Abstract

Table 1

Experimental details

Crystal data	
Chemical formula	La_2Ni_2
M_r	395.24
Crystal system, space group	Orthorhombic, *Cmcm*
Temperature (K)	300
a, *b*, *c* (Å)	3.9014 (4), 10.7782 (12), 4.3854 (5)
V (Å^3)	184.41 (3)
Z	2
Radiation type	Mo *K*α
μ (mm^{-1})	32.47
Crystal size (mm)	0.10 × 0.08 × 0.02
Data collection	
Diffractometer	Bruker D8 Venture Photon 100 CMOS
Absorption correction	Multi-scan (*SADABS*; Krause et al., 2015)
T_{min}, T_{max}	0.314, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	2438, 109, 104
R_{int}	0.066
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.594
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.015, 0.033, 1.24
No. of reflections	109
No. of parameters	9
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.57, −1.06

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

References

NOT FOUND

full crystallographic data

Computing details

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

(240929_a)

Crystal data

La_2Ni_2
M_r = 395.24
Orthorhombic, *Cmcm*
a = 3.9014 (4) Å
b = 10.7782 (12) Å
c = 4.3854 (5) Å
V = 184.41 (3) Å^3
Z = 2
F(000) = 340
D_x = 7.118 Mg m^{-3}
Mo *K*α radiation, λ = 0.71073 Å
Cell parameters from 1883 reflections
θ = 3.8–27.5°
μ = 32.47 mm^{-1}
T = 300 K
Lump, gray
0.10 × 0.08 × 0.02 mm

Data collection

Bruker D8 Venture Photon 100 CMOS diffractometer
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Krause et al., 2015)
T_{min} = 0.314, T_{max} = 0.746
2438 measured reflections
109 independent reflections
104 reflections with $I > 2\sigma(I)$
R_{int} = 0.066
θ_{max} = 25.0°, θ_{min} = 3.8°
h = −4→4
k = −12→12
l = −5→5

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.015
$wR(F^2)$ = 0.033
S = 1.24
109 reflections
9 parameters
0 restraints
$w = 1/[\sigma^2(F_o^2) + (0.0072P)^2 + 1.5679P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ < 0.001
$\Delta\rho_{max}$ = 0.57 e Å^{-3}
$\Delta\rho_{min}$ = −1.06 e Å^{-3}

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 (Å^2) for (240929_a)

	x	*y*	*z*	U_{iso}*/U_{eq}
La1	0.000000	0.13715 (5)	0.250000	0.0116 (2)
Ni1	0.000000	0.42884 (13)	0.250000	0.0173 (4)

Atomic displacement parameters (Å^2) for (240929_a)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
La1	0.0106 (3)	0.0126 (3)	0.0116 (3)	0.000	0.000	0.000
Ni1	0.0178 (7)	0.0203 (8)	0.0139 (7)	0.000	0.000	0.000

Geometric parameters (Å, º) for (240929_a)

La1—Ni1^{i}	2.9743 (11)	La1—La1^{vii}	3.6808 (10)
La1—Ni1^{ii}	2.9743 (11)	La1—La1^{viii}	3.6808 (10)
La1—Ni1^{iii}	3.0198 (4)	La1—La1^{iv}	3.8120 (8)
La1—Ni1^{iv}	3.0198 (4)	La1—La1^{vi}	3.8120 (8)
La1—Ni1^{v}	3.0198 (4)	La1—La1^{v}	3.8120 (8)
La1—Ni1^{vi}	3.0198 (4)	Ni1—Ni1^{ix}	2.6761 (16)
La1—Ni1	3.1439 (15)	Ni1—Ni1^{x}	2.6761 (16)
Ni1^{i}—La1—Ni1^{ii}	81.97 (4)	Ni1—La1—La1^{vi}	50.344 (14)
Ni1^{i}—La1—Ni1^{iii}	53.03 (3)	La1^{vii}—La1—La1^{vi}	148.786 (11)
Ni1^{ii}—La1—Ni1^{iii}	104.235 (19)	La1^{viii}—La1—La1^{vi}	99.783 (9)
Ni1^{i}—La1—Ni1^{iv}	104.235 (19)	La1^{iv}—La1—La1^{vi}	61.558 (15)
Ni1^{ii}—La1—Ni1^{iv}	53.03 (3)	Ni1^{i}—La1—La1^{v}	144.822 (8)
Ni1^{iii}—La1—Ni1^{iv}	152.76 (6)	Ni1^{ii}—La1—La1^{v}	98.403 (17)
Ni1^{i}—La1—Ni1^{v}	104.235 (19)	Ni1^{iii}—La1—La1^{v}	93.623 (18)
Ni1^{ii}—La1—Ni1^{v}	53.03 (3)	Ni1^{iv}—La1—La1^{v}	103.733 (18)
Ni1^{iii}—La1—Ni1^{v}	80.478 (14)	Ni1^{v}—La1—La1^{v}	53.28 (3)
Ni1^{iv}—La1—Ni1^{v}	93.124 (17)	Ni1^{vi}—La1—La1^{v}	153.97 (4)
Ni1^{i}—La1—Ni1^{vi}	53.03 (3)	Ni1—La1—La1^{v}	50.344 (14)
Ni1^{ii}—La1—Ni1^{vi}	104.235 (19)	La1^{vii}—La1—La1^{v}	99.783 (9)
Ni1^{iii}—La1—Ni1^{vi}	93.124 (17)	La1^{viii}—La1—La1^{v}	148.786 (11)
Ni1^{iv}—La1—Ni1^{vi}	80.478 (14)	La1^{iv}—La1—La1^{v}	70.229 (17)
Ni1^{v}—La1—Ni1^{vi}	152.76 (6)	La1^{vi}—La1—La1^{v}	100.69 (3)
Ni1^{i}—La1—Ni1	139.015 (19)	Ni1^{ix}—Ni1—Ni1^{x}	110.04 (10)
Ni1^{ii}—La1—Ni1	139.015 (19)	Ni1^{ix}—Ni1—La1^{xi}	64.36 (4)
Ni1^{iii}—La1—Ni1	103.62 (3)	Ni1^{x}—Ni1—La1^{xi}	64.36 (4)
Ni1^{iv}—La1—Ni1	103.62 (3)	Ni1^{ix}—Ni1—La1^{xii}	64.36 (4)
Ni1^{v}—La1—Ni1	103.62 (3)	Ni1^{x}—Ni1—La1^{xii}	64.36 (4)
Ni1^{vi}—La1—Ni1	103.62 (3)	La1^{xi}—Ni1—La1^{xii}	81.97 (4)
Ni1^{i}—La1—La1^{vii}	52.676 (16)	Ni1^{ix}—Ni1—La1^{iii}	136.88 (3)
Ni1^{ii}—La1—La1^{vii}	52.676 (16)	Ni1^{x}—Ni1—La1^{iii}	62.615 (16)
Ni1^{iii}—La1—La1^{vii}	51.56 (2)	La1^{xi}—Ni1—La1^{iii}	126.97 (3)
Ni1^{iv}—La1—La1^{vii}	104.09 (3)	La1^{xii}—Ni1—La1^{iii}	75.765 (19)
Ni1^{v}—La1—La1^{vii}	51.56 (2)	Ni1^{ix}—Ni1—La1^{iv}	62.615 (16)
Ni1^{vi}—La1—La1^{vii}	104.09 (3)	Ni1^{x}—Ni1—La1^{iv}	136.88 (3)
Ni1—La1—La1^{vii}	143.436 (12)	La1^{xi}—Ni1—La1^{iv}	75.765 (19)
Ni1^{i}—La1—La1^{viii}	52.676 (16)	La1^{xii}—Ni1—La1^{iv}	126.97 (3)
Ni1^{ii}—La1—La1^{viii}	52.676 (16)	La1^{iii}—Ni1—La1^{iv}	152.76 (6)
Ni1^{iii}—La1—La1^{viii}	104.09 (3)	Ni1^{ix}—Ni1—La1^{v}	136.88 (3)
Ni1^{iv}—La1—La1^{viii}	51.56 (2)	Ni1^{x}—Ni1—La1^{v}	62.615 (16)
Ni1^{v}—La1—La1^{viii}	104.09 (3)	La1^{xi}—Ni1—La1^{v}	75.765 (19)
Ni1^{vi}—La1—La1^{viii}	51.56 (2)	La1^{xii}—Ni1—La1^{v}	126.97 (3)
Ni1—La1—La1^{viii}	143.436 (12)	La1^{iii}—Ni1—La1^{v}	80.478 (14)

$La1^{vii}—La1—La1^{viii}$	73.13 (2)	$La1^{iv}—Ni1—La1^{v}$	93.124 (17)
$Ni1^{i}—La1—La1^{iv}$	144.822 (8)	$Ni1^{ix}—Ni1—La1^{vi}$	62.615 (16)
$Ni1^{ii}—La1—La1^{iv}$	98.403 (17)	$Ni1^{x}—Ni1—La1^{vi}$	136.88 (3)
$Ni1^{iii}—La1—La1^{iv}$	153.97 (4)	$La1^{xi}—Ni1—La1^{vi}$	126.97 (3)
$Ni1^{iv}—La1—La1^{iv}$	53.28 (3)	$La1^{xii}—Ni1—La1^{vi}$	75.765 (19)
$Ni1^{v}—La1—La1^{iv}$	103.733 (18)	$La1^{iii}—Ni1—La1^{vi}$	93.124 (17)
$Ni1^{vi}—La1—La1^{iv}$	93.623 (18)	$La1^{iv}—Ni1—La1^{vi}$	80.478 (14)
$Ni1—La1—La1^{iv}$	50.344 (14)	$La1^{v}—Ni1—La1^{vi}$	152.76 (6)
$La1^{vii}—La1—La1^{iv}$	148.786 (11)	$Ni1^{ix}—Ni1—La1$	124.98 (5)
$La1^{viii}—La1—La1^{iv}$	99.783 (9)	$Ni1^{x}—Ni1—La1$	124.98 (5)
$Ni1^{i}—La1—La1^{vi}$	98.403 (17)	$La1^{xi}—Ni1—La1$	139.015 (19)
$Ni1^{ii}—La1—La1^{vi}$	144.822 (8)	$La1^{xii}—Ni1—La1$	139.015 (19)
$Ni1^{iii}—La1—La1^{vi}$	103.733 (18)	$La1^{iii}—Ni1—La1$	76.38 (3)
$Ni1^{iv}—La1—La1^{vi}$	93.623 (18)	$La1^{iv}—Ni1—La1$	76.38 (3)
$Ni1^{v}—La1—La1^{vi}$	153.97 (4)	$La1^{v}—Ni1—La1$	76.38 (3)
$Ni1^{vi}—La1—La1^{vi}$	53.28 (3)	$La1^{vi}—Ni1—La1$	76.38 (3)

Symmetry codes: (i) *x*−1/2, *y*−1/2, *z*; (ii) *x*+1/2, *y*−1/2, *z*; (iii) −*x*−1/2, −*y*+1/2, −*z*; (iv) −*x*+1/2, −*y*+1/2, −*z*+1; (v) −*x*+1/2, −*y*+1/2, −*z*; (vi) −*x*−1/2, −*y*+1/2, −*z*+1; (vii) −*x*, −*y*, −*z*; (viii) −*x*, −*y*, −*z*+1; (ix) −*x*, −*y*+1, −*z*+1; (x) −*x*, −*y*+1, −*z*; (xi) *x*+1/2, *y*+1/2, *z*; (xii) *x*−1/2, *y*+1/2, *z*.