

Al_{80.6}Cr_{10.7}Fe_{8.7} v-phase [1]

Structural features: A dense 3D-framework with mainly icosahedral coordination.

Zou X.D. et al. (2003) [1]

Al₂₃₇Cr_{29.70}Fe_{24.30} $a = 4.0687$, $c = 1.2546$ nm, $c/a = 0.308$, $V = 17.9865$ nm³, $Z = 4$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Al1	12i	1	0.0025	0.1663	0.1333		pseudo Frank-Kasper Al ₁₀ Cr ₃
Al2	12i	1	0.0025	0.263	0.0583		12-vertex polyhedron Al ₁₀ Cr ₂
Al3	12i	1	0.0199	0.4764	0.0667		tricapped pentagonal prism Cr ₂ Al ₁₁
Al4	12i	1	0.0223	0.3375	0.1333		pseudo Frank-Kasper Al ₁₀ Cr ₃
Al5	12i	1	0.0323	0.072	0.15		14-vertex Frank-Kasper Al ₁₃ Cr
Al6	12i	1	0.0422	0.4094	0.0667		tricapped pentagonal prism Cr ₂ Al ₁₁
Al7	12i	1	0.0471	0.5533	0.05		pseudo Frank-Kasper Al ₁₀ Cr ₃
Al8	12i	1	0.0571	0.0422	0.0583		pseudo Frank-Kasper Al ₁₃
Al9	12i	1	0.0571	0.1414	0.0583		14-vertex Frank-Kasper Cr ₂ Al ₁₂
Al10	12i	1	0.062	0.2457	0.1333		pseudo Frank-Kasper Al ₁₀ Cr ₃
M11	12i	1	0.0794	0.3176	0.0667		icosahedron Al ₁₁ Cr
Al12	12i	1	0.0943	0.531	0.1417		pseudo Frank-Kasper Cr ₂ Al ₁₁
Al13	12i	1	0.0993	0.0124	0.0583		14-vertex Frank-Kasper Al ₁₂ Cr ₂
Al14	12i	1	0.0993	0.3921	0.0583		pseudo Frank-Kasper Al ₁₀ Cr ₃
Al15	12i	1	0.1141	0.6129	0.05		14-vertex Frank-Kasper Cr ₂ Al ₁₂
Al16	12i	1	0.1166	0.4665	0.125		pseudo Frank-Kasper Cr ₃ Al ₁₀
Al17	12i	1	0.1191	0.2258	0.0667		12-vertex polyhedron Cr ₂ Al ₁₀
Al18	12i	1	0.1216	0.0893	0.1333		14-vertex Frank-Kasper Al ₁₂ Cr ₂
Al19	12i	1	0.1365	0.3002	0.0583		tricapped pentagonal prism Al ₁₀ Cr ₃
Al20	12i	1	0.1414	0.1663	0.0583		12-vertex polyhedron Cr ₂ Al ₁₀
Al21	12i	1	0.1563	0.3747	0.1333		15-vertex Frank-Kasper Al ₁₂ Cr ₃
Al22	12i	1	0.1737	0.4442	0.0583		14-vertex Frank-Kasper Cr ₃ Al ₁₁
M23	12i	1	0.1762	0.0695	0.0583		icosahedron Al ₁₁ Cr
Al24	12i	1	0.18	0.585	0.0583		icosahedron Al ₉ Cr ₃
Al25	12i	1	0.1935	0.2829	0.1417		12-vertex polyhedron Al ₁₀ Cr ₂
Al26	12i	1	0.196	0.1414	0.0583		pseudo Frank-Kasper Cr ₃ Al ₁₀
M27	12i	1	0.198	0.521	0.0677		pseudo Frank-Kasper Al ₁₀ Cr
Al28	12i	1	0.2084	0.3548	0.0583		pseudo Frank-Kasper Cr ₂ Al ₁₁
Al29	12i	1	0.2134	0.2208	0.1333		12-vertex polyhedron Cr ₂ Al ₁₀
Al30	12i	1	0.2333	0.0496	0.05		12-vertex polyhedron Al ₁₀ Cr ₂
Al31	12i	1	0.235	0.44	0.0667		icosahedron Al ₉ Cr ₃
Al32	12i	1	0.248	0.505	0.1417		icosahedron Al ₉ Cr ₃
Al33	12i	1	0.2531	0.1266	0.1333		pseudo Frank-Kasper Al ₁₀ Cr ₃
Al34	12i	1	0.255	0.61	0.0583		12-vertex polyhedron Al ₁₀ Cr ₂
Al35	12i	1	0.2705	0.201	0.0667		icosahedron Cr ₂ Al ₁₀
Al36	12i	1	0.2754	0.3027	0.125		icosahedron Al ₁₀ Cr ₂
Al37	12i	1	0.2953	0.3797	0.0667		icosahedron Cr ₂ Al ₁₀
Al38	12i	1	0.3102	0.072	0.0583		12-vertex polyhedron Al ₁₀ Cr ₂
Al39	12i	1	0.3102	0.5906	0.1417		icosahedron Al ₁₁ Cr
Al40	12i	1	0.315	0.46	0.0667		icosahedron Al ₉ Cr ₃
Al41	12i	1	0.3325	0.1489	0.1333		pseudo Frank-Kasper Al ₁₀ Cr ₃
Al42	12i	1	0.335	0.2854	0.0667		12-vertex polyhedron Cr ₂ Al ₁₀
Al43	12i	1	0.335	0.53	0.1417		icosahedron Al ₉ Cr ₃

Al44	12i	1	0.3524	0.2258	0.0667	12-vertex polyhedron Cr ₂ Al ₁₀
Al45	12i	1	0.3524	0.3623	0.0583	pseudo Frank-Kasper Cr ₃ Al ₁₀
Al46	12i	1	0.3672	0.0521	0.1333	pseudo Frank-Kasper Al ₁₀ Cr ₃
Al47	12i	1	0.3697	0.4367	0.1333	15-vertex Frank-Kasper Al ₁₂ Cr ₃
M48	12i	1	0.3896	0.1315	0.0667	pseudo Frank-Kasper Al ₁₂ Cr
Al49	12i	1	0.4069	0.206	0.0583	pseudo Frank-Kasper Al ₁₀ Cr ₃
Al50	12i	1	0.4069	0.34	0.1333	pseudo Frank-Kasper Al ₁₀ Cr ₃
Al51	12i	1	0.4243	0.2804	0.1333	icosahedron Al ₉ Cr ₃
Al52	12i	1	0.4268	0.0323	0.0583	12-vertex polyhedron Cr ₂ Al ₁₀
Al53	12i	1	0.4392	0.1067	0.0583	pseudo Frank-Kasper Al ₁₀ Cr ₃
Al54	12i	1	0.464	0.1861	0.1333	15-vertex Frank-Kasper Al ₁₂ Cr ₃
M55	12i	1	0.4864	0.263	0.0667	pseudo Frank-Kasper Al ₁₁ Cr ₂
Al56	12i	1	0.5012	0.0918	0.1417	pseudo Frank-Kasper Al ₁₀ Cr ₃
Al57	12i	1	0.5186	0.3548	0.0667	bicapped square prism Cr ₃ Al ₇
M58	12i	1	0.5211	0.1663	0.0667	pseudo Frank-Kasper Al ₁₂ Cr
Al59	12i	1	0.5285	0.0297	0.1417	pseudo Frank-Kasper Cr ₃ Al ₁₀
Al60	12i	1	0.536	0.2382	0.0583	icosahedron Cr ₃ Al ₉
Al61	12i	1	0.5583	0.3201	0.1333	pseudo Frank-Kasper Cr ₄ Al ₉
Al62	12i	1	0.5757	0.139	0.0667	pseudo Frank-Kasper Al ₉ Cr ₂
M63	12i	1	0.5856	0.0124	0.0667	icosahedron Al ₁₁ Cr
Al64	12i	1	0.598	0.2208	0.1417	pseudo Frank-Kasper Cr ₃ Al ₁₀
Al65	12i	1	0.603	0.0869	0.0583	icosahedron Cr ₂ Al ₁₀
Al66	12i	1	0.6129	0.2953	0.0667	icosahedron CrAl ₁₁
Al67	6h	m..	0.0	0.3821	$\frac{1}{4}$	12-vertex polyhedron Cr ₂ Al ₁₀
Al68	6h	m..	0.0224	0.5658	$\frac{1}{4}$	icosahedron Al ₇ Cr ₅
M69	6h	m..	0.0298	0.1241	$\frac{1}{4}$	icosahedron Al ₁₂
M70	6h	m..	0.0323	0.5062	$\frac{1}{4}$	icosahedron Al ₁₁ Cr
M71	6h	m..	0.0397	0.2903	$\frac{1}{4}$	icosahedron Al ₁₀ Cr ₂
Al72	6h	m..	0.0521	0.4591	$\frac{1}{4}$	12-vertex polyhedron Cr ₂ Al ₁₀
Al73	6h	m..	0.0645	0.0298	$\frac{1}{4}$	pseudo Frank-Kasper Al ₁₂ Cr
M74	6h	m..	0.067	0.4069	$\frac{1}{4}$	icosahedron Al ₁₁ Cr
Al75	6h	m..	0.0744	0.1911	$\frac{1}{4}$	12-vertex polyhedron Cr ₂ Al ₁₀
Al76	6h	m..	0.0918	0.3573	$\frac{1}{4}$	icosahedron Al ₇ Cr ₅
M77	6h	m..	0.0918	0.5906	$\frac{1}{4}$	icosahedron Al ₁₁ Cr
Al78	6h	m..	0.0993	0.139	$\frac{1}{4}$	12-vertex polyhedron Cr ₂ Al ₁₀
Al79	6h	m..	0.1092	0.3077	$\frac{1}{4}$	icosahedron Al ₇ Cr ₅
M80	6h	m..	0.1266	0.2556	$\frac{1}{4}$	icosahedron Al ₁₁ Cr
Al81	6h	m..	0.134	0.0397	$\frac{1}{4}$	icosahedron Cr ₄ Al ₈
M82	6h	m..	0.1439	0.4293	$\frac{1}{4}$	icosahedron Al ₁₁ Cr
Al83	6h	m..	0.1514	0.2109	$\frac{1}{4}$	12-vertex polyhedron Cr ₂ Al ₁₀
Al84	6h	m..	0.1563	0.5955	$\frac{1}{4}$	icosahedron Al ₁₀ Cr ₂
Al85	6h	m..	0.1613	0.5385	$\frac{1}{4}$	12-vertex polyhedron Al ₉ Cr ₃
M86	6h	m..	0.1667	0.1563	$\frac{1}{4}$	icosahedron Al ₁₁ Cr
M87	6h	m..	0.1787	0.3325	$\frac{1}{4}$	icosahedron Al ₁₁ Cr
Al88	6h	m..	0.1861	0.1067	$\frac{1}{4}$	icosahedron Al ₇ Cr ₅
Al89	6h	m..	0.1861	0.4988	$\frac{1}{4}$	icosahedron Al ₉ Cr ₃
Al90	6h	m..	0.206	0.4442	$\frac{1}{4}$	icosahedron Cr ₂ Al ₁₀
M91	6h	m..	0.2084	0.0596	$\frac{1}{4}$	icosahedron Al ₁₀ Cr ₂
Al92	6h	m..	0.2208	0.0025	$\frac{1}{4}$	12-vertex polyhedron Cr ₂ Al ₁₀
M93	6h	m..	0.2258	0.6253	$\frac{1}{4}$	12-vertex polyhedron Al ₁₂
Al94	6h	m..	0.2283	0.3995	$\frac{1}{4}$	pseudo Frank-Kasper Al ₉ Cr ₂
M95	6h	m..	0.2382	0.1811	$\frac{1}{4}$	icosahedron Al ₁₁ Cr
Al96	6h	m..	0.2432	0.5633	$\frac{1}{4}$	12-vertex polyhedron Al ₉ Cr ₃
Al97	6h	m..	0.2457	0.3424	$\frac{1}{4}$	12-vertex polyhedron Cr ₂ Al ₁₀

Al98	6h	m..	0.2779	0.0868	$\frac{1}{4}$	12-vertex polyhedron Cr ₂ Al ₁₀
M99	6h	m..	0.2779	0.4665	$\frac{1}{4}$	12-vertex polyhedron Al ₁₂
Al100	6h	m..	0.2829	0.2481	$\frac{1}{4}$	12-vertex polyhedron Cr ₂ Al ₁₀
Al101	6h	m..	0.2903	0.6377	$\frac{1}{4}$	icosahedron CrAl ₁₁
Al102	6h	m..	0.3027	0.0298	$\frac{1}{4}$	12-vertex polyhedron Cr ₂ Al ₁₀
Al103	6h	m..	0.3052	0.1911	$\frac{1}{4}$	12-vertex polyhedron Cr ₂ Al ₁₀
Al104	6h	m..	0.3077	0.4218	$\frac{1}{4}$	pseudo Frank-Kasper Cr ₂ Al ₉
M105	6h	m..	0.3151	0.3672	$\frac{1}{4}$	icosahedron Al ₁₁ Cr
M106	6h	m..	0.3375	0.3151	$\frac{1}{4}$	icosahedron Al ₁₁ Cr
M107	6h	m..	0.3449	0.0968	$\frac{1}{4}$	icosahedron Al ₁₀ Cr ₂
Al108	6h	m..	0.3499	0.4888	$\frac{1}{4}$	icosahedron Cr ₂ Al ₁₀
Al109	6h	m..	0.3648	0.273	$\frac{1}{4}$	12-vertex polyhedron Cr ₂ Al ₁₀
M110	6h	m..	0.3722	0.2159	$\frac{1}{4}$	icosahedron Al ₁₂
Al111	6h	m..	0.3871	0.3921	$\frac{1}{4}$	icosahedron Al ₇ Cr ₅
Al112	6h	m..	0.4	0.17	$\frac{1}{4}$	icosahedron Al ₈ Cr ₄
Al113	6h	m..	0.4169	0.1216	$\frac{1}{4}$	icosahedron Al ₈ Cr ₄
M114	6h	m..	0.4342	0.062	$\frac{1}{4}$	icosahedron Al ₁₂
Al115	6h	m..	0.4491	0.2407	$\frac{1}{4}$	icosahedron Al ₈ Cr ₄
Al116	6h	m..	0.4615	0.0248	$\frac{1}{4}$	12-vertex polyhedron Cr ₂ Al ₁₀
Al117	6h	m..	0.464	0.3474	$\frac{1}{4}$	12-vertex polyhedron Cr ₂ Al ₁₀
Al118	6h	m..	0.4814	0.134	$\frac{1}{4}$	icosahedron Al ₈ Cr ₄
M119	6h	m..	0.4963	0.3077	$\frac{1}{4}$	icosahedron Al ₁₀ Cr ₂
Al120	6h	m..	0.5136	0.2556	$\frac{1}{4}$	icosahedron Al ₈ Cr ₄
Al121	6h	m..	0.531	0.2035	$\frac{1}{4}$	icosahedron Cr ₄ Al ₈
M122	6h	m..	0.5534	0.1563	$\frac{1}{4}$	icosahedron Al ₁₀ Cr ₂
Al123	6h	m..	0.5682	0.0967	$\frac{1}{4}$	12-vertex polyhedron Cr ₂ Al ₁₀
M124	6h	m..	0.5881	0.2779	$\frac{1}{4}$	icosahedron Al ₁₂
M125	6h	m..	0.5931	0.0522	$\frac{1}{4}$	icosahedron Al ₁₀ Cr ₂
Al126	6h	m..	0.6228	0.1687	$\frac{1}{4}$	12-vertex polyhedron Al ₁₀ Cr ₂
Al127	6h	m..	0.6303	0.3424	$\frac{1}{4}$	12-vertex polyhedron Cr ₂ Al ₁₀
Al128	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.0583	icosahedron Al ₁₂
Al129	2a	-6..	0	0	$\frac{1}{4}$	15-vertex Frank-Kasper Al ₁₅

M11 = 0.55Cr + 0.45Fe; M23 = 0.55Cr + 0.45Fe; M27 = 0.55Cr + 0.45Fe; M48 = 0.55Cr + 0.45Fe; M55 = 0.55Cr + 0.45Fe; M58 = 0.55Cr + 0.45Fe; M63 = 0.55Cr + 0.45Fe; M69 = 0.55Cr + 0.45Fe; M70 = 0.55Cr + 0.45Fe; M71 = 0.55Cr + 0.45Fe; M74 = 0.55Cr + 0.45Fe; M77 = 0.55Cr + 0.45Fe; M80 = 0.55Cr + 0.45Fe; M82 = 0.55Cr + 0.45Fe; M86 = 0.55Cr + 0.45Fe; M87 = 0.55Cr + 0.45Fe; M91 = 0.55Cr + 0.45Fe; M93 = 0.55Cr + 0.45Fe; M95 = 0.55Cr + 0.45Fe; M99 = 0.55Cr + 0.45Fe; M105 = 0.55Cr + 0.45Fe; M106 = 0.55Cr + 0.45Fe; M107 = 0.55Cr + 0.45Fe; M110 = 0.55Cr + 0.45Fe; M114 = 0.55Cr + 0.45Fe; M119 = 0.55Cr + 0.45Fe; M122 = 0.55Cr + 0.45Fe; M124 = 0.55Cr + 0.45Fe; M125 = 0.55Cr + 0.45Fe

Transformation from published data: y,x,-z

Experimental: thin film, electron diffraction

Remarks: Hexagonal approximant of quasicrystals. We assigned an approximate value to the Cr/Fe ratio of sites M based on the nominal composition. The structure was refined on single-crystal X-ray diffraction data in [2].

References: [1] Zou X.D., Mo Z.M., Hovmöller S., Li X.Z., Kuo K.H. (2003), Acta Crystallogr. A 59, 526-539. [2] Mo Z.M., Zhou H.Y., Kuo K.H. (2000), Acta Crystallogr. B 56, 392-401.