$Cr_{63.4}Fe_{51.4}Al_{477.4}$	*hP*1192	(176) $P6_3/m$ – $i^{69}h^{59}fea$

$Al_{80.6}Cr_{10.7}Fe_{8.7}$ ν-phase [1]
Structural features: A dense 3D-framework with mainly icosahedral coordination.

Mo Z.M. et al. (2000) [1]
$Al_{477.44}Cr_{63.42}Fe_{51.42}$
$a = 4.068$, $c = 1.2546$ nm, $c/a = 0.308$, $V = 17.9803$ nm^3, $Z = 2$

site	Wyck.	sym.	*x*	*y*	*z*	occ.	atomic environment
M1	12*i*	1	0.01312	0.58373	0.0754		icosahedron $Al_{11}Cr$
Al2	12*i*	1	0.01769	0.10777	0.056		14-vertex Frank-Kasper $Al_{12}Cr_2$
Al3	12*i*	1	0.03015	0.52845	0.1359		pseudo Frank-Kasper $Al_{10}Cr_3$
Al4	12*i*	1	0.03463	0.42895	0.0692		tricapped pentagonal prism Cr_3Al_{10}
M5	12*i*	1	0.04531	0.06444	0.0464		tricapped trigonal prism Al_9
Al6	12*i*	1	0.05171	0.23478	0.0574		12-vertex polyhedron Cr_2Al_{10}
Al7	12*i*	1	0.0569	0.3723	0.1367		pseudo Frank-Kasper $Al_{10}Cr_3$
M8	12*i*	1	0.07075	0.1804	0.0751		icosahedron $Al_{11}Cr$
Al9	12*i*	1	0.0736	0.0326	0.1458		14-vertex Frank-Kasper $Al_{13}Cr$
Al10	12*i*	1	0.07369	0.31484	0.0572		12-vertex polyhedron Cr_2Al_{10}
Al11	12*i*	1	0.08619	0.6029	0.0552		pseudo Frank-Kasper $FeCr_2Al_{10}$
Al12	12*i*	1	0.0899	0.5029	0.1357		tricapped pentagonal prism Cr_3Al_{10}
Al13	12*i*	1	0.0919	0.1255	0.1375		pseudo Frank-Kasper $Al_{11}Cr_2$
Al14	12*i*	1	0.10882	0.44576	0.0598		14-vertex Frank-Kasper Cr_3Al_{11}
Al15	12*i*	1	0.126	0.2529	0.1361		pseudo Frank-Kasper $Al_{10}Cr_3$
Cr16	12*i*	1	0.12994	0.39043	0.0766		icosahedron $Al_{11}Cr$
Al17	12*i*	1	0.13897	0.5726	0.0605		tricapped pentagonal prism $FeCr_2Al_{10}$
Al18	12*i*	1	0.14501	0.05941	0.0651		tricapped pentagonal prism Cr_2Al_{11}
Al19	12*i*	1	0.14683	0.19805	0.0656		pseudo Frank-Kasper $Al_{10}Cr_3$
Al20	12*i*	1	0.1486	0.3346	0.139		pseudo Frank-Kasper $Al_{10}Cr_3$
Al21	12*i*	1	0.1633	0.0028	0.1365		pseudo Frank-Kasper $Al_{10}Cr_3$
Al22	12*i*	1	0.16719	0.14257	0.0693		12-vertex polyhedron Cr_2Al_{10}
Al23	12*i*	1	0.16902	0.52509	0.0623		pseudo Frank-Kasper $FeCr_2Al_{10}$
Al24	12*i*	1	0.1849	0.4655	0.1306		15-vertex Frank-Kasper $FeAl_{13}Cr$
Al25	12*i*	1	0.20256	0.27249	0.0696		12-vertex polyhedron Cr_2Al_{10}
Al26	12*i*	1	0.20399	0.40675	0.0641		pseudo Frank-Kasper $Al_{11}Cr_2$
Al27	12*i*	1	0.21344	0.59807	0.1374		pseudo Frank-Kasper Fe_2CrAl_{10}
Al28	12*i*	1	0.2216	0.21668	0.1341		12-vertex polyhedron Cr_2Al_{10}
Al29	12*i*	1	0.2251	0.35184	0.0701		12-vertex polyhedron Cr_2Al_{10}
Al30	12*i*	1	0.22539	0.11879	0.0705		12-vertex polyhedron Cr_2Al_{10}
Fe31	12*i*	1	0.23518	0.53229	0.0733		pseudo Frank-Kasper Al_{11}
Al32	12*i*	1	0.2454	0.0613	0.1347		pseudo Frank-Kasper $Al_{10}Cr_3$
Al33	12*i*	1	0.26177	0.48719	0.0657		pseudo Frank-Kasper $FeAl_{11}Cr$
Al34	12*i*	1	0.26296	0.00535	0.0569		12-vertex polyhedron Cr_2Al_{10}
Fe35	12*i*	1	0.26525	0.64938	0.0534		bicapped square antiprism Al_{10}
Al36	12*i*	1	0.2801	0.1939	0.1328		12-vertex polyhedron Cr_2Al_{10}
Al37	12*i*	1	0.2817	0.4269	0.1369		pseudo Frank-Kasper $Al_{11}Cr_2$
Al38	12*i*	1	0.28295	0.59902	0.1195		pseudo Frank-Kasper Fe_3Al_{10}
Al39	12*i*	1	0.28525	0.33166	0.0702		12-vertex polyhedron Cr_2Al_{10}
Al40	12*i*	1	0.29918	0.13639	0.0647		pseudo Frank-Kasper $Al_{10}Cr_3$
Al41	12*i*	1	0.30319	0.27552	0.1327		12-vertex polyhedron Cr_2Al_{10}
M42	12*i*	1	0.31785	0.07945	0.0748		icosahedron $Al_{11}Cr$
Al43	12*i*	1	0.31908	0.55654	0.1378		tricapped pentagonal prism Fe_2CrAl_{10}

Al44	12*i*	1	0.33443	0.49941	0.0656		tricapped pentagonal prism $FeCrAl_{11}$
Al45	12*i*	1	0.3375	0.02517	0.1361		pseudo Frank-Kasper $Al_{10}Cr_3$
Al46	12*i*	1	0.34271	0.40795	0.1359		pseudo Frank-Kasper $Al_{10}Cr_3$
Al47	12*i*	1	0.35396	0.21199	0.0677		12-vertex polyhedron Cr_2Al_{10}
Al48	12*i*	1	0.36034	0.35193	0.0641		pseudo Frank-Kasper $Al_{10}Cr_3$
Al49	12*i*	1	0.37085	0.1531	0.1377		14-vertex Frank-Kasper $Al_{12}Cr_2$
Al50	12*i*	1	0.37767	0.29474	0.067		12-vertex polyhedron Cr_2Al_{10}
Al51	12*i*	1	0.39115	0.09837	0.0614		pseudo Frank-Kasper $Al_{11}Cr_2$
Al52	12*i*	1	0.41319	0.04435	0.0694		12-vertex polyhedron Cr_2Al_{10}
Al53	12*i*	1	0.4319	0.2678	0.0717		pseudo Frank-Kasper Cr_2Al_9
Al54	12*i*	1	0.4345	0.3731	0.1358		14-vertex Frank-Kasper Cr_3Al_{11}
M55	12*i*	1	0.43858	0.17214	0.0587		10-vertex polyhedron Al_{10}
Al56	12*i*	1	0.4626	0.118	0.1371		tricapped pentagonal prism $FeCrAl_{11}$
Al57	12*i*	1	0.4754	0.0217	0.0694		12-vertex polyhedron Cr_2Al_{10}
Al58	12*i*	1	0.4871	0.337	0.137	0.87	12-vertex polyhedron Cr_2Al_{10}
Al59	12*i*	1	0.5018	0.2744	0.0922	0.84	icosahedron $FeAl_{10}Cr$
Al60	12*i*	1	0.5061	0.1959	0.1335		14-vertex Frank-Kasper $Al_{13}Fe$
Fe61	12*i*	1	0.52366	0.1424	0.0633		tricapped trigonal prism Al_9
Al62	12*i*	1	0.5326	0.0932	0.1327		tricapped pentagonal prism $FeCr_2Al_{10}$
Al63	12*i*	1	0.55257	0.04292	0.0581		pseudo Frank-Kasper Cr_3Al_{10}
Al64	12*i*	1	0.56339	0.27069	0.0562		pseudo Frank-Kasper Fe_2Al_{11}
Al65	12*i*	1	0.5765	0.2077	0.0557		rhombic dodecahedron $Fe_2Al_{11}Cr$
Al66	12*i*	1	0.58208	0.34727	0.0537		pseudo Frank-Kasper Fe_2CrAl_{10}
Al67	12*i*	1	0.59957	0.16097	0.1375		tricapped pentagonal prism $Cr_2Al_{10}Fe$
M68	12*i*	1	0.60862	0.10926	0.053		11-vertex polyhedron Al_{11}
Al69	12*i*	1	0.6345	0.2864	0.1311		icosahedron $FeAl_{10}Cr$
Al70	6*h*	*m*..	0.0018	0.3811	$^1/_4$		12-vertex polyhedron Cr_2Al_{10}
Al71	6*h*	*m*..	0.0071	0.2243	$^1/_4$		12-vertex polyhedron Cr_2Al_{10}
Al72	6*h*	*m*..	0.0238	0.4655	$^1/_4$		12-vertex polyhedron Cr_2Al_{10}
Al73	6*h*	*m*..	0.029	0.3031	$^1/_4$		12-vertex polyhedron Cr_2Al_{10}
M74	6*h*	*m*..	0.0358	0.0711	$^1/_4$		8-vertex polyhedron Al_8
Al75	6*h*	*m*..	0.0398	0.1388	$^1/_4$		icosahedron Cr_4Al_8
M76	6*h*	*m*..	0.05536	0.59504	$^1/_4$		icosahedron $Al_{10}Cr_2$
M77	6*h*	*m*..	0.06002	0.21149	$^1/_4$		icosahedron $Al_{10}Cr_2$
M78	6*h*	*m*..	0.06518	0.43681	$^1/_4$		icosahedron Al_{12}
Al79	6*h*	*m*..	0.0856	0.2808	$^1/_4$		12-vertex polyhedron Cr_2Al_{10}
Al80	6*h*	*m*..	0.0969	0.5648	$^1/_4$		12-vertex polyhedron Cr_2Al_{10}
Cr81	6*h*	*m*..	0.09767	0.34702	$^1/_4$		icosahedron $Al_{10}Cr_2$
Al82	6*h*	*m*..	0.1107	0.19	$^1/_4$		icosahedron Cr_5Al_7
M83	6*h*	*m*..	0.1178	0.4187	$^1/_4$		icosahedron Al_8Cr_4
Cr84	6*h*	*m*..	0.1247	0.03193	$^1/_4$		icosahedron Al_{12}
Al85	6*h*	*m*..	0.1346	0.0962	$^1/_4$		12-vertex polyhedron Cr_2Al_{10}
Al86	6*h*	*m*..	0.1361	0.4885	$^1/_4$		icosahedron $Al_{10}Cr_2$
Cr87	6*h*	*m*..	0.15519	0.55852	$^1/_4$		icosahedron Al_{12}
Cr88	6*h*	*m*..	0.15933	0.16598	$^1/_4$		icosahedron $Al_{11}Cr$
M89	6*h*	*m*..	0.1682	0.3974	$^1/_4$		icosahedron Al_8Cr_4
Al90	6*h*	*m*..	0.1706	0.6247	$^1/_4$		12-vertex polyhedron Cr_2Al_{10}
Cr91	6*h*	*m*..	0.18129	0.24119	$^1/_4$		icosahedron $Al_{11}Cr$
Al92	6*h*	*m*..	0.1897	0.3063	$^1/_4$		12-vertex polyhedron Cr_2Al_{10}
Al93	6*h*	*m*..	0.1924	0.0722	$^1/_4$		12-vertex polyhedron Cr_2Al_{10}
Al94	6*h*	*m*..	0.2091	0.5411	$^1/_4$		pseudo Frank-Kasper $Al_{10}Fe_2Cr$
Al95	6*h*	*m*..	0.2129	0.1538	$^1/_4$		12-vertex polyhedron Cr_2Al_{10}
Cr96	6*h*	*m*..	0.21868	0.37594	$^1/_4$		icosahedron Al_{12}
Al97	6*h*	*m*..	0.2372	0.4463	$^1/_4$		icosahedron $Al_{10}Cr_2$

Al98	6*h*	*m*..	0.2497	0.2841	$^1/_4$		12-vertex polyhedron Cr_2Al_{10}
Al99	6*h*	*m*..	0.2554	0.5199	$^1/_4$		pseudo Frank-Kasper $Al_{10}Fe_2Cr$
M100	6*h*	*m*..	0.25692	0.12878	$^1/_4$		icosahedron $Al_{11}Cr$
Al101	6*h*	*m*..	0.2744	0.3656	$^1/_4$		12-vertex polyhedron Cr_2Al_{10}
Al102	6*h*	*m*..	0.2841	0.6538	$^1/_4$		14-vertex polyhedron Fe_2Al_{12}
M103	6*h*	*m*..	0.28622	0.03669	$^1/_4$		icosahedron $Al_{10}Cr_2$
Al104	6*h*	*m*..	0.3061	0.1081	$^1/_4$		icosahedron Cr_5Al_7
M105	6*h*	*m*..	0.30749	0.49887	$^1/_4$		icosahedron Al_{12}
Cr106	6*h*	*m*..	0.31594	0.3367	$^1/_4$		icosahedron $Al_{11}Cr$
Cr107	6*h*	*m*..	0.32996	0.18049	$^1/_4$		icosahedron $Al_{11}Cr$
Al108	6*h*	*m*..	0.3422	0.2475	$^1/_4$		12-vertex polyhedron Cr_2Al_{10}
Al109	6*h*	*m*..	0.3484	0.468	$^1/_4$		12-vertex polyhedron Cr_2Al_{10}
Al110	6*h*	*m*..	0.3563	0.0881	$^1/_4$		icosahedron Al_8Cr_4
M111	6*h*	*m*..	0.36948	0.31882	$^1/_4$		icosahedron $Al_{11}Cr$
Al112	6*h*	*m*..	0.3867	0.3896	$^1/_4$		icosahedron Al_7Cr_5
Al113	6*h*	*m*..	0.3981	0.2234	$^1/_4$		pseudo Frank-Kasper Cr_2Al_9
M114	6*h*	*m*..	0.40747	0.06812	$^1/_4$		icosahedron Al_{12}
Al115	6*h*	*m*..	0.4197	0.3039	$^1/_4$		12-vertex polyhedron Cr_2Al_{10}
M116	6*h*	*m*..	0.42528	0.14507	$^1/_4$		pseudo Frank-Kasper $Al_{12}Cr$
Al117	6*h*	*m*..	0.4598	0.2147	$^1/_4$	0.84	bicapped square prism Al_9Cr
Al118	6*h*	*m*..	0.4616	0.0567	$^1/_4$		12-vertex polyhedron Cr_2Al_{10}
M119	6*h*	*m*..	0.46495	0.27959	$^1/_4$		pseudo Frank-Kasper Al_{11}
M120	6*h*	*m*..	0.50693	0.03379	$^1/_4$		icosahedron Al_{12}
M121	6*h*	*m*..	0.52623	0.25518	$^1/_4$		pseudo Frank-Kasper $Al_{10}Cr$
Al122	6*h*	*m*..	0.5386	0.326	$^1/_4$		12-vertex polyhedron Cr_2Al_{10}
Al123	6*h*	*m*..	0.5394	0.1576	$^1/_4$		14-vertex polyhedron $Fe_2Al_{11}Cr$
Al124	6*h*	*m*..	0.5588	0.0157	$^1/_4$		icosahedron Cr_4Al_8
M125	6*h*	*m*..	0.5702	0.2387	$^1/_4$		icosahedron $Al_{11}Cr$
M126	6*h*	*m*..	0.5883	0.0911	$^1/_4$		14-vertex polyhedron Cr_3Al_{11}
Al127	6*h*	*m*..	0.5934	0.312	$^1/_4$		12-vertex polyhedron $Al_{11}Cr$
M128	6*h*	*m*..	0.62096	0.22191	$^1/_4$		icosahedron Al_{12}
Al129	4*f*	3..	$^1/_3$	$^2/_3$	0.0426		icosahedron Fe_3Al_9
Al130	4*e*	3..	0	0	0.1099	0.5	single atom Al
M131	2*a*	-6..	0	0	$^1/_4$	0.5	colinear Al_2

M1 = 0.5Cr + 0.5Fe; M5 = 0.53Al + 0.235Cr + 0.235Fe; M8 = 0.5Cr + 0.5Fe; M42 = 0.5Cr + 0.5Fe; M55 = 0.71Al + 0.145Cr + 0.145Fe; M68 = 0.405Cr + 0.405Fe + 0.19Al; M74 = 0.52Al + 0.24Cr + 0.24Fe; M76 = 0.5Cr + 0.5Fe; M77 = 0.5Cr + 0.5Fe; M78 = 0.5Cr + 0.5Fe; M83 = 0.87Al + 0.065Cr + 0.065Fe; M89 = 0.92Al + 0.04Cr + 0.04Fe; M100 = 0.5Cr + 0.5Fe; M103 = 0.5Cr + 0.5Fe; M105 = 0.5Cr + 0.5Fe; M111 = 0.5Cr + 0.5Fe; M114 = 0.5Cr + 0.5Fe; M116 = 0.40Al + 0.30Cr + 0.30Fe; M119 = 0.5Cr + 0.5Fe; M120 = 0.5Cr + 0.5Fe; M121 = 0.38Al + 0.31Cr + 0.31Fe; M125 = 0.76Al + 0.12Cr + 0.12Fe; M126 = 0.83Al + 0.085Cr + 0.085Fe; M128 = 0.405Cr + 0.405Fe + 0.19Al; M131 = 0.94Al + 0.03Cr + 0.03Fe

Transformation from published data: origin shift 0 0 $^1/_2$

Experimental: single crystal, diffractometer, X-rays, R = 0.075, T = 293 K

Remarks: Hexagonal approximant of quasicrystals. Short interatomic distances for partly occupied site(s). The structure was studied by electron diffraction in [2].

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