

Mn₈Al₃₉ [1]

Structural features: Commensurate approximant of icosahedral quasicrystals.

Hansen V., Gjonnes J. (1996) [1]

Al₃₉Mn₈ $a = 2.0516 \text{ nm}$, $V = 8.6353 \text{ nm}^3$, $Z = 12$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Al1	12b	1	0.0	0.1	0.03		11-vertex polyhedron Al ₁₀ Mn
Al2	12b	1	0.01	0.09	0.66		11-vertex polyhedron MnAl ₁₀
Al3	12b	1	0.01	0.1	0.53		11-vertex polyhedron MnAl ₁₀
Al4	12b	1	0.01	0.59	0.34		11-vertex polyhedron Al ₁₀ Mn
Al5	12b	1	0.02	0.03	0.41		13-vertex polyhedron Mn ₃ Al ₁₀
Al6	12b	1	0.02	0.17	0.41		14-vertex polyhedron Mn ₃ Al ₁₁
Mn7	12b	1	0.02	0.29	0.6		bicapped square prism Al ₁₀
Al8	12b	1	0.02	0.4	0.17		13-vertex polyhedron Al ₁₀ Mn ₃
Al9	12b	1	0.02	0.53	0.22		tricapped pentagonal prism Al ₁₀ Mn ₃
Al10	12b	1	0.02	0.66	0.22		tricapped pentagonal prism Al ₁₀ Mn ₃
Al11	12b	1	0.02	0.79	0.17		pseudo Frank-Kasper Mn ₃ Al ₁₀
Al12	12b	1	0.03	0.2	0.1		11-vertex polyhedron MnAl ₁₀
Al13	12b	1	0.03	0.28	0.21		tricapped pentagonal prism Mn ₂ Al ₁₁
Mn14	12b	1	0.03	0.39	0.4		icosahedron Al ₁₂
Mn15	12b	1	0.03	0.8	0.4		11-vertex polyhedron Al ₁₁
Al16	12b	1	0.09	0.1	0.33		tricapped pentagonal prism Mn ₃ Al ₁₀
Al17	12b	1	0.09	0.21	0.52		14-vertex polyhedron Mn ₂ Al ₁₂
Al18	12b	1	0.09	0.21	0.67		12-vertex polyhedron Al ₁₀ Mn ₂
Al19	12b	1	0.09	0.29	0.39		icosahedron Mn ₂ Al ₁₀
Al20	12b	1	0.09	0.48	0.33		tricapped pentagonal prism Mn ₃ Al ₁₀
Al21	12b	1	0.09	0.48	0.48		tricapped pentagonal prism Al ₁₀ Mn ₃
Al22	12b	1	0.09	0.59	0.14		tricapped pentagonal prism Al ₁₀ Mn ₃
Al23	12b	1	0.09	0.71	0.34		12-vertex polyhedron Al ₁₀ Mn ₂
Al24	12b	1	0.09	0.71	0.47		tricapped pentagonal prism Mn ₂ Al ₁₁
Mn25	12b	1	0.09	0.72	0.1		11-vertex polyhedron Al ₁₁
Mn26	12b	1	0.1	0.1	0.47		11-vertex polyhedron Al ₁₁
Al27	12b	1	0.1	0.16	0.2		11-vertex polyhedron MnAl ₁₀
Mn28	12b	1	0.1	0.22	0.3		icosahedron Al ₁₂
Al29	12b	1	0.1	0.36	0.29		14-vertex polyhedron Mn ₃ Al ₁₁
Al30	12b	1	0.11	0.36	0.49		bicapped square prism Mn ₃ Al ₇
Mn31	12b	1	0.11	0.59	0.28		11-vertex polyhedron Al ₁₁
Al32	12b	1	0.12	0.81	0.29		pseudo Frank-Kasper Al ₁₁ Mn ₂
Al33	12b	1	0.13	0.6	0.41		tricapped pentagonal prism Mn ₃ Al ₁₀
Al34	12b	1	0.15	0.5	0.22		14-vertex Frank-Kasper Mn ₃ Al ₁₁
Al35	12b	1	0.16	0.18	0.4		pseudo Frank-Kasper Al ₁₀ Mn ₃
Al36	12b	1	0.16	0.68	0.21		pseudo Frank-Kasper Al ₁₁ Mn ₂
Al37	12b	1	0.17	0.28	0.21		tricapped pentagonal prism Mn ₃ Al ₁₀
Al38	12b	1	0.17	0.4	0.4		14-vertex polyhedron Al ₁₁ Mn ₃
Al39	12b	1	0.2	0.67	0.32		icosahedron Al ₁₀ Mn ₂
Al40	12b	1	0.21	0.27	0.63		pseudo Frank-Kasper Al ₁₁ Mn ₂
Mn41	12b	1	0.21	0.41	0.28		11-vertex polyhedron Al ₁₁
Al42	12b	1	0.22	0.29	0.33		14-vertex polyhedron Mn ₃ Al ₁₁
Al43	12b	1	0.22	0.29	0.48		14-vertex Frank-Kasper Mn ₂ Al ₁₂

Al44	12b	1	0.22	0.52	0.33	14-vertex polyhedron Mn ₃ Al ₁₁
Al45	12b	1	0.22	0.52	0.48	14-vertex polyhedron Mn ₃ Al ₁₁
Al46	12b	1	0.3	0.4	0.47	11-vertex polyhedron MnAl ₁₀
Al47	12b	1	0.3	0.41	0.34	11-vertex polyhedron MnAl ₁₀

Transformation from published data: $1/4+y, 1/4+x, 1/4+z$

Experimental: polycrystalline sample, electron diffraction

Remarks: Model tested on diffraction data from [2].

References: [1] Hansen V., Gjonnes J. (1996), Acta Crystallogr. A 52, 125-132. [2] Gratias D., Cahn J.W., Mozer B. (1988), Phys. Rev. B: Condens. Matter 38, 1643-1646.