Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Redetermination of dysprosium trinickel from single-crystal X-ray data

Volodymyr Levytskyy,[a]* Volodymyr Babizhetskyy,[a] Bohdan Kotur[a] and Volodymyr Smetana[b]

[a]Department of Inorganic Chemistry, Ivan Franko National University of Lviv, Kyryla & Mefodiya street 6, 79005 Lviv, Ukraine, and [b]344 Spedding Hall, Ames Laboratory, Ames, IA 50011-3020, USA
Correspondence e-mail: v.levyckyy@gmail.com

Received 28 September 2012; accepted 22 October 2012

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(Dy–Ni) = 0.002 Å; R factor = 0.022; wR factor = 0.043; data-to-parameter ratio = 11.6.

The crystal structure of the title compound, $DyNi_3$, was redetermined from single-crystal X-ray diffraction data. In comparison with previous studies based on powder X-ray diffraction data [Lemaire & Paccard (1969). *Bull. Soc. Fr. Minéral. Cristallogr.* **92**, 9–16; Tsai *et al.* (1974). *J. Appl. Phys.* **45**, 3582–3586], the present redetermination revealed refined coordinates and anisotropic displacement parameters for all atoms. The crystal structure of $DyNi_3$ adopts the $PuNi_3$ structure type and can be derived from the $CaCu_5$ structure type as an intergrowth structure. The asymmetric unit contains two Dy sites (site symmetries $3m$ and $\overline{3}m$) and three Ni sites (m, $3m$ and $\overline{3}m$). The two different coordination polyhedra of Dy are a Frank–Kasper polyhedron formed by four Dy and 12 Ni atoms and a pseudo-Frank–Kasper polyhedron formed by two Dy and 18 Ni atoms. The three different coordination polyhedra of Ni are Frank–Kasper icosahedra formed by five Dy and seven Ni atoms, three Dy and nine Ni atoms, and six Dy and six Ni atoms.

Related literature

For the $PuNi_3$ structure type, see: Cromer & Olsen (1959). For previous powder diffraction studies of the title compoud, see: Paccard & Pauthenet (1967); Lemaire & Paccard (1969); Virkar & Raman (1969); Buschow & van der Goot (1970); Yakinthos & Paccard (1972); Tsai *et al.* (1974). For related compounds, see: Virkar & Raman (1969); Buschow & van der Goot (1970); Levytskyy *et al.* (2012). For the $CaCu_5$ structure type, see: Haucke (1940); Nowotny (1942). For the $MgCu_2$ structure type, see: Friauf (1927); Ohba *et al.* (1984). For intergrowth structures, see: Parthé *et al.* (1985); Grin (1992).

Experimental

Crystal data

$DyNi_3$
M_r = 338.63
Trigonal, $R\overline{3}m$
a = 4.966 (2) Å
c = 24.37 (1) Å
V = 520.5 (4) Å^3
Z = 9
Mo $K\alpha$ radiation
μ = 55.52 mm^{-1}
T = 293 K
0.13 × 0.08 × 0.06 mm

Data collection

Stoe IPDS II diffractometer
Absorption correction: multi-scan (*PLATON*, Spek, 2009)
T_{min} = 0.071, T_{max} = 0.182
1516 measured reflections
197 independent reflections
163 reflections with $I > 2\sigma(I)$
R_{int} = 0.058

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.022
$wR(F^2)$ = 0.043
S = 1.01
197 reflections
17 parameters
$\Delta\rho_{max}$ = 2.77 e Å^{-3}
$\Delta\rho_{min}$ = −1.33 e Å^{-3}

Data collection: *X-AREA* (Stoe & Cie, 2009); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SIR2011* (Burla *et al.*, 2012); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008) and *WinGX* (Farrugia, 1999); molecular graphics: *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2688).

References

Brandenburg, K. (2006). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Burla, M. C., Caliandro, R., Camalli, M., Carrozzini, B., Cascarano, G. L., Giacovazzo, C., Mallamo, M., Mazzone, A., Polidori, G. & Spagna, R. (2012). *J. Appl. Cryst.* **45**, 357–361.
Buschow, K. H. J. & van der Goot, A. S. (1970). *J. Less Common Met.* **22**, 419–428.
Cromer, D. T. & Olsen, C. E. (1959). *Acta Cryst.* **12**, 689–694.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Friauf, J. B. (1927). *J. Am. Chem. Soc.* **49**, 3107–3114.
Grin, Yu. (1992). *Modern Perspectives in Inorganic Crystal Chemistry*, edited by E. Parthé, pp. 77–95. Dordrecht: Kluwer Academic Publishers.
Haucke, W. (1940). *Z. Anorg. Allg. Chem.* **244**, 17–22.
Lemaire, R. & Paccard, D. (1969). *Bull. Soc. Fr. Minéral. Cristallogr.* **92**, 9–16.
Levytskyy, V., Babizhetskyy, V., Kotur, B. & Smetana, V. (2012). *Acta Cryst.* E**68**, i20.
Nowotny, H. (1942). *Z. Metallkd.* **34**, 247–253.
Ohba, T., Kitano, Y. & Komura, Y. (1984). *Acta Cryst.* C**40**, 1–5.
Paccard, D. & Pauthenet, R. (1967). *Compt. Rend. Sci. Ser. B.* **264**, 1056–1059.
Parthé, E., Chabot, B. A. & Censual, K. (1985). *Chimia*, **39**, 164–174.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Stoe & Cie. (2009). *X-AREA*. Stoe & Cie, Darmstadt, Germany.
Tsai, S. C., Narasimhan, K. S. V. L., Kemesh, C. J. & Butera, R. A. (1974). *J. Appl. Phys.* **45**, 3582–3586.
Virkar, A. V. & Raman, A. (1969). *J. Less Common Met.* **18**, 59–66.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.
Yakinthos, J. & Paccard, D. (1972). *Solid State Commun.* **10**, 989–993.

supporting information

Acta Cryst. (2012). E**68**, i83 [doi:10.1107/S1600536812043747]

Redetermination of dysprosium trinickel from single-crystal X-ray data

Volodymyr Levytskyy, Volodymyr Babizhetskyy, Bohdan Kotur and Volodymyr Smetana

S1. Comment

The existence of the intermetallic phase with composition $DyNi_3$ has been long known before. The first structure report (Paccard & Pauthenet, 1967) of the title compound revealed isotypism with the $PuNi_3$ structure type (Cromer & Olsen, 1959). Lattice parameters were determined from X-ray powder diffraction data without specifying atomic coordinates (Paccard & Pauthenet, 1967; Lemaire & Paccard, 1969; Virkar & Raman, 1969; Buschow & van der Goot, 1970; Tsai *et al.*, 1974). Yakinthos & Paccard (1972) reported crystal structure data for RNi_3 compounds (R = Pr, Nd, Tb, Dy, Tm) from powder neutron diffraction data.

The present work contains the results of the full single-crystal X-ray determination of $DyNi_3$, including refinement of the atomic coordinates and the temperature factors for all atoms. These results confirm the belonging to the $PuNi_3$ structure type in space group $R\overline{3}m$. A view of the crystal structure of $DyNi_3$ is shown in Fig. 1. As has been noted previously (Yakinthos & Paccard, 1972), the crystal structure of $DyNi_3$ can be derived from the $CaCu_5$ structure type (Haucke, 1940; Nowotny, 1942). It consists of stacks of RX_5 blocks ($CaCu_5$-type) and R_2X_4 blocks ($MgCu_2$-type (Friauf, 1927; Ohba *et al.*, 1984)). Both types have the same Kagome net of Ni atoms that allows a combination of both structural motifs along the 3-fold inversion axis. As a result, it can be considered as an intergrowth structure: $R_2X_4 + RX_5 = 3RX_3$ (Parthé *et al.*, 1985; Grin, 1992).

In Fig. 2 the projection of the unit cell on the *ab* plane and the resulting coordination polyhedra for all atom types are shown. The coordination number for the Dy1 atom (Wyckoff site 6*c*, site symmetry 3*m*). The coordination polyhedron for this atom is a Frank-Kasper polyhedron formed by 4 Dy and 12 Ni atoms. The coordination number for the Dy2 atom (Wyckoff site 3*a*, site symmetry $\overline{3}m$) is 20. The coordination polyhedron of Dy2 is a pseudo-Frank-Kasper polyhedron formed by 2 Dy and 18 Ni atoms. Although the site symmetries for all Ni atoms are different, the coordination number for all Ni atoms is 12, with Frank-Kasper icosahedra as coordination polyhedra. The Ni1 atom (Wyckoff site 18*h*, site symmetry .*m*) is surrounded by 5 Dy atoms and 7 Ni atoms. The Ni2 atom (Wyckoff site 6*c*, site symmetry 3*m*) is surrounded by 3 Dy atoms and 9 Ni atoms. The Ni3 atom (Wyckoff site 3*b*, site symmetry $\overline{3}m$) is surrounded by 6 Dy atoms and 6 Ni atoms.

The interatomic distances in $DyNi_3$ are similar than those in Di_2Ni_7 (Levytskyy *et al.*, 2012).

S2. Experimental

The sample was prepared of the powdered commercially available pure elements: sublimed bulk pieces of dysprosium metal with a claimed purity of 99.99 at.% (Alfa Aesar, Johnson Matthey) and electrolytic nickel (99.99% pure) piece (Aldrich). A mixture of the powders was compacted in stainless steel dies. The pellet was arc-melted under an argon atmosphere on a water-cooled copper hearth. The alloy button (~1 g) was turned over and remolten three times to improve homogeneity. Subsequently, the sample was annealed in an evacuated silica tube under an argon atmosphere for four weeks at 1070 K. Shiny grey irregular-shaped crystals were isolated mechanically with a help of microscope by crushing the sample.

S3. Refinement

The atomic positions found from the direct methods structure solution were in good agreement with those from the $PuNi_3$ structure type and were used as starting parameters for the structure refinement. The highest Fourier difference peak of 2.77 e Å^{-3} is at (0 0 0.1019) and 0.91 Å away from the Dy1 atom. The deepest hole of -1.33 e Å^{-3} is at (0.8263 0.9132 0.0194) and 0.88 Å away from the Dy2 atom.

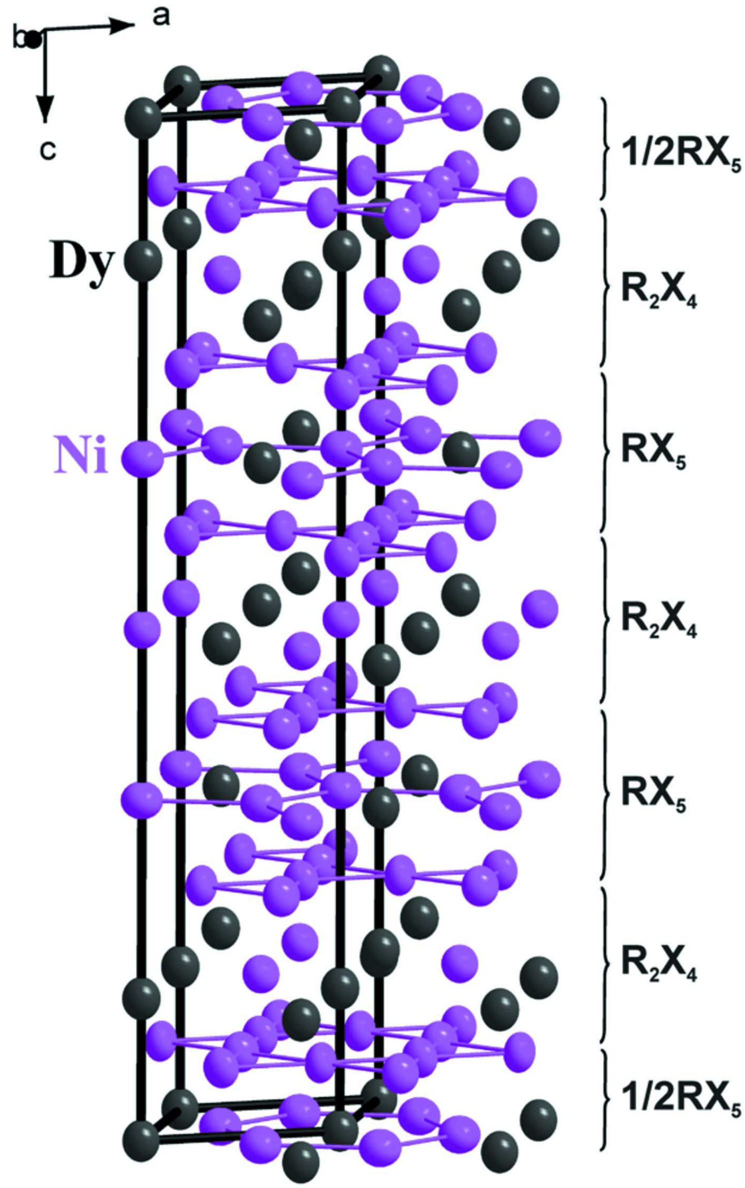

Figure 1

Perspective view of the crystal structure of $DyNi_3$. The unit cell and the blocks of RX_5 and R_2X_4 are emphasized. Atoms are represented by their anisotropic displacement ellipsoids at the 99.9% probability level

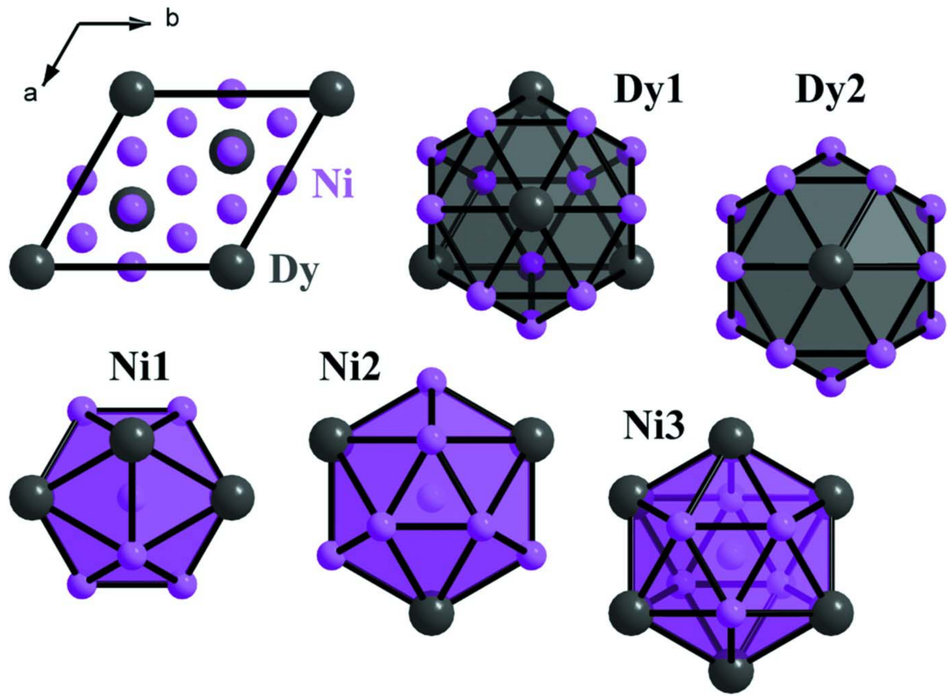

Figure 2

The *ab* projection of the unit cell and coordination polyhedra for all types of atoms in the $DyNi_3$ structure

Disprosium trinickel

Crystal data

$DyNi_3$
M_r = 338.63
Trigonal, $R\overline{3}m$
Hall symbol: -R 3 2"
a = 4.966 (2) Å
c = 24.37 (1) Å
V = 520.5 (4) Å^3
Z = 9
F(000) = 1350
D_x = 9.723 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71069 Å
Cell parameters from 1064 reflections
θ = 0.8–28.4°
μ = 55.52 mm^{-1}
T = 293 K
Irregular, grey
0.13 × 0.08 × 0.06 mm

Data collection

Stoe IPDS II diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*PLATON*, Spek, 2009)
T_{min} = 0.071, T_{max} = 0.182
1516 measured reflections
197 independent reflections
163 reflections with $I > 2\sigma(I)$
R_{int} = 0.058
θ_{max} = 28.4°, θ_{min} = 2.5°
h = −6→6
k = −6→6
l = −32→30

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.022
$wR(F^2)$ = 0.043
S = 1.01
197 reflections
17 parameters
0 restraints

Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
$w = 1/[\sigma^2(F_o^2) + (0.0207P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 2.77$ e Å^{-3}
$\Delta\rho_{min} = -1.33$ e Å^{-3}

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	y	z	U_{iso}*/U_{eq}
Ni1	0.50038 (13)	0.49962 (13)	0.08188 (5)	0.0116 (3)
Dy1	0.0000	0.0000	0.13920 (4)	0.0135 (2)
Ni2	0.0000	0.0000	0.33306 (9)	0.0143 (5)
Ni3	0.0000	0.0000	0.5000	0.0118 (7)
Dy2	0.0000	0.0000	0.0000	0.0128 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0112 (5)	0.0112 (5)	0.0141 (7)	0.0069 (6)	0.0003 (3)	−0.0003 (3)
Dy1	0.0125 (3)	0.0125 (3)	0.0157 (5)	0.00623 (15)	0.000	0.000
Ni2	0.0153 (7)	0.0153 (7)	0.0123 (12)	0.0077 (4)	0.000	0.000
Ni3	0.0115 (10)	0.0115 (10)	0.0124 (17)	0.0057 (5)	0.000	0.000
Dy2	0.0117 (4)	0.0117 (4)	0.0151 (6)	0.00584 (19)	0.000	0.000

Geometric parameters (Å, º)

Ni1—Ni2^{i}	2.450 (2)	Ni2—Dy2^{xviii}	2.8671 (12)
Ni1—Ni2^{ii}	2.464 (2)	Ni2—Dy2^{xv}	2.8671 (12)
Ni1—Ni1^{iii}	2.477 (2)	Ni2—Ni2^{xix}	2.8671 (12)
Ni1—Ni1^{iv}	2.477 (2)	Ni2—Ni2^{xx}	2.8671 (12)
Ni1—Ni1^{v}	2.489 (2)	Ni2—Dy2^{xxi}	2.8672 (12)
Ni1—Ni1^{vi}	2.489 (2)	Ni2—Ni2^{xxii}	2.8672 (12)
Ni1—Ni3^{ii}	2.5166 (14)	Ni3—Ni1^{xx}	2.5166 (14)
Ni1—Dy1^{vii}	2.8489 (11)	Ni3—Ni1^{xv}	2.5166 (14)
Ni1—Dy1	2.8489 (11)	Ni3—Ni1^{xxiii}	2.5166 (14)
Ni1—Dy1^{i}	3.0869 (18)	Ni3—Ni1^{xvii}	2.5166 (14)
Ni1—Dy2	3.1855 (12)	Ni3—Ni1^{xxiv}	2.5166 (14)
Ni1—Dy2^{vii}	3.1855 (12)	Ni3—Ni1^{xvi}	2.5166 (14)
Dy1—Ni1^{viii}	2.8489 (11)	Ni3—Dy1^{xx}	2.9442 (11)
Dy1—Ni1^{ix}	2.8489 (11)	Ni3—Dy1^{xv}	2.9442 (11)

Dy1—Ni1^{x}	2.8489 (11)	Ni3—Dy1^{xix}	2.9442 (11)
Dy1—Ni1^{vi}	2.8489 (11)	Ni3—Dy1^{xviii}	2.9442 (11)
Dy1—Ni1^{iv}	2.8489 (11)	Ni3—Dy1^{xxii}	2.9442 (11)
Dy1—Ni3^{ii}	2.9442 (11)	Ni3—Dy1^{xxi}	2.9442 (11)
Dy1—Ni3^{xi}	2.9442 (11)	Dy2—Ni2^{i}	2.8671 (12)
Dy1—Ni3^{xii}	2.9442 (11)	Dy2—Ni2^{xxv}	2.8671 (12)
Dy1—Ni1^{i}	3.0869 (18)	Dy2—Ni2^{ii}	2.8671 (12)
Dy1—Ni1^{xiii}	3.0869 (18)	Dy2—Ni2^{xi}	2.8671 (12)
Dy1—Ni1^{xiv}	3.0869 (18)	Dy2—Ni2^{xxvi}	2.8672 (12)
Ni2—Ni1^{i}	2.450 (2)	Dy2—Ni2^{xii}	2.8672 (12)
Ni2—Ni1^{xiv}	2.450 (2)	Dy2—Ni1^{xxvii}	3.1855 (12)
Ni2—Ni1^{xiii}	2.450 (2)	Dy2—Ni1^{vi}	3.1855 (12)
Ni2—Ni1^{xv}	2.464 (2)	Dy2—Ni1^{iv}	3.1855 (12)
Ni2—Ni1^{xvi}	2.464 (2)	Dy2—Ni1^{xxviii}	3.1855 (12)
Ni2—Ni1^{xvii}	2.464 (2)	Dy2—Ni1^{viii}	3.1855 (12)

Ni2^{i}—Ni1—Ni2^{ii}	71.39 (4)	Ni1^{xvii}—Ni2—Ni2^{xix}	54.07 (7)
Ni2^{i}—Ni1—Ni1^{iii}	59.63 (4)	Dy2^{xviii}—Ni2—Ni2^{xix}	179.60 (14)
Ni2^{ii}—Ni1—Ni1^{iii}	120.32 (4)	Dy2^{xv}—Ni2—Ni2^{xix}	60.0
Ni2^{i}—Ni1—Ni1^{iv}	59.63 (4)	Ni1^{i}—Ni2—Ni2^{xx}	107.20 (9)
Ni2^{ii}—Ni1—Ni1^{iv}	120.32 (4)	Ni1^{xiv}—Ni2—Ni2^{xx}	107.20 (9)
Ni1^{iii}—Ni1—Ni1^{iv}	60.0	Ni1^{xiii}—Ni2—Ni2^{xx}	54.54 (7)
Ni2^{i}—Ni1—Ni1^{v}	120.37 (4)	Ni1^{xv}—Ni2—Ni2^{xx}	106.72 (9)
Ni2^{ii}—Ni1—Ni1^{v}	59.68 (4)	Ni1^{xvi}—Ni2—Ni2^{xx}	54.07 (7)
Ni1^{iii}—Ni1—Ni1^{v}	120.0	Ni1^{xvii}—Ni2—Ni2^{xx}	106.72 (9)
Ni1^{iv}—Ni1—Ni1^{v}	180.0	Dy2^{xviii}—Ni2—Ni2^{xx}	60.0
Ni2^{i}—Ni1—Ni1^{vi}	120.37 (4)	Dy2^{xv}—Ni2—Ni2^{xx}	179.60 (14)
Ni2^{ii}—Ni1—Ni1^{vi}	59.68 (4)	Ni2^{xix}—Ni2—Ni2^{xx}	119.999 (2)
Ni1^{iii}—Ni1—Ni1^{vi}	180.00 (5)	Ni1^{i}—Ni2—Dy2^{xxi}	125.86 (8)
Ni1^{iv}—Ni1—Ni1^{vi}	120.0	Ni1^{xiv}—Ni2—Dy2^{xxi}	73.14 (3)
Ni1^{v}—Ni1—Ni1^{vi}	60.0	Ni1^{xiii}—Ni2—Dy2^{xxi}	73.14 (3)
Ni2^{i}—Ni1—Ni3^{ii}	179.09 (6)	Ni1^{xv}—Ni2—Dy2^{xxi}	125.53 (8)
Ni2^{ii}—Ni1—Ni3^{ii}	109.52 (6)	Ni1^{xvi}—Ni2—Dy2^{xxi}	72.94 (3)
Ni1^{iii}—Ni1—Ni3^{ii}	119.63 (2)	Ni1^{xvii}—Ni2—Dy2^{xxi}	72.94 (3)
Ni1^{iv}—Ni1—Ni3^{ii}	119.63 (2)	Dy2^{xviii}—Ni2—Dy2^{xxi}	119.999 (1)
Ni1^{v}—Ni1—Ni3^{ii}	60.37 (2)	Dy2^{xv}—Ni2—Dy2^{xxi}	119.999 (1)
Ni1^{vi}—Ni1—Ni3^{ii}	60.37 (2)	Ni2^{xix}—Ni2—Dy2^{xxi}	60.0
Ni2^{i}—Ni1—Dy1^{vii}	113.50 (3)	Ni2^{xx}—Ni2—Dy2^{xxi}	60.0
Ni2^{ii}—Ni1—Dy1^{vii}	113.43 (3)	Ni1^{i}—Ni2—Ni2^{xxii}	54.54 (7)
Ni1^{iii}—Ni1—Dy1^{vii}	64.23 (2)	Ni1^{xiv}—Ni2—Ni2^{xxii}	107.20 (9)
Ni1^{iv}—Ni1—Dy1^{vii}	115.90 (2)	Ni1^{xiii}—Ni2—Ni2^{xxii}	107.20 (9)
Ni1^{v}—Ni1—Dy1^{vii}	64.10 (2)	Ni1^{xv}—Ni2—Ni2^{xxii}	54.07 (7)
Ni1^{vi}—Ni1—Dy1^{vii}	115.77 (2)	Ni1^{xvi}—Ni2—Ni2^{xxii}	106.72 (9)
Ni3^{ii}—Ni1—Dy1^{vii}	66.22 (3)	Ni1^{xvii}—Ni2—Ni2^{xxii}	106.72 (9)
Ni2^{i}—Ni1—Dy1	113.50 (3)	Dy2^{xviii}—Ni2—Ni2^{xxii}	60.0
Ni2^{ii}—Ni1—Dy1	113.43 (3)	Dy2^{xv}—Ni2—Ni2^{xxii}	60.0
Ni1^{iii}—Ni1—Dy1	115.90 (2)	Ni2^{xix}—Ni2—Ni2^{xxii}	119.997 (2)
Ni1^{iv}—Ni1—Dy1	64.23 (2)	Ni2^{xx}—Ni2—Ni2^{xxii}	119.997 (2)

Ni1^{v}—Ni1—Dy1	115.77 (2)	Dy2^{xxi}—Ni2—Ni2^{xxii}	179.60 (14)
Ni1^{vi}—Ni1—Dy1	64.10 (2)	Ni1^{xx}—Ni3—Ni1^{xv}	180.00 (3)
Ni3^{ii}—Ni1—Dy1	66.22 (3)	Ni1^{xx}—Ni3—Ni1^{xxiii}	59.27 (5)
Dy1^{vii}—Ni1—Dy1	121.28 (6)	Ni1^{xv}—Ni3—Ni1^{xxiii}	120.73 (5)
Ni2^{i}—Ni1—Dy1^{i}	116.67 (6)	Ni1^{xx}—Ni3—Ni1^{xvii}	120.73 (5)
Ni2^{ii}—Ni1—Dy1^{i}	171.94 (6)	Ni1^{xv}—Ni3—Ni1^{xvii}	59.27 (5)
Ni1^{iii}—Ni1—Dy1^{i}	66.34 (2)	Ni1^{xxiii}—Ni3—Ni1^{xvii}	180.0
Ni1^{iv}—Ni1—Dy1^{i}	66.34 (2)	Ni1^{xx}—Ni3—Ni1^{xxiv}	59.27 (5)
Ni1^{v}—Ni1—Dy1^{i}	113.66 (2)	Ni1^{xv}—Ni3—Ni1^{xxiv}	120.73 (5)
Ni1^{vi}—Ni1—Dy1^{i}	113.66 (2)	Ni1^{xxiii}—Ni3—Ni1^{xxiv}	59.27 (5)
Ni3^{ii}—Ni1—Dy1^{i}	62.42 (4)	Ni1^{xvii}—Ni3—Ni1^{xxiv}	120.73 (5)
Dy1^{vii}—Ni1—Dy1^{i}	64.28 (3)	Ni1^{xx}—Ni3—Ni1^{xvi}	120.73 (5)
Dy1—Ni1—Dy1^{i}	64.28 (3)	Ni1^{xv}—Ni3—Ni1^{xvi}	59.27 (5)
Ni2^{i}—Ni1—Dy2	59.47 (3)	Ni1^{xxiii}—Ni3—Ni1^{xvi}	120.73 (5)
Ni2^{ii}—Ni1—Dy2	59.37 (3)	Ni1^{xvii}—Ni3—Ni1^{xvi}	59.27 (5)
Ni1^{iii}—Ni1—Dy2	112.99 (2)	Ni1^{xxiv}—Ni3—Ni1^{xvi}	180.0
Ni1^{iv}—Ni1—Dy2	67.12 (2)	Ni1^{xx}—Ni3—Dy1^{xx}	62.314 (16)
Ni1^{v}—Ni1—Dy2	112.88 (2)	Ni1^{xv}—Ni3—Dy1^{xx}	117.686 (16)
Ni1^{vi}—Ni1—Dy2	67.01 (2)	Ni1^{xxiii}—Ni3—Dy1^{xx}	62.314 (16)
Ni3^{ii}—Ni1—Dy2	120.91 (3)	Ni1^{xvii}—Ni3—Dy1^{xx}	117.686 (16)
Dy1^{vii}—Ni1—Dy2	170.57 (4)	Ni1^{xxiv}—Ni3—Dy1^{xx}	111.68 (4)
Dy1—Ni1—Dy2	68.15 (3)	Ni1^{xvi}—Ni3—Dy1^{xx}	68.32 (4)
Dy1^{i}—Ni1—Dy2	123.75 (3)	Ni1^{xx}—Ni3—Dy1^{xv}	117.686 (16)
Ni2^{i}—Ni1—Dy2^{vii}	59.47 (3)	Ni1^{xv}—Ni3—Dy1^{xv}	62.314 (16)
Ni2^{ii}—Ni1—Dy2^{vii}	59.37 (3)	Ni1^{xxiii}—Ni3—Dy1^{xv}	117.686 (16)
Ni1^{iii}—Ni1—Dy2^{vii}	67.12 (2)	Ni1^{xvii}—Ni3—Dy1^{xv}	62.314 (16)
Ni1^{iv}—Ni1—Dy2^{vii}	112.99 (2)	Ni1^{xxiv}—Ni3—Dy1^{xv}	68.32 (4)
Ni1^{v}—Ni1—Dy2^{vii}	67.01 (2)	Ni1^{xvi}—Ni3—Dy1^{xv}	111.68 (4)
Ni1^{vi}—Ni1—Dy2^{vii}	112.88 (2)	Dy1^{xx}—Ni3—Dy1^{xv}	180.0
Ni3^{ii}—Ni1—Dy2^{vii}	120.91 (3)	Ni1^{xx}—Ni3—Dy1^{xix}	62.314 (16)
Dy1^{vii}—Ni1—Dy2^{vii}	68.15 (3)	Ni1^{xv}—Ni3—Dy1^{xix}	117.686 (16)
Dy1—Ni1—Dy2^{vii}	170.57 (4)	Ni1^{xxiii}—Ni3—Dy1^{xix}	111.68 (4)
Dy1^{i}—Ni1—Dy2^{vii}	123.75 (3)	Ni1^{xvii}—Ni3—Dy1^{xix}	68.32 (4)
Dy2—Ni1—Dy2^{vii}	102.42 (5)	Ni1^{xxiv}—Ni3—Dy1^{xix}	62.314 (16)
Ni1^{viii}—Dy1—Ni1^{ix}	51.80 (5)	Ni1^{xvi}—Ni3—Dy1^{xix}	117.686 (16)
Ni1^{viii}—Dy1—Ni1^{x}	51.54 (5)	Dy1^{xx}—Ni3—Dy1^{xix}	114.993 (13)
Ni1^{ix}—Dy1—Ni1^{x}	98.01 (4)	Dy1^{xv}—Ni3—Dy1^{xix}	65.007 (13)
Ni1^{viii}—Dy1—Ni1	121.28 (6)	Ni1^{xx}—Ni3—Dy1^{xviii}	117.686 (16)
Ni1^{ix}—Dy1—Ni1	98.01 (4)	Ni1^{xv}—Ni3—Dy1^{xviii}	62.314 (16)
Ni1^{x}—Dy1—Ni1	98.01 (4)	Ni1^{xxiii}—Ni3—Dy1^{xviii}	68.32 (4)
Ni1^{viii}—Dy1—Ni1^{vi}	98.01 (4)	Ni1^{xvii}—Ni3—Dy1^{xviii}	111.68 (4)
Ni1^{ix}—Dy1—Ni1^{vi}	51.54 (5)	Ni1^{xxiv}—Ni3—Dy1^{xviii}	117.686 (16)
Ni1^{x}—Dy1—Ni1^{vi}	121.28 (6)	Ni1^{xvi}—Ni3—Dy1^{xviii}	62.314 (16)
Ni1—Dy1—Ni1^{vi}	51.80 (5)	Dy1^{xx}—Ni3—Dy1^{xviii}	65.007 (13)
Ni1^{viii}—Dy1—Ni1^{iv}	98.01 (4)	Dy1^{xv}—Ni3—Dy1^{xviii}	114.993 (13)
Ni1^{ix}—Dy1—Ni1^{iv}	121.28 (6)	Dy1^{xix}—Ni3—Dy1^{xviii}	180.00 (3)
Ni1^{x}—Dy1—Ni1^{iv}	51.80 (5)	Ni1^{xx}—Ni3—Dy1^{xxii}	111.68 (4)
Ni1—Dy1—Ni1^{iv}	51.54 (5)	Ni1^{xv}—Ni3—Dy1^{xxii}	68.32 (4)

$Ni1^{vi}$—Dy1—$Ni1^{iv}$	98.01 (4)	$Ni1^{xxiii}$—Ni3—$Dy1^{xxii}$	62.314 (16)
$Ni1^{viii}$—Dy1—$Ni3^{ii}$	147.89 (3)	$Ni1^{xvii}$—Ni3—$Dy1^{xxii}$	117.686 (16)
$Ni1^{ix}$—Dy1—$Ni3^{ii}$	96.33 (2)	$Ni1^{xxiv}$—Ni3—$Dy1^{xxii}$	62.314 (16)
$Ni1^{x}$—Dy1—$Ni3^{ii}$	147.89 (3)	$Ni1^{xvi}$—Ni3—$Dy1^{xxii}$	117.686 (16)
Ni1—Dy1—$Ni3^{ii}$	51.46 (3)	$Dy1^{xx}$—Ni3—$Dy1^{xxii}$	114.992 (13)
$Ni1^{vi}$—Dy1—$Ni3^{ii}$	51.46 (3)	$Dy1^{xv}$—Ni3—$Dy1^{xxii}$	65.008 (13)
$Ni1^{iv}$—Dy1—$Ni3^{ii}$	96.33 (2)	$Dy1^{xix}$—Ni3—$Dy1^{xxii}$	114.992 (13)
$Ni1^{viii}$—Dy1—$Ni3^{xi}$	51.46 (3)	$Dy1^{xviii}$—Ni3—$Dy1^{xxii}$	65.008 (13)
$Ni1^{ix}$—Dy1—$Ni3^{xi}$	51.46 (3)	$Ni1^{xx}$—Ni3—$Dy1^{xxi}$	68.32 (4)
$Ni1^{x}$—Dy1—$Ni3^{xi}$	96.33 (2)	$Ni1^{xv}$—Ni3—$Dy1^{xxi}$	111.68 (4)
Ni1—Dy1—$Ni3^{xi}$	147.89 (3)	$Ni1^{xxiii}$—Ni3—$Dy1^{xxi}$	117.686 (16)
$Ni1^{vi}$—Dy1—$Ni3^{xi}$	96.33 (2)	$Ni1^{xvii}$—Ni3—$Dy1^{xxi}$	62.314 (16)
$Ni1^{iv}$—Dy1—$Ni3^{xi}$	147.89 (3)	$Ni1^{xxiv}$—Ni3—$Dy1^{xxi}$	117.686 (16)
$Ni3^{ii}$—Dy1—$Ni3^{xi}$	114.993 (13)	$Ni1^{xvi}$—Ni3—$Dy1^{xxi}$	62.314 (16)
$Ni1^{viii}$—Dy1—$Ni3^{xii}$	96.33 (2)	$Dy1^{xx}$—Ni3—$Dy1^{xxi}$	65.008 (13)
$Ni1^{ix}$—Dy1—$Ni3^{xii}$	147.89 (3)	$Dy1^{xv}$—Ni3—$Dy1^{xxi}$	114.992 (13)
$Ni1^{x}$—Dy1—$Ni3^{xii}$	51.46 (3)	$Dy1^{xix}$—Ni3—$Dy1^{xxi}$	65.008 (13)
Ni1—Dy1—$Ni3^{xii}$	96.33 (2)	$Dy1^{xviii}$—Ni3—$Dy1^{xxi}$	114.992 (13)
$Ni1^{vi}$—Dy1—$Ni3^{xii}$	147.89 (3)	$Dy1^{xxii}$—Ni3—$Dy1^{xxi}$	180.00 (3)
$Ni1^{iv}$—Dy1—$Ni3^{xii}$	51.46 (3)	$Ni2^{i}$—Dy2—$Ni2^{xxv}$	120.0
$Ni3^{ii}$—Dy1—$Ni3^{xii}$	114.992 (13)	$Ni2^{i}$—Dy2—$Ni2^{ii}$	60.0
$Ni3^{xi}$—Dy1—$Ni3^{xii}$	114.992 (13)	$Ni2^{xxv}$—Dy2—$Ni2^{ii}$	180.0
$Ni1^{viii}$—Dy1—$Ni1^{i}$	115.72 (3)	$Ni2^{i}$—Dy2—$Ni2^{xi}$	180.0
$Ni1^{ix}$—Dy1—$Ni1^{i}$	141.67 (2)	$Ni2^{xxv}$—Dy2—$Ni2^{xi}$	60.0
$Ni1^{x}$—Dy1—$Ni1^{i}$	94.88 (4)	$Ni2^{ii}$—Dy2—$Ni2^{xi}$	120.0
Ni1—Dy1—$Ni1^{i}$	115.72 (3)	$Ni2^{i}$—Dy2—$Ni2^{xxvi}$	120.0
$Ni1^{vi}$—Dy1—$Ni1^{i}$	141.67 (2)	$Ni2^{xxv}$—Dy2—$Ni2^{xxvi}$	120.0
$Ni1^{iv}$—Dy1—$Ni1^{i}$	94.88 (4)	$Ni2^{ii}$—Dy2—$Ni2^{xxvi}$	60.0
$Ni3^{ii}$—Dy1—$Ni1^{i}$	91.38 (3)	$Ni2^{xi}$—Dy2—$Ni2^{xxvi}$	60.0
$Ni3^{xi}$—Dy1—$Ni1^{i}$	91.38 (3)	$Ni2^{i}$—Dy2—$Ni2^{xii}$	60.0
$Ni3^{xii}$—Dy1—$Ni1^{i}$	49.26 (2)	$Ni2^{xxv}$—Dy2—$Ni2^{xii}$	60.0
$Ni1^{viii}$—Dy1—$Ni1^{xiii}$	141.67 (2)	$Ni2^{ii}$—Dy2—$Ni2^{xii}$	120.0
$Ni1^{ix}$—Dy1—$Ni1^{xiii}$	115.72 (3)	$Ni2^{xi}$—Dy2—$Ni2^{xii}$	120.0
$Ni1^{x}$—Dy1—$Ni1^{xiii}$	141.67 (2)	$Ni2^{xxvi}$—Dy2—$Ni2^{xii}$	180.0
Ni1—Dy1—$Ni1^{xiii}$	94.88 (4)	$Ni2^{i}$—Dy2—Ni1	47.39 (4)
$Ni1^{vi}$—Dy1—$Ni1^{xiii}$	94.88 (4)	$Ni2^{xxv}$—Dy2—Ni1	132.30 (4)
$Ni1^{iv}$—Dy1—$Ni1^{xiii}$	115.72 (3)	$Ni2^{ii}$—Dy2—Ni1	47.70 (4)
$Ni3^{ii}$—Dy1—$Ni1^{xiii}$	49.26 (2)	$Ni2^{xi}$—Dy2—Ni1	132.61 (4)
$Ni3^{xi}$—Dy1—$Ni1^{xiii}$	91.38 (3)	$Ni2^{xxvi}$—Dy2—Ni1	89.97 (4)
$Ni3^{xii}$—Dy1—$Ni1^{xiii}$	91.39 (3)	$Ni2^{xii}$—Dy2—Ni1	90.03 (4)
$Ni1^{i}$—Dy1—$Ni1^{xiii}$	47.32 (4)	$Ni2^{i}$—Dy2—$Ni1^{xxvii}$	132.61 (4)
$Ni1^{viii}$—Dy1—$Ni1^{xiv}$	94.88 (4)	$Ni2^{xxv}$—Dy2—$Ni1^{xxvii}$	47.70 (4)
$Ni1^{ix}$—Dy1—$Ni1^{xiv}$	94.88 (4)	$Ni2^{ii}$—Dy2—$Ni1^{xxvii}$	132.30 (4)
$Ni1^{x}$—Dy1—$Ni1^{xiv}$	115.72 (3)	$Ni2^{xi}$—Dy2—$Ni1^{xxvii}$	47.39 (4)
Ni1—Dy1—$Ni1^{xiv}$	141.67 (2)	$Ni2^{xxvi}$—Dy2—$Ni1^{xxvii}$	90.03 (4)
$Ni1^{vi}$—Dy1—$Ni1^{xiv}$	115.72 (3)	$Ni2^{xii}$—Dy2—$Ni1^{xxvii}$	89.97 (4)
$Ni1^{iv}$—Dy1—$Ni1^{xiv}$	141.67 (2)	Ni1—Dy2—$Ni1^{xxvii}$	180.00 (3)
$Ni3^{ii}$—Dy1—$Ni1^{xiv}$	91.38 (3)	$Ni2^{i}$—Dy2—$Ni1^{vi}$	89.97 (4)

Ni3^{xi}—Dy1—Ni1^{xiv}	49.26 (2)	Ni2^{xxv}—Dy2—Ni1^{vi}	132.30 (4)
Ni3^{xii}—Dy1—Ni1^{xiv}	91.39 (3)	Ni2^{ii}—Dy2—Ni1^{vi}	47.70 (4)
Ni1^{i}—Dy1—Ni1^{xiv}	47.32 (4)	Ni2^{xi}—Dy2—Ni1^{vi}	90.03 (4)
Ni1^{xiii}—Dy1—Ni1^{xiv}	47.32 (4)	Ni2^{xxvi}—Dy2—Ni1^{vi}	47.39 (4)
Ni1^{i}—Ni2—Ni1^{xiv}	60.75 (7)	Ni2^{xii}—Dy2—Ni1^{vi}	132.61 (4)
Ni1^{i}—Ni2—Ni1^{xiii}	60.75 (7)	Ni1—Dy2—Ni1^{vi}	45.99 (4)
Ni1^{xiv}—Ni2—Ni1^{xiii}	60.75 (7)	Ni1^{xxvii}—Dy2—Ni1^{vi}	134.01 (4)
Ni1^{i}—Ni2—Ni1^{xv}	108.61 (4)	Ni2^{i}—Dy2—Ni1^{iv}	47.39 (4)
Ni1^{xiv}—Ni2—Ni1^{xv}	146.078 (19)	Ni2^{xxv}—Dy2—Ni1^{iv}	89.97 (4)
Ni1^{xiii}—Ni2—Ni1^{xv}	146.078 (19)	Ni2^{ii}—Dy2—Ni1^{iv}	90.03 (4)
Ni1^{i}—Ni2—Ni1^{xvi}	146.078 (19)	Ni2^{xi}—Dy2—Ni1^{iv}	132.61 (4)
Ni1^{xiv}—Ni2—Ni1^{xvi}	146.077 (19)	Ni2^{xxvi}—Dy2—Ni1^{iv}	132.30 (4)
Ni1^{xiii}—Ni2—Ni1^{xvi}	108.61 (4)	Ni2^{xii}—Dy2—Ni1^{iv}	47.70 (4)
Ni1^{xv}—Ni2—Ni1^{xvi}	60.65 (7)	Ni1—Dy2—Ni1^{iv}	45.77 (4)
Ni1^{i}—Ni2—Ni1^{xvii}	146.078 (19)	Ni1^{xxvii}—Dy2—Ni1^{iv}	134.23 (4)
Ni1^{xiv}—Ni2—Ni1^{xvii}	108.61 (4)	Ni1^{vi}—Dy2—Ni1^{iv}	84.91 (3)
Ni1^{xiii}—Ni2—Ni1^{xvii}	146.077 (19)	Ni2^{i}—Dy2—Ni1^{xxviii}	90.03 (4)
Ni1^{xv}—Ni2—Ni1^{xvii}	60.65 (7)	Ni2^{xxv}—Dy2—Ni1^{xxviii}	47.70 (4)
Ni1^{xvi}—Ni2—Ni1^{xvii}	60.65 (7)	Ni2^{ii}—Dy2—Ni1^{xxviii}	132.30 (4)
Ni1^{i}—Ni2—Dy2^{xviii}	73.14 (3)	Ni2^{xi}—Dy2—Ni1^{xxviii}	89.97 (4)
Ni1^{xiv}—Ni2—Dy2^{xviii}	125.86 (8)	Ni2^{xxvi}—Dy2—Ni1^{xxviii}	132.61 (4)
Ni1^{xiii}—Ni2—Dy2^{xviii}	73.14 (3)	Ni2^{xii}—Dy2—Ni1^{xxviii}	47.39 (4)
Ni1^{xv}—Ni2—Dy2^{xviii}	72.94 (3)	Ni1—Dy2—Ni1^{xxviii}	134.01 (4)
Ni1^{xvi}—Ni2—Dy2^{xviii}	72.94 (3)	Ni1^{xxvii}—Dy2—Ni1^{xxviii}	45.99 (4)
Ni1^{xvii}—Ni2—Dy2^{xviii}	125.53 (8)	Ni1^{vi}—Dy2—Ni1^{xxviii}	180.00 (5)
Ni1^{i}—Ni2—Dy2^{xv}	73.14 (3)	Ni1^{iv}—Dy2—Ni1^{xxviii}	95.09 (3)
Ni1^{xiv}—Ni2—Dy2^{xv}	73.14 (3)	Ni2^{i}—Dy2—Ni1^{viii}	132.30 (4)
Ni1^{xiii}—Ni2—Dy2^{xv}	125.86 (8)	Ni2^{xxv}—Dy2—Ni1^{viii}	47.39 (4)
Ni1^{xv}—Ni2—Dy2^{xv}	72.94 (3)	Ni2^{ii}—Dy2—Ni1^{viii}	132.61 (4)
Ni1^{xvi}—Ni2—Dy2^{xv}	125.53 (8)	Ni2^{xi}—Dy2—Ni1^{viii}	47.70 (4)
Ni1^{xvii}—Ni2—Dy2^{xv}	72.94 (3)	Ni2^{xxvi}—Dy2—Ni1^{viii}	89.97 (4)
Dy2^{xviii}—Ni2—Dy2^{xv}	120.000 (1)	Ni2^{xii}—Dy2—Ni1^{viii}	90.03 (4)
Ni1^{i}—Ni2—Ni2^{xix}	107.20 (9)	Ni1—Dy2—Ni1^{viii}	102.42 (5)
Ni1^{xiv}—Ni2—Ni2^{xix}	54.54 (7)	Ni1^{xxvii}—Dy2—Ni1^{viii}	77.58 (5)
Ni1^{xiii}—Ni2—Ni2^{xix}	107.20 (9)	Ni1^{vi}—Dy2—Ni1^{viii}	84.91 (3)
Ni1^{xv}—Ni2—Ni2^{xix}	106.72 (9)	Ni1^{iv}—Dy2—Ni1^{viii}	84.91 (3)
Ni1^{xvi}—Ni2—Ni2^{xix}	106.72 (9)	Ni1^{xxviii}—Dy2—Ni1^{viii}	95.09 (3)

Symmetry codes: (i) −*x*+2/3, −*y*+1/3, −*z*+1/3; (ii) *x*+1/3, *y*+2/3, *z*−1/3; (iii) −*x*+*y*+1, −*x*+1, *z*; (iv) −*y*+1, *x*−*y*, *z*; (v) −*y*+1, *x*−*y*+1, *z*; (vi) −*x*+*y*, −*x*+1, *z*; (vii) *x*+1, *y*+1, *z*; (viii) *x*−1, *y*−1, *z*; (ix) −*y*, *x*−*y*, *z*; (x) −*x*+*y*, −*x*, *z*; (xi) *x*−2/3, *y*−1/3, *z*−1/3; (xii) *x*+1/3, *y*−1/3, *z*−1/3; (xiii) *y*−1/3, −*x*+*y*+1/3, −*z*+1/3; (xiv) *x*−*y*−1/3, *x*−2/3, −*z*+1/3; (xv) *x*−1/3, *y*−2/3, *z*+1/3; (xvi) −*y*+2/3, *x*−*y*+1/3, *z*+1/3; (xvii) −*x*+*y*−1/3, −*x*+1/3, *z*+1/3; (xviii) *x*+2/3, *y*+1/3, *z*+1/3; (xix) −*x*−2/3, −*y*−1/3, −*z*+2/3; (xx) −*x*+1/3, −*y*+2/3, −*z*+2/3; (xxi) *x*−1/3, *y*+1/3, *z*+1/3; (xxii) −*x*+1/3, −*y*−1/3, −*z*+2/3; (xxiii) *x*−*y*+1/3, *x*−1/3, −*z*+2/3; (xxiv) *y*−2/3, −*x*+*y*−1/3, −*z*+2/3; (xxv) −*x*−1/3, −*y*−2/3, −*z*+1/3; (xxvi) −*x*−1/3, −*y*+1/3, −*z*+1/3; (xxvii) −*x*, −*y*, −*z*; (xxviii) *x*−*y*, *x*−1, −*z*.