

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<sup>3</sup>

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 Å<sup>3</sup>

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 <sup>2</sup> )
( 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 Å<sup>3</sup>

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 = 48 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 Å<sup>3</sup>

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 Å<sup>3</sup>

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 Å<sup>3</sup>

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 Å<sup>3</sup>

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					

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