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Crystal structure of ytterbium nickel aluminium, Yb₄Ni₆Al₂₃

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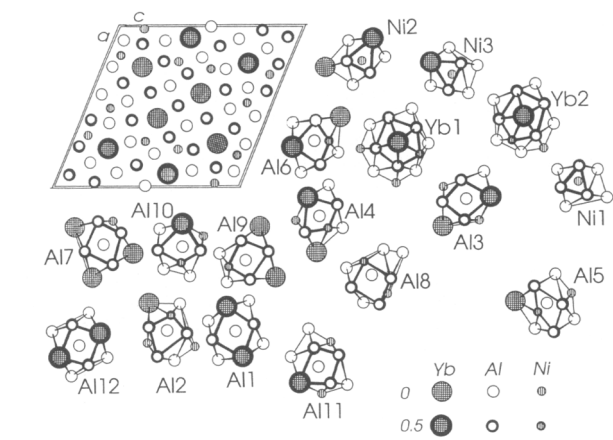


Table 1. Parameters used for the X-ray data collection

Crystal:	metallic needle, size 0.016 x 0.016 x 0.128 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	232.5 cm ⁻¹
Diffractometer:	Philips PW1100
Scan mode:	ω -2 θ
$T_{\text{measurement}}$:	293 K
2 θ_{max} :	50°
$N(hkl)_{\text{unique}}$:	1086
Criterion for F_o :	$F_o > 3 \sigma(F_o)$
$N(\text{param})_{\text{refined}}$:	102
Program:	XTAL 3.2

Source of material: Synthesis from elements by arc melting.
Nominal composition Yb₁₀Ni₁₅Al₇₅.
Yb₄Ni₆Al₂₃ crystallizes with Y₄Ni₆Al₂₃ structure type (see ref. 1).

Al₂₃Ni₆Yb₄, monoclinic, $C2/m$ (No. 12), $a = 15.834(7)$ Å,
 $b = 4.069(1)$ Å, $c = 18.18(1)$ Å, $\beta = 112.84(4)^\circ$, $V = 1080$ Å³, $Z = 2$,
 $R(F) = 0.046$, $R_w(F) = 0.034$.

Table 2. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> ₁₁	<i>U</i> ₂₂	<i>U</i> ₃₃	<i>U</i> ₁₂	<i>U</i> ₁₃	<i>U</i> ₂₃
Yb(1)	4i	0.26372(9)	0	0.21808(8)	0.0078(7)	0.0048(8)	0.0064(8)	0	0.0016(6)	0
Yb(2)	4i	0.57506(9)	0	0.40731(8)	0.0078(7)	0.0053(8)	0.0066(8)	0	0.0010(6)	0
Ni(1)	4i	0.0074(3)	0	0.1369(3)	0.010(2)	0.009(3)	0.010(3)	0	0.005(2)	0
Ni(2)	4i	0.2282(3)	0	0.3986(3)	0.008(2)	0.007(3)	0.008(2)	0	0.003(2)	0
Ni(3)	4i	0.6893(3)	0	0.0674(3)	0.005(2)	0.004(2)	0.006(2)	0	−0.002(2)	0
Al(1)	4i	0.0811(7)	0	0.6861(6)	0.005(4)	0.009(5)	0.004(4)	0	−0.002(4)	0
Al(2)	4i	0.0900(6)	0	0.0510(6)	0.006(5)	0.009(6)	0.011(5)	0	0.000(4)	0
Al(3)	4i	0.0919(6)	0	0.2812(6)	0.007(5)	0.010(6)	0.008(5)	0	−0.006(4)	0
Al(4)	4i	0.1998(6)	0	0.5195(6)	0.011(5)	0.001(5)	0.011(5)	0	0.007(4)	0
Al(5)	4i	0.2556(6)	0	0.0468(5)	0.011(5)	0.011(6)	−0.001(5)	0	0.000(4)	0
Al(6)	4i	0.2726(7)	0	0.6763(6)	0.013(5)	0.001(5)	0.011(5)	0	0.004(4)	0
Al(7)	4i	0.3793(6)	0	0.4052(6)	0.006(5)	0.017(6)	0.007(5)	0	−0.001(4)	0
Al(8)	4i	0.4326(6)	0	0.0596(6)	0.011(5)	0.022(7)	−0.001(5)	0	−0.006(4)	0
Al(9)	4i	0.4676(7)	0	0.2203(6)	0.017(5)	0.008(6)	0.008(5)	0	0.006(5)	0
Al(10)	4i	0.6115(6)	0	0.1640(6)	0.008(5)	0.007(5)	0.012(5)	0	0.004(4)	0
Al(11)	4i	0.8554(7)	0	0.1438(6)	0.010(5)	0.005(6)	0.008(5)	0	0.000(4)	0
Al(12)	2c	0	0	1/2	0.007(7)	0.022(9)	0.016(8)	0	0.007(6)	0

Reference
1. Gladyshevskii, R. E; Parthé, E.: Structure of Monoclinic Y₄Ni₆Al₂₃. Acta Crystallogr. C48 (1992) 232-236.