

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

Tetraaquabis[3-(3-pyridyl)-5-(4-pyridyl)-1,2,4-triazolido]nickel(II) dihydrate

Yun-Liang Zhang,* Ti-Lou Liu and Shuang-Jiao Sun

Department of Pharmacy, Shaoyang Medical College, Shaoyang, Hunan 422000, People's Republic of China

Correspondence e-mail: yunliangz2009@163.com

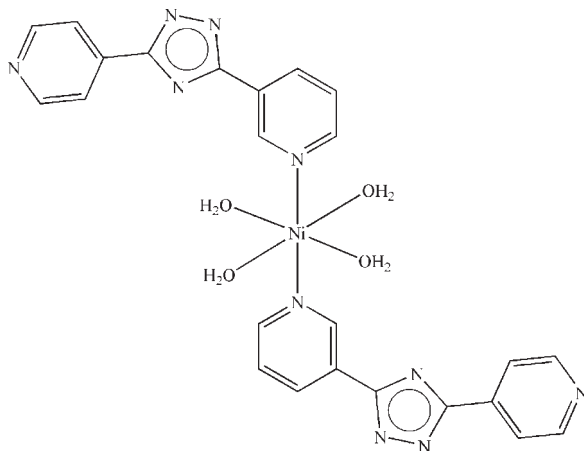
Received 25 October 2009; accepted 7 November 2009

Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.052; wR factor = 0.150; data-to-parameter ratio = 11.5.

In the title compound, $[\text{Ni}(\text{C}_{12}\text{H}_8\text{N}_5)_2(\text{H}_2\text{O})_4] \cdot 2\text{H}_2\text{O}$, the Ni^{II} atom is coordinated by the two N atoms [$\text{Ni}-\text{N} = 2.094$ (3) Å] and four O atoms [$\text{Ni}-\text{O} = 2.063$ (3)– 2.083 (2) Å] in a distorted octahedral geometry. The molecule is centrosymmetric and the Ni^{II} atom is located on an inversion center. Intermolecular $\text{O}-\text{H} \cdots \text{N}$ and $\text{O}-\text{H} \cdots \text{O}$ hydrogen bonds link the complex into a three-dimensional supramolecular framework.

Related literature

For hydrogen-bond interactions in biological systems, see: Deisenhofer & Michel (1989). For supramolecular assembly through hydrogen bonds, see: Beatty (2003); Li *et al.* (2006); Russell & Ward (1996). For related structures, see: Liu *et al.* (2008); Liu & Zhang (2009); Rarig *et al.* (2001).



Experimental

Crystal data

 $[\text{Ni}(\text{C}_{12}\text{H}_8\text{N}_5)_2(\text{H}_2\text{O})_4] \cdot 2\text{H}_2\text{O}$ $M_r = 611.25$

Triclinic, $P\bar{1}$
 $a = 8.2240$ (16) Å
 $b = 9.1990$ (18) Å
 $c = 9.3850$ (19) Å
 $\alpha = 90.70$ (3)°
 $\beta = 104.96$ (3)°
 $\gamma = 96.47$ (3)°

$V = 680.9$ (2) Å³
 $Z = 1$
 Mo $K\alpha$ radiation
 $\mu = 0.77$ mm⁻¹
 $T = 293$ K
 $0.20 \times 0.12 \times 0.08$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 1998)
 $T_{\text{min}} = 0.866$, $T_{\text{max}} = 0.943$

4042 measured reflections
 2437 independent reflections
 2258 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.040$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.052$
 $wR(F^2) = 0.150$
 $S = 0.99$
 2437 reflections
 211 parameters
 9 restraints

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.55$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.85$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$\text{O1}-\text{H1A} \cdots \text{N5}^{\text{i}}$	0.83 (2)	1.92 (3)	2.751 (4)	179 (3)
$\text{O1}-\text{H1B} \cdots \text{N3}^{\text{ii}}$	0.83 (3)	1.95 (3)	2.750 (4)	162 (3)
$\text{O2}-\text{H2A} \cdots \text{O3}^{\text{iii}}$	0.83 (3)	1.93 (3)	2.751 (4)	171 (3)
$\text{O2}-\text{H2B} \cdots \text{N4}^{\text{iv}}$	0.84 (3)	1.96 (3)	2.791 (4)	169 (3)
$\text{O3}-\text{H3A} \cdots \text{N2}^{\text{v}}$	0.82 (5)	2.10 (5)	2.911 (4)	170 (3)
$\text{O3}-\text{H3B} \cdots \text{N4}^{\text{vi}}$	0.82 (4)	2.20 (5)	2.944 (4)	151 (3)

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

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1998); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); software used to prepare material for publication: SHELXTL.

We acknowledge financial support from the Foundation of Shaoyang Medical College (grant No. XK200804) and the Science & Technology Foundation of Shaoyang (grant Nos. 56 J08 & J0966)

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BG2306).

References

- Beatty, A. M. (2003). *Coord. Chem. Rev.* **246**, 131–143.
 Bruker (1998). SMART, SAINT and SADABS. Bruker AXS Inc., Madison, Wisconsin, USA.
 Deisenhofer, J. & Michel, H. (1989). *EMBO J.* **8**, 2149–2154.
 Li, F., Su, T.-H., Gao, W. & Cao, R. (2006). *Eur. J. Inorg. Chem.* pp. 1582–1587.
 Liu, N., Wang, Y.-Q., Gao, E.-Q., Chen, Z.-X. & Weng, L.-H. (2008). *CrystEngComm*, **10**, 915–922.
 Liu, T.-L. & Zhang, Y.-L. (2009). *Acta Cryst.* **E65**, m913.
 Rarig, R. S. & Zubietta, J. J. (2001). *J. Chem. Soc. Dalton Trans.* pp. 3446–3452.
 Russell, V. A. & Ward, M. D. (1996). *Chem. Mater.* **8**, 1654–1666.
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.

supporting information

Acta Cryst. (2009). E65, m1590 [doi:10.1107/S1600536809047102]

Tetraaquabis[3-(3-pyridyl)-5-(4-pyridyl)-1,2,4-triazolido]nickel(II) dihydrate**Yun-Liang Zhang, Ti-Lou Liu and Shuang-Jiao Sun****S1. Comment**

The hydrogen bond interaction plays an important role in some biological systems (Deisenhofer & Michel, 1989). Supramolecular assembly through hydrogen bonds has been extensively exploited to generate extended one-, two- and three-dimensional structures (Beatty *et al.*, 2003; Li *et al.*, 2006; Russell & Ward, 1996). As part of this ongoing work (Liu *et al.*, 2009), we present here the synthesis and structural characterization of the title nickel complex, $[\text{Ni}(\text{C}_{12}\text{H}_8\text{N}_5)_2(\text{H}_2\text{O})_4]\cdot 2\text{H}_2\text{O}$, (**I**).

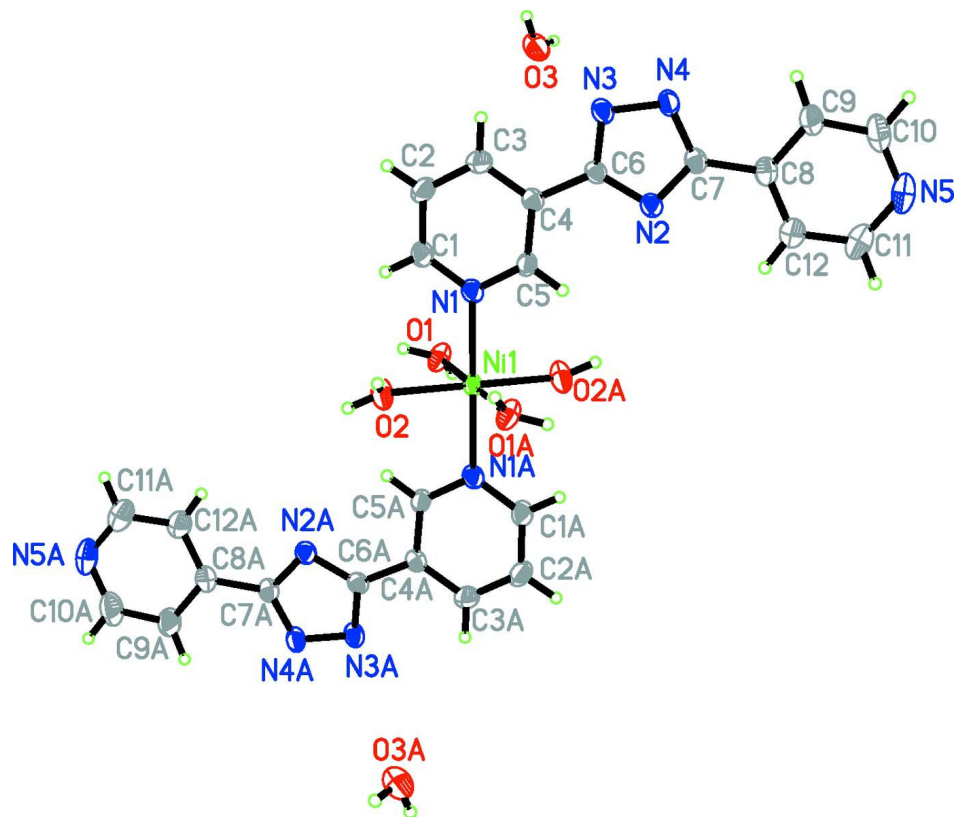
The molecule of the title complex, (Fig. 1), is centrosymmetric, so pairs of equivalent ligands lie *trans* to each other in a slightly distorted octahedral coordination geometry, *cis* angles deviating from 90° by less than 2°. with Ni—O bond length in the range 2.063–2.083 Å and Ni—N bond length 2.094 Å. These bond distances compare well with those in the literature (Liu *et al.*, 2008; Rarig *et al.*, 2001). Molecules are linked by O—H···O and O—H···N hydrogen bonds (Fig. 2, Table 1).

S2. Experimental

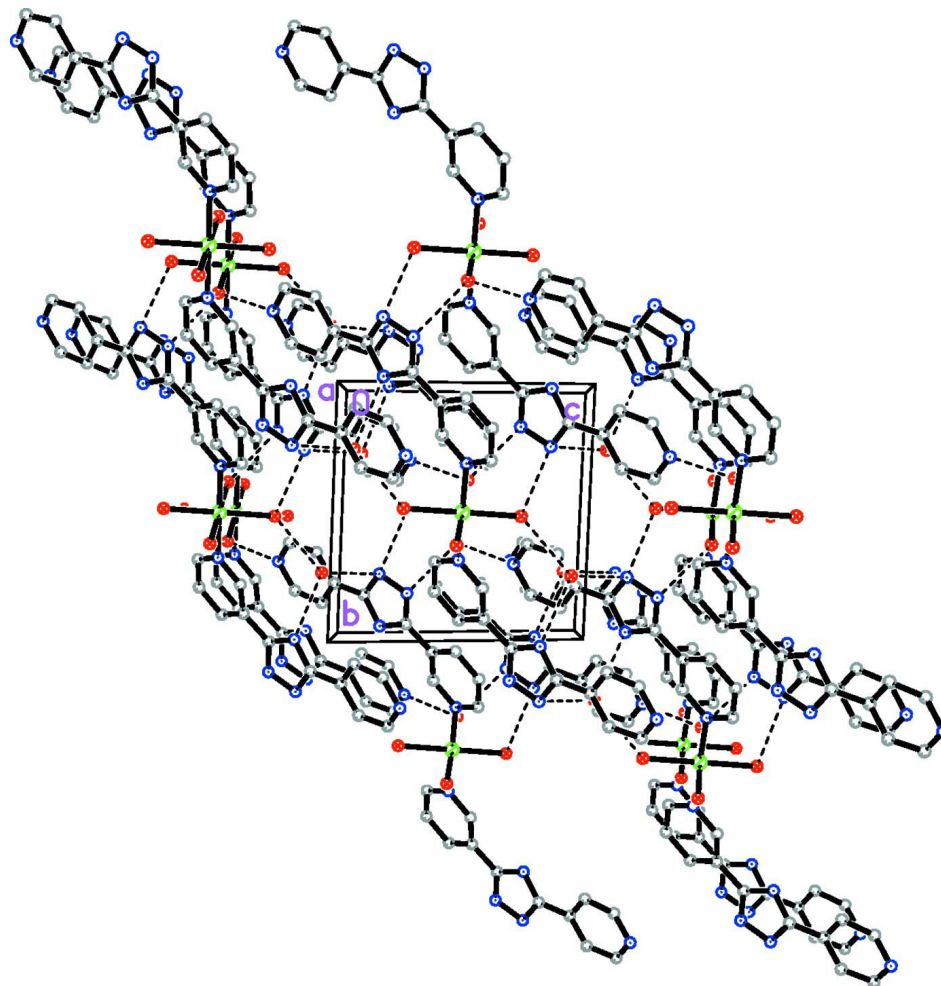
$\text{Ni}(\text{NO}_3)_2\cdot 4\text{H}_2\text{O}$ (0.5 mmol, 0.145 g), 1*H*-3-(3-pyridyl)-5-(4-pyridyl)-1,2,4-triazole (0.5 mmol, 0.112 g), and water (12 ml) were placed in a 23-ml Teflon-lined Parr bomb. The bomb was heated at 453 K for 3 d. The green block-shaped crystals were filtered off and washed with water and acetone (yield 33%, based on Ni).

S3. Refinement

Hydrogen atoms of water molecules were located in a difference Fourier map and refined with distance restraints of O—H = 0.82 (2) Å and H···H = 1.35 (2) Å. H atoms on C atom were positioned geometrically and refined using a riding model, with C—H = 0.93 Å, in all cases with $U(\text{H}) = 1.2/1.5 \times U_{\text{equiv}}(\text{Host})$

**Figure 1**

A view of the molecular structure of (I) with the atom-numbering scheme and 50% displacement ellipsoids (arbitrary spheres for the H atoms). Atoms with the suffix A are generated by the symmetry operation $(-x, -y + 1, -z + 1)$.

**Figure 2**

The 3-D network of (I).

Tetraaquabis[3-(3-pyridyl)-5-(4-pyridyl)-1,2,4-triazolido]nickel(II) dihydrate

Crystal data

$[\text{Ni}(\text{C}_{12}\text{H}_8\text{N}_5)_2(\text{H}_2\text{O})_4] \cdot 2\text{H}_2\text{O}$

$M_r = 611.25$

Triclinic, $P\bar{1}$

Hall symbol: $-P\ 1$

$a = 8.2240$ (16) Å

$b = 9.1990$ (18) Å

$c = 9.3850$ (19) Å

$\alpha = 90.70$ (3)°

$\beta = 104.96$ (3)°

$\gamma = 96.47$ (3)°

$V = 680.9$ (2) Å³

$Z = 1$

$F(000) = 318$

$D_x = 1.491$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 2567 reflections

$\theta = 1.5$ – 25.3 °

$\mu = 0.77$ mm⁻¹

$T = 293$ K

Block, green

$0.20 \times 0.12 \times 0.08$ mm

Data collection

Bruker SMART CCD area-detector
diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
 φ and ω scans
Absorption correction: multi-scan
(*SADABS*; Bruker, 1998)
 $T_{\min} = 0.866$, $T_{\max} = 0.943$

4042 measured reflections
2437 independent reflections
2258 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.040$
 $\theta_{\max} = 25.2^\circ$, $\theta_{\min} = 3.1^\circ$
 $h = -9 \rightarrow 9$
 $k = -9 \rightarrow 11$
 $l = -11 \rightarrow 11$

Refinement

Refinement on F^2
Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.052$
 $wR(F^2) = 0.150$
 $S = 0.99$
2437 reflections
211 parameters
9 restraints
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
 $w = 1/[\sigma^2(F_o^2) + (0.0912P)^2 + 0.8P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.55 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.85 \text{ e } \text{\AA}^{-3}$

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Ni1	0.0000	0.5000	0.5000	0.0217 (2)
C1	0.2767 (4)	0.3042 (4)	0.6004 (4)	0.0291 (7)
H1	0.3256	0.3814	0.6683	0.035*
C2	0.3637 (5)	0.1847 (4)	0.5989 (4)	0.0347 (8)
H2	0.4679	0.1806	0.6663	0.042*
C3	0.2938 (4)	0.0712 (4)	0.4959 (4)	0.0299 (8)
H3	0.3508	-0.0100	0.4928	0.036*
C4	0.1385 (4)	0.0799 (3)	0.3976 (3)	0.0211 (6)
C5	0.0578 (4)	0.2022 (3)	0.4086 (3)	0.0235 (7)
H5A	-0.0480	0.2078	0.3440	0.028*
C6	0.0580 (4)	-0.0361 (3)	0.2837 (3)	0.0214 (6)
C7	-0.1047 (4)	-0.1550 (3)	0.1011 (3)	0.0231 (7)
C8	-0.2408 (4)	-0.2007 (4)	-0.0305 (4)	0.0270 (7)
C9	-0.2480 (5)	-0.3324 (4)	-0.1091 (4)	0.0382 (9)
H9A	-0.1643	-0.3938	-0.0785	0.046*

C10	-0.3798 (6)	-0.3703 (5)	-0.2319 (5)	0.0480 (11)
H10A	-0.3804	-0.4570	-0.2841	0.058*
C11	-0.4989 (5)	-0.1649 (5)	-0.2061 (4)	0.0428 (10)
H11A	-0.5863	-0.1074	-0.2379	0.051*
C12	-0.3699 (5)	-0.1149 (4)	-0.0848 (4)	0.0363 (8)
H12A	-0.3689	-0.0242	-0.0395	0.044*
N1	0.1255 (4)	0.3132 (3)	0.5083 (3)	0.0253 (6)
N2	-0.0797 (3)	-0.0233 (3)	0.1726 (3)	0.0243 (6)
N3	0.1159 (4)	-0.1651 (3)	0.2840 (3)	0.0263 (6)
N4	0.0088 (4)	-0.2439 (3)	0.1640 (3)	0.0276 (6)
N5	-0.5067 (4)	-0.2906 (4)	-0.2810 (4)	0.0442 (9)
O1	0.2181 (3)	0.6258 (3)	0.4839 (3)	0.0321 (6)
O2	0.0796 (4)	0.5155 (3)	0.7297 (3)	0.0353 (6)
O3	0.8076 (4)	0.2539 (3)	0.0662 (3)	0.0405 (7)
H1A	0.302 (4)	0.650 (5)	0.555 (3)	0.059 (15)*
H2A	0.122 (5)	0.580 (3)	0.796 (4)	0.043 (12)*
H3A	0.850 (8)	0.182 (5)	0.103 (6)	0.12 (3)*
H1B	0.210 (5)	0.695 (3)	0.427 (4)	0.043 (12)*
H2B	0.051 (6)	0.440 (3)	0.771 (4)	0.049 (13)*
H3B	0.836 (7)	0.274 (5)	-0.009 (4)	0.069 (17)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0260 (4)	0.0160 (3)	0.0190 (3)	0.0037 (2)	-0.0020 (2)	-0.0023 (2)
C1	0.0293 (18)	0.0210 (17)	0.0308 (18)	0.0002 (13)	-0.0018 (15)	-0.0049 (13)
C2	0.0247 (18)	0.031 (2)	0.040 (2)	0.0061 (14)	-0.0065 (15)	-0.0046 (15)
C3	0.0285 (18)	0.0260 (18)	0.0344 (19)	0.0079 (14)	0.0048 (15)	-0.0010 (14)
C4	0.0249 (16)	0.0183 (16)	0.0203 (15)	0.0011 (12)	0.0068 (13)	0.0007 (12)
C5	0.0241 (17)	0.0199 (16)	0.0223 (16)	0.0026 (12)	-0.0016 (13)	-0.0007 (12)
C6	0.0260 (16)	0.0171 (15)	0.0211 (15)	0.0023 (12)	0.0062 (13)	0.0001 (12)
C7	0.0277 (17)	0.0209 (16)	0.0197 (16)	0.0004 (12)	0.0054 (13)	0.0008 (12)
C8	0.0285 (18)	0.0289 (18)	0.0218 (16)	-0.0021 (14)	0.0057 (14)	0.0005 (13)
C9	0.038 (2)	0.032 (2)	0.036 (2)	0.0010 (16)	-0.0030 (17)	-0.0087 (16)
C10	0.049 (3)	0.051 (3)	0.035 (2)	-0.005 (2)	0.0004 (19)	-0.0144 (18)
C11	0.031 (2)	0.052 (3)	0.039 (2)	-0.0002 (17)	-0.0001 (17)	0.0073 (18)
C12	0.033 (2)	0.038 (2)	0.034 (2)	0.0034 (16)	0.0022 (16)	-0.0022 (16)
N1	0.0311 (15)	0.0184 (14)	0.0242 (14)	0.0033 (11)	0.0031 (12)	-0.0016 (11)
N2	0.0275 (15)	0.0193 (14)	0.0239 (14)	0.0022 (11)	0.0030 (12)	-0.0017 (11)
N3	0.0363 (16)	0.0175 (14)	0.0217 (14)	0.0035 (11)	0.0015 (12)	-0.0013 (10)
N4	0.0356 (16)	0.0224 (15)	0.0203 (14)	0.0040 (12)	-0.0009 (12)	-0.0031 (11)
N5	0.0390 (19)	0.054 (2)	0.0289 (17)	-0.0109 (16)	-0.0033 (14)	0.0008 (15)
O1	0.0298 (13)	0.0263 (13)	0.0320 (14)	0.0000 (10)	-0.0057 (11)	0.0068 (11)
O2	0.0554 (17)	0.0220 (14)	0.0216 (12)	-0.0001 (12)	-0.0001 (12)	0.0005 (10)
O3	0.0514 (18)	0.0363 (16)	0.0345 (15)	0.0052 (13)	0.0128 (14)	-0.0034 (12)

Geometric parameters (Å, °)

Ni1—O1 ⁱ	2.063 (3)	C7—N2	1.347 (4)
Ni1—O1	2.063 (3)	C7—C8	1.456 (5)
Ni1—O2	2.083 (2)	C8—C12	1.389 (5)
Ni1—O2 ⁱ	2.083 (2)	C8—C9	1.398 (5)
Ni1—N1	2.094 (3)	C9—C10	1.373 (6)
Ni1—N1 ⁱ	2.094 (3)	C9—H9A	0.9300
C1—N1	1.330 (4)	C10—N5	1.331 (6)
C1—C2	1.379 (5)	C10—H10A	0.9300
C1—H1	0.9300	C11—N5	1.333 (5)
C2—C3	1.381 (5)	C11—C12	1.373 (5)
C2—H2	0.9300	C11—H11A	0.9300
C3—C4	1.380 (5)	C12—H12A	0.9300
C3—H3	0.9300	N3—N4	1.376 (4)
C4—C5	1.385 (4)	O1—H1A	0.836 (19)
C4—C6	1.472 (4)	O1—H1B	0.830 (18)
C5—N1	1.345 (4)	O2—H2A	0.828 (18)
C5—H5A	0.9300	O2—H2B	0.836 (19)
C6—N3	1.327 (4)	O3—H3A	0.82 (5)
C6—N2	1.344 (4)	O3—H3B	0.81 (4)
C7—N4	1.337 (4)		
O1 ⁱ —Ni1—O1	180.00 (15)	N4—C7—N2	113.1 (3)
O1 ⁱ —Ni1—O2	88.62 (11)	N4—C7—C8	121.9 (3)
O1—Ni1—O2	91.38 (11)	N2—C7—C8	125.0 (3)
O1 ⁱ —Ni1—O2 ⁱ	91.38 (11)	C12—C8—C9	116.5 (3)
O1—Ni1—O2 ⁱ	88.62 (11)	C12—C8—C7	121.6 (3)
O2—Ni1—O2 ⁱ	180.0	C9—C8—C7	121.9 (3)
O1 ⁱ —Ni1—N1	90.86 (11)	C10—C9—C8	119.4 (4)
O1—Ni1—N1	89.14 (11)	C10—C9—H9A	120.3
O2—Ni1—N1	87.82 (11)	C8—C9—H9A	120.3
O2 ⁱ —Ni1—N1	92.18 (11)	N5—C10—C9	124.1 (4)
O1 ⁱ —Ni1—N1 ⁱ	89.14 (11)	N5—C10—H10A	118.0
O1—Ni1—N1 ⁱ	90.86 (11)	C9—C10—H10A	118.0
O2—Ni1—N1 ⁱ	92.18 (11)	N5—C11—C12	124.1 (4)
O2 ⁱ —Ni1—N1 ⁱ	87.82 (11)	N5—C11—H11A	117.9
N1—Ni1—N1 ⁱ	180.000 (1)	C12—C11—H11A	117.9
N1—C1—C2	122.5 (3)	C11—C12—C8	119.5 (4)
N1—C1—H1	118.7	C11—C12—H12A	120.2
C2—C1—H1	118.7	C8—C12—H12A	120.2
C1—C2—C3	119.1 (3)	C1—N1—C5	118.1 (3)
C1—C2—H2	120.5	C1—N1—Ni1	122.7 (2)
C3—C2—H2	120.5	C5—N1—Ni1	118.9 (2)
C4—C3—C2	119.2 (3)	C6—N2—C7	101.9 (3)
C4—C3—H3	120.4	C6—N3—N4	105.3 (3)
C2—C3—H3	120.4	C7—N4—N3	105.8 (3)
C3—C4—C5	118.1 (3)	C10—N5—C11	116.3 (3)

C3—C4—C6	122.0 (3)	Ni1—O1—H1A	125 (3)
C5—C4—C6	119.9 (3)	Ni1—O1—H1B	119 (3)
N1—C5—C4	122.9 (3)	H1A—O1—H1B	107 (3)
N1—C5—H5A	118.5	Ni1—O2—H2A	138 (3)
C4—C5—H5A	118.5	Ni1—O2—H2B	114 (3)
N3—C6—N2	114.0 (3)	H2A—O2—H2B	107 (3)
N3—C6—C4	121.9 (3)	H3A—O3—H3B	111 (3)
N2—C6—C4	124.1 (3)		
N1—C1—C2—C3	1.6 (6)	C4—C5—N1—C1	-0.1 (5)
C1—C2—C3—C4	-0.3 (5)	C4—C5—N1—Ni1	174.5 (2)
C2—C3—C4—C5	-1.0 (5)	O1 ⁱ —Ni1—N1—C1	-129.6 (3)
C2—C3—C4—C6	179.1 (3)	O1—Ni1—N1—C1	50.4 (3)
C3—C4—C5—N1	1.3 (5)	O2—Ni1—N1—C1	-41.0 (3)
C6—C4—C5—N1	-178.8 (3)	O2 ⁱ —Ni1—N1—C1	139.0 (3)
C3—C4—C6—N3	11.2 (5)	O1 ⁱ —Ni1—N1—C5	56.0 (2)
C5—C4—C6—N3	-168.7 (3)	O1—Ni1—N1—C5	-124.0 (2)
C3—C4—C6—N2	-169.8 (3)	O2—Ni1—N1—C5	144.6 (2)
C5—C4—C6—N2	10.3 (5)	O2 ⁱ —Ni1—N1—C5	-35.4 (2)
N4—C7—C8—C12	172.1 (3)	N3—C6—N2—C7	-0.4 (4)
N2—C7—C8—C12	-7.2 (5)	C4—C6—N2—C7	-179.4 (3)
N4—C7—C8—C9	-8.3 (5)	N4—C7—N2—C6	0.5 (4)
N2—C7—C8—C9	172.4 (3)	C8—C7—N2—C6	179.8 (3)
C12—C8—C9—C10	-0.7 (6)	N2—C6—N3—N4	0.1 (4)
C7—C8—C9—C10	179.7 (4)	C4—C6—N3—N4	179.2 (3)
C8—C9—C10—N5	-1.7 (7)	N2—C7—N4—N3	-0.5 (4)
N5—C11—C12—C8	-2.7 (6)	C8—C7—N4—N3	-179.8 (3)
C9—C8—C12—C11	2.8 (5)	C6—N3—N4—C7	0.2 (3)
C7—C8—C12—C11	-177.6 (3)	C9—C10—N5—C11	2.0 (6)
C2—C1—N1—C5	-1.3 (5)	C12—C11—N5—C10	0.2 (6)
C2—C1—N1—Ni1	-175.7 (3)		

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

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

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
O1—H1A \cdots N5 ⁱⁱ	0.83 (2)	1.92 (3)	2.751 (4)	179 (3)
O1—H1B \cdots N3 ⁱⁱⁱ	0.83 (3)	1.95 (3)	2.750 (4)	162 (3)
O2—H2A \cdots O3 ^{iv}	0.83 (3)	1.93 (3)	2.751 (4)	171 (3)
O2—H2B \cdots N4 ^v	0.84 (3)	1.96 (3)	2.791 (4)	169 (3)
O3—H3A \cdots N2 ^{vi}	0.82 (5)	2.10 (5)	2.911 (4)	170 (3)
O3—H3B \cdots N4 ^{vii}	0.82 (4)	2.20 (5)	2.944 (4)	151 (3)

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