O     0.425950     0.575260     0.727022
16 O     0.424740     0.574050     0.227022
17 O     0.575260     0.425950     0.727022
18 O     0.736964     0.234018     0.288604
19 O     0.263036     0.765982     0.788604
20 O     0.234018     0.736964     0.288604
21 O     0.765982     0.263036     0.788604
```

```
22 O     0.234752     0.234752     0.975836
23 O     0.765248     0.765248     0.475836
24 O     0.919295     0.086038     0.725661
25 O     0.080705     0.913962     0.225661
26 O     0.086038     0.919295     0.725661
27 O     0.913962     0.080705     0.225661
```

E. $LiScAs_2O_7$

Non-polar
ICSD 161499[7]

```
Space Group = 5
Full Formula (Li1 Sc1 As2 O7)
Reduced Formula: LiScAs2O7
abc   :   5.479358   5.479358   4.886724
angles:  81.380919  98.619081  76.658134
Sites (11)
0 Li     0.248257     0.248257     0.500000
1 Sc     0.629209     0.629209     0.500000
2 As     0.744375     0.181808     0.091957
3 As     0.181808     0.744375     0.908043
4 O     0.860982     0.355948     0.317506
5 O     0.355948     0.860982     0.682494
6 O     0.610499     0.964711     0.250562
7 O     0.964711     0.610499     0.749438
8 O     0.039454     0.039454     0.000000
9 O     0.550202     0.338414     0.778226
10 O     0.338414     0.550202     0.221774
```

Polar

```
Space Group = 1
Full Formula (Li1 Sc1 As2 O7)
Reduced Formula: LiScAs2O7
abc   :   4.904965   5.502197   5.426075
angles: 103.017926  98.384543  98.313286
Sites (11)
0 Li     0.400711     0.261942     0.794925
1 Sc     0.504527     0.628371     0.370512
2 As     0.915986     0.176805     0.249631
3 As     0.099622     0.743621     0.809983
4 O     0.678828     0.343520     0.140753
5 O     0.318668     0.865493     0.631307
6 O     0.770055     0.937703     0.361935
7 O     0.262256     0.595945     0.016441
8 O     0.055813     0.054739     0.971764
9 O     0.210073     0.350736     0.460435
10 O     0.775042     0.572400     0.674873
```

F. YSF

Non-polar
ICSD 2597[1]

```
Space Group = 194
Full Formula (Y4 S4 F4)
Reduced Formula: YSF
abc   :   4.008530   4.008530  16.634373
angles:  90.000000  90.000000 120.000000
Sites (12)
0 Y     0.666667     0.333333     0.750000
1 Y     0.333333     0.666667     0.250000
2 Y     0.000000     0.000000     0.500000
3 Y     0.000000     0.000000     0.000000
4 S     0.666667     0.333333     0.585895
5 S     0.333333     0.666667     0.414105
6 S     0.333333     0.666667     0.085895
7 S     0.666667     0.333333     0.914105
8 F     0.666667     0.333333     0.250000
9 F     0.333333     0.666667     0.750000
10 F     0.000000     0.000000     0.750000
11 F     0.000000     0.000000     0.250000
```

Polar

```
Space Group = 186
Full Formula (Y4 S4 F4)
Reduced Formula: YSF
abc   :   3.963361   3.963361  16.755899
angles:  90.000000  90.000000 120.000000
Sites (12)
0 Y     0.666667     0.333333     0.749842
1 Y     0.333333     0.666667     0.249842
2 Y     0.000000     0.000000     0.499582
3 Y     0.000000     0.000000     0.999582
4 S     0.666667     0.333333     0.586677
5 S     0.333333     0.666667     0.413442
6 S     0.333333     0.666667     0.086677
7 S     0.666667     0.333333     0.913442
8 F     0.666667     0.333333     0.228329
9 F     0.333333     0.666667     0.728329
10 F     0.000000     0.000000     0.772287
11 F     0.000000     0.000000     0.272287
```

Anti-polar

```
Space Group = 164
Full Formula (Y4 S4 F4)
Reduced Formula: YSF
abc   :   3.965357   3.965357  16.760398
angles:  90.000000  90.000000 120.000000
Sites (12)
0 Y     0.333333     0.666667     0.250301
1 Y     0.666667     0.333333     0.749699
2 Y     0.000000     0.000000     0.500000
3 Y     0.000000     0.000000     0.000000
4 S     0.333333     0.666667     0.413553
5 S     0.666667     0.333333     0.586447
6 S     0.666667     0.333333     0.913219
7 S     0.333333     0.666667     0.086781
```

```
8 F     0.333333     0.666667     0.771576
9 F     0.666667     0.333333     0.228424
10 F     0.000000     0.000000     0.272384
11 F     0.000000     0.000000     0.727616
```

G. $CuBiW_2O_8$

Non-polar

```
Space Group = 2
Full Formula (Cu1 Bi1 W2 O8)
Reduced Formula: CuBi(WO4)2
abc   :   4.954784   6.002433   6.057345
angles: 109.232204  91.907057 113.168425
Sites (12)
0 Cu     0.000000     0.000000     0.000000
1 Bi     0.500000     0.000000     0.500000
2 W     0.256161     0.523911     0.833206
3 W     0.743839     0.476089     0.166794
4 O     0.467319     0.310039     0.835525
5 O     0.532681     0.689961     0.164475
6 O     0.003780     0.276267     0.565620
7 O     0.996220     0.723733     0.434380
8 O     0.036832     0.704840     0.981538
9 O     0.963168     0.295160     0.018462
10 O     0.512774     0.758107     0.731189
11 O     0.487226     0.241893     0.268811
```

Polar
ICSD 67569[8]

```
Space Group = 1
Full Formula (Cu1 Bi1 W2 O8)
Reduced Formula: CuBi(WO4)2
abc   :   4.952819   6.062362   5.998570
angles: 109.259503 113.207528  91.708300
Sites (12)
0 Cu     0.177536     0.245262     0.122987
1 Bi     0.634674     0.709085     0.095901
2 W     0.392890     0.042142     0.620538
3 W     0.881866     0.375136     0.574592
4 O     0.175435     0.193418     0.803232
5 O     0.639700     0.933500     0.852003
6 O     0.136291     0.777285     0.370075
7 O     0.102540     0.230932     0.393192
8 O     0.615018     0.471235     0.336001
9 O     0.127222     0.645307     0.818895
10 O     0.607054     0.041943     0.408491
11 O     0.670973     0.370656     0.788294
```

H. $PbGa_2O_4$

Non-polar

```
Space Group = 190
Full Formula (Ga4 Pb2 O8)
Reduced Formula: Ga2PbO4
abc   :   5.232320   5.232320   8.880171
angles:  90.000000  90.000000 120.000000
Sites (14)
0 Ga     0.666667     0.333333     0.546082
1 Ga     0.333333     0.666667     0.453918
2 Ga     0.666667     0.333333     0.953918
3 Ga     0.333333     0.666667     0.046082
4 Pb     0.000000     0.000000     0.750000
5 Pb     0.000000     0.000000     0.250000
6 O     0.666667     0.333333     0.750000
7 O     0.333333     0.666667     0.250000
8 O     0.685705     0.685705     0.000000
9 O     0.000000     0.314295     0.000000
10 O     0.314295     0.000000     0.000000
11 O     0.314295     0.000000     0.500000
12 O     0.685705     0.685705     0.500000
13 O     0.000000     0.314295     0.500000
```

Polar
ICSD 80129, 33533

```
Space Group = 40
Full Formula (Ga4 Pb2 O8)
Reduced Formula: Ga2PbO4
abc   :   5.376237   5.376237   8.570045
angles:  90.000000  90.000000 121.472135
Sites (14)
0 Ga     0.300293     0.646664     0.052211
1 Ga     0.300293     0.646664     0.447789
2 Ga     0.646664     0.300293     0.947789
3 Ga     0.646664     0.300293     0.552211
4 Pb     0.987157     0.039054     0.250000
5 Pb     0.039054     0.987157     0.750000
6 O     0.003787     0.641350     0.560950
7 O     0.003787     0.641350     0.939050
8 O     0.641350     0.003787     0.439050
9 O     0.641350     0.003787     0.060950
10 O     0.522080     0.136299     0.750000
11 O     0.136299     0.522080     0.250000
12 O     0.329665     0.329665     0.500000
13 O     0.329665     0.329665     0.000000
```

I. $PbAl_2O_4$

Non-polar

```
Space Group = 190
Full Formula (Al4 Pb2 O8)
Reduced Formula: Al2PbO4
abc   :   5.111914   5.111914   8.729952
angles:  90.000000  90.000000 120.000000
```

```
Sites (14)
0 Al     0.666667     0.333333     0.551620
1 Al     0.333333     0.666667     0.448380
2 Al     0.666667     0.333333     0.948380
3 Al     0.333333     0.666667     0.051620
4 Pb     0.000000     0.000000     0.750000
5 Pb     0.000000     0.000000     0.250000
6 O     0.666667     0.333333     0.750000
7 O     0.333333     0.666667     0.250000
8 O     0.665287     0.665287     0.000000
9 O     0.000000     0.334713     0.000000
10 O     0.334713     0.000000     0.000000
11 O     0.334713     0.000000     0.500000
12 O     0.665287     0.665287     0.500000
13 O     0.000000     0.334713     0.500000
```

Polar
ICSD 80128, 33532

```
Space Group = 40
Full Formula (Al4 Pb2 O8)
Reduced Formula: Al2PbO4
abc   :   5.267321   5.267321   8.469406
angles:  90.000000  90.000000 122.123141
Sites (14)
0 Al     0.295736     0.640325     0.054038
1 Al     0.295736     0.640325     0.445962
2 Al     0.640325     0.295736     0.945962
3 Al     0.640325     0.295736     0.554038
4 Pb     0.974379     0.030932     0.250000
5 Pb     0.030932     0.974379     0.750000
6 O     0.001784     0.624613     0.555812
7 O     0.001784     0.624613     0.944188
8 O     0.624613     0.001784     0.444188
9 O     0.624613     0.001784     0.055812
10 O     0.535785     0.159651     0.750000
11 O     0.159651     0.535785     0.250000
12 O     0.351220     0.351220     0.500000
13 O     0.351220     0.351220     1.000000
```

J. LiV_2O_5

Non-polar

```
Space Group = 59
Full Formula (Li2 V4 O10)
Reduced Formula: LiV2O5
abc   :   3.557338   4.592446  11.260591
angles:  90.000000  90.000000  90.000000
Sites (16)
0 Li     0.000000     0.278366     0.500000
1 Li     0.500000     0.721634     0.000000
2 V     0.000000     0.113061     0.151304
3 V     0.500000     0.886939     0.651304
```

```
4 V     0.500000     0.886939     0.348696
5 V     0.000000     0.113061     0.848696
6 O     0.000000     0.018665     0.322835
7 O     0.500000     0.981335     0.822835
8 O     0.500000     0.981335     0.177165
9 O     0.000000     0.018665     0.677165
10 O     0.500000     0.023139     0.500000
11 O     0.000000     0.976861     0.000000
12 O     0.500000     0.539234     0.366075
13 O     0.000000     0.460766     0.866075
14 O     0.000000     0.460766     0.133925
15 O     0.500000     0.539234     0.633925
```

Polar
ICSD 88641,88642, 88643[9]

```
Space Group = 31
Full Formula (Li2 V4 O10)
Reduced Formula: LiV2O5
abc   :   3.534100   4.636708  11.339180
angles:  90.000000  90.000000  90.000000
Sites (16)
0 Li     0.000000     0.303744     0.290003
1 Li     0.500000     0.696256     0.790003
2 V     0.500000     0.907894     0.100472
3 V     0.000000     0.092106     0.600472
4 V     0.000000     0.124728     0.900233
5 V     0.500000     0.875272     0.400233
6 O     0.000000     0.470708     0.877523
7 O     0.500000     0.529292     0.377523
8 O     0.000000     0.033999     0.069893
9 O     0.500000     0.966001     0.569893
10 O     0.500000     0.563874     0.111757
11 O     0.000000     0.436126     0.611757
12 O     0.500000     0.026744     0.252137
13 O     0.000000     0.973256     0.752137
14 O     0.500000     0.990438     0.926682
15 O     0.000000     0.009562     0.426682
```

K. $NaVO_2F_2$

Non-polar

```
Space Group = 11
Full Formula (Na2 V2 O4 F4)
Reduced Formula: NaV(OF)2
abc   :   6.451637   3.516552   7.214677
angles:  90.000000 109.429458  90.000000
Sites (12)
0 Na     0.372057     0.250000     0.782104
1 Na     0.627943     0.750000     0.217896
2 V     0.867255     0.750000     0.790643
3 V     0.132745     0.250000     0.209357
4 O     0.092023     0.750000     0.136970
5 O     0.907977     0.250000     0.863030
```

```
6 O     0.279484     0.250000     0.435597
7 O     0.720516     0.750000     0.564403
8 F     0.859206     0.250000     0.240436
9 F     0.140794     0.750000     0.759564
10 F     0.373255     0.250000     0.110634
11 F     0.626745     0.750000     0.889366
```

Polar
ICSD 75418[10]

```
Space Group = 4
Full Formula (Na2 V2 O4 F4)
Reduced Formula: NaV(OF)2
abc   :   6.417150   3.552008   7.202376
angles:  90.000000 109.411802  90.000000
Sites (12)
0 Na     0.372117     0.224124     0.781141
1 Na     0.627883     0.724124     0.218859
2 V     0.867873     0.765980     0.791285
3 V     0.132127     0.265980     0.208715
4 O     0.090989     0.737530     0.137277
5 O     0.909011     0.237530     0.862723
6 O     0.278897     0.268370     0.435809
7 O     0.721103     0.768370     0.564191
8 F     0.857291     0.222259     0.237581
9 F     0.142709     0.722259     0.762419
10 F     0.372090     0.222637     0.110345
11 F     0.627910     0.722637     0.889655
```

L. SbW_2O_6

Non-polar

```
Space Group = 14
Full Formula (Sb4 W2 O12)
Reduced Formula: Sb2WO6
abc   :   5.523370   4.937108   9.248750
angles:  90.000000  94.847812  90.000000
Sites (18)
0 Sb     0.854223     0.455433     0.666649
1 Sb     0.645777     0.955433     0.333351
2 Sb     0.145777     0.544567     0.333351
3 Sb     0.354223     0.044567     0.666649
4 W     0.000000     0.000000     0.000000
5 W     0.500000     0.500000     0.000000
6 O     0.730483     0.761247     0.943209
7 O     0.769517     0.261247     0.056791
8 O     0.269517     0.238753     0.056791
9 O     0.230483     0.738753     0.943209
10 O     0.012914     0.853484     0.189566
11 O     0.487086     0.353484     0.810434
12 O     0.987086     0.146516     0.810434
13 O     0.512914     0.646516     0.189566
14 O     0.642763     0.176526     0.561105
15 O     0.857237     0.676526     0.438895
```

```
16 O     0.357237     0.823474     0.438895
17 O     0.142763     0.323474     0.561105
```

Polar
ICSD 75595[11]

```
Space Group = 4
Full Formula (Sb4 W2 O12)
Reduced Formula: Sb2WO6
abc   :   5.557749   4.990369   9.198174
angles:  90.000000  95.389320  90.000000
Sites (18)
0 Sb     0.107099     0.952317     0.666038
1 Sb     0.892901     0.452317     0.333962
2 Sb     0.605096     0.548741     0.667591
3 Sb     0.394904     0.048741     0.332409
4 W     0.755418     0.963650     0.008139
5 W     0.244582     0.463650     0.991861
6 O     0.736893     0.860887     0.809320
7 O     0.263107     0.360887     0.190680
8 O     0.970164     0.268410     0.941003
9 O     0.029836     0.768410     0.058997
10 O     0.389040     0.817103     0.557543
11 O     0.610960     0.317103     0.442457
12 O     0.471971     0.225733     0.942583
13 O     0.528029     0.725733     0.057417
14 O     0.892421     0.675639     0.562651
15 O     0.107579     0.175639     0.437349
16 O     0.759007     0.148071     0.188505
17 O     0.240993     0.648071     0.811495
```

M. V_2MoO_8

Non-polar

```
Space Group = 65
Full Formula (V2 Mo1 O8)
Reduced Formula: V2MoO8
abc   :  10.011173  10.011173   3.662590
angles:  90.000000  90.000000 158.303585
Sites (11)
0 V     0.813557     0.186443     0.000000
1 V     0.186443     0.813557     0.000000
2 Mo     0.000000     0.000000     0.000000
3 O     0.810497     0.189503     0.500000
4 O     0.189503     0.810497     0.500000
5 O     0.292653     0.707347     0.000000
6 O     0.707347     0.292653     0.000000
7 O     0.000000     0.000000     0.500000
8 O     0.903284     0.096716     0.000000
9 O     0.096716     0.903284     0.000000
10 O     0.500000     0.500000     0.000000
```

Polar
ICSD 25378[12]

```
Space Group = 35
Full Formula (V2 Mo1 O8)
Reduced Formula: V2MoO8
abc   :   9.759683   9.759683   4.058949
angles:  90.000000  90.000000 158.426990
Sites (11)
0 V     0.811827     0.188173     0.958236
1 V     0.188173     0.811827     0.958236
2 Mo     0.000000     0.000000     0.982470
3 O     0.812838     0.187162     0.565521
4 O     0.187162     0.812838     0.565521
5 O     0.902124     0.097876     0.053157
6 O     0.097876     0.902124     0.053157
7 O     0.000000     0.000000     0.561671
8 O     0.290918     0.709082     0.040288
9 O     0.709082     0.290918     0.040288
10 O     0.500000     0.500000     0.074453
```

Anti-polar 28471[13]

```
Space Group = 12
Full Formula (V2 Mo1 O8)
Reduced Formula: V2MoO8
abc   :   9.775701   9.775701   3.842561
angles:  89.741754  90.258246 158.122438
Sites (11)
0 V     0.189764     0.810236     0.088884
1 V     0.810236     0.189764     0.911116
2 Mo     0.000000     0.000000     0.000000
3 O     0.291238     0.708762     0.992766
4 O     0.708762     0.291238     0.007234
5 O     0.500000     0.500000     0.000000
6 O     0.098812     0.901188     0.005565
7 O     0.901188     0.098812     0.994435
8 O     0.188971     0.811029     0.505827
9 O     0.811029     0.188971     0.494173
10 O     0.000000     1.000000     0.500000
```

N. Zn_2BrN

Non-polar

```
Space Group = 62
Full Formula (Zn8 Br4 N4)
Reduced Formula: Zn2BrN
abc   :   6.055989   6.181249   7.584113
angles:  90.000000  90.000000  90.000000
Sites (16)
0 Zn     0.250000     0.881036     0.675358
1 Zn     0.750000     0.118964     0.324642
2 Zn     0.750000     0.618964     0.175358
3 Zn     0.250000     0.381036     0.824642
4 Zn     0.500000     0.000000     0.000000
5 Zn     0.500000     0.500000     0.500000
```

```
6 Zn     0.000000     0.000000     0.000000
7 Zn     0.000000     0.500000     0.500000
8 Br     0.250000     0.089065     0.383681
9 Br     0.750000     0.910935     0.616319
10 Br     0.750000     0.410935     0.883681
11 Br     0.250000     0.589065     0.116319
12 N     0.250000     0.576744     0.627947
13 N     0.750000     0.423256     0.372053
14 N     0.750000     0.923256     0.127947
15 N     0.250000     0.076744     0.872053
```

Polar
ICSD 425736[14]

```
Space Group = 33
Full Formula (Zn8 Br4 N4)
Reduced Formula: Zn2BrN
abc   :   6.028627   6.190893   7.526637
angles:  90.000000  90.000000  90.000000
Sites (16)
0 Zn     0.407114     0.020372     0.966621
1 Zn     0.407114     0.520372     0.533379
2 Zn     0.907114     0.979628     0.033379
3 Zn     0.907114     0.479628     0.466621
4 Zn     0.088408     0.871921     0.680893
5 Zn     0.088408     0.371921     0.819107
6 Zn     0.588408     0.128079     0.319107
7 Zn     0.588408     0.628079     0.180893
8 Br     0.127831     0.084973     0.380191
9 Br     0.127831     0.584973     0.119809
10 Br     0.627831     0.915027     0.619809
11 Br     0.627831     0.415027     0.880191
12 N     0.124696     0.572675     0.627404
13 N     0.124696     0.072675     0.872596
14 N     0.624696     0.427325     0.372596
15 N     0.624696     0.927325     0.127404
```

O. Zn_2BrN

Non-polar

```
Space Group = 62
Full Formula (Zn8 N4 Cl4)
Reduced Formula: Zn2NCl
abc   :   5.957168   6.090093   7.412435
angles:  90.000000  90.000000  90.000000
Sites (16)
0 Zn     0.250000     0.101155     0.337185
1 Zn     0.750000     0.898845     0.662815
2 Zn     0.750000     0.398845     0.837185
3 Zn     0.250000     0.601155     0.162815
4 Zn     0.500000     0.000000     0.000000
5 Zn     0.500000     0.500000     0.500000
6 Zn     0.000000     0.000000     0.000000
7 Zn     0.000000     0.500000     0.500000
```

```
8 N     0.250000     0.413056     0.370896
9 N     0.750000     0.586944     0.629104
10 N     0.750000     0.086944     0.870896
11 N     0.250000     0.913056     0.129104
12 Cl     0.250000     0.907146     0.612393
13 Cl     0.750000     0.092854     0.387607
14 Cl     0.750000     0.592854     0.112393
15 Cl     0.250000     0.407146     0.887607
```

Polar
ICSD 425734[14]

```
Space Group = 33
Full Formula (Zn8 N4 Cl4)
Reduced Formula: Zn2NCl
abc   :   5.895180   6.102977   7.278818
angles:  90.000000  90.000000  90.000000
Sites (16)
0 Zn     0.574308     0.115385     0.828615
1 Zn     0.574308     0.615385     0.671385
2 Zn     0.074308     0.884615     0.171385
3 Zn     0.074308     0.384615     0.328615
4 Zn     0.920855     0.971716     0.547057
5 Zn     0.920855     0.471716     0.952943
6 Zn     0.420855     0.028284     0.452943
7 Zn     0.420855     0.528284     0.047057
8 N     0.124792     0.080968     0.372195
9 N     0.124792     0.580968     0.127805
10 N     0.624792     0.919032     0.627805
11 N     0.624792     0.419032     0.872195
12 Cl     0.128096     0.585889     0.620540
13 Cl     0.128096     0.085889     0.879460
14 Cl     0.628096     0.414111     0.379460
15 Cl     0.628096     0.914111     0.120540
```

P. $AlAgO_2$

Non-polar

```
Space Group = 62
Full Formula (Al4 Ag4 O8)
Reduced Formula: AlAgO2
abc   :   5.274923   5.696013   6.676147
angles:  90.000000  90.000000  90.000000
Sites (16)
0 Al     0.400286     0.250000     0.370442
1 Al     0.599714     0.750000     0.629558
2 Al     0.099714     0.750000     0.870442
3 Al     0.900286     0.250000     0.129558
4 Ag     0.416658     0.250000     0.828669
5 Ag     0.583342     0.750000     0.171331
6 Ag     0.083342     0.750000     0.328669
7 Ag     0.916658     0.250000     0.671331
8 O     0.065520     0.250000     0.359415
9 O     0.934480     0.750000     0.640585
```

```
10 O     0.434480     0.750000     0.859415
11 O     0.565520     0.250000     0.140585
12 O     0.000000     0.500000     0.000000
13 O     0.500000     0.500000     0.500000
14 O     0.000000     0.000000     0.000000
15 O     0.500000     0.000000     0.500000
```

Polar
ICSD 99688[15]

```
Space Group = 33
Full Formula (Al4 Ag4 O8)
Reduced Formula: AlAgO2
abc   :   5.355008   5.452759   6.910347
angles:  90.000000  90.000000  90.000000
Sites (16)
0 Al     0.071100     0.122459     0.375838
1 Al     0.571100     0.122459     0.124162
2 Al     0.928900     0.622459     0.624162
3 Al     0.428900     0.622459     0.875838
4 Ag     0.557787     0.130267     0.643986
5 Ag     0.057787     0.130267     0.856014
6 Ag     0.442213     0.630267     0.356014
7 Ag     0.942213     0.630267     0.143986
8 O     0.109072     0.558503     0.833631
9 O     0.609072     0.558503     0.666369
10 O     0.890928     0.058503     0.166369
11 O     0.390928     0.058503     0.333631
12 O     0.965947     0.936740     0.568412
13 O     0.465947     0.936740     0.931588
14 O     0.034053     0.436740     0.431588
15 O     0.534053     0.436740     0.068412
```


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