

$\text{La}_{16.25}\text{Al}_{12.75}$ $hP29$ $(189) P-62m - i^2hg^2fec$ **La_5Al_4 [1]**

Belyavina N.M. et al. (2004) [1]

 $\text{Al}_{12.75}\text{La}_{16.25}$ $a = 0.91628, c = 1.12309 \text{ nm}, c/a = 1.226, V = 0.8166 \text{ nm}^3, Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Al1	$6i$	$..m$	0.286	0	0.294		bicapped square prism Al_2La_8
La2	$6i$	$..m$	0.6109	0	0.164		14-vertex Frank-Kasper Al_7La_7
La3	$4h$	$3..$	$\frac{1}{3}$	$\frac{2}{3}$	0.3428		14-vertex Frank-Kasper Al_7La_7
M4	$3g$	$m2m$	0.428	0	$\frac{1}{2}$		tricapped trigonal prism Al_2La_7
La5	$3g$	$m2m$	0.763	0	$\frac{1}{2}$		7-capped pentagonal prism Al_9La_8
La6	$3f$	$m2m$	0.2601	0	0		14-vertex Frank-Kasper Al_6La_8
Al7	$2e$	$3.m$	0	0	0.232		icosahedron Al_3La_9
M8	$2c$	$-6..$	$\frac{1}{3}$	$\frac{2}{3}$	0		pseudo Frank-Kasper La_{11}

 $\text{M4} = 0.95\text{Al} + 0.05\text{La}; \text{M8} = 0.95\text{Al} + 0.05\text{La}$ Transformation from published data: $-x, -y, -z$; origin shift $0 \ 0 \ \frac{1}{2}$ Experimental: powder, diffractometer, X-rays, $wR_p = 0.042$ Remarks: Approximate composition. Identical to the phase called La_3Al_2 in [2].

References: [1] Belyavina N.M., Markiv V.Y., Zavodyanny V.V. (2004), J. Alloys Compd. 367, 132-136.

[2] Chaban N.F., Kuz'ma Y.B. (1971), Dopov. Akad. Nauk Ukr. RSR, Ser. A 1971, 1048-1050.