

(3,3'-{(1*E*,1'*E*)-1,1'-[Ethane-1,2-diylbis(azan-1-yl-1-ylidene- κ N)]bis(ethan-1-yl-1-ylidene)}dipyrazine 1-oxide- κ N⁴)bis-(nitrate- κ O)nickel(II) monohydrate

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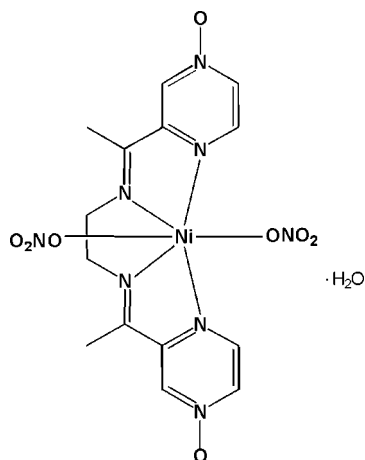
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.032; wR factor = 0.070; data-to-parameter ratio = 12.1.

In the title complex, $[\text{Ni}(\text{NO}_3)_2(\text{C}_{14}\text{H}_{16}\text{N}_6\text{O}_2)] \cdot \text{H}_2\text{O}$, the Ni^{II} atom, lying on a twofold rotation axis, is coordinated by a tetradentate 3,3'-{(1*E*,1'*E*)-1,1'-[ethane-1,2-diylbis(azan-1-yl-1-ylidene)]bis(ethan-1-yl-1-ylidene)}dipyrazine 1-oxide ligand and two mutually *trans* monodentate nitrate anions in a distorted octahedral geometry. The lattice water molecule is located on a twofold rotation axis. The complex molecules are linked by the water molecules through O—H...O hydrogen bonds into a chain along [001]. Further C—H...O hydrogen bonds lead to the formation of a three-dimensional network.

Related literature

For background to complexes with heterocyclic aromatic *N*-oxide ligands, see: Chupakhin *et al.* (2011); Karayannis *et al.* (1973); Nizhnik *et al.* (2008); Sarma *et al.* (2010). For related structures, see: Banerjee *et al.* (2004); Padhi & Manivannan (2007).



Experimental

Crystal data

$[\text{Ni}(\text{NO}_3)_2(\text{C}_{14}\text{H}_{16}\text{N}_6\text{O}_2)] \cdot \text{H}_2\text{O}$	$V = 1960.8 (10) \text{ \AA}^3$
$M_r = 501.05$	$Z = 4$
Monoclinic, $C2/c$	Mo $K\alpha$ radiation
$a = 16.993 (5) \text{ \AA}$	$\mu = 1.06 \text{ mm}^{-1}$
$b = 16.218 (5) \text{ \AA}$	$T = 293 \text{ K}$
$c = 7.754 (2) \text{ \AA}$	$0.23 \times 0.21 \times 0.19 \text{ mm}$
$\beta = 113.427 (3)^\circ$	

Data collection

Bruker APEXII CCD diffractometer	6930 measured reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	1828 independent reflections
$T_{\min} = 0.793$, $T_{\max} = 0.824$	1515 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.034$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.032$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.070$	$\Delta\rho_{\text{max}} = 0.26 \text{ e \AA}^{-3}$
$S = 1.04$	$\Delta\rho_{\text{min}} = -0.23 \text{ e \AA}^{-3}$
1828 reflections	
151 parameters	
1 restraint	

Table 1

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$\text{O5}-\text{H1W} \cdots \text{O2}^{\text{i}}$	0.78 (12)	2.46 (14)	3.086 (4)	139 (14)
$\text{C3}-\text{H3A} \cdots \text{O2}^{\text{ii}}$	0.93	2.58	3.389 (3)	146
$\text{C6}-\text{H6A} \cdots \text{O1}^{\text{iii}}$	0.96	2.56	3.453 (4)	156

 Symmetry codes: (i) $x + 1, y, z$; (ii) $x + \frac{1}{2}, -y + \frac{1}{2}, z + \frac{1}{2}$; (iii) $-x + \frac{1}{2}, y + \frac{1}{2}, -z + \frac{1}{2}$.

Data collection: APEX2 (Bruker, 2007); cell refinement: SAINT (Bruker, 2007); data reduction: SAINT; 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: SHELXTL (Sheldrick, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2621).

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supporting information

Acta Cryst. (2013). E69, m263–m264 [https://doi.org/10.1107/S1600536813009355]

(3,3'-{(1*E*,1'*E*)-1,1'-[Ethane-1,2-diylbis(azan-1-yl-1-ylidene- κ N)]bis(ethan-1-yl-1-ylidene)}dipyrazine 1-oxide- κ N⁴)bis(nitrato- κ O)nickel(II) monohydrate

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S1. Comment

Interest in heterocyclic aromatic N-oxides has flourished because of their practical impact on biological activity (Sarma *et al.*, 2010). Several aromatic N-oxide derivatives capable of forming biologically active metal complexes have been reported (Nizhnik *et al.*, 2008). Indeed, most coordinative studies of N-oxide donors have been carried out using pyridine-*N*-oxide (Karayannis *et al.*, 1973) or bipyridine-*N,N'*-bisoxide. However, complexes containing ligands with pyrazine single N-oxide site are few (Chupakhin *et al.*, 2011). Herein, we synthesize a new bipyrazine N-oxide Schiff base 3,3'-(1*E*,1'*E*)-1,1'-[ethane-1,2-diylbis(azan-1-yl-1-ylidene)] bis(ethan-1-yl-1-ylidene)dipyrazine-1-oxide (*L*) and its Ni(II) complex.

In the title complex, the Ni^{II} atom, lying on a twofold rotation axis, exhibits a distorted octahedral geometry, defined by four N atoms from the *L* ligand, occupying the equatorial plane, and two axial O atoms from two monodentate nitrate anions (Fig. 1). The equatorial Ni—N distances [Ni1—N1 = 2.0855 (19) and Ni1—N3 = 2.0183 (19) Å] are in a normal range for this class of compounds and also very similar to those of Ni—N(pyridine) and Ni—N(imine) found in analogue complexes (Banerjee *et al.*, 2004; Padhi & Manivannan, 2007). Hydrogen bonding plays an important role in the formation of the crystal structure (Table 1). The lattice water molecule is located on a twofold rotation axis and connect two symmetry-related complex molecules through O—H \cdots O hydrogen bonds, so forming a chain structure along [001] (Fig. 2). C—H \cdots O hydrogen bonds lead to a three-dimensional network (Fig. 3).

S2. Experimental

Synthesis of 2-acetylpyrazine-*N*-oxide: 2-Acetylpyrazine (12.2 g, 0.1 mol), glacial acetic acid (75 ml) and 30% hydrogen peroxide (14 ml) were heated with reflux at 70–80°C for 3 h. Additional 30% H₂O₂ (10 ml) was added and the temperature was maintained at 70–80°C for a further 10 h. The solvent was removed by rotary evaporation and upon standing brown yellow solid was formed, filtered and dried.

Synthesis of the *L* ligand : 1,2-Diaminoethane (0.100 g, 1.66 mmol) in 5 cm³ methanol was added dropwise to a hot stirred solution of 2-acetylpyrazine-*N*-oxide (0.455 g, 3.3 mmol) in 25 ml of methanol. The mixture was refluxed for 5 h. Brown precipitate was filtered, washed with methanol and air dried (yield: 0.68 g, 68.7%).

Synthesis of the title complex: Ni(NO₃)₂·6H₂O (0.290 g, 0.1 mmol) in 5 cm³ of CH₃CN was added dropwise to a hot stirred solution of the ligand *L* (0.030 g, 0.1 mmol) in a mixture of CH₃OH/CH₃CN (*v/v* = 2:1) and the mixture was stirred for 30 min. Diethyl ether was slowly diffused into the solution and block brown crystals suitable for X-ray diffraction analysis were collected by filtration within two weeks.

S3. Refinement

C-bound H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 (aromatic), 0.97 (CH₂) and 0.96 (CH₃) Å and with $U_{\text{iso}}(\text{H}) = 1.2(1.5 \text{ for methyl})U_{\text{eq}}(\text{C})$. The water H atom was located on a difference Fourier map and refined isotropically.

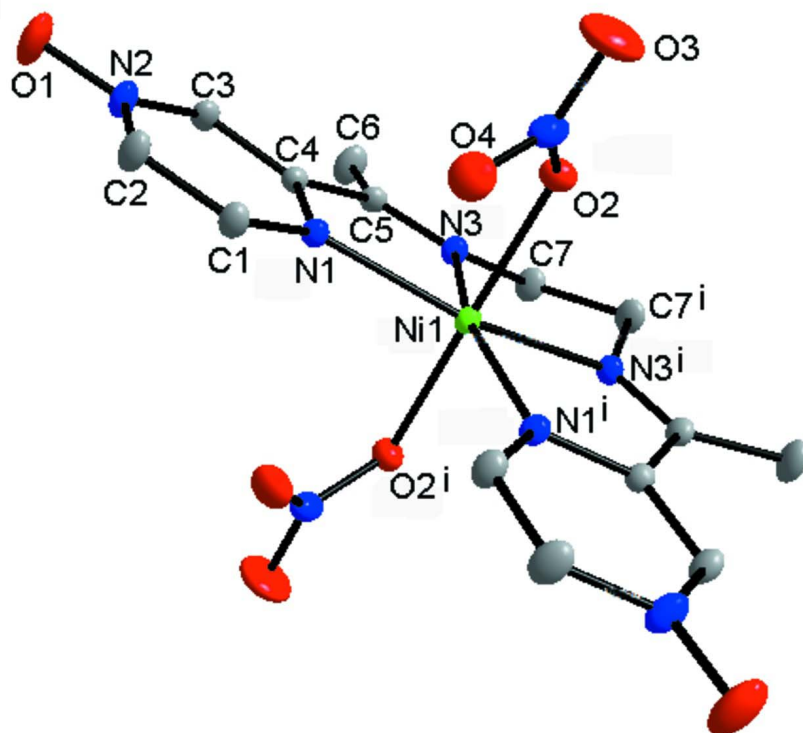


Figure 1

The molecular structure of the title complex. Displacement ellipsoids are drawn at the 30% probability level. H atoms and water molecule have been omitted for clarity. [Symmetry code: (i) $-x, y, -z+1/2$.]

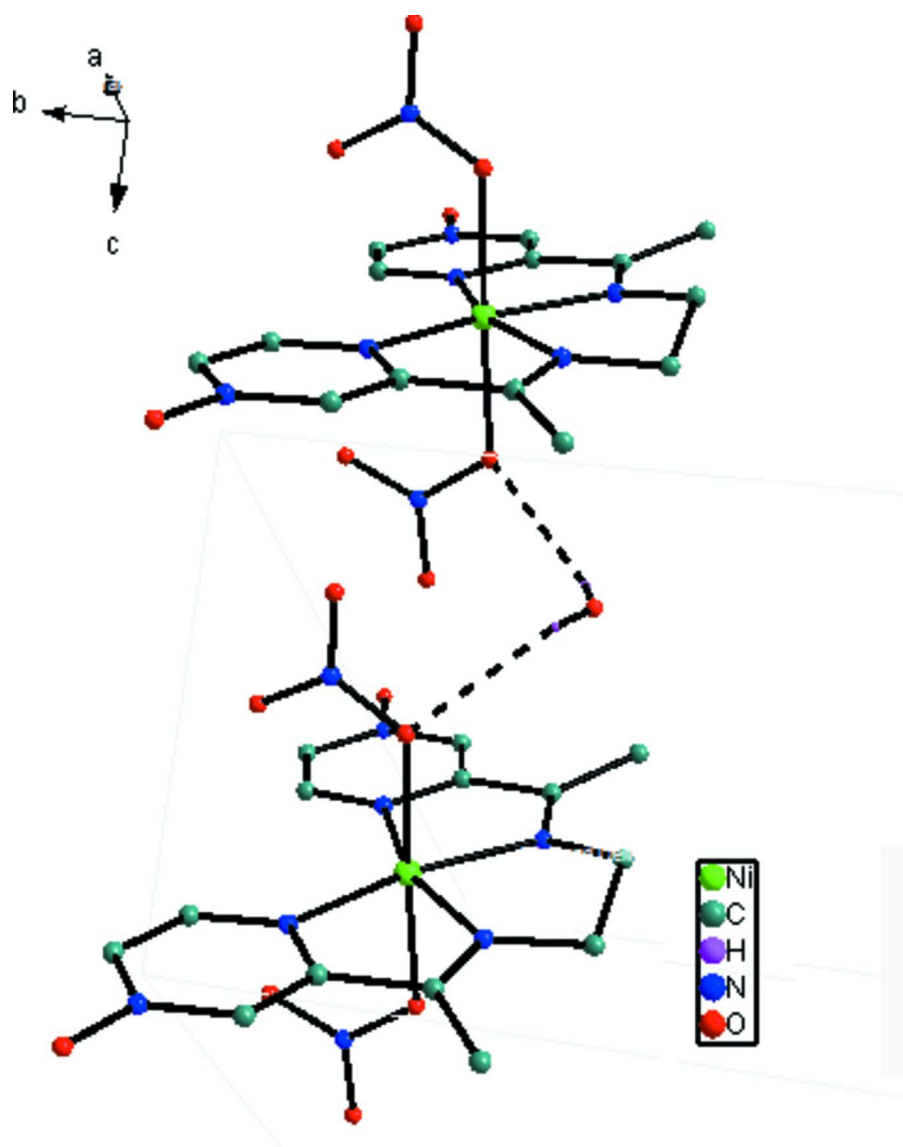


Figure 2

O—H...O hydrogen bonds (dashed lines) between water molecule and two adjacent complex molecules, which lead to a chain along [001]. H atoms not involved in hydrogen bonds are omitted for clarity.

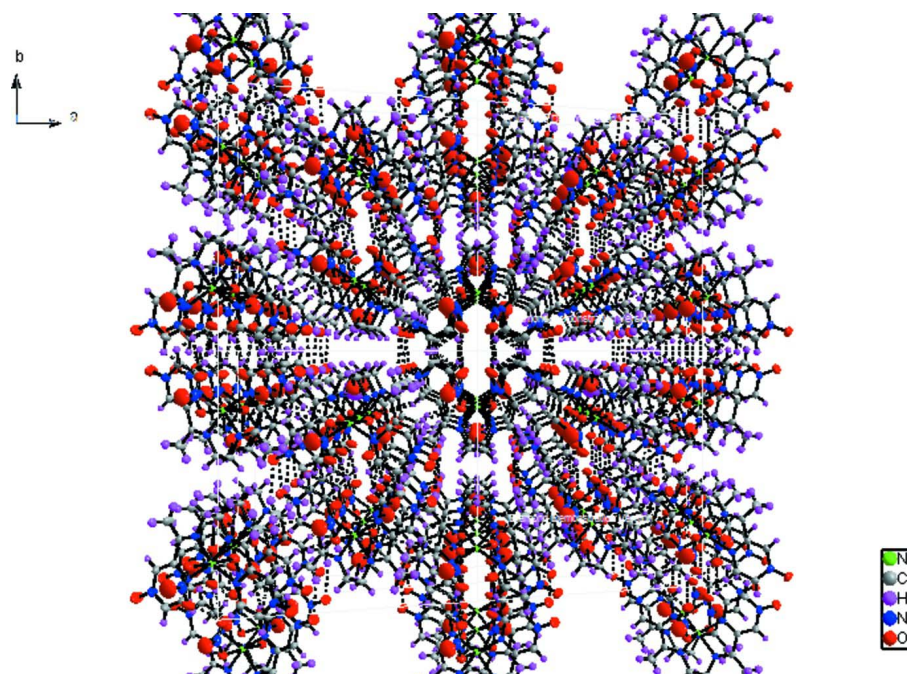


Figure 3

The crystal packing of the title complex, viewed along the c axis. Hydrogen bonds are shown as dashed lines.

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Crystal data

[Ni(NO₃)₂(C₁₄H₁₆N₆O₂)]·H₂O

$M_r = 501.05$

Monoclinic, $C2/c$

Hall symbol: $-C\ 2yc$

$a = 16.993\ (5)\ \text{\AA}$

$b = 16.218\ (5)\ \text{\AA}$

$c = 7.754\ (2)\ \text{\AA}$

$\beta = 113.427\ (3)^\circ$

$V = 1960.8\ (10)\ \text{\AA}^3$

$Z = 4$

$F(000) = 1032$

$D_x = 1.697\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 2097 reflections

$\theta = 2.5\text{--}23.4^\circ$

$\mu = 1.06\ \text{mm}^{-1}$

$T = 293\ \text{K}$

Block, brown

$0.23 \times 0.21 \times 0.19\ \text{mm}$

Data collection

Bruker APEXII CCD
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan
(*SADABS*; Sheldrick, 1996)

$T_{\min} = 0.793$, $T_{\max} = 0.824$

6930 measured reflections

1828 independent reflections

1515 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.034$

$\theta_{\max} = 25.5^\circ$, $\theta_{\min} = 2.5^\circ$

$h = -20 \rightarrow 20$

$k = -19 \rightarrow 18$

$l = -9 \rightarrow 9$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.032$
 $wR(F^2) = 0.070$
 $S = 1.04$
 1828 reflections
 151 parameters
 1 restraint
 Primary atom site location: structure-invariant
 direct methods

Secondary atom site location: difference Fourier
 map
 Hydrogen site location: inferred from
 neighbouring sites
 H atoms treated by a mixture of independent
 and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0282P)^2 + 1.9388P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.26 \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{\min} = -0.23 \text{ e } \text{Å}^{-3}$

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 (Å^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Ni1	0.0000	0.22687 (3)	0.2500	0.02616 (14)
C1	0.11963 (16)	0.08324 (15)	0.4745 (4)	0.0364 (6)
H1	0.0798	0.0464	0.3947	0.044*
C2	0.19290 (17)	0.05229 (17)	0.6107 (4)	0.0461 (7)
H2	0.2022	-0.0043	0.6214	0.055*
C3	0.23627 (16)	0.18666 (15)	0.7095 (3)	0.0352 (6)
H3A	0.2760	0.2238	0.7884	0.042*
C4	0.16163 (14)	0.21473 (14)	0.5717 (3)	0.0282 (5)
C5	0.13925 (15)	0.30501 (15)	0.5473 (3)	0.0308 (5)
C6	0.19245 (18)	0.36564 (17)	0.6900 (4)	0.0528 (8)
H6A	0.1707	0.4202	0.6515	0.079*
H6B	0.2507	0.3625	0.7015	0.079*
H6C	0.1902	0.3533	0.8091	0.079*
C7	0.03112 (17)	0.40247 (15)	0.3526 (4)	0.0397 (6)
H7A	0.0746	0.4444	0.3731	0.048*
H7B	0.0006	0.4150	0.4319	0.048*
H1W	0.961 (7)	0.337 (9)	0.670 (19)	0.65 (10)*
N1	0.10253 (12)	0.16371 (12)	0.4506 (3)	0.0289 (5)
N2	0.25192 (14)	0.10433 (13)	0.7301 (3)	0.0437 (6)
N3	0.07187 (12)	0.32112 (11)	0.4021 (3)	0.0302 (5)
N4	-0.08220 (14)	0.16354 (17)	0.4974 (3)	0.0462 (6)
O1	0.32056 (13)	0.07731 (13)	0.8616 (3)	0.0739 (7)
O2	-0.06595 (11)	0.22970 (11)	0.4291 (2)	0.0413 (4)
O3	-0.11896 (19)	0.16980 (18)	0.6043 (4)	0.0997 (10)

O4	-0.06439 (14)	0.09594 (13)	0.4506 (3)	0.0603 (6)
O5	1.0000	0.3575 (3)	0.7500	0.0993 (13)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0253 (2)	0.0206 (2)	0.0280 (2)	0.000	0.00583 (18)	0.000
C1	0.0348 (14)	0.0261 (14)	0.0407 (14)	-0.0021 (11)	0.0071 (12)	0.0025 (11)
C2	0.0413 (16)	0.0265 (14)	0.0576 (18)	0.0033 (12)	0.0059 (14)	0.0085 (13)
C3	0.0284 (14)	0.0325 (14)	0.0376 (14)	-0.0053 (11)	0.0055 (11)	0.0030 (11)
C4	0.0262 (12)	0.0287 (13)	0.0288 (12)	-0.0019 (10)	0.0100 (10)	0.0012 (10)
C5	0.0292 (14)	0.0282 (13)	0.0336 (13)	-0.0052 (11)	0.0110 (11)	-0.0025 (10)
C6	0.0490 (18)	0.0387 (17)	0.0501 (17)	-0.0044 (14)	-0.0021 (14)	-0.0097 (14)
C7	0.0454 (17)	0.0208 (13)	0.0458 (15)	0.0011 (11)	0.0106 (13)	-0.0029 (11)
N1	0.0278 (11)	0.0226 (10)	0.0336 (11)	-0.0015 (9)	0.0092 (9)	0.0011 (9)
N2	0.0331 (13)	0.0363 (13)	0.0476 (13)	0.0022 (10)	0.0011 (11)	0.0110 (10)
N3	0.0330 (12)	0.0218 (11)	0.0330 (11)	-0.0011 (9)	0.0102 (10)	-0.0021 (9)
N4	0.0339 (13)	0.0634 (17)	0.0408 (13)	-0.0025 (12)	0.0144 (11)	0.0077 (12)
O1	0.0487 (13)	0.0509 (14)	0.0815 (16)	0.0081 (11)	-0.0169 (12)	0.0172 (12)
O2	0.0453 (11)	0.0378 (10)	0.0453 (10)	0.0033 (9)	0.0226 (9)	0.0051 (9)
O3	0.118 (2)	0.125 (2)	0.100 (2)	0.0031 (19)	0.090 (2)	0.0153 (17)
O4	0.0714 (15)	0.0405 (12)	0.0721 (15)	-0.0098 (11)	0.0319 (12)	0.0052 (11)
O5	0.126 (4)	0.113 (3)	0.068 (2)	0.000	0.047 (2)	0.000

Geometric parameters (Å, °)

Ni1—N3	2.0183 (19)	C5—C6	1.488 (3)
Ni1—N1	2.0855 (19)	C6—H6A	0.9600
Ni1—O2	2.1032 (17)	C6—H6B	0.9600
C1—N1	1.334 (3)	C6—H6C	0.9600
C1—C2	1.368 (3)	C7—N3	1.468 (3)
C1—H1	0.9300	C7—C7 ⁱ	1.521 (5)
C2—N2	1.355 (3)	C7—H7A	0.9700
C2—H2	0.9300	C7—H7B	0.9700
C3—N2	1.358 (3)	N2—O1	1.283 (3)
C3—C4	1.371 (3)	N4—O3	1.224 (3)
C3—H3A	0.9300	N4—O4	1.230 (3)
C4—N1	1.351 (3)	N4—O2	1.275 (3)
C4—C5	1.506 (3)	O5—H1W	0.780 (5)
C5—N3	1.274 (3)		
N3—Ni1—N3 ⁱ	81.53 (11)	N3—C5—C4	113.8 (2)
N3—Ni1—N1 ⁱ	160.01 (8)	C6—C5—C4	120.1 (2)
N3 ⁱ —Ni1—N1 ⁱ	78.71 (8)	C5—C6—H6A	109.5
N3—Ni1—N1	78.71 (8)	C5—C6—H6B	109.5
N3 ⁱ —Ni1—N1	160.01 (8)	H6A—C6—H6B	109.5
N1 ⁱ —Ni1—N1	121.17 (11)	C5—C6—H6C	109.5
N3—Ni1—O2 ⁱ	90.67 (7)	H6A—C6—H6C	109.5

N3 ⁱ —Ni1—O2 ⁱ	87.44 (7)	H6B—C6—H6C	109.5
N1 ⁱ —Ni1—O2 ⁱ	91.42 (7)	N3—C7—C7 ⁱ	109.44 (14)
N1—Ni1—O2 ⁱ	89.81 (7)	N3—C7—H7A	109.8
N3—Ni1—O2	87.44 (7)	C7 ⁱ —C7—H7A	109.8
N3 ⁱ —Ni1—O2	90.67 (7)	N3—C7—H7B	109.8
N1 ⁱ —Ni1—O2	89.81 (7)	C7 ⁱ —C7—H7B	109.8
N1—Ni1—O2	91.42 (7)	H7A—C7—H7B	108.2
O2 ⁱ —Ni1—O2	177.50 (10)	C1—N1—C4	116.2 (2)
N1—C1—C2	123.2 (2)	C1—N1—Ni1	130.95 (16)
N1—C1—H1	118.4	C4—N1—Ni1	112.79 (15)
C2—C1—H1	118.4	O1—N2—C2	121.5 (2)
N2—C2—C1	119.9 (2)	O1—N2—C3	120.2 (2)
N2—C2—H2	120.1	C2—N2—C3	118.3 (2)
C1—C2—H2	120.1	C5—N3—C7	125.5 (2)
N2—C3—C4	119.7 (2)	C5—N3—Ni1	118.92 (16)
N2—C3—H3A	120.2	C7—N3—Ni1	114.52 (15)
C4—C3—H3A	120.2	O3—N4—O4	121.7 (3)
N1—C4—C3	122.7 (2)	O3—N4—O2	117.7 (3)
N1—C4—C5	115.32 (19)	O4—N4—O2	120.6 (2)
C3—C4—C5	122.0 (2)	N4—O2—Ni1	121.09 (16)
N3—C5—C6	126.1 (2)		
N1—C1—C2—N2	0.4 (4)	C4—C3—N2—O1	-178.2 (2)
N2—C3—C4—N1	-1.4 (4)	C4—C3—N2—C2	0.8 (4)
N2—C3—C4—C5	177.5 (2)	C6—C5—N3—C7	-3.4 (4)
N1—C4—C5—N3	-7.4 (3)	C4—C5—N3—C7	174.4 (2)
C3—C4—C5—N3	173.6 (2)	C6—C5—N3—Ni1	-170.6 (2)
N1—C4—C5—C6	170.5 (2)	C4—C5—N3—Ni1	7.1 (3)
C3—C4—C5—C6	-8.5 (3)	C7 ⁱ —C7—N3—C5	164.2 (3)
C2—C1—N1—C4	-1.0 (4)	C7 ⁱ —C7—N3—Ni1	-28.1 (3)
C2—C1—N1—Ni1	176.96 (19)	N3 ⁱ —Ni1—N3—C5	179.1 (2)
C3—C4—N1—C1	1.4 (3)	N1 ⁱ —Ni1—N3—C5	170.39 (19)
C5—C4—N1—C1	-177.5 (2)	N1—Ni1—N3—C5	-3.94 (17)
C3—C4—N1—Ni1	-176.86 (18)	O2 ⁱ —Ni1—N3—C5	-93.61 (18)
C5—C4—N1—Ni1	4.2 (2)	O2—Ni1—N3—C5	88.02 (18)
N3—Ni1—N1—C1	-178.5 (2)	N3 ⁱ —Ni1—N3—C7	10.46 (13)
N3 ⁱ —Ni1—N1—C1	-169.8 (2)	N1 ⁱ —Ni1—N3—C7	1.8 (3)
N1 ⁱ —Ni1—N1—C1	3.71 (19)	N1—Ni1—N3—C7	-172.56 (17)
O2 ⁱ —Ni1—N1—C1	-87.8 (2)	O2 ⁱ —Ni1—N3—C7	97.77 (17)
O2—Ni1—N1—C1	94.4 (2)	O2—Ni1—N3—C7	-80.60 (17)
N3—Ni1—N1—C4	-0.56 (15)	O3—N4—O2—Ni1	178.3 (2)
N3 ⁱ —Ni1—N1—C4	8.2 (3)	O4—N4—O2—Ni1	-4.6 (3)
N1 ⁱ —Ni1—N1—C4	-178.30 (17)	N3—Ni1—O2—N4	-134.41 (18)
O2 ⁱ —Ni1—N1—C4	90.16 (15)	N3 ⁱ —Ni1—O2—N4	144.10 (18)
O2—Ni1—N1—C4	-87.66 (15)	N1 ⁱ —Ni1—O2—N4	65.39 (18)

C1—C2—N2—O1	178.7 (3)	N1—Ni1—O2—N4	-55.78 (18)
C1—C2—N2—C3	-0.3 (4)		

Symmetry code: (i) $-x, y, -z+1/2$.

Hydrogen-bond geometry (Å, °)

<i>D—H...A</i>	<i>D—H</i>	<i>H...A</i>	<i>D...A</i>	<i>D—H...A</i>
O5—H1 <i>W</i> ...O2 ⁱⁱ	0.78 (12)	2.46 (14)	3.086 (4)	139 (14)
C3—H3 <i>A</i> ...O2 ⁱⁱⁱ	0.93	2.58	3.389 (3)	146
C6—H6 <i>A</i> ...O1 ^{iv}	0.96	2.56	3.453 (4)	156

Symmetry codes: (ii) $x+1, y, z$; (iii) $x+1/2, -y+1/2, z+1/2$; (iv) $-x+1/2, y+1/2, -z+3/2$.