

MnAl₄ λ [1]

Structural features: A dense 3D-framework with mainly icosahedral coordination. So-called I3 units consisting of three vertex-linked icosahedra.

Kreiner G., Franzen H.F. (1997) [1]

Al_{230.75}Mn_{53.30}

$a = 2.8382$, $c = 1.2389$ nm, $c/a = 0.437$, $V = 8.6428$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Al1	12i	1	0.0095	0.5635	0.0692		12-vertex polyhedron Mn ₂ Al ₁₀
Al2	12i	1	0.0231	0.4721	0.1348		tricapped pentagonal prism Al ₁₀ Mn ₃
Al3	12i	1	0.0273	0.2416	0.1361		tricapped pentagonal prism Al ₁₀ Mn ₃
Al4	12i	1	0.0405	0.3884	0.055		12-vertex polyhedron Mn ₂ Al ₁₀
Al5	12i	1	0.0406	0.1543	0.0578		14-vertex Frank-Kasper Al ₁₂ Mn ₂
Al6	12i	1	0.0696	0.0871	0.0496	0.6	icosahedron Al ₁₂
Al7	12i	1	0.0999	0.0424	0.1411	0.75	tricapped pentagonal prism Al ₁₂ Mn
Al8	12i	1	0.1121	0.343	0.0571		12-vertex polyhedron Mn ₂ Al ₁₀
Mn9	12i	1	0.12742	0.25706	0.0744		icosahedron Al ₁₁ Mn
Al10	12i	1	0.1435	0.1705	0.1363		14-vertex Frank-Kasper Al ₁₂ Mn ₂
Al11	12i	1	0.144	0.5474	0.135		tricapped pentagonal prism Al ₁₀ Mn ₃
Al12	12i	1	0.157	0.4616	0.0564		12-vertex polyhedron Mn ₂ Al ₁₀
Al13	12i	1	0.2011	0.063	0.0677		tricapped pentagonal prism Mn ₂ Al ₁₁
Al14	12i	1	0.2134	0.3552	0.1349		tricapped pentagonal prism Al ₁₀ Mn ₃
Al15	12i	1	0.232	0.2714	0.0629		tricapped pentagonal prism Al ₁₀ Mn ₃
Mn16	12i	1	0.24449	0.56317	0.071		icosahedron Al ₁₁ Mn
Al17	12i	1	0.2465	0.1834	0.0695		12-vertex polyhedron Mn ₂ Al ₁₀
Al18	12i	1	0.2594	0.4759	0.1358		tricapped pentagonal prism Al ₁₀ Mn ₃
Al19	12i	1	0.3172	0.3719	0.0677		12-vertex polyhedron Mn ₂ Al ₁₀
Al20	12i	1	0.3188	0.1362	0.0692		12-vertex polyhedron Mn ₂ Al ₁₀
Al21	12i	1	0.3332	0.2858	0.1341		12-vertex polyhedron Mn ₂ Al ₁₀
Al22	12i	1	0.3344	0.0463	0.1356		pseudo Frank-Kasper Al ₁₀ Mn ₃
Al23	12i	1	0.3479	0.5802	0.057		14-vertex Frank-Kasper Mn ₃ Al ₁₁
Al24	12i	1	0.3636	0.4906	0.0682		12-vertex polyhedron Mn ₂ Al ₁₀
Al25	12i	1	0.4082	0.2398	0.1367		12-vertex polyhedron Mn ₂ Al ₁₀
Al26	12i	1	0.4207	0.1494	0.0624		tricapped pentagonal prism Al ₁₀ Mn ₃
Mn27	12i	1	0.43473	0.06194	0.0743		icosahedron Al ₁₁ Mn
Al28	12i	1	0.4506	0.3564	0.1363		12-vertex polyhedron Al ₁₀ Mn ₂
Al29	12i	1	0.5072	0.2497	0.0681		12-vertex polyhedron Mn ₂ Al ₁₀
Al30	12i	1	0.5188	0.1606	0.1372		
Al31	12i	1	0.537	0.0767	0.0652		tricapped pentagonal prism Al ₁₀ Mn ₃
Al32	12i	1	0.6099	0.3269	0.1	0.78	
Al33	12i	1	0.622	0.1771	0.068		12-vertex polyhedron Mn ₂ Al ₁₀
Al34	6h	m..	0.0517	0.3364	$\frac{1}{4}$		12-vertex polyhedron Mn ₂ Al ₁₀
M35	6h	m..	0.0531	0.1007	$\frac{1}{4}$		14-vertex polyhedron Al ₁₃ Mn
Al36	6h	m..	0.0723	0.5711	$\frac{1}{4}$		12-vertex polyhedron Mn ₂ Al ₁₀
Al37	6h	m..	0.0785	0.205	$\frac{1}{4}$		icosahedron Mn ₄ Al ₈
Al38	6h	m..	0.0957	0.4529	$\frac{1}{4}$		12-vertex polyhedron Mn ₂ Al ₁₀
Mn39	6h	m..	0.1188	0.3079	$\frac{1}{4}$		icosahedron Al ₁₀ Mn ₂
Al40	6h	m..	0.1646	0.4068	$\frac{1}{4}$		12-vertex polyhedron Mn ₂ Al ₁₀
Mn41	6h	m..	0.1661	0.022	$\frac{1}{4}$		icosahedron Al ₁₂
M42	6h	m..	0.1823	0.2661	$\frac{1}{4}$		icosahedron Mn ₅ Al ₇

Mn43	6h	m..	0.1922	0.5012	$\frac{1}{4}$	icosahedron Al ₁₀ Mn ₂
Al44	6h	m..	0.1952	0.1213	$\frac{1}{4}$	12-vertex polyhedron Mn ₂ Al ₁₀
Al45	6h	m..	0.2328	0.6036	$\frac{1}{4}$	icosahedron Al ₈ Mn ₄
Mn46	6h	m..	0.2418	0.2192	$\frac{1}{4}$	icosahedron Al ₁₁ Mn
Al47	6h	m..	0.2665	0.0728	$\frac{1}{4}$	12-vertex polyhedron Mn ₂ Al ₁₀
Mn48	6h	m..	0.2854	0.3315	$\frac{1}{4}$	icosahedron Al ₁₁ Mn
M49	6h	m..	0.295	0.5668	$\frac{1}{4}$	icosahedron Al ₈ Mn ₄
Al50	6h	m..	0.306	0.4257	$\frac{1}{4}$	12-vertex polyhedron Mn ₂ Al ₁₀
Al51	6h	m..	0.3102	0.1918	$\frac{1}{4}$	12-vertex polyhedron Mn ₂ Al ₁₀
Mn52	6h	m..	0.3599	0.527	$\frac{1}{4}$	icosahedron Al ₁₂
Mn53	6h	m..	0.362	0.1455	$\frac{1}{4}$	icosahedron Al ₁₁ Mn
Al54	6h	m..	0.3815	0.3796	$\frac{1}{4}$	12-vertex polyhedron Mn ₂ Al ₁₀
Mn55	6h	m..	0.384	0.0019	$\frac{1}{4}$	icosahedron Al ₁₀ Mn ₂
M56	6h	m..	0.4223	0.1055	$\frac{1}{4}$	icosahedron Mn ₅ Al ₇
Mn57	6h	m..	0.4724	0.2119	$\frac{1}{4}$	
Al58	6h	m..	0.4872	0.0667	$\frac{1}{4}$	icosahedron Mn ₅ Al ₇
Al59	6h	m..	0.5079	0.3105	$\frac{1}{4}$	14-vertex polyhedron Mn ₂ Al ₁₂
Mn60	6h	m..	0.5498	0.0272	$\frac{1}{4}$	icosahedron Al ₁₁ Mn
Al61	6h	m..	0.5773	0.2487	$\frac{1}{4}$	0.53
Mn62	6h	m..	0.5897	0.1364	$\frac{1}{4}$	icosahedron Al ₁₁ Mn
Al63	6h	m..	0.5991	0.2382	$\frac{1}{4}$	0.4
M64	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.1188	16-vertex Frank-Kasper Al ₁₃ Mn ₃
Al65	4e	3..	0	0	0.1378	0.74 10-vertex polyhedron Al ₁₀
Mn66	2d	-6..	$\frac{2}{3}$	$\frac{1}{3}$	$\frac{1}{4}$	

M35 = 0.85Al + 0.15Mn; M42 = 0.95Al + 0.05Mn; M49 = 0.88Al + 0.12Mn; M56 = 0.94Al + 0.06Mn;
M64 = 0.92Al + 0.08Mn

Experimental: single crystal, diffractometer, X-rays, wR = 0.059

Remarks: Short interatomic distances for partly occupied site(s). Preliminary account in [2].

References: [1] Kreiner G., Franzen H.F. (1997), J. Alloys Compd. 261, 83-104. [2] Franzen H.F., Kreiner G. (1993), J. Alloys Compd. 202, L21-L23.