

La₂Ni₂I*hP5*(187) *P-6m2* – icba**La₂Ni₂I** [1]

Structural features: NiLa₆ trigonal prisms share edges to form AlB₂-type infinite slabs, which alternate with close-packed I layers along [001].

Hong S.T. et al. (1998) [1]

ILa₂Ni₂ $a = 0.41387$, $c = 0.8814$ nm, $c/a = 2.130$, $V = 0.1307$ nm³, $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
La1	2 <i>i</i>	3 <i>m</i> .	$\frac{2}{3}$	$\frac{1}{3}$	0.2124		16-vertex polyhedron Ni ₆ I ₃ La ₇
Ni2	1 <i>c</i>	-6 <i>m2</i>	$\frac{1}{3}$	$\frac{2}{3}$	0		tricapped trigonal prism Ni ₃ La ₆
I3	1 <i>b</i>	-6 <i>m2</i>	0	0	$\frac{1}{2}$		trigonal prism La ₆
Ni4	1 <i>a</i>	-6 <i>m2</i>	0	0	0		tricapped trigonal prism Ni ₃ La ₆

Transformation from published data: origin shift $\frac{1}{3} \frac{2}{3} \frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays, R = 0.018, T = 296 K

Remarks: Additional reflections could be indexed with a 2-fold supercell (new axes a,b,2c).

References: [1] Hong S.T., Martin J.D., Corbett J.D. (1998), Inorg. Chem. 37, 3385-3390.