OpenGL version: 2.1 NVIDIA-10.2.34 310.90.10.05b54
Video configuration: NVIDIA GeForce GT 330M OpenGL Engine
Maximum supported width and height of the viewport: 8192 x 8192
OpenGL depth buffer bit: 16

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================================================================================
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Title               Ag4 Mn Sb2 S6

Lattice type        P
Space group name    P 21/n
Space group number  14
Setting number      2

Lattice parameters

   a        b        c       alpha    beta     gamma
10.38610  8.11080  6.66300  90.0000  92.6390  90.0000

Unit-cell volume = 560.693037 Å^3

Structure parameters

                        x          y          z          Occ.     U
Site      Sym.
   1 Ag  Ag1          0.30800    0.24380    0.57230    1.000    0.043
4e          1
   2 Ag  Ag2          0.50140    0.96600    0.76260    1.000    0.063
4e          1
   3 Mn  Mn           0.00000    0.00000    0.50000    1.000    0.017
2b         -1
   4 Sb  Sb           0.18404    0.16448    0.03847    1.000    0.016
4e          1
   5 S   S1           0.09171    0.26901    0.34369    1.000    0.016
4e          1
   6 S   S2           0.51791    0.67354    0.66932    1.000    0.016
4e          1
   7 S   S3           0.26400    0.42128   -0.11123    1.000    0.018
4e          1
================================================================================
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Number of polygons and unique vertices on isosurface = 0 (0)
64 atoms, 82 bonds, 20 polyhedra; CPU time = 204 ms

64 atoms, 82 bonds, 20 polyhedra; CPU time = 61 ms

64 atoms, 82 bonds, 20 polyhedra; CPU time = 2 ms

64 atoms, 82 bonds, 20 polyhedra; CPU time = 2 ms
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64 atoms, 82 bonds, 20 polyhedra; CPU time = 2 ms

64 atoms, 82 bonds, 20 polyhedra; CPU time = 2 ms

64 atoms, 82 bonds, 20 polyhedra; CPU time = 2 ms

64 atoms, 82 bonds, 20 polyhedra; CPU time = 2 ms

64 atoms, 82 bonds, 20 polyhedra; CPU time = 2 ms

64 atoms, 82 bonds, 20 polyhedra; CPU time = 2 ms

64 atoms, 82 bonds, 20 polyhedra; CPU time = 2 ms

64 atoms, 82 bonds, 20 polyhedra; CPU time = 2 ms

84 atoms, 194 bonds, 20 polyhedra; CPU time = 5 ms

84 atoms, 194 bonds, 20 polyhedra; CPU time = 5 ms

84 atoms, 194 bonds, 20 polyhedra; CPU time = 5 ms

84 atoms, 194 bonds, 20 polyhedra; CPU time = 5 ms

84 atoms, 194 bonds, 20 polyhedra; CPU time = 3 ms

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Title Ag4 Mn Sb2 S6

Lattice type P
Space group name P 21/n
Space group number 14
Setting number 2

Lattice parameters

a	b	c	alpha	beta	gamma
3.00000	6.00000	9.00000	90.0000	92.6390	90.0000

Unit-cell volume = 161.828193 Å^3

Structure parameters

			x	y	z	Occ.	U	Site	Sym.
1	Ag	Ag1	0.30800	0.24380	0.57230	1.000	0.043	4e	1
2	Ag	Ag2	0.50140	0.96600	0.76260	1.000	0.063		

```
4e         1
   3 Mn  Mn          0.00000    0.00000    0.50000    1.000    0.017
2b        -1
   4 Sb  Sb          0.18404    0.16448    0.03847    1.000    0.016
4e         1
   5 S   S1          0.09171    0.26901    0.34369    1.000    0.016
4e         1
   6 S   S2          0.51791    0.67354    0.66932    1.000    0.016
4e         1
   7 S   S3          0.26400    0.42128   -0.11123    1.000    0.018
4e         1
================================================================================
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Faces of crystal shape
  (  h   k   l)       d (Å)      area (Å^2)
  (  3   1   1)            2       15.2036
  ( -3  -1  -1)            2       15.2036
  ( -3   1  -1)            2       15.2036
  (  3  -1   1)            2       15.2036
  (  1   6   1)            3       5.99784
  ( -1  -6  -1)            3       5.99784
  ( -1   6  -1)            3       5.99784
  (  1  -6   1)            3       5.99784
  (  1   1   3)            2       18.4116
  ( -1  -1  -3)            2       18.4116
  ( -1   1  -3)            2       18.4116
  (  1  -1   3)            2       18.4116
================================================================================
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Number of polygons and unique vertices on isosurface = 0 (0)
84 atoms, 194 bonds, 20 polyhedra; CPU time = 4 ms

================================================================================
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Title               O5 Si Al2

Lattice type        P
Space group name    P n n m
Space group number  58
Setting number      1

Lattice parameters

   a        b        c       alpha    beta     gamma
 7.76000  7.90000  5.56000  90.0000  90.0000  90.0000

Unit-cell volume = 340.850251 Å^3
```

Structure parameters

Site		Sym.	x	y	z	Occ.	B
1	O	O1	0.08000	−0.14000	0.00000	1.000	1.000
4g		..m					
2	O	O2	0.04000	−0.17000	0.50000	1.000	1.000
4g		..m					
3	O	O3	0.14000	0.40000	0.00000	1.000	1.000
4g		..m					
4	O	O4	0.21000	0.14000	0.25000	1.000	1.000
8h		1					
5	Si	Si1	0.28000	0.25000	0.00000	1.000	1.000
4g		..m					
6	Al	Al1	0.00000	0.00000	0.25000	1.000	1.000
4e		..2					
7	Al	Al2	−0.14000	0.36000	0.00000	1.000	1.000
4g		..m					

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Number of polygons and unique vertices on isosurface = 0 (0)
88 atoms, 108 bonds, 22 polyhedra; CPU time = 48 ms

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Title O5 Si Al2

Lattice type P
Space group name P n n m
Space group number 58
Setting number 1

Lattice parameters

a	b	c	alpha	beta	gamma
7.76000	7.90000	5.56000	90.0000	90.0000	90.0000

Unit-cell volume = 340.850251 Å^3

Structure parameters

Site		Sym.	x	y	z	Occ.	B
1	O	O1	0.08000	−0.14000	0.00000	1.000	1.000
4g		..m					
2	O	O2	0.04000	−0.17000	0.50000	1.000	1.000
4g		..m					
3	O	O3	0.14000	0.40000	0.00000	1.000	1.000
4g		..m					

```
   4 O   O4          0.21000    0.14000    0.25000    1.000    1.000
8h         1
   5 Si  Si1         0.28000    0.25000    0.00000    1.000    1.000
4g        ..m
   6 Al  Al1         0.00000    0.00000    0.25000    1.000    1.000
4e        ..2
   7 Al  Al2        -0.14000    0.36000    0.00000    1.000    1.000
4g        ..m
================================================================================
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Number of polygons and unique vertices on isosurface = 0 (0)
88 atoms, 108 bonds, 22 polyhedra; CPU time = 1 ms

================================================================================
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Title               O5 Si Al2

Lattice type        P
Space group name    P n n m
Space group number  58
Setting number      1

Lattice parameters

   a        b        c       alpha    beta     gamma
 7.76000  7.90000  5.56000  90.0000  90.0000  90.0000

Unit-cell volume = 340.850251 Å^3

Structure parameters

                        x          y          z          Occ.      B
Site      Sym.
   1 O   O1          0.08000   -0.14000    0.00000    1.000    1.000
4g        ..m
   2 O   O2          0.04000   -0.17000    0.50000    1.000    1.000
4g        ..m
   3 O   O3          0.14000    0.40000    0.00000    1.000    1.000
4g        ..m
   4 O   O4          0.21000    0.14000    0.25000    1.000    1.000
8h         1
   5 Si  Si1         0.28000    0.25000    0.00000    1.000    1.000
4g        ..m
   6 Al  Al1         0.00000    0.00000    0.25000    1.000    1.000
4e        ..2
   7 Al  Al2        -0.14000    0.36000    0.00000    1.000    1.000
4g        ..m
================================================================================
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```

Number of polygons and unique vertices on isosurface = 0 (0)
88 atoms, 108 bonds, 22 polyhedra; CPU time = 2 ms

==========
Title O5 Si Al2

Lattice type P
Space group name P n n m
Space group number 58
Setting number 1

Lattice parameters

a	b	c	alpha	beta	gamma
7.76000	7.90000	5.56000	90.0000	90.0000	90.0000

Unit-cell volume = 340.850251 Å^3

Structure parameters

		Site	Sym.	x	y	z	Occ.	B
1	O	O1	4g ..m	0.08000	-0.14000	0.00000	1.000	1.000
2	O	O2	4g ..m	0.04000	-0.17000	0.50000	1.000	1.000
3	O	O3	4g ..m	0.14000	0.40000	0.00000	1.000	1.000
4	O	O4	8h 1	0.21000	0.14000	0.25000	1.000	1.000
5	Si	Si1	4g ..m	0.28000	0.25000	0.00000	1.000	1.000
6	Al	Al1	4e ..2	0.00000	0.00000	0.25000	1.000	1.000
7	Al	Al2	4g ..m	-0.14000	0.36000	0.00000	1.000	1.000

==========

Number of polygons and unique vertices on isosurface = 0 (0)
88 atoms, 108 bonds, 22 polyhedra; CPU time = 5 ms

==========
Title Si6.111 Be2.859 Li.027 Al1.311 Fe.366 Mg.328 O18 Na.406 Cs.012

Lattice type P

Space group name   P 6/m c c
Space group number 192
Setting number   1

Lattice parameters

a	b	c	alpha	beta	gamma
9.27360	9.27360	9.19100	90.0000	90.0000	120.0000

Unit-cell volume = 684.526209 Å^3

Structure parameters

			x	y	z	Occ.	U	Site	Sym.
1	Si	Si1	0.38520	0.11220	0.00000	1.000	0.005	12l	m..
2	Be	Be	0.50000	0.00000	0.25000	0.953	0.006	6f	222
3	Li	Li	0.50000	0.00000	0.25000	0.009	0.006	6f	222
4	Si	Si2	0.50000	0.00000	0.25000	0.037	0.006	6f	222
5	Al	Al1	0.50000	0.00000	0.25000	0.001	0.006	6f	222
6	Al	Al2	0.66667	0.33333	0.25000	0.654	0.007	4c	3.2
7	Fe	Fe1	0.66667	0.33333	0.25000	0.037	0.007	4c	3.2
8	Fe	Fe2	0.66667	0.33333	0.25000	0.146	0.007	4c	3.2
9	Mg	Mg	0.66667	0.33333	0.25000	0.164	0.007	4c	3.2
10	O	O1	0.30620	0.23150	0.00000	1.000	0.013	12l	m..
11	O	O2	0.49510	0.14180	0.14500	1.000	0.009	24m	1
12	Na	Na	0.00000	0.00000	0.25000	0.406	0.049	2a	622
13	Cs	Cs	0.00000	0.00000	0.25000	0.012	0.049	2a	622

Number of polygons and unique vertices on isosurface = 0 (0)
122 atoms, 136 bonds, 32 polyhedra; CPU time = 4 ms

Title   Al1.98 Cr.02 Be O4

```
Lattice type        P
Space group name    P n m a
Space group number  62
Setting number      1

Lattice parameters

   a        b        c       alpha    beta     gamma
 9.40820  5.47900  4.42880  90.0000  90.0000  90.0000

Unit-cell volume = 228.293707 Å^3

Structure parameters

                        x          y          z          Occ.     U
Site      Sym.
   1 Al  Al1         0.00000    0.00000    0.00000    1.000    0.003
4a         -1
   2 Al  Al2         0.27282    0.25000   -0.00503    0.980    0.004
4c        .m.
   3 Cr  Cr2         0.27282    0.25000   -0.00503    0.020    0.004
4c        .m.
   4 Be  Be          0.09289    0.25000    0.43360    1.000    0.005
4c        .m.
   5 O   O1          0.09022    0.25000    0.78822    1.000    0.003
4c        .m.
   6 O   O2          0.43316    0.25000    0.24167    1.000    0.004
4c        .m.
   7 O   O3          0.16324    0.01554    0.25728    1.000    0.004
8d          1
================================================================================
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Number of polygons and unique vertices on isosurface = 0 (0)
99 atoms, 138 bonds, 25 polyhedra; CPU time = 1 ms

================================================================================
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Title               Al2 O3

Lattice type        R
Space group name    R -3 c
Space group number  167
Setting number      1

Lattice parameters

   a        b        c       alpha    beta     gamma
 4.75400  4.75400 12.99000  90.0000  90.0000 120.0000
```

Unit-cell volume = 254.248362 Å^3

Structure parameters

		x	y	z	Occ.	U	Site	Sym.
1	Al Al	0.00000	0.00000	0.35228	1.000	0.004	12c	3.
2	O O	0.30640	0.00000	0.25000	1.000	0.004	18e	.2

Number of polygons and unique vertices on isosurface = 0 (0)
102 atoms, 144 bonds, 24 polyhedra; CPU time = 2 ms

Title C

Lattice type F
Space group name F d -3 m
Space group number 227
Setting number 1

Lattice parameters

a	b	c	alpha	beta	gamma
3.56700	3.56700	3.56700	90.0000	90.0000	90.0000

Unit-cell volume = 45.384682 Å^3

Structure parameters

		x	y	z	Occ.	B	Site	Sym.
1	C C	0.00000	0.00000	0.00000	1.000	1.000	8a	-43m

Number of polygons and unique vertices on isosurface = 0 (0)
46 atoms, 56 bonds, 14 polyhedra; CPU time = 3 ms

Title Na.549 Ca.018 Al7.606 Mn.031 Li1.363 Si6 B3 O30.681 F.319 H3.762

Lattice type   R
Space group name   R 3 m
Space group number 160
Setting number   1

Lattice parameters

a	b	c	alpha	beta	gamma
15.83180	15.83180	7.09980	90.0000	90.0000	120.0000

Unit-cell volume = 1541.123236 Å^3

Structure parameters

Site		Sym.	x	y	z	Occ.	U	
1	Na	NaX	0.00000	0.00000	0.23136	0.549	0.021	3a 3m
2	Ca	CaX	0.00000	0.00000	0.23136	0.018	0.021	3a 3m
3	Al	AlY	0.12312	0.06156	0.63440	0.535	0.007	9b .m
4	Mn	MnY	0.12312	0.06156	0.63440	0.010	0.007	9b .m
5	Li	LiY	0.12312	0.06156	0.63440	0.454	0.007	9b .m
6	Al	AlZ	0.29670	0.25987	0.60996	1.000	0.005	18c 1
7	Si	SiT	0.19197	0.18988	0.00000	1.000	0.004	18c 1
8	B	B	0.10903	0.21806	0.45468	1.000	0.005	9b .m
9	O	O-H1W	0.00000	0.00000	0.78239	0.681	0.041	3a 3m
10	F	F1W	0.00000	0.00000	0.78239	0.319	0.041	3a 3m
11	O	O2	0.06015	0.12030	0.48966	0.973	0.014	9b .m
12	O	O-H2	0.06015	0.12030	0.48966	0.027	0.014	9b .m
13	O	O-H3V	0.26544	0.13272	0.50744	1.000	0.012	9b .m
14	O	O4	0.09365	0.18730	0.07309	1.000	0.008	9b .m
15	O	O5	0.18746	0.09373	0.09545	1.000	0.008	9b .m
16	O	O6	0.19541	0.18490	0.77503	1.000	0.007	18c 1
17	O	O7	0.28626	0.28609	0.07879	1.000	0.006	18c 1

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  18 O   O8          0.20937    0.26983    0.43938    1.000    0.007
18c         1
================================================================================

Number of polygons and unique vertices on isosurface = 0 (0)
243 atoms, 333 bonds, 67 polyhedra; CPU time = 7 ms

================================================================================
Title               Ca F2

Lattice type        F
Space group name    F m -3 m
Space group number  225
Setting number      1

Lattice parameters

   a        b        c       alpha    beta     gamma
 5.46310  5.46310  5.46310  90.0000  90.0000  90.0000

Unit-cell volume = 163.048737 Å^3

Structure parameters

                        x          y          z          Occ.     B
Site      Sym.
   1 Ca  Ca          0.00000    0.00000    0.00000    1.000    1.000
4a      m-3m
   2 F   F           0.25000    0.25000    0.25000    1.000    1.000
8c      -43m
================================================================================

Number of polygons and unique vertices on isosurface = 0 (0)
78 atoms, 112 bonds, 14 polyhedra; CPU time = 3 ms

================================================================================
Title               Al4 Si5 (Mg1.54 Fe.46) O18.48 Li.12 Na.1 Ca.03 K.
02 H.96

Lattice type        C
Space group name    C c c m
Space group number  66
Setting number      1

Lattice parameters
```

a	b	c	alpha	beta	gamma
17.08300	9.73800	9.33500	90.0000	90.0000	90.0000

Unit-cell volume = 1552.916971 Å^3

Structure parameters

Site		Sym.	x	y	z	Occ.	U	
1	Al	Al1	0.25000	0.25000	0.25000	1.000	0.003	8k ..2
2	Si	Si2	0.00000	0.50000	0.25000	0.920	0.003	4b 222
3	Al	Al2	0.00000	0.50000	0.25000	0.080	0.003	4b 222
4	Si	Si3	0.19230	0.07810	0.00000	1.000	0.003	8l ..m
5	Si	Si4	0.13510	−0.23720	0.00000	1.000	0.003	8l ..m
6	Al	Al5	0.05060	0.30840	0.00000	0.960	0.003	8l ..m
7	Si	Si5	0.05060	0.30840	0.00000	0.040	0.003	8l ..m
8	Mg	Mg	0.33740	0.00000	0.25000	0.770	0.003	8g 2..
9	Fe	Fe	0.33740	0.00000	0.25000	0.230	0.003	8g 2..
10	O	O1	0.24660	−0.10400	0.35910	1.000	0.003	16m 1
11	O	O2	0.06160	−0.41670	0.34940	1.000	0.003	16m 1
12	O	O3	−0.17300	−0.30910	0.35830	1.000	0.004	16m 1
13	O	O4	0.04340	−0.24530	0.00000	1.000	0.003	8l ..m
14	O	O5	0.12240	0.18480	0.00000	1.000	0.008	8l ..m
15	O	O6	0.16390	−0.07880	0.00000	1.000	0.007	8l ..m
16	O	Wat	0.00000	0.00000	0.25000	0.480	0.090	4a 222
17	Li	Li	0.00000	0.00000	0.25000	0.120	0.090	4a 222
18	Na	Na	0.00000	0.00000	0.25000	0.100	0.090	4a 222
19	Ca	Ca	0.00000	0.00000	0.25000	0.030	0.090	4a 222
20	K	K	0.00000	0.00000	0.25000	0.020	0.090	4a 222

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Number of polygons and unique vertices on isosurface = 0 (0)
226 atoms, 280 bonds, 64 polyhedra; CPU time = 7 ms

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Title   K Si3 Al3 O12 H2

Lattice type   C
Space group name   C 2/c
Space group number 15
Setting number   1

Lattice parameters

   a   b   c   alpha   beta   gamma
 5.19880 9.02660 20.10580 90.0000 95.7820 90.0000

Unit-cell volume = 938.714508 Å^3

Structure parameters

                        x   y   z   Occ.   B
Site   Sym.
   1 K   K   0.00000   0.09920   0.25000   1.000   2.637
4e   2
   2 Si Si1   0.45100   0.25870   0.13550   0.750   1.708
8f   1
   3 Al Al1   0.45100   0.25870   0.13550   0.250   1.711
8f   1
   4 Si Si2   0.03540   0.42980   0.36460   0.750   1.652
8f   1
   5 Al Al2   0.03540   0.42980   0.36460   0.250   1.652
8f   1
   6 Al Al3   0.25060   0.08380   0.00020   1.000   1.447
8f   1
   7 O   O1   0.38720   0.25250   0.05430   1.000   2.245
8f   1
   8 O   O2   0.03660   0.44310   0.44590   1.000   2.198
8f   1
   9 O   O3   0.41780   0.09310   0.16850   1.000   2.721
8f   1
  10 O   O4   0.24750   0.37120   0.16850   1.000   2.577
8f   1
  11 O   O5   0.25090   0.31320   0.34240   1.000   2.966
8f   1
  12 O   O-H6   0.04220   0.06220   0.44920   1.000   2.528
8f   1
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Number of polygons and unique vertices on isosurface = 0 (0)
130 atoms, 148 bonds, 30 polyhedra; CPU time = 4 ms