

Abstract

Table 1

Experimental details

Crystal data	
Chemical formula	LaNi ₅
M_r	432.47
Crystal system, space group	Hexagonal, $P6/mmm$
Temperature (K)	300
a, c (Å)	5.0149 (4), 3.9751 (5)
V (Å ³)	86.58 (2)
Z	1
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	38.41
Crystal size (mm)	0.14 × 0.08 × 0.07
Data collection	
Diffractometer	Bruker D8 Venture Photon 100 CMOS
Absorption correction	Multi-scan (<i>SADABS</i> ; Krause et al., 2015)
T_{\min}, T_{\max}	0.171, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	1897, 47, 47
R_{int}	0.067
$(\sin \theta/\lambda)_{\max}$ (Å ⁻¹)	0.589
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.029, 0.071, 1.37
No. of reflections	47
No. of parameters	9
$\Delta\rho_{\max}, \Delta\rho_{\min}$ (e Å ⁻³)	1.19, -1.07

Computer programs: *SHELXL2019/1* (Sheldrick, 2019).

References

NOT FOUND

full crystallographic data

Computing details

Program(s) used to refine structure: *SHELXL2019/1* (Sheldrick, 2019).

(242006_a)

Crystal data

LaNi ₅	$D_x = 8.295 \text{ Mg m}^{-3}$
$M_r = 432.47$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
Hexagonal, $P6/mmm$	Cell parameters from 1868 reflections
$a = 5.0149 (4) \text{ \AA}$	$\theta = 4.7\text{--}27.5^\circ$
$c = 3.9751 (5) \text{ \AA}$	$\mu = 38.41 \text{ mm}^{-1}$
$V = 86.58 (2) \text{ \AA}^3$	$T = 300 \text{ K}$
$Z = 1$	Lump, gray
$F(000) = 197$	$0.14 \times 0.08 \times 0.07 \text{ mm}$

Data collection

Bruker D8 Venture Photon 100 CMOS diffractometer	47 independent reflections
phi and ω scans	47 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (<i>SADABS</i> ; Krause et al., 2015)	$R_{\text{int}} = 0.067$
$T_{\text{min}} = 0.171$, $T_{\text{max}} = 0.746$	$\theta_{\text{max}} = 24.8^\circ$, $\theta_{\text{min}} = 4.7^\circ$
1897 measured reflections	$h = -5 \rightarrow 5$
	$k = -5 \rightarrow 5$
	$l = -4 \rightarrow 4$

Refinement

Refinement on F^2	0 restraints
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.035P)^2 + 1.6892P]$
$R[F^2 > 2\sigma(F^2)] = 0.029$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.071$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.37$	$\Delta\rho_{\text{max}} = 1.19 \text{ e \AA}^{-3}$
47 reflections	$\Delta\rho_{\text{min}} = -1.07 \text{ e \AA}^{-3}$
9 parameters	

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2) for (242006_a)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
La1	0.000000	0.000000	0.000000	0.0061 (10)
Ni1	0.333333	0.666667	0.000000	0.0078 (12)
Ni2	0.500000	0.000000	0.500000	0.0063 (11)

Atomic displacement parameters (\AA^2) for (242006_a)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
La1	0.0041 (11)	0.0041 (11)	0.0100 (15)	0.0021 (6)	0.000	0.000
Ni1	0.0083 (15)	0.0083 (15)	0.007 (2)	0.0042 (7)	0.000	0.000
Ni2	0.0066 (14)	0.0034 (18)	0.0078 (16)	0.0017 (9)	0.000	0.000

Geometric parameters (\AA , $^\circ$) for (242006_a)

La1—Ni1 ⁱ	2.8953 (2)	Ni1—Ni2 ^{xii}	2.4589 (2)
La1—Ni1 ⁱⁱ	2.8953 (2)	Ni1—Ni2 ^{viii}	2.4589 (2)
La1—Ni1 ⁱⁱⁱ	2.8953 (2)	Ni1—Ni2 ^{xiii}	2.4589 (2)
La1—Ni1	2.8954 (2)	Ni1—Ni2 ^{vi}	2.4589 (2)
La1—Ni1 ^{iv}	2.8954 (2)	Ni1—Ni2 ^{xiv}	2.4589 (2)
La1—Ni1 ^v	2.8954 (2)	Ni1—Ni1 ⁱ	2.8953 (2)
La1—Ni2 ^{vi}	3.1996 (2)	Ni1—Ni1 ^{iv}	2.8954 (2)
La1—Ni2 ^{vii}	3.1996 (2)	Ni1—Ni1 ^{xv}	2.8954 (2)
La1—Ni2	3.1996 (2)	Ni2—Ni2 ^{xvi}	2.5075 (2)
La1—Ni2 ^{viii}	3.1996 (2)	Ni2—Ni2 ^{xvii}	2.5075 (2)
La1—Ni2 ^{ix}	3.1996 (2)	Ni2—Ni2 ^{vi}	2.5075 (2)
La1—Ni2 ^x	3.1996 (2)	Ni2—Ni2 ^{xviii}	2.5075 (2)
Ni1—Ni2 ^{xi}	2.4589 (2)		
Ni1 ⁱ —La1—Ni1 ⁱⁱ	120.0	Ni2 ^{xiv} —Ni1—La1 ^{xix}	72.880 (1)
Ni1 ⁱ —La1—Ni1 ⁱⁱⁱ	180.0	Ni1 ⁱ —Ni1—La1 ^{xix}	60.0
Ni1 ⁱⁱ —La1—Ni1 ⁱⁱⁱ	60.0	La1 ^{xii} —Ni1—La1 ^{xix}	120.0
Ni1 ⁱ —La1—Ni1	60.0	Ni2 ^{xi} —Ni1—La1	72.880 (1)
Ni1 ⁱⁱ —La1—Ni1	180.0	Ni2 ^{xii} —Ni1—La1	126.069 (4)
Ni1 ⁱⁱⁱ —La1—Ni1	120.0	Ni2 ^{viii} —Ni1—La1	72.880 (1)
Ni1 ⁱ —La1—Ni1 ^{iv}	120.0	Ni2 ^{xiii} —Ni1—La1	126.069 (4)
Ni1 ⁱⁱ —La1—Ni1 ^{iv}	120.0	Ni2 ^{vi} —Ni1—La1	72.880 (1)
Ni1 ⁱⁱⁱ —La1—Ni1 ^{iv}	60.0	Ni2 ^{xiv} —Ni1—La1	72.880 (2)
Ni1—La1—Ni1 ^{iv}	60.0	Ni1 ⁱ —Ni1—La1	60.0
Ni1 ⁱ —La1—Ni1 ^v	60.0	La1 ^{xii} —Ni1—La1	120.0
Ni1 ⁱⁱ —La1—Ni1 ^v	60.0	La1 ^{xix} —Ni1—La1	120.0
Ni1 ⁱⁱⁱ —La1—Ni1 ^v	120.0	Ni2 ^{xi} —Ni1—Ni1 ^{iv}	53.931 (4)
Ni1—La1—Ni1 ^v	120.0	Ni2 ^{xii} —Ni1—Ni1 ^{iv}	107.120 (1)
Ni1 ^{iv} —La1—Ni1 ^v	180.0	Ni2 ^{viii} —Ni1—Ni1 ^{iv}	53.931 (4)
Ni1 ⁱ —La1—Ni2 ^{vi}	47.259 (3)	Ni2 ^{xiii} —Ni1—Ni1 ^{iv}	107.120 (2)
Ni1 ⁱⁱ —La1—Ni2 ^{vi}	132.741 (3)	Ni2 ^{vi} —Ni1—Ni1 ^{iv}	107.120 (2)
Ni1 ⁱⁱⁱ —La1—Ni2 ^{vi}	132.741 (3)	Ni2 ^{xiv} —Ni1—Ni1 ^{iv}	107.120 (2)
Ni1—La1—Ni2 ^{vi}	47.260 (3)	Ni1 ⁱ —Ni1—Ni1 ^{iv}	120.0
Ni1 ^{iv} —La1—Ni2 ^{vi}	90.0	La1 ^{xii} —Ni1—Ni1 ^{iv}	60.0
Ni1 ^v —La1—Ni2 ^{vi}	90.0	La1 ^{xix} —Ni1—Ni1 ^{iv}	180.0
Ni1 ⁱ —La1—Ni2 ^{vii}	132.741 (3)	La1—Ni1—Ni1 ^{iv}	60.0
Ni1 ⁱⁱ —La1—Ni2 ^{vii}	47.259 (3)	Ni2 ^{xi} —Ni1—Ni1 ^{xv}	107.120 (1)
Ni1 ⁱⁱⁱ —La1—Ni2 ^{vii}	47.259 (3)	Ni2 ^{xii} —Ni1—Ni1 ^{xv}	53.931 (4)
Ni1—La1—Ni2 ^{vii}	132.740 (3)	Ni2 ^{viii} —Ni1—Ni1 ^{xv}	107.120 (2)
Ni1 ^{iv} —La1—Ni2 ^{vii}	90.0	Ni2 ^{xiii} —Ni1—Ni1 ^{xv}	53.931 (4)
Ni1 ^v —La1—Ni2 ^{vii}	90.0	Ni2 ^{vi} —Ni1—Ni1 ^{xv}	107.120 (1)
Ni2 ^{vi} —La1—Ni2 ^{vii}	180.0	Ni2 ^{xiv} —Ni1—Ni1 ^{xv}	107.120 (2)

Ni1 ⁱ —La1—Ni2	47.260 (3)	Ni1 ⁱ —Ni1—Ni1 ^{xv}	120.0
Ni1 ⁱⁱ —La1—Ni2	90.0	La1 ^{xii} —Ni1—Ni1 ^{xv}	60.0
Ni1 ⁱⁱⁱ —La1—Ni2	132.740 (4)	La1 ^{xix} —Ni1—Ni1 ^{xv}	60.0
Ni1—La1—Ni2	90.0	La1—Ni1—Ni1 ^{xv}	180.0
Ni1 ^{iv} —La1—Ni2	132.740 (3)	Ni1 ^{iv} —Ni1—Ni1 ^{xv}	120.0
Ni1 ^v —La1—Ni2	47.260 (3)	Ni1 ^{xx} —Ni2—Ni1 ^v	180.0
Ni2 ^{vi} —La1—Ni2	46.137 (3)	Ni1 ^{xx} —Ni2—Ni1 ⁱ	107.862 (8)
Ni2 ^{vii} —La1—Ni2	133.863 (3)	Ni1 ^v —Ni2—Ni1 ⁱ	72.138 (8)
Ni1 ⁱ —La1—Ni2 ^{viii}	90.0	Ni1 ^{xx} —Ni2—Ni1 ^{xxi}	72.138 (8)
Ni1 ⁱⁱ —La1—Ni2 ^{viii}	132.740 (4)	Ni1 ^v —Ni2—Ni1 ^{xxi}	107.862 (8)
Ni1 ⁱⁱⁱ —La1—Ni2 ^{viii}	90.0	Ni1 ⁱ —Ni2—Ni1 ^{xxi}	180.0
Ni1—La1—Ni2 ^{viii}	47.260 (4)	Ni1 ^{xx} —Ni2—Ni2 ^{xvi}	59.345 (3)
Ni1 ^{iv} —La1—Ni2 ^{viii}	47.260 (3)	Ni1 ^v —Ni2—Ni2 ^{xvi}	120.655 (3)
Ni1 ^v —La1—Ni2 ^{viii}	132.740 (3)	Ni1 ⁱ —Ni2—Ni2 ^{xvi}	59.345 (4)
Ni2 ^{vi} —La1—Ni2 ^{viii}	46.137 (3)	Ni1 ^{xxi} —Ni2—Ni2 ^{xvi}	120.655 (4)
Ni2 ^{vii} —La1—Ni2 ^{viii}	133.863 (3)	Ni1 ^{xx} —Ni2—Ni2 ^{xvii}	120.655 (3)
Ni2—La1—Ni2 ^{viii}	85.481 (6)	Ni1 ^v —Ni2—Ni2 ^{xvii}	59.345 (3)
Ni1 ⁱ —La1—Ni2 ^{ix}	132.740 (4)	Ni1 ⁱ —Ni2—Ni2 ^{xvii}	120.655 (4)
Ni1 ⁱⁱ —La1—Ni2 ^{ix}	90.0	Ni1 ^{xxi} —Ni2—Ni2 ^{xvii}	59.345 (4)
Ni1 ⁱⁱⁱ —La1—Ni2 ^{ix}	47.260 (3)	Ni2 ^{xvi} —Ni2—Ni2 ^{xvii}	180.0
Ni1—La1—Ni2 ^{ix}	90.0	Ni1 ^{xx} —Ni2—Ni2 ^{vi}	59.344 (4)
Ni1 ^{iv} —La1—Ni2 ^{ix}	47.260 (3)	Ni1 ^v —Ni2—Ni2 ^{vi}	120.656 (4)
Ni1 ^v —La1—Ni2 ^{ix}	132.740 (3)	Ni1 ⁱ —Ni2—Ni2 ^{vi}	59.344 (4)
Ni2 ^{vi} —La1—Ni2 ^{ix}	133.863 (3)	Ni1 ^{xxi} —Ni2—Ni2 ^{vi}	120.656 (4)
Ni2 ^{vii} —La1—Ni2 ^{ix}	46.137 (3)	Ni2 ^{xvi} —Ni2—Ni2 ^{vi}	60.0
Ni2—La1—Ni2 ^{ix}	180.0	Ni2 ^{xvii} —Ni2—Ni2 ^{vi}	120.0
Ni2 ^{viii} —La1—Ni2 ^{ix}	94.519 (6)	Ni1 ^{xx} —Ni2—Ni2 ^{xviii}	120.656 (4)
Ni1 ⁱ —La1—Ni2 ^x	90.0	Ni1 ^v —Ni2—Ni2 ^{xviii}	59.344 (4)
Ni1 ⁱⁱ —La1—Ni2 ^x	47.260 (3)	Ni1 ⁱ —Ni2—Ni2 ^{xviii}	120.656 (4)
Ni1 ⁱⁱⁱ —La1—Ni2 ^x	90.0	Ni1 ^{xxi} —Ni2—Ni2 ^{xviii}	59.344 (4)
Ni1—La1—Ni2 ^x	132.740 (4)	Ni2 ^{xvi} —Ni2—Ni2 ^{xviii}	120.0
Ni1 ^{iv} —La1—Ni2 ^x	132.740 (3)	Ni2 ^{xvii} —Ni2—Ni2 ^{xviii}	60.0
Ni1 ^v —La1—Ni2 ^x	47.260 (3)	Ni2 ^{vi} —Ni2—Ni2 ^{xviii}	180.0
Ni2 ^{vi} —La1—Ni2 ^x	133.863 (3)	Ni1 ^{xx} —Ni2—La1	120.139 (5)
Ni2 ^{vii} —La1—Ni2 ^x	46.137 (3)	Ni1 ^v —Ni2—La1	59.861 (5)
Ni2—La1—Ni2 ^x	94.519 (6)	Ni1 ⁱ —Ni2—La1	59.860 (5)
Ni2 ^{viii} —La1—Ni2 ^x	180.0	Ni1 ^{xxi} —Ni2—La1	120.140 (4)
Ni2 ^{ix} —La1—Ni2 ^x	85.481 (6)	Ni2 ^{xvi} —Ni2—La1	113.069 (1)
Ni2 ^{xi} —Ni1—Ni2 ^{xii}	145.760 (4)	Ni2 ^{xvii} —Ni2—La1	66.931 (1)
Ni2 ^{xi} —Ni1—Ni2 ^{viii}	107.863 (8)	Ni2 ^{vi} —Ni2—La1	66.931 (2)
Ni2 ^{xii} —Ni1—Ni2 ^{viii}	61.311 (7)	Ni2 ^{xviii} —Ni2—La1	113.069 (2)
Ni2 ^{xi} —Ni1—Ni2 ^{xiii}	61.311 (7)	Ni1 ^{xx} —Ni2—La1 ^{xxii}	59.861 (5)
Ni2 ^{xii} —Ni1—Ni2 ^{xiii}	107.863 (8)	Ni1 ^v —Ni2—La1 ^{xxii}	120.139 (5)
Ni2 ^{viii} —Ni1—Ni2 ^{xiii}	145.760 (4)	Ni1 ⁱ —Ni2—La1 ^{xxii}	120.140 (5)
Ni2 ^{xi} —Ni1—Ni2 ^{vi}	145.760 (4)	Ni1 ^{xxi} —Ni2—La1 ^{xxii}	59.860 (4)
Ni2 ^{xii} —Ni1—Ni2 ^{vi}	61.311 (7)	Ni2 ^{xvi} —Ni2—La1 ^{xxii}	66.931 (1)
Ni2 ^{viii} —Ni1—Ni2 ^{vi}	61.311 (7)	Ni2 ^{xvii} —Ni2—La1 ^{xxii}	113.069 (1)
Ni2 ^{xiii} —Ni1—Ni2 ^{vi}	145.760 (4)	Ni2 ^{vi} —Ni2—La1 ^{xxii}	113.069 (2)
Ni2 ^{xi} —Ni1—Ni2 ^{xiv}	61.311 (7)	Ni2 ^{xviii} —Ni2—La1 ^{xxii}	66.931 (1)
Ni2 ^{xii} —Ni1—Ni2 ^{xiv}	145.760 (4)	La1—Ni2—La1 ^{xxii}	180.0
Ni2 ^{viii} —Ni1—Ni2 ^{xiv}	145.760 (4)	Ni1 ^{xx} —Ni2—La1 ^{xxiii}	59.860 (4)

Ni2 ^{xiii} —Ni1—Ni2 ^{xiv}	61.311 (7)	Ni1 ^v —Ni2—La1 ^{xxiii}	120.140 (4)
Ni2 ^{vi} —Ni1—Ni2 ^{xiv}	107.863 (8)	Ni1 ⁱ —Ni2—La1 ^{xxiii}	120.139 (5)
Ni2 ^{xi} —Ni1—Ni1 ⁱ	107.120 (2)	Ni1 ^{xxi} —Ni2—La1 ^{xxiii}	59.861 (5)
Ni2 ^{xii} —Ni1—Ni1 ⁱ	107.120 (2)	Ni2 ^{xvi} —Ni2—La1 ^{xxiii}	113.069 (1)
Ni2 ^{viii} —Ni1—Ni1 ⁱ	107.120 (2)	Ni2 ^{xvii} —Ni2—La1 ^{xxiii}	66.931 (1)
Ni2 ^{xiii} —Ni1—Ni1 ⁱ	107.120 (2)	Ni2 ^{vi} —Ni2—La1 ^{xxiii}	66.931 (1)
Ni2 ^{vi} —Ni1—Ni1 ⁱ	53.931 (4)	Ni2 ^{xviii} —Ni2—La1 ^{xxiii}	113.069 (1)
Ni2 ^{xiv} —Ni1—Ni1 ⁱ	53.931 (4)	La1—Ni2—La1 ^{xxiii}	76.805 (8)
Ni2 ^{xi} —Ni1—La1 ^{xii}	72.880 (2)	La1 ^{xxii} —Ni2—La1 ^{xxiii}	103.195 (8)
Ni2 ^{xii} —Ni1—La1 ^{xii}	72.880 (1)	Ni1 ^{xx} —Ni2—La1 ^{xxiv}	120.140 (5)
Ni2 ^{viii} —Ni1—La1 ^{xii}	72.880 (2)	Ni1 ^v —Ni2—La1 ^{xxiv}	59.860 (4)
Ni2 ^{xiii} —Ni1—La1 ^{xii}	72.880 (2)	Ni1 ⁱ —Ni2—La1 ^{xxiv}	59.861 (5)
Ni2 ^{vi} —Ni1—La1 ^{xii}	126.069 (4)	Ni1 ^{xxi} —Ni2—La1 ^{xxiv}	120.139 (5)
Ni2 ^{xiv} —Ni1—La1 ^{xii}	126.069 (4)	Ni2 ^{xvi} —Ni2—La1 ^{xxiv}	66.931 (2)
Ni1 ⁱ —Ni1—La1 ^{xii}	180.0	Ni2 ^{xvii} —Ni2—La1 ^{xxiv}	113.069 (1)
Ni2 ^{xi} —Ni1—La1 ^{xix}	126.069 (4)	Ni2 ^{vi} —Ni2—La1 ^{xxiv}	113.069 (1)
Ni2 ^{xii} —Ni1—La1 ^{xix}	72.880 (1)	Ni2 ^{xviii} —Ni2—La1 ^{xxiv}	66.931 (1)
Ni2 ^{viii} —Ni1—La1 ^{xix}	126.069 (4)	La1—Ni2—La1 ^{xxiv}	103.195 (8)
Ni2 ^{xiii} —Ni1—La1 ^{xix}	72.880 (1)	La1 ^{xxii} —Ni2—La1 ^{xxiv}	76.805 (8)
Ni2 ^{vi} —Ni1—La1 ^{xix}	72.880 (2)	La1 ^{xxiii} —Ni2—La1 ^{xxiv}	180.0

Symmetry codes: (i) $-x+1, -y+1, -z$; (ii) $-x, -y, -z$; (iii) $x-1, y-1, z$; (iv) $-x, -y+1, -z$; (v) $x, y-1, z$; (vi) $-x+y+1, -x+1, z$; (vii) $-x+y, -x, z-1$; (viii) $-y, x-y, z$; (ix) $x-1, y, z-1$; (x) $-y, x-y-1, z-1$; (xi) $-y, x-y, z-1$; (xii) $x, y+1, z$; (xiii) $x, y+1, z-1$; (xiv) $-x+y+1, -x+1, z-1$; (xv) $-x+1, -y+2, -z$; (xvi) $-y+1, x-y, z$; (xvii) $-y, x-y-1, z$; (xviii) $-x+y+1, -x, z$; (xix) $x+1, y+1, z$; (xx) $-x+1, -y+1, -z+1$; (xxi) $x, y-1, z+1$; (xxii) $x+1, y, z+1$; (xxiii) $x, y, z+1$; (xxiv) $x+1, y, z$.