

Mg₃FeAl₉Si₅*hP*18(189) *P*-62*m* – ihgfba**Mg₃FeAl₉Si₅** [1], Strukturbericht notation E9_b

Structural features: Infinite columns of base-linked Si(Mg₃Al₃) trigonal prisms share edges to form a 3D-framework; single columns of base-linked SiAl₆ and FeAl₆ trigonal prisms in channels parallel to [001] (partial substitution ignored). Ordering variant of Ti₄Ni₂Ga₃.

Krendelsberger R. et al. (1998) [1]

Al_{8.64}FeMg_{3.36}Si₅ $a = 0.6652$, $c = 0.791$ nm, $c/a = 1.189$, $V = 0.3031$ nm³, $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
M1	6 <i>i</i>	.. <i>m</i>	0.24981	0	0.2209		pseudo Frank-Kasper FeSi ₃ Al ₆ Mg ₃
Si2	4 <i>h</i>	3.. ₂	¹ / ₃	² / ₃	0.24205		tricapped trigonal prism Al ₆ Mg ₃
Mg3	3 <i>g</i>	<i>m</i> 2 <i>m</i>	0.58241	0	¹ / ₂		pseudo Frank-Kasper Si ₆ Al ₈ Mg ₄
Al4	3 <i>f</i>	<i>m</i> 2 <i>m</i>	0.62251	0	0		11-vertex polyhedron FeAl ₆ Si ₄
Si5	1 <i>b</i>	-62 <i>m</i>	0	0	¹ / ₂		tricapped trigonal prism Al ₆ Mg ₃
Fe6	1 <i>a</i>	-62 <i>m</i>	0	0	0		tricapped trigonal prism Al ₉

 $M1 = 0.94Al + 0.06Mg$ Experimental: single crystal, diffractometer, X-rays, $R = 0.064$, $T = 297$ K

Remarks: Phase referred to as π -(AlFeMgSi), experimental composition Mg₃FeAl_{9.5}Si₅. The structure type was originally reported for so-called Mg₃FeAl₈Si₆ in [2], however, the atom distribution proposed in [2] is superseded.

References: [1] Krendelsberger R., Rogl P., Leithe Jasper A., Simensen C.J. (1998), J. Alloys Compd. 264, 236-239. [2] Perlitz H., Westgren A. (1942), Ark. Kemi Mineral. Geol. 15B(16), 1-8.