

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	0.30640	0.00000	0.25000	1.000	0.004
18e	0	.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