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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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

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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
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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					

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   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

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

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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

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