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Nickel hexayttrium decaiodide, [NiY<sub>6</sub>I<sub>10</sub>]

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Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(I-Y) = 0.001$  Å;  
 R factor = 0.034; wR factor = 0.091; data-to-parameter ratio = 41.2.

Comproportionation reactions of yttrium triiodide, yttrium and nickel led to the formation of the compound [NiY<sub>6</sub>I<sub>10</sub>], which is isostructural with the prototypical [RuY<sub>6</sub>I<sub>10</sub>]. In particular, [NiY<sub>6</sub>I<sub>10</sub>] is composed of isolated nickel centered yttrium octahedra (site symmetry  $\bar{1}$ ) that are further surrounded by iodide ligands to construct a three-dimensional cluster complex framework. Although this compound has been previously detected by powder X-ray diffraction techniques [Payne & Corbett (1990). *Inorg. Chem.* **29**, 2246–2251], details of the crystal structure for triclinic [NiY<sub>6</sub>I<sub>10</sub>] were not provided.

## Related literature

For a report of the prototypical [RuY<sub>6</sub>I<sub>10</sub>], see: Hughbanks *et al.* (1989). For the determination of the lattice parameters of [NiY<sub>6</sub>I<sub>10</sub>] from PXRD data, see: Payne & Corbett (1990). For a survey of isotypic structures, see: Rustige *et al.* (2012). For the synthesis of the starting material YI<sub>3</sub>, see: Corbett (1983); Meyer (1991). The symmetry of the refined structure was checked using the *PLATON* software package (Spek, 2009).

## Experimental

## Crystal data

[NiY <sub>6</sub> I <sub>10</sub> ]	$\gamma = 107.540$ (5)°
$M_r = 1861.17$	$V = 613.06$ (8) Å <sup>3</sup>
Triclinic, $P\bar{1}$	$Z = 1$
$a = 9.4904$ (7) Å	Mo $K\alpha$ radiation
$b = 9.4990$ (7) Å	$\mu = 27.35$ mm <sup>-1</sup>
$c = 7.5702$ (5) Å	$T = 293$ K
$\alpha = 97.056$ (6)°	$0.1 \times 0.1 \times 0.1$ mm
$\beta = 105.096$ (6)°	

## Data collection

Stoe IPDS 2T diffractometer	11699 measured reflections
Absorption correction: numerical	3294 independent reflections
[ <i>X-SHAPE</i> (Stoe & Cie, 1999)	2873 reflections with $I > 2\sigma(I)$
and <i>X-RED</i> (Stoe & Cie, 2001)]	$R_{int} = 0.106$
$T_{min} = 0.031$ , $T_{max} = 0.084$	

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.034$	80 parameters
$wR(F^2) = 0.091$	$\Delta\rho_{max} = 1.37$ e Å <sup>-3</sup>
$S = 1.05$	$\Delta\rho_{min} = -1.64$ e Å <sup>-3</sup>
3294 reflections	

Table 1

Averaged Y–Ni, Y–Y and Y–I distances (Å) in triclinic [NiY<sub>6</sub>I<sub>10</sub>].

Interaction	Y–Ni	Y–Y	Y–I
Distance	2.649	3.746	3.143

Data collection: *X-AREA* (Stoe & Cie, 2003); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXL97* and local programs.

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Supporting information for this paper is available from the IUCr electronic archives (Reference: HP2066).

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## supporting information

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## Nickel hexayttrium decaiodide, [NiY<sub>6</sub>]I<sub>10</sub>

Simon Steinberg and Gerd Meyer

### S1. Comment

[NiY<sub>6</sub>]I<sub>10</sub> crystallizes with the triclinic [RuY<sub>6</sub>]I<sub>10</sub> type of structure (Hughbanks *et al.*, 1989) and may be depicted as cubic closest packings of nickel and iodine atoms with yttrium atoms residing in 6/11 of all octahedral holes. Particularly, the yttrium atoms occupy those voids surrounding the nickel atoms to aggregate to octahedral [NiY<sub>6</sub>] clusters (Fig. 1). The twelve edges of each [NiY<sub>6</sub>] octahedron are capped by inner iodido ligands forming cuboctahedra around the endohedral nickel atoms. Additionally, the yttrium atoms bond to outer iodido ligands that reside in the inner coordination spheres of like clusters. More specifically, the iodido ligands interconnect the [NiY<sub>6</sub>] clusters *via* (i)–(i)–, (i)–(a)– and (a)–(i)– functionalities (Fig. 2), which can be emphasized by the formula [NiY<sub>6</sub>]I<sub>2/1</sub><sup>i</sup>I<sub>4/2</sub><sup>i-i</sup>I<sub>6/2</sub><sup>i-a</sup>I<sub>6/2</sub><sup>a-i</sup> (Rustige *et al.*, 2012 and lit. cited therein). The averaged Y–Y and Y–I (see below) distances correlate well with data of recently reported yttrium cluster iodides (Rustige *et al.*, 2012).

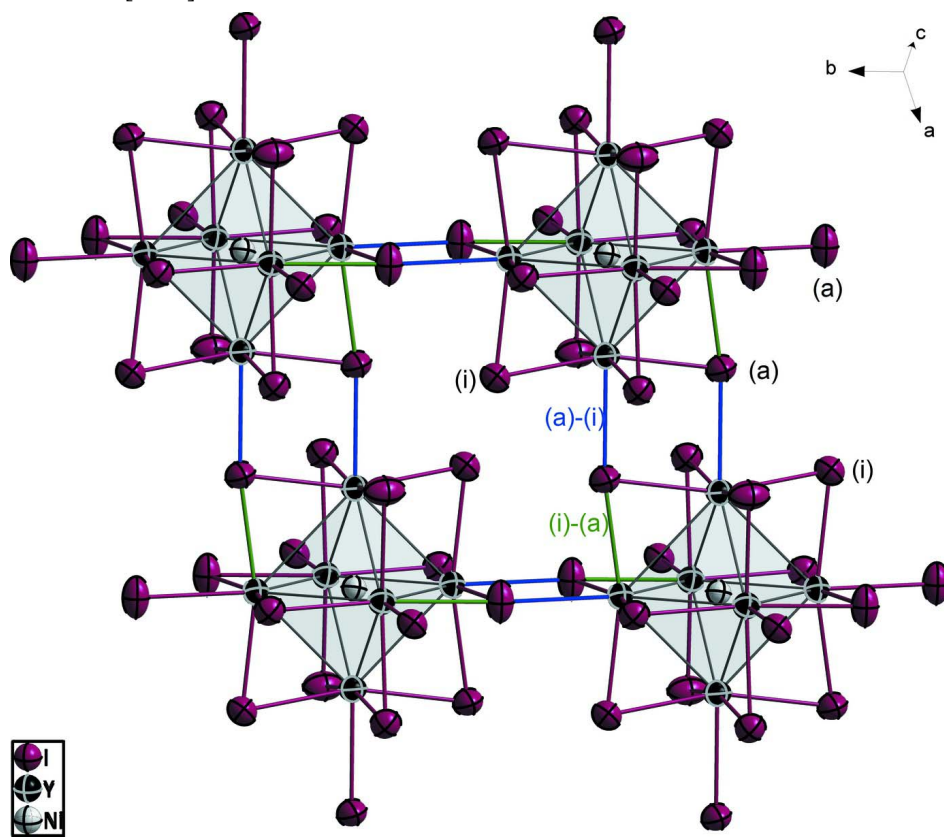
### S2. Experimental

[NiY<sub>6</sub>]I<sub>10</sub> was obtained from comproportionation reactions of yttrium triiodide, yttrium and nickel. Yttrium triiodide was synthesized from reactions of the pure elements (Corbett, 1983; Meyer, 1991), while the metals were obtained from commercial sources (Y, smart elements, 99.99%; Ni, Riedel–de Haen, 99.8%) and used without further purification. Due to the sensitivity of the used chemicals and products to air and moisture, all sample preparations were performed under a nitrogen atmosphere in a glove box with strict exclusion of air and water (< 0.1 p.p.m.). The reaction mixtures were loaded as {NiY<sub>3</sub>}I<sub>3</sub> in pre-cleaned, one-side He-arc welded tantalum tubes, which were closed inside a glove box, arc-welded at the other end and jacketed by evacuated, fused silica tubes. The mixtures were first heated to 1050 °C, kept at that temperature for one week, slowly-annealed to 700 °C and, then, rapidly cooled to room temperature. The product appeared as a black powder containing small crystals of polyhedral shape. Single crystals were selected from the bulk and fixed in capillaries, which were closed inside a glove box. The crystals were subsequently transferred to a Stoe IPDS 2 T diffractometer and complete sets of intensity data were collected at room temperature (293 (2) K).

### S3. Refinement

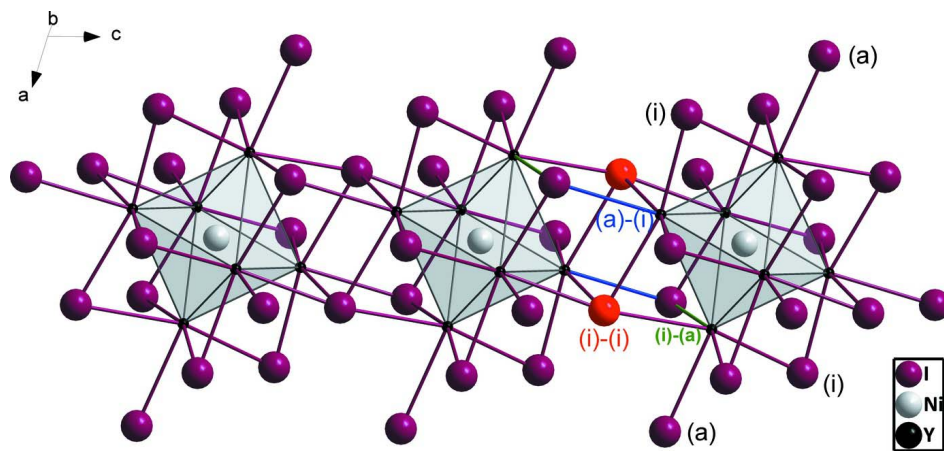
The intensity data sets were corrected for Lorentz and polarization effects. The structure was solved using direct methods (*SHELXS97*, Sheldrick, 2008) and refined on F<sup>2</sup> (*SHELXL97*, Sheldrick, 2008). A numerical absorption correction and a crystal shape optimization were carried out with the programs *X-RED* (Stoe & Cie, 2001) and *X-SHAPE* (Stoe & Cie, 1999), respectively. The *PLATON* software package (Spek, 2009) was utilized to check the symmetry of the refined structure and no higher symmetry was identified. As the largest difference peaks (1.365 and -1.635 e.Å) are located 0.73 Å and 0.81 Å near to the I2 and I1 sites, respectively, and all thermal ellipsoids are reasonable in shape and size (Rustige *et al.*, 2012), the presence of further atom sites was excluded. To compare the lattice parameters of the title compound to those of more recently reported yttrium cluster iodides (Rustige *et al.*, 2012), a lattice setting unlike the standard setting

was chosen for the triclinic  $[\text{NiY}_6]\text{I}_{10}$ .



**Figure 1**

Representation of isolated  $[\text{NiY}_6]$  octahedra. The edges are capped by the iodido ligands, whereas each yttrium atom bonds to one outer iodido ligand (90% probability thermal ellipsoids).



**Figure 2**

View on the (i)-(i)-, (i)-a- and (a)-(i)-interconnections as seen in the triclinic  $[\text{NiY}_6]\text{I}_{10}$ .

## Hexayttrium nickel decaiodide

## Crystal data

$Y_6Ni_{10}$	$Z = 1$
$M_r = 1861.17$	$F(000) = 792$
Triclinic, $P\bar{1}$	$D_x = 5.041 \text{ Mg m}^{-3}$
Hall symbol: $-P\ 1$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$a = 9.4904 (7) \text{ \AA}$	Cell parameters from 7675 reflections
$b = 9.4990 (7) \text{ \AA}$	$\theta = 2.3\text{--}29.7^\circ$
$c = 7.5702 (5) \text{ \AA}$	$\mu = 27.35 \text{ mm}^{-1}$
$\alpha = 97.056 (6)^\circ$	$T = 293 \text{ K}$
$\beta = 105.096 (6)^\circ$	Polyhedral, black
$\gamma = 107.540 (5)^\circ$	$0.1 \times 0.1 \times 0.1 \text{ mm}$
$V = 613.06 (8) \text{ \AA}^3$	

## Data collection

Stoe IPDS 2T diffractometer	$T_{\min} = 0.031, T_{\max} = 0.084$
Radiation source: fine-focus sealed tube	11699 measured reflections
Graphite monochromator	3294 independent reflections
Detector resolution: not measured pixels $\text{mm}^{-1}$	2873 reflections with $I > 2\sigma(I)$
$\omega$ and $\phi$ scans	$R_{\text{int}} = 0.106$
Absorption correction: numerical	$\theta_{\max} = 29.2^\circ, \theta_{\min} = 2.3^\circ$
[ <i>X-SHAPE</i> (Stoe & Cie, 1999) and <i>X-RED</i> (Stoe & Cie, 2001)]	$h = -12 \rightarrow 12$
	$k = -12 \rightarrow 12$
	$l = -10 \rightarrow 10$

## Refinement

Refinement on $F^2$	Secondary atom site location: difference Fourier map
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0426P)^2]$
$R[F^2 > 2\sigma(F^2)] = 0.034$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.091$	$(\Delta/\sigma)_{\max} = 0.001$
$S = 1.05$	$\Delta\rho_{\max} = 1.37 \text{ e \AA}^{-3}$
3294 reflections	$\Delta\rho_{\min} = -1.64 \text{ e \AA}^{-3}$
80 parameters	Extinction correction: <i>SHELXL</i> ,
0 restraints	$F_c^* = kFc[1 + 0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0065 (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 ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
I1	0.46133 (4)	0.27745 (5)	0.36198 (5)	0.03196 (12)
I2	0.09092 (5)	-0.53117 (5)	-0.73275 (5)	0.03117 (12)
I3	0.62560 (4)	0.18495 (5)	-0.08746 (6)	0.03022 (12)

I4	0.18872 (4)	-0.09482 (4)	-0.45161 (4)	0.02376 (11)
I5	0.26512 (4)	0.35524 (4)	-0.21790 (6)	0.02461 (11)
Y1	0.03920 (6)	-0.24090 (6)	-0.88682 (7)	0.01994 (13)
Y2	0.28566 (6)	0.08659 (6)	-0.02824 (7)	0.02070 (13)
Y3	0.12577 (6)	0.16546 (6)	-0.65217 (7)	0.02003 (13)
Ni1	0.0000	0.0000	0.0000	0.01763 (19)

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
I1	0.0218 (2)	0.0379 (3)	0.02921 (19)	0.00438 (18)	0.00735 (15)	-0.00074 (17)
I2	0.0445 (3)	0.0225 (2)	0.02586 (18)	0.01531 (18)	0.00550 (16)	0.00573 (15)
I3	0.0238 (2)	0.0314 (2)	0.0443 (2)	0.01372 (17)	0.01644 (16)	0.01687 (19)
I4	0.02514 (19)	0.0264 (2)	0.02106 (17)	0.01056 (16)	0.00748 (13)	0.00530 (14)
I5	0.02516 (19)	0.0237 (2)	0.02650 (17)	0.00764 (14)	0.01043 (13)	0.00798 (13)
Y1	0.0214 (2)	0.0197 (3)	0.0214 (2)	0.00886 (18)	0.00798 (17)	0.00681 (18)
Y2	0.0188 (2)	0.0232 (3)	0.0223 (2)	0.00806 (18)	0.00821 (17)	0.00681 (19)
Y3	0.0212 (2)	0.0205 (3)	0.0198 (2)	0.00802 (18)	0.00750 (16)	0.00500 (17)
Ni1	0.0174 (4)	0.0184 (5)	0.0191 (4)	0.0072 (3)	0.0070 (3)	0.0060 (3)

*Geometric parameters (Å, °)*

I1—Y3 <sup>i</sup>	3.0062 (7)	Y1—Y2 <sup>vii</sup>	3.7458 (8)
I1—Y2	3.0150 (7)	Y1—Y3	3.7913 (8)
I2—Y1 <sup>ii</sup>	3.0839 (7)	Y2—Ni1	2.6595 (5)
I2—Y3 <sup>iii</sup>	3.1124 (7)	Y2—I3 <sup>iv</sup>	3.0999 (6)
I2—Y1	3.2421 (6)	Y2—Y3 <sup>i</sup>	3.6579 (8)
I3—Y2 <sup>iv</sup>	3.0999 (6)	Y2—Y1 <sup>vi</sup>	3.7404 (8)
I3—Y1 <sup>v</sup>	3.1255 (7)	Y2—Y1 <sup>i</sup>	3.7458 (8)
I3—Y2	3.2437 (7)	Y2—Y3 <sup>vi</sup>	3.8540 (8)
I4—Y1	3.1700 (6)	Y3—Ni1 <sup>vii</sup>	2.6540 (5)
I4—Y3	3.1805 (6)	Y3—I1 <sup>vii</sup>	3.0062 (7)
I4—Y3 <sup>vi</sup>	3.1811 (7)	Y3—I2 <sup>ix</sup>	3.1124 (7)
I4—Y2	3.1999 (6)	Y3—I4 <sup>vi</sup>	3.1811 (7)
I5—Y1 <sup>vi</sup>	3.1085 (7)	Y3—Y2 <sup>vii</sup>	3.6579 (8)
I5—Y2	3.1091 (6)	Y3—Y1 <sup>viii</sup>	3.6863 (7)
I5—Y3	3.2633 (7)	Y3—Y2 <sup>vi</sup>	3.8540 (8)
Y1—Ni1 <sup>vii</sup>	2.6339 (5)	Ni1—Y1 <sup>i</sup>	2.6339 (5)
Y1—I2 <sup>ii</sup>	3.0839 (7)	Ni1—Y1 <sup>vi</sup>	2.6339 (5)
Y1—I5 <sup>vi</sup>	3.1085 (7)	Ni1—Y3 <sup>vi</sup>	2.6540 (5)
Y1—I3 <sup>v</sup>	3.1255 (7)	Ni1—Y3 <sup>i</sup>	2.6540 (5)
Y1—Y3 <sup>viii</sup>	3.6863 (7)	Ni1—Y2 <sup>x</sup>	2.6595 (5)
Y1—Y2 <sup>vi</sup>	3.7404 (8)		
Y3 <sup>i</sup> —I1—Y2	74.819 (17)	I1—Y2—Y1 <sup>vi</sup>	95.963 (18)
Y1 <sup>ii</sup> —I2—Y3 <sup>iii</sup>	73.012 (17)	I3 <sup>iv</sup> —Y2—Y1 <sup>vi</sup>	142.723 (19)
Y1 <sup>ii</sup> —I2—Y1	97.915 (17)	I5—Y2—Y1 <sup>vi</sup>	53.010 (13)
Y3 <sup>iii</sup> —I2—Y1	170.822 (19)	I4—Y2—Y1 <sup>vi</sup>	95.321 (16)

Y2 <sup>iv</sup> —I3—Y1 <sup>v</sup>	73.981 (17)	I3—Y2—Y1 <sup>vi</sup>	134.546 (18)
Y2 <sup>iv</sup> —I3—Y2	97.455 (17)	Y3 <sup>i</sup> —Y2—Y1 <sup>vi</sup>	59.759 (14)
Y1 <sup>v</sup> —I3—Y2	171.270 (19)	Ni1—Y2—Y1 <sup>i</sup>	44.682 (11)
Y1—I4—Y3	73.313 (16)	I1—Y2—Y1 <sup>i</sup>	96.665 (18)
Y1—I4—Y3 <sup>vi</sup>	97.782 (17)	I3 <sup>iv</sup> —Y2—Y1 <sup>i</sup>	53.322 (14)
Y3—I4—Y3 <sup>vi</sup>	92.193 (17)	I5—Y2—Y1 <sup>i</sup>	141.452 (18)
Y1—I4—Y2	167.857 (18)	I4—Y2—Y1 <sup>i</sup>	93.299 (17)
Y3—I4—Y2	97.453 (17)	I3—Y2—Y1 <sup>i</sup>	135.838 (19)
Y3 <sup>vi</sup> —I4—Y2	74.310 (16)	Y3 <sup>i</sup> —Y2—Y1 <sup>i</sup>	61.592 (15)
Y1 <sup>vi</sup> —I5—Y2	73.966 (16)	Y1 <sup>vi</sup> —Y2—Y1 <sup>i</sup>	89.447 (15)
Y1 <sup>vi</sup> —I5—Y3	97.326 (18)	Ni1—Y2—Y3 <sup>vi</sup>	43.448 (11)
Y2—I5—Y3	97.588 (18)	I1—Y2—Y3 <sup>vi</sup>	142.34 (2)
Ni1 <sup>vii</sup> —Y1—I2 <sup>ii</sup>	99.864 (17)	I3 <sup>iv</sup> —Y2—Y3 <sup>vi</sup>	93.585 (17)
Ni1 <sup>vii</sup> —Y1—I5 <sup>vi</sup>	97.898 (17)	I5—Y2—Y3 <sup>vi</sup>	91.241 (16)
I2 <sup>ii</sup> —Y1—I5 <sup>vi</sup>	94.416 (18)	I4—Y2—Y3 <sup>vi</sup>	52.622 (13)
Ni1 <sup>vii</sup> —Y1—I3 <sup>v</sup>	97.912 (18)	I3—Y2—Y3 <sup>vi</sup>	133.462 (18)
I2 <sup>ii</sup> —Y1—I3 <sup>v</sup>	88.724 (19)	Y3 <sup>i</sup> —Y2—Y3 <sup>vi</sup>	89.881 (16)
I5 <sup>vi</sup> —Y1—I3 <sup>v</sup>	163.10 (2)	Y1 <sup>vi</sup> —Y2—Y3 <sup>vi</sup>	59.875 (14)
Ni1 <sup>vii</sup> —Y1—I4	97.867 (18)	Y1 <sup>i</sup> —Y2—Y3 <sup>vi</sup>	58.011 (13)
I2 <sup>ii</sup> —Y1—I4	162.27 (2)	Ni1 <sup>vii</sup> —Y3—I1 <sup>vii</sup>	99.248 (19)
I5 <sup>vi</sup> —Y1—I4	83.191 (17)	Ni1 <sup>vii</sup> —Y3—I2 <sup>ix</sup>	98.706 (17)
I3 <sup>v</sup> —Y1—I4	88.768 (17)	I1 <sup>vii</sup> —Y3—I2 <sup>ix</sup>	90.954 (19)
Ni1 <sup>vii</sup> —Y1—I2	178.04 (2)	Ni1 <sup>vii</sup> —Y3—I4	97.190 (17)
I2 <sup>ii</sup> —Y1—I2	82.085 (17)	I1 <sup>vii</sup> —Y3—I4	88.952 (18)
I5 <sup>vi</sup> —Y1—I2	81.656 (16)	I2 <sup>ix</sup> —Y3—I4	163.91 (2)
I3 <sup>v</sup> —Y1—I2	82.341 (16)	Ni1 <sup>vii</sup> —Y3—I4 <sup>vi</sup>	96.629 (17)
I4—Y1—I2	80.185 (15)	I1 <sup>vii</sup> —Y3—I4 <sup>vi</sup>	164.07 (2)
Ni1 <sup>vii</sup> —Y1—Y3 <sup>viii</sup>	46.028 (12)	I2 <sup>ix</sup> —Y3—I4 <sup>vi</sup>	87.890 (18)
I2 <sup>ii</sup> —Y1—Y3 <sup>viii</sup>	53.849 (14)	I4—Y3—I4 <sup>vi</sup>	87.807 (17)
I5 <sup>vi</sup> —Y1—Y3 <sup>viii</sup>	98.781 (17)	Ni1 <sup>vii</sup> —Y3—I5	176.74 (2)
I3 <sup>v</sup> —Y1—Y3 <sup>viii</sup>	96.476 (18)	I1 <sup>vii</sup> —Y3—I5	83.500 (17)
I4—Y1—Y3 <sup>viii</sup>	143.879 (19)	I2 <sup>ix</sup> —Y3—I5	82.942 (16)
I2—Y1—Y3 <sup>viii</sup>	135.914 (19)	I4—Y3—I5	81.059 (15)
Ni1 <sup>vii</sup> —Y1—Y2 <sup>vi</sup>	45.319 (11)	I4 <sup>vi</sup> —Y3—I5	80.592 (16)
I2 <sup>ii</sup> —Y1—Y2 <sup>vi</sup>	95.733 (17)	Ni1 <sup>vii</sup> —Y3—Y2 <sup>vii</sup>	46.558 (12)
I5 <sup>vi</sup> —Y1—Y2 <sup>vi</sup>	53.024 (13)	I1 <sup>vii</sup> —Y3—Y2 <sup>vii</sup>	52.700 (15)
I3 <sup>v</sup> —Y1—Y2 <sup>vi</sup>	143.204 (19)	I2 <sup>ix</sup> —Y3—Y2 <sup>vii</sup>	96.907 (18)
I4—Y1—Y2 <sup>vi</sup>	96.770 (17)	I4—Y3—Y2 <sup>vii</sup>	95.821 (17)
I2—Y1—Y2 <sup>vi</sup>	134.455 (19)	I4 <sup>vi</sup> —Y3—Y2 <sup>vii</sup>	143.186 (18)
Y3 <sup>viii</sup> —Y1—Y2 <sup>vi</sup>	59.009 (14)	I5—Y3—Y2 <sup>vii</sup>	136.194 (19)
Ni1 <sup>vii</sup> —Y1—Y2 <sup>vii</sup>	45.234 (12)	Ni1 <sup>vii</sup> —Y3—Y1 <sup>viii</sup>	45.581 (11)
I2 <sup>ii</sup> —Y1—Y2 <sup>vii</sup>	98.116 (18)	I1 <sup>vii</sup> —Y3—Y1 <sup>viii</sup>	97.251 (19)
I5 <sup>vi</sup> —Y1—Y2 <sup>vii</sup>	142.547 (19)	I2 <sup>ix</sup> —Y3—Y1 <sup>viii</sup>	53.138 (14)
I3 <sup>v</sup> —Y1—Y2 <sup>vii</sup>	52.697 (13)	I4—Y3—Y1 <sup>viii</sup>	142.755 (19)
I4—Y1—Y2 <sup>vii</sup>	94.288 (17)	I4 <sup>vi</sup> —Y3—Y1 <sup>viii</sup>	94.750 (17)
I2—Y1—Y2 <sup>vii</sup>	134.926 (19)	I5—Y3—Y1 <sup>viii</sup>	136.052 (19)
Y3 <sup>viii</sup> —Y1—Y2 <sup>vii</sup>	62.465 (15)	Y2 <sup>vii</sup> —Y3—Y1 <sup>viii</sup>	61.232 (14)
Y2 <sup>vi</sup> —Y1—Y2 <sup>vii</sup>	90.553 (16)	Ni1 <sup>vii</sup> —Y3—Y1	43.984 (11)

Ni1 <sup>vii</sup> —Y1—Y3	44.407 (11)	I1 <sup>vii</sup> —Y3—Y1	95.871 (19)
I2 <sup>ii</sup> —Y1—Y3	144.254 (18)	I2 <sup>ix</sup> —Y3—Y1	142.674 (18)
I5 <sup>vi</sup> —Y1—Y3	92.436 (17)	I4—Y3—Y1	53.216 (13)
I3 <sup>v</sup> —Y1—Y3	94.680 (17)	I4 <sup>vi</sup> —Y3—Y1	94.652 (16)
I4—Y1—Y3	53.471 (13)	I5—Y3—Y1	134.247 (18)
I2—Y1—Y3	133.650 (17)	Y2 <sup>vii</sup> —Y3—Y1	60.346 (15)
Y3 <sup>viii</sup> —Y1—Y3	90.435 (16)	Y1 <sup>viii</sup> —Y3—Y1	89.565 (16)
Y2 <sup>vi</sup> —Y1—Y3	61.551 (14)	Ni1 <sup>vii</sup> —Y3—Y2 <sup>vi</sup>	43.561 (12)
Y2 <sup>vii</sup> —Y1—Y3	58.063 (14)	I1 <sup>vii</sup> —Y3—Y2 <sup>vi</sup>	142.796 (19)
Ni1—Y2—I1	98.905 (19)	I2 <sup>ix</sup> —Y3—Y2 <sup>vi</sup>	95.413 (17)
Ni1—Y2—I3 <sup>iv</sup>	97.985 (17)	I4—Y3—Y2 <sup>vi</sup>	94.365 (16)
I1—Y2—I3 <sup>iv</sup>	90.836 (17)	I4 <sup>vi</sup> —Y3—Y2 <sup>vi</sup>	53.068 (13)
Ni1—Y2—I5	97.335 (17)	I5—Y3—Y2 <sup>vi</sup>	133.637 (19)
I1—Y2—I5	95.806 (19)	Y2 <sup>vii</sup> —Y3—Y2 <sup>vi</sup>	90.119 (16)
I3 <sup>iv</sup> —Y2—I5	162.14 (2)	Y1 <sup>viii</sup> —Y3—Y2 <sup>vi</sup>	59.523 (14)
Ni1—Y2—I4	96.070 (17)	Y1—Y3—Y2 <sup>vi</sup>	58.574 (14)
I1—Y2—I4	165.00 (2)	Y1 <sup>i</sup> —Ni1—Y1 <sup>vi</sup>	180.0
I3 <sup>iv</sup> —Y2—I4	86.140 (18)	Y1 <sup>i</sup> —Ni1—Y3 <sup>vi</sup>	88.391 (16)
I5—Y2—I4	83.167 (16)	Y1 <sup>vi</sup> —Ni1—Y3 <sup>vi</sup>	91.609 (16)
Ni1—Y2—I3	176.84 (2)	Y1 <sup>i</sup> —Ni1—Y3 <sup>i</sup>	91.609 (16)
I1—Y2—I3	84.194 (17)	Y1 <sup>vi</sup> —Ni1—Y3 <sup>i</sup>	88.391 (16)
I3 <sup>iv</sup> —Y2—I3	82.545 (17)	Y3 <sup>vi</sup> —Ni1—Y3 <sup>i</sup>	180.00 (2)
I5—Y2—I3	81.665 (16)	Y1 <sup>i</sup> —Ni1—Y2	90.083 (17)
I4—Y2—I3	80.844 (17)	Y1 <sup>vi</sup> —Ni1—Y2	89.917 (17)
Ni1—Y2—Y3 <sup>i</sup>	46.433 (12)	Y3 <sup>vi</sup> —Ni1—Y2	92.991 (17)
I1—Y2—Y3 <sup>i</sup>	52.481 (14)	Y3 <sup>i</sup> —Ni1—Y2	87.009 (17)
I3 <sup>iv</sup> —Y2—Y3 <sup>i</sup>	97.823 (18)	Y1 <sup>i</sup> —Ni1—Y2 <sup>x</sup>	89.917 (17)
I5—Y2—Y3 <sup>i</sup>	99.371 (18)	Y1 <sup>vi</sup> —Ni1—Y2 <sup>x</sup>	90.083 (17)
I4—Y2—Y3 <sup>i</sup>	142.503 (18)	Y3 <sup>vi</sup> —Ni1—Y2 <sup>x</sup>	87.009 (17)
I3—Y2—Y3 <sup>i</sup>	136.648 (19)	Y3 <sup>i</sup> —Ni1—Y2 <sup>x</sup>	92.991 (17)
Ni1—Y2—Y1 <sup>vi</sup>	44.765 (11)	Y2—Ni1—Y2 <sup>x</sup>	180.000 (7)

Symmetry codes: (i)  $x, y, z+1$ ; (ii)  $-x, -y-1, -z-2$ ; (iii)  $x, y-1, z$ ; (iv)  $-x+1, -y, -z$ ; (v)  $-x+1, -y, -z-1$ ; (vi)  $-x, -y, -z-1$ ; (vii)  $x, y, z-1$ ; (viii)  $-x, -y, -z-2$ ; (ix)  $x, y+1, z$ ; (x)  $-x, -y, -z$ .