

$\text{Y}_3\text{NiAl}_3\text{Ge}_2$	$hP9$	(189) $P\text{-}62m - \text{gfd}$
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**$\text{Y}_3\text{NiAl}_3\text{Ge}_2$  [1]**

Structural features: Infinite columns of base-linked  $\text{GeY}_6$  trigonal prisms share edges to form a 3D-framework; single columns of base-linked  $\text{NiAl}_6$  trigonal prisms in channels parallel to  $[001]$  (capping atoms ignored). Ordering variant of  $\text{Fe}_2\text{P}$ .

Zhao J.T., Parthé E. (1990) [1]

$\text{Al}_3\text{Ge}_2\text{NiY}_3$

$a = 0.69481$ ,  $c = 0.41565$  nm,  $c/a = 0.598$ ,  $V = 0.1738$  nm<sup>3</sup>,  $Z = 1$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Al1	$3g$	$m2m$	0.2268	0	$\frac{1}{2}$		cuboctahedron $\text{Ni}_2\text{Al}_2\text{Ge}_2\text{Y}_6$
Y2	$3f$	$m2m$	0.5963	0	0		pseudo Frank-Kasper $\text{Ni}_2\text{Ge}_4\text{Al}_6\text{Y}_6$
Ge3	$2d$	$-6..$	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$		tricapped trigonal prism $\text{Al}_3\text{Y}_6$
Ni4	$1a$	$-62m$	0	0	0		tricapped trigonal prism $\text{Al}_6\text{Y}_3$

Experimental: single crystal, diffractometer, X-rays,  $wR = 0.048$ ,  $T = 300$  K

References: [1] Zhao J.T., Parthé E. (1990), Acta Crystallogr. C 46, 2273-2276.