

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 Å³

Structure parameters

Site	Sym.	x	y	z	Occ.	U
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

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 Å³

Structure parameters

Site	Sym.	x	y	z	Occ.	U
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 05 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 Å³

Structure parameters

Site		Sym.	x	y	z	Occ.	B
1	0	01	0.08000	-0.14000	0.00000	1.000	1.000
4g		..m					
2	0	02	0.04000	-0.17000	0.50000	1.000	1.000
4g		..m					
3	0	03	0.14000	0.40000	0.00000	1.000	1.000
4g		..m					
4	0	04	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 05 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 Å³

Structure parameters

Site		Sym.	x	y	z	Occ.	B
1	0	01	0.08000	-0.14000	0.00000	1.000	1.000
4g		..m					
2	0	02	0.04000	-0.17000	0.50000	1.000	1.000
4g		..m					
3	0	03	0.14000	0.40000	0.00000	1.000	1.000
4g		..m					

8h	4 0	04	0.21000	0.14000	0.25000	1.000	1.000
		1					
4g	5 Si	Si1	0.28000	0.25000	0.00000	1.000	1.000
		..m					
4e	6 Al	Al1	0.00000	0.00000	0.25000	1.000	1.000
		..2					
4g	7 Al	Al2	-0.14000	0.36000	0.00000	1.000	1.000
		..m					

Number of polygons and unique vertices on isosurface = 0 (0)
 88 atoms, 108 bonds, 22 polyhedra; CPU time = 1 ms

Title 05 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 Å³

Structure parameters

Site	Sym.	x	y	z	Occ.	B
1 0	01	0.08000	-0.14000	0.00000	1.000	1.000
4g	..m					
2 0	02	0.04000	-0.17000	0.50000	1.000	1.000
4g	..m					
3 0	03	0.14000	0.40000	0.00000	1.000	1.000
4g	..m					
4 0	04	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					

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

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=====
Title 05 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 Å³

Structure parameters

Site		Sym.	x	y	z	Occ.	B
1	0	01	0.08000	-0.14000	0.00000	1.000	1.000
4g		..m					
2	0	02	0.04000	-0.17000	0.50000	1.000	1.000
4g		..m					
3	0	03	0.14000	0.40000	0.00000	1.000	1.000
4g		..m					
4	0	04	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 = 5 ms

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Title Si6.111 Be2.859 Li.027 Al1.311 Fe.366 Mg.328 018
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 Å³

Structure parameters

Site	Sym.	x	y	z	Occ.	U
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 04

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 Å³

Structure parameters

Site	Sym.	x	y	z	Occ.	U
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 Å³

Structure parameters

Site		Sym.	x	y	z	Occ.	U
1	Al	Al	0.00000	0.00000	0.35228	1.000	0.004
12c	2	0 0	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 Å³

Structure parameters

Site		Sym.	x	y	z	Occ.	B
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
030.681 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 Å³

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					

18 0 08 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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=====
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 Å³

Structure parameters

Site	Sym.	x	y	z	Occ.	B
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					

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

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=====
Title Al4 Si5 (Mg1.54 Fe.46) 018.48 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 Å³

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	0	01	0.24660	-0.10400	0.35910	1.000	0.003
16m		1					
11	0	02	0.06160	-0.41670	0.34940	1.000	0.003
16m		1					
12	0	03	-0.17300	-0.30910	0.35830	1.000	0.004
16m		1					
13	0	04	0.04340	-0.24530	0.00000	1.000	0.003
8l		..m					
14	0	05	0.12240	0.18480	0.00000	1.000	0.008
8l		..m					
15	0	06	0.16390	-0.07880	0.00000	1.000	0.007
8l		..m					
16	0	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 Å³

Structure parameters

Site		Sym.	x	y	z	Occ.	B
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

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Title Si3 Al3 Ca2 O13 H

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
16.05390	5.46090	9.84370	90.0000	90.0000	90.0000

Unit-cell volume = 862.984797 Å³

Structure parameters

Site	Sym.	x	y	z	Occ.	U
1 Si	Si1	0.41022	0.75000	0.27960	1.000	0.011
4c	.m.					
2 Si	Si2	0.08005	0.25000	0.10580	1.000	0.012
4c	.m.					
3 Si	Si3	0.15990	0.25000	0.43560	1.000	0.010
4c	.m.					
4 Al	Al12	0.24902	0.99890	0.18730	1.000	0.011
8d	1					
5 Al	Al3	0.10533	0.75000	0.29930	1.000	0.011
4c	.m.					
6 Ca	Ca1	0.36544	0.25000	0.43590	1.000	0.014
4c	.m.					
7 Ca	Ca2	0.45481	0.25000	0.11030	1.000	0.013
4c	.m.					
8 O	O1	0.12800	0.99360	0.14720	1.000	0.012
8d	1					
9 O	O2	0.10090	0.01280	0.43210	1.000	0.013
8d	1					
10 O	O3	0.35840	0.99400	0.24110	1.000	0.011
8d	1					
11 O	O4	0.21940	0.75000	0.30330	1.000	0.015
4c	.m.					
12 O	O5	0.22670	0.25000	0.31100	1.000	0.007
4c	.m.					
13 O	O6	0.27020	0.75000	0.05750	1.000	0.012

4c	.m.						
14	0	07	0.98930	0.25000	0.16660	1.000	0.019
4c	.m.						
15	0	08	0.99530	0.75000	0.30240	1.000	0.014
4c	.m.						
16	0	09	0.42070	0.75000	0.44310	1.000	0.028
4c	.m.						
17	0	0-H10	0.26210	0.25000	0.06600	1.000	0.013
4c	.m.						

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Number of polygons and unique vertices on isosurface = 0 (0)
124 atoms, 176 bonds, 32 polyhedra; CPU time = 3 ms