

La₂₁Ni_{10.49}Si₁₅

hP98

(176) $P6_3/m - h^{15}eca$ **La₂₁Ni_{10.49}Si₁₅** [1]

Structural features: Infinite columns of base-linked SiLa₆Ni₃, SiLa₆(LaNi₂) and SiLa₆(La₂Ni) tricapped trigonal prisms share atoms to form a 3D-framework with AlB₂-type (BaLiSi) columns (25 prisms in the triangular cross-section); additional Ni in channels of hexagonal cross-section parallel to [001] (partial disorder).

Prots' Y.M., Jeitschko W. (1998) [1]

La₂₁Ni_{10.50}Si₁₅ $a = 2.4277$, $c = 0.4352$ nm, $c/a = 0.179$, $V = 2.2213$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Si1	6h	m..	0.0432	0.2123	$\frac{1}{4}$		tricapped trigonal prism NiLa ₈
Si2	6h	m..	0.0772	0.3987	$\frac{1}{4}$		tricapped trigonal prism Ni ₂ La ₇
La3	6h	m..	0.10837	0.12769	$\frac{1}{4}$		
Si4	6h	m..	0.1117	0.5848	$\frac{1}{4}$		tricapped trigonal prism Ni ₂ La ₇
Ni5	6h	m..	0.1173	0.3272	$\frac{1}{4}$		tricapped trigonal prism Si ₃ La ₆
Ni6	6h	m..	0.1498	0.5117	$\frac{1}{4}$		tricapped trigonal prism Si ₃ La ₆
Si7	6h	m..	0.2318	0.3733	$\frac{1}{4}$		tricapped trigonal prism Ni ₂ La ₇
Si8	6h	m..	0.2618	0.5527	$\frac{1}{4}$		tricapped trigonal prism Ni ₃ La ₆
La9	6h	m..	0.26894	0.11175	$\frac{1}{4}$		7-capped pentagonal prism Ni ₂ Si ₅ La ₁₀
La10	6h	m..	0.29214	0.275	$\frac{1}{4}$		7-capped pentagonal prism Ni ₂ Si ₅ La ₁₀
Ni11	6h	m..	0.303	0.4838	$\frac{1}{4}$		tricapped trigonal prism Si ₃ La ₆
La12	6h	m..	0.4228	0.0835	$\frac{1}{4}$		7-capped pentagonal prism Ni ₂ Si ₅ La ₁₀
La13	6h	m..	0.44425	0.25318	$\frac{1}{4}$		pseudo Frank-Kasper Ni ₆ Si ₆ La ₈
La14	6h	m..	0.57502	0.05055	$\frac{1}{4}$		7-capped pentagonal prism Ni ₂ Si ₅ La ₁₀
La15	6h	m..	0.59675	0.22312	$\frac{1}{4}$		pseudo Frank-Kasper Ni ₆ Si ₆ La ₈
Ni16	4e	3..	0	0	0.11	0.08	
Ni17	2c	-6..	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		tricapped trigonal prism Si ₃ La ₆
Ni18	2a	-6..	0	0	$\frac{1}{4}$	0.34	

Experimental: single crystal, diffractometer, X-rays, wR = 0.027, T = 295 K

Remarks: Short interatomic distances for partly occupied site(s).

References: [1] Prots' Y.M., Jeitschko W. (1998), Inorg. Chem. 37, 5431-5438.