



$\text{Ni}_3\text{Te}_2\text{O}_2(\text{PO}_4)_2(\text{OH})_4$, an open-framework structure isotypic with $\text{Co}_3\text{Te}_2\text{O}_2(\text{PO}_4)_2(\text{OH})_4$

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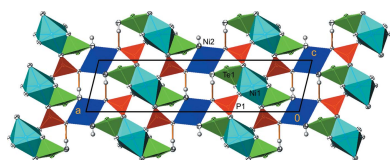
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Single crystals of $\text{Ni}_3(\text{TeO}(\text{OH})_2)_2(\text{PO}_4)_2$, trinickel(II) bis[(oxidodihydroxidotellurate(IV)) bis(phosphate)], were obtained by hydrothermal synthesis at 483 K, starting from $\text{NiCO}_3 \cdot 2\text{Ni}(\text{OH})_2$, TeO_2 and H_3PO_4 in a molar ratio of 1:2:2. The crystal structure of $\text{Ni}_3\text{Te}_2\text{O}_2(\text{PO}_4)_2(\text{OH})_4$ is isotypic with that of $\text{Co}_3\text{Te}_2\text{O}_2(\text{PO}_4)_2(\text{OH})_4$ [Zimmermann *et al.* (2011). *J. Solid State Chem.* **184**, 3080–3084]. The asymmetric unit comprises two Ni (site symmetries $\bar{1}$, $2/m$) one Te (m), one P (m), five O (three m , two 1) and one H (1) sites. The tellurium(IV) atom shows a coordination number of five, with the corresponding $[\text{TeO}_3(\text{OH})_2]$ polyhedron having a distorted square-pyramidal shape. The two Ni^{II} atoms are both octahedrally coordinated but form different structural elements: one constitutes chains made up from edge-sharing $[\text{NiO}_6]$ octahedra extending parallel to $[010]$, and the other isolated $[\text{NiO}_2(\text{OH})_4]$ octahedra. The two kinds of nickel/oxygen octahedra are connected by the $[\text{TeO}_3(\text{OH})_2]$ pyramids and the $[\text{PO}_4]$ tetrahedra through edge- and corner-sharing into a three-dimensional framework structure with channels extending parallel to $[010]$. Hydrogen bonds of medium strength between the hydroxy groups and one of the phosphate O atoms consolidate the packing. A quantitative structure comparison between $\text{Ni}_3\text{Te}_2\text{O}_2(\text{PO}_4)_2(\text{OH})_4$ and $\text{Co}_3\text{Te}_2\text{O}_2(\text{PO}_4)_2(\text{OH})_4$ is made.

1. Chemical context

The crystal chemistry of Te^{IV} -containing compounds is very diverse and strongly influenced by the stereochemically active $5s^2$ lone pair. The space requirement of the latter frequently results in one-sided and low-symmetric coordination spheres around Te^{IV} , as surveyed recently for the vast family of oxidotellurates(IV) (Christy *et al.*, 2016). The polarities and shapes of corresponding oxidotellurate(IV) anions can be utilized in the search for new compounds with non-centrosymmetric structures. The absence of an inversion centre is a precondition for a substance to have ferro-, pyro- or piezoelectric properties or to have non-linear optical properties (Ok *et al.*, 2006). Combining oxidotellurates(IV) with additional (transition) metal cations often leads to open-framework structures because of the space required for the $5s^2$ lone pair. This way, either channels can be integrated within three-dimensional frameworks, or layers, chains or clusters of building blocks can be formed (Stöger & Weil, 2013). Incorporating additional anions into transition-metal oxidotellurates(IV) increases the possibilities for structural diversification. Following this strategy, several mixed-anion oxidotellurates(IV) have been characterized over the last decade, including sulfates [*e.g.* $\text{Cd}_4(\text{SO}_4)(\text{TeO}_3)_3$; Weil & Shir Khanlou, 2017], selenates [*e.g.* $\text{Hg}_3(\text{SeO}_4)(\text{TeO}_3)$; Weil &



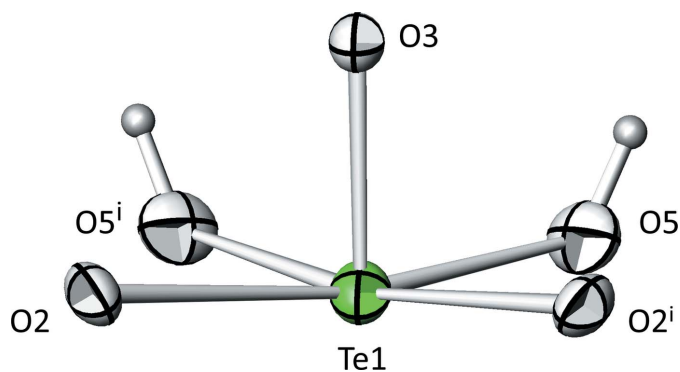


Figure 1
The square-pyramidal $[\text{TeO}_3(\text{OH})_2]$ polyhedron in the title compound. Displacement ellipsoids are drawn at the 90% probability level. [Symmetry code: (i) $x, -y + 1, z$.]

Shirkhanlou, 2015], nitrates [e.g. $\text{Ca}_6\text{Te}_5\text{O}_{15}(\text{NO}_3)_2$; Stöger & Weil, 2013] or phosphates [e.g. $\text{Co}_3\text{Te}_2\text{O}_2(\text{PO}_4)_2(\text{OH})_4$; Zimmermann *et al.*, 2011].

In this communication we describe the synthesis and crystal structure analysis of $\text{Ni}_3\text{Te}_2\text{O}_2(\text{PO}_4)_2(\text{OH})_4$, which is isotopic with its cobalt(II) analogue. The two structures are quantitatively compared.

2. Structural commentary

Of the ten atoms in the asymmetric unit (2 Ni, 1 Te, 1 P, 5 O, 1 H), seven are situated on special positions. Ni1 is located on an inversion centre (Wyckoff position 4 *f*), Ni2 on a site with symmetry 2/*m* (2 *b*), Te1 and P1 both possess site symmetry *m* (4 *i*), and three of the oxygen sites (O1, O3, O4) are likewise located on a mirror plane (4 *i*) while the other two oxygen atoms and the hydrogen atom (O2, O5, H1) are located on general positions (8 *j*).

Both nickel atoms are coordinated octahedrally but otherwise show a different environment. Ni1 is surrounded by six

Table 1
Comparison of bond lengths (Å) in the isotopic $M_3\text{Te}_2\text{O}_2(\text{PO}_4)_2(\text{OH})_4$ compounds ($M = \text{Ni}, \text{Co}^{\text{II}}$).

	$M = \text{Ni}$	$M = \text{Co}$
Te1—O3	1.866 (2)	1.861 (4)
Te1—O5	2.0002 (18)	1.994 (3)
Te1—O2	2.3093 (18)	2.331 (3)
M1—O1	2.0343 (16)	2.051 (3)
M1—O2	2.0457 (18)	2.079 (3)
M1—O3	2.0940 (18)	2.143 (3)
M2—O4	2.061 (2)	2.076 (4)
M2—O5	2.0928 (19)	2.147 (3)
P1—O4	1.534 (3)	1.530 (4)
P1—O1	1.538 (2)	1.541 (5)
P1—O2	1.5449 (18)	1.550 (3)

(a) Unit-cell parameters: $a = 19.4317$ (10), $b = 6.0249$ (3), $c = 4.7788$ (2) Å, $\beta = 103.139$ (5)°, $V = 544.83$ (5) Å³ (Zimmermann *et al.*, 2011).

oxygen atoms (O1, O2, O3 and their symmetry-related counterparts) and forms chains of edge-sharing $[\text{Ni1O}_6]$ octahedra extending parallel to [010]. The $\infty^1[\text{Ni1O}_{4/2}\text{O}_{2/1}]$ chains are not entirely straight; the octahedra are tilted against each other with every second unit being oriented in the same direction. The three pairs of Ni1—O bond lengths are rather similar (Table 1), with an average length of 2.058 Å. The distance between neighbouring Ni1 atoms in a chains amounts to 2.9717 (11) Å. Ni2 is coordinated by two O atoms (O4 and its symmetry-related counterpart) in axial positions and by four hydroxide groups (O5 and its three symmetry-related counterparts) in the equatorial positions. The latter have a slightly longer bond than the former ($\Delta = 0.032$ Å), with an average bond length of 2.084 Å for the six O atoms. The $[\text{Ni2O}_2(\text{OH})_4]$ octahedra are isolated from each other and are also not linked to the $\infty^1[\text{Ni1O}_{4/2}\text{O}_{2/1}]$ chains.

Te1 is coordinated by five oxygen atoms, two of them being hydroxide groups. The surrounding atoms form a distorted square pyramid (Fig. 1), a coordination polyhedron that is comparatively rare in the crystal chemistry of oxidotellur-

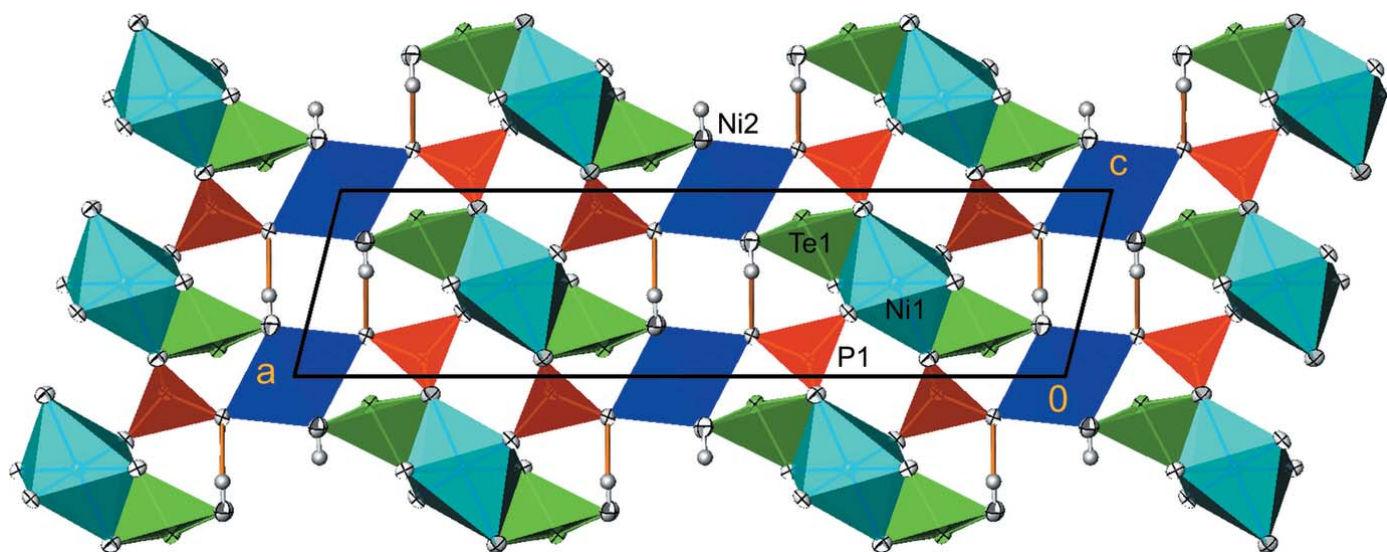


Figure 2
The crystal structure of $\text{Ni}_3\text{Te}_2\text{O}_2(\text{PO}_4)_2(\text{OH})_4$ in a projection along [010]. Displacement ellipsoids are drawn at the 90% probability level; hydrogen bonds are shown as orange lines.

Table 2
Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$O5-H1\cdots O4^i$	0.80 (5)	2.03 (5)	2.812 (3)	164 (6)

Symmetry code: (i) $x, y + 1, z$.

ates(IV), with a trigonal pyramid (TeO_3^{2-}) as the most commonly observed type of anion (Christy *et al.*, 2016). The Te1 atom is displaced from the basal plane of the pyramid by 0.1966 (2) Å. The two symmetry-related O2 atoms defining one side of the basal plane exhibit a significantly larger distance [2.3094 (18) Å] from Te than the two hydroxy groups [2.0002 (18) Å] on the other side. The oxygen atom closest [O3, 1.866 (2) Å] to Te1 lies at the apex of the pyramid. The calculated bond-valence sum (BVS; Brown, 2002) of Te1 is 4.05 valence units (v.u.) based on the parameters of Brese & O’Keeffe (1991). Using the revised parameters of Mills & Christy (2013), a BVS of 3.93 v.u. was calculated. The $[TeO_3(OH)_2]$ units are not connected to each other but share two edges with $[Ni1O_6]$ octahedra and two corners, being the hydroxide groups, with $[Ni2O_2(OH)_4]$ octahedra, as well as a corner of the phosphate tetrahedra. In this way, a three-dimensional framework structure is obtained with channels running parallel to [010]. The free-electron pairs point into the smaller type of channels whereas the hydrogen atoms of the hydroxy group protrude into the larger type of channels. This results in hydrogen bonds of medium strength, with the OH groups linking to opposite O atoms (Fig. 2; Table 2).

As a result of the similar ionic radii (Shannon, 1976) of six-coordinated Ni^{2+} (0.69 Å) and Co^{2+} (0.75 Å, assuming a high-spin d^7 state), the comparable bond lengths in the two isotopic structures differ only marginally (Table 1). The two structures were also quantitatively compared using the program *compstru* (de la Flor *et al.*, 2016). The absolute distances between paired atoms are 0 Å for Ni1/Co1, 0 Å for Ni2/Co2, 0.0213 Å for P1, 0.0289 Å for O1, 0.0289 Å for O2, 0.0342 Å for O3, 0.0192 Å for O4 and 0.0271 Å for O5. The degree of lattice distortion is 0.0072, the arithmetic mean of the distance between paired atoms is 0.0227 Å, and the measure of similarity is 0.011.

3. Synthesis and crystallization

Crystals of $Ni_3Te_2O_2(PO_4)_2(OH)_4$ were obtained under hydrothermal conditions. The starting materials, 0.1796 g (0.591 mmol) $NiCO_3 \cdot 2Ni(OH)_2$, 0.1870 g TeO_2 (1.172 mmol) and 0.16 g 85% H_3PO_4 (1.4 mmol), were weighed into a small Teflon vessel with a volume of *ca* 3 ml. The reactants were mixed, and the vessel filled to about two thirds with deionized water. The reaction vessel was heated inside a steel autoclave at 483 K for 7 d; the autoclave was removed from the oven and allowed to cool to room temperature over about four hours. A bright-green solid besides small amounts of a pale-yellow powder was obtained as the reaction product. X-ray powder diffraction of the bulk revealed $Ni_3Te_2O_2(PO_4)_2(OH)_4$ as the

Table 3
Experimental details.

Crystal data	$Ni_3Te_2O_2(PO_4)_2(OH)_4$
Chemical formula	721.30
M_r	Monoclinic, $C2/m$
Crystal system, space group	300
Temperature (K)	19.241 (7), 5.943 (2), 4.7808 (18)
a, b, c (Å)	104.094 (8)
β (°)	530.3 (3)
V (Å ³)	2
Z	Mo $K\alpha$
Radiation type	11.05
μ (mm ⁻¹)	0.08 × 0.06 × 0.03
Crystal size (mm)	
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (<i>SADABS</i> ; Bruker, 2016)
T_{min}, T_{max}	0.600, 0.747
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	12917, 1292, 1212
R_{int}	0.054
$(\sin \theta/\lambda)_{max}$ (Å ⁻¹)	0.820
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.022, 0.058, 1.11
No. of reflections	1292
No. of parameters	63
H-atom treatment	All H-atom parameters refined
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å ⁻³)	3.84, -1.39

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXL* (Sheldrick, 2015), *ATOMS* (Dowty, 2006) and *pubCIF* (Westrip, 2010).

main product and TeO_2 (corresponding to the pale-yellow powder) as a side product. A light-green block-shaped single crystal of $Ni_3Te_2O_2(PO_4)_2(OH)_4$ was selected for the diffraction experiment.

4. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. Atom labels and starting coordinates for refinement were adopted from the isotopic $Co_3Te_2O_2(PO_4)_2(OH)_4$ structure (Zimmermann *et al.*, 2011). The hydrogen atom of the hydroxy group was located in a difference-Fourier map and was refined freely. The remaining maximum electron density of $3.6 e^- \text{Å}^{-3}$ is located 0.71 Å from P1. Modelling the corresponding site as a minor disorder component lead to unrealistic P—O distances and physically non-reasonable displacement parameters. We therefore did not consider this site in the final model.

Acknowledgements

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Ni₃Te₂O₂(PO₄)₂(OH)₄, an open-framework structure isotypic with Co₃Te₂O₂(PO₄)₂(OH)₄

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Computing details

Data collection: *APEX3* (Bruker, 2016); cell refinement: *SAINTE* (Bruker, 2016); data reduction: *SAINTE* (Bruker, 2016); program(s) used to solve structure: coordinates from isotypic structure; program(s) used to refine structure: *SHELXL* (Sheldrick, 2015); molecular graphics: *ATOMS* (Dowty, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Trinickel(II) bis(oxidodihydroxidotellurate(IV)) bis(phosphate)

Crystal data

Ni₃Te₂O₂(PO₄)₂(OH)₄
M_r = 721.30
 Monoclinic, *C2/m*
a = 19.241 (7) Å
b = 5.943 (2) Å
c = 4.7808 (18) Å
 β = 104.094 (8)°
V = 530.3 (3) Å³
Z = 2

F(000) = 668
D_x = 4.518 Mg m⁻³
 Mo *K*α radiation, λ = 0.71073 Å
 Cell parameters from 8089 reflections
 θ = 3.6–35.3°
 μ = 11.05 mm⁻¹
T = 300 K
 Block, light green
 0.08 × 0.06 × 0.03 mm

Data collection

Bruker APEXII CCD
 diffractometer
 ω - and φ -scan
 Absorption correction: multi-scan
 (*SADABS*; Bruker, 2016)
T_{min} = 0.600, *T_{max}* = 0.747
 12917 measured reflections

1292 independent reflections
 1212 reflections with *I* > 2σ(*I*)
R_{int} = 0.054
 θ_{\max} = 35.7°, θ_{\min} = 3.6°
h = -31→31
k = -9→9
l = -7→7

Refinement

Refinement on *F*²
 Least-squares matrix: full
R[*F*² > 2σ(*F*²)] = 0.022
wR(*F*²) = 0.058
S = 1.11
 1292 reflections
 63 parameters
 0 restraints

Primary atom site location: isomorphous
 structure methods
 Hydrogen site location: difference Fourier map
 All H-atom parameters refined
 $w = 1/[\sigma^2(F_o^2) + (0.0264P)^2 + 2.8929P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 3.84 \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{\min} = -1.39 \text{ e } \text{Å}^{-3}$

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Te1	0.39329 (2)	0.500000	0.84942 (4)	0.00797 (6)
Ni1	0.250000	0.250000	0.500000	0.00608 (8)
Ni2	0.500000	1.000000	1.000000	0.00680 (11)
P1	0.33875 (4)	0.000000	0.09068 (16)	0.00516 (13)
O1	0.30175 (13)	0.000000	0.3417 (5)	0.0075 (4)
O2	0.31714 (9)	0.2109 (3)	0.9006 (4)	0.0085 (3)
O3	0.32631 (13)	0.500000	0.4940 (5)	0.0075 (4)
O4	0.42002 (13)	0.000000	0.2189 (5)	0.0093 (4)
O5	0.45243 (10)	0.7393 (3)	0.7251 (4)	0.0110 (3)
H1	0.441 (3)	0.790 (10)	0.565 (11)	0.043 (14)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Te1	0.00681 (10)	0.00738 (9)	0.00868 (10)	0.000	-0.00009 (7)	0.000
Ni1	0.00630 (17)	0.00493 (16)	0.00686 (16)	0.00020 (12)	0.00132 (13)	-0.00027 (12)
Ni2	0.0063 (2)	0.0062 (2)	0.0081 (2)	0.000	0.00213 (19)	0.000
P1	0.0061 (3)	0.0051 (3)	0.0049 (3)	0.000	0.0026 (2)	0.000
O1	0.0095 (10)	0.0062 (9)	0.0084 (9)	0.000	0.0051 (8)	0.000
O2	0.0094 (7)	0.0071 (6)	0.0084 (6)	-0.0011 (5)	0.0009 (5)	0.0023 (5)
O3	0.0085 (10)	0.0060 (9)	0.0074 (9)	0.000	0.0008 (8)	0.000
O4	0.0062 (9)	0.0137 (10)	0.0077 (9)	0.000	0.0013 (7)	0.000
O5	0.0098 (7)	0.0118 (7)	0.0109 (7)	-0.0046 (6)	0.0017 (6)	-0.0004 (6)

Geometric parameters (\AA , $^\circ$)

Te1—O3	1.866 (2)	Ni1—Ni1 ^{iv}	2.9717 (11)
Te1—O5	2.0002 (18)	Ni2—O4 ^v	2.061 (2)
Te1—O5 ⁱ	2.0002 (18)	Ni2—O4 ^{vi}	2.061 (2)
Te1—O2 ⁱ	2.3093 (18)	Ni2—O5 ^{vii}	2.0928 (19)
Te1—O2	2.3094 (18)	Ni2—O5 ^{viii}	2.0928 (19)
Ni1—O1	2.0343 (16)	Ni2—O5 ^{ix}	2.0928 (19)
Ni1—O1 ⁱⁱ	2.0343 (16)	Ni2—O5	2.0928 (19)
Ni1—O2 ⁱⁱ	2.0457 (18)	P1—O4	1.534 (3)
Ni1—O2	2.0457 (18)	P1—O1	1.538 (2)
Ni1—O3 ⁱⁱ	2.0940 (18)	P1—O2 ^x	1.5449 (18)
Ni1—O3	2.0940 (18)	P1—O2 ^{xi}	1.5449 (18)
Ni1—Ni1 ⁱⁱⁱ	2.9717 (11)		

O3—Te1—O5	92.64 (8)	O4 ^{vi} —Ni2—O5 ^{viii}	93.01 (7)
O3—Te1—O5 ⁱ	92.64 (8)	O5 ^{vii} —Ni2—O5 ^{viii}	84.49 (11)
O5—Te1—O5 ⁱ	90.65 (11)	O4 ^v —Ni2—O5 ^{ix}	93.01 (7)
O3—Te1—O2 ⁱ	77.35 (7)	O4 ^{vi} —Ni2—O5 ^{ix}	86.99 (7)
O5—Te1—O2 ⁱ	85.64 (8)	O5 ^{vii} —Ni2—O5 ^{ix}	95.51 (11)
O5 ⁱ —Te1—O2 ⁱ	169.13 (7)	O5 ^{viii} —Ni2—O5 ^{ix}	180.0
O3—Te1—O2	77.35 (7)	O4 ^v —Ni2—O5	86.99 (7)
O5—Te1—O2	169.13 (7)	O4 ^{vi} —Ni2—O5	93.01 (7)
O5 ⁱ —Te1—O2	85.64 (8)	O5 ^{vii} —Ni2—O5	180.0
O2 ⁱ —Te1—O2	96.14 (9)	O5 ^{viii} —Ni2—O5	95.51 (11)
O1—Ni1—O1 ⁱⁱ	180.0	O5 ^{ix} —Ni2—O5	84.49 (11)
O1—Ni1—O2 ⁱⁱ	89.40 (9)	O4—P1—O1	107.98 (14)
O1 ⁱⁱ —Ni1—O2 ⁱⁱ	90.60 (9)	O4—P1—O2 ^x	109.71 (9)
O1—Ni1—O2	90.60 (9)	O1—P1—O2 ^x	110.48 (9)
O1 ⁱⁱ —Ni1—O2	89.40 (9)	O4—P1—O2 ^{xi}	109.71 (9)
O2 ⁱⁱ —Ni1—O2	180.0	O1—P1—O2 ^{xi}	110.48 (9)
O1—Ni1—O3 ⁱⁱ	83.98 (8)	O2 ^x —P1—O2 ^{xi}	108.48 (14)
O1 ⁱⁱ —Ni1—O3 ⁱⁱ	96.02 (8)	P1—O1—Ni1 ^{iv}	130.69 (6)
O2 ⁱⁱ —Ni1—O3 ⁱⁱ	78.95 (8)	P1—O1—Ni1	130.69 (6)
O2—Ni1—O3 ⁱⁱ	101.05 (8)	Ni1 ^{iv} —O1—Ni1	93.84 (10)
O1—Ni1—O3	96.02 (8)	P1 ^{xii} —O2—Ni1	131.38 (11)
O1 ⁱⁱ —Ni1—O3	83.98 (8)	P1 ^{xii} —O2—Te1	125.39 (10)
O2 ⁱⁱ —Ni1—O3	101.05 (8)	Ni1—O2—Te1	95.09 (6)
O2—Ni1—O3	78.95 (8)	Te1—O3—Ni1	108.58 (9)
O3 ⁱⁱ —Ni1—O3	180.0	Te1—O3—Ni1 ⁱⁱⁱ	108.58 (9)
O4 ^v —Ni2—O4 ^{vi}	180.00 (7)	Ni1—O3—Ni1 ⁱⁱⁱ	90.40 (10)
O4 ^v —Ni2—O5 ^{vii}	93.01 (7)	P1—O4—Ni2 ^{xiii}	127.69 (15)
O4 ^{vi} —Ni2—O5 ^{vii}	86.99 (7)	Te1—O5—Ni2	122.22 (9)
O4 ^v —Ni2—O5 ^{viii}	86.99 (7)		

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

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O5—H1 \cdots O4 ^{xiv}	0.80 (5)	2.03 (5)	2.812 (3)	164 (6)

Symmetry code: (xiv) $x, y+1, z$.