

Triaqua(2,2'-bipyridine)(5-nitroisophthalato- κ O)nickel(II) monohydrate

Ying Liu,* Qingpeng He, Xianxi Zhang, Zechun Xue and Chunyan Lv

College of Chemistry and Chemical Engineering, Liaocheng University, Liaocheng 252059, People's Republic of China

Correspondence e-mail: yllctu@yahoo.com.cn

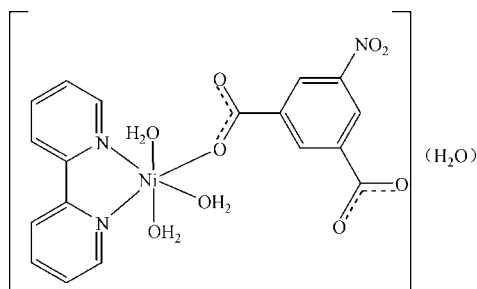
Received 9 November 2008; accepted 17 November 2008

Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.043; wR factor = 0.122; data-to-parameter ratio = 12.2.

In the title compound, $[\text{Ni}(\text{C}_8\text{H}_3\text{NO}_6)(\text{C}_{10}\text{H}_8\text{N}_2)(\text{H}_2\text{O})_3]\cdot\text{H}_2\text{O}$, the Ni^{II} cation is six-coordinated by a chelating 2,2'-bipyridine ligand, one carboxylate O atom from a 5-nitroisophthalate dianion and three water molecules, with a slightly distorted *cis*- NiN_2O_4 octahedral geometry. The neutral complex is isolated, in contrast to coordination polymers formed by Mn^{II} , Co^{II} and Cu^{II} with the same ligand set, but forms an extensive network of $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds between the coordinated and uncoordinated water molecules and carboxylate groups of the 5-nitroisophthalate ions.

Related literature

For the related coordination polymers containing Co^{II} , Mn^{II} and Cu^{II} , see: Xiao *et al.* (2005); Xie *et al.* (2005, 2006), respectively. For background, see: Kim *et al.* (2001).



Experimental

Crystal data

$[\text{Ni}(\text{C}_8\text{H}_3\text{NO}_6)(\text{C}_{10}\text{H}_8\text{N}_2)(\text{H}_2\text{O})_3]\cdot\text{H}_2\text{O}$

$M_r = 496.05$

Triclinic, $P\bar{1}$

$a = 7.4867$ (10) Å

$b = 10.717$ (3) Å

$c = 12.773$ (2) Å

$\alpha = 89.798$ (10)°

$\beta = 87.89$ (2)°

$\gamma = 74.675$ (10)°

$V = 987.7$ (3) Å³

$Z = 2$

Mo $K\alpha$ radiation

$\mu = 1.05$ mm⁻¹

$T = 293$ (2) K

0.12 × 0.10 × 0.08 mm

Data collection

Bruker APEXII CCD diffractometer

Absorption correction: multi-scan (SADABS; Bruker, 2001)

$T_{\text{min}} = 0.885$, $T_{\text{max}} = 0.921$

5649 measured reflections

3823 independent reflections

3271 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.016$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.043$

$wR(F^2) = 0.122$

$S = 1.01$

3823 reflections

314 parameters

12 restraints

H atoms treated by a mixture of independent and constrained refinement

$\Delta\rho_{\text{max}} = 0.99$ e Å⁻³

$\Delta\rho_{\text{min}} = -0.73$ e Å⁻³

Table 1

Selected bond lengths (Å).

Ni1—O1	2.051 (2)	Ni1—O3W	2.142 (2)
Ni1—O2W	2.079 (2)	Ni1—N2	2.097 (2)
Ni1—O1W	2.088 (2)	Ni1—N3	2.100 (2)

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1W—H1W ⁽ⁱ⁾ ···O2	0.81 (3)	2.00 (3)	2.727 (3)	150 (5)
O1W—H2W ⁽ⁱ⁾ ···O4 ⁱ	0.82 (4)	1.96 (5)	2.715 (3)	154 (4)
O2W—H3W ⁽ⁱ⁾ ···O4W ⁱⁱ	0.82 (3)	1.82 (4)	2.614 (4)	166 (4)
O2W—H4W ⁽ⁱ⁾ ···O4 ⁱⁱⁱ	0.82 (4)	1.96 (4)	2.757 (3)	164 (4)
O3W—H5W ⁽ⁱ⁾ ···O4W ^{iv}	0.82 (4)	2.42 (2)	3.185 (7)	156 (5)
O3W—H6W ⁽ⁱ⁾ ···O4 ^v	0.82 (3)	1.97 (2)	2.735 (3)	155 (4)
O4W—H7W ⁽ⁱ⁾ ···O2 ^{vi}	0.81 (4)	1.91 (2)	2.697 (4)	161 (5)
O4W—H8W ⁽ⁱ⁾ ···O3 ^{vii}	0.81 (3)	1.98 (4)	2.639 (4)	138 (5)

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

Data collection: APEX2 (Bruker, 2004); cell refinement: SAINT-Plus (Bruker, 2001); data reduction: SAINT-Plus; 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.

The authors thank the NSFC (grant No. 20501011) and Liaocheng University for financial support (grant No. X071011).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2841).

References

- Bruker (2001). SAINT-Plus and SADABS. Bruker AXS Inc., Madison, Wisconsin, USA.
- Bruker (2004). APEX2. Bruker AXS Inc., Madison, Wisconsin, USA.
- Kim, Y., Lee, E. & Jung, D. Y. (2001). *Chem. Mater.* **13**, 2684–2689.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Xiao, H. P., Li, X.-H. & Cheng, Y.-Q. (2005). *Acta Cryst.* **E61**, m158–m159.
- Xie, G., Zeng, M.-H., Chen, S.-P. & Gao, S.-L. (2005). *Acta Cryst.* **E61**, m2273–m2275.
- Xie, G., Zeng, M.-H., Chen, S.-P. & Gao, S.-L. (2006). *Acta Cryst.* **E62**, m397–m399.

supplementary materials

Acta Cryst. (2009). E65, m27 [doi:10.1107/S1600536808038233]

Triaqua(2,2'-bipyridine)(5-nitroisophthalato- κO)nickel(II) monohydrate

Y. Liu, Q. He, X. Zhang, Z. Xue and C. Lv

Comment

In recent years, carboxylic acids have been widely used in materials science as polydentate ligands which can coordinate to transition-metal or rare-earth cations to yield complexes with interesting or useful properties. For example, Kim *et al.* (2001) have focused on the syntheses of transition-metal complexes containing benzene carboxylate and rigid aromatic pyridine ligands in order to study their electronic conductivity and magnetic properties. The importance of transition-metal dicarboxylate complexes motivated us to pursue synthetic strategies for these compounds, using 5-nitroisophthalic acid as a polydentate ligand and we now report the synthesis and structure of the title compound, (I) (Fig. 1).

The Ni^{II} cation in (I) is hexa-coordinated by a chelating 2,2'-bipyridine ligand, one carboxylate O atom from a 5-nitroisophthalate dianion and three water molecules, with a slightly distorted cis-NiN₂O₄ octahedral geometry (Table 1). The neutral complex is isolated, in contrast to coordination polymers formed by Mn^{II}, Co^{II} and Cu^{II} with the same ligand set, but forms an extensive network of O—H \cdots O hydrogen bonds (Table 2) between the coordinated and uncoordinated water molecules and carboxylate groups of the 5-nitroisophthalate ions.

Experimental

A mixture of nickel dichloride (0.5 mmol), 2,2'-bipyridine (0.5 mmol), and 5-nitroisophthalic acid (0.5 mmol) in H₂O (8 ml) and ethanol (8 ml) was sealed in a 25-ml Teflon-lined stainless steel autoclave and heated to 413 K for three days. Green blocks of (I) were obtained after cooling to room temperature with a yield of 27%.

Refinement

The H atoms of the water molecule were located from difference density maps and were refined with distance restraints of H \cdots H = 1.38 (2) Å, O— = 0.88 (2) Å, and with a fixed U_{iso} of 0.80 Å². All other H atoms were placed in calculated positions with a C—H bond distance of 0.93 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}$ of the carrier atom.

Figures

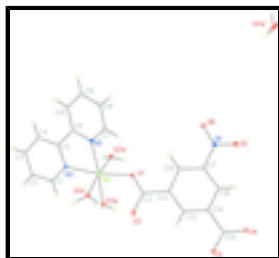


Fig. 1. A view of the molecular structure of (I), showing 30% probability displacement ellipsoids for the non-hydrogen atoms.

Triaqua(2,2'-bipyridine)(5-nitroisophthalato- κ O)nickel(II) monohydrate

Crystal data

$[\text{Ni}(\text{C}_8\text{H}_3\text{NO}_6)(\text{C}_{10}\text{H}_8\text{N}_2)(\text{H}_2\text{O})_3]\cdot\text{H}_2\text{O}$	$Z = 2$
$M_r = 496.05$	$F(000) = 512$
Triclinic, $P\bar{1}$	$D_x = 1.668 \text{ Mg m}^{-3}$
Hall symbol: -P 1	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$a = 7.4867 (10) \text{ \AA}$	Cell parameters from 3823 reflections
$b = 10.717 (3) \text{ \AA}$	$\theta = 1.6\text{--}26.0^\circ$
$c = 12.773 (2) \text{ \AA}$	$\mu = 1.05 \text{ mm}^{-1}$
$\alpha = 89.798 (10)^\circ$	$T = 293 \text{ K}$
$\beta = 87.89 (2)^\circ$	Block, green
$\gamma = 74.675 (10)^\circ$	$0.12 \times 0.10 \times 0.08 \text{ mm}$
$V = 987.7 (3) \text{ \AA}^3$	

Data collection

Bruker APEXII CCD diffractometer	3823 independent reflections
Radiation source: fine-focus sealed tube graphite	3271 reflections with $I > 2\sigma(I)$
ω scans	$R_{\text{int}} = 0.016$
Absorption correction: multi-scan (SADABS; Bruker, 2001)	$\theta_{\text{max}} = 26.0^\circ$, $\theta_{\text{min}} = 1.6^\circ$
$T_{\text{min}} = 0.885$, $T_{\text{max}} = 0.921$	$h = -8 \rightarrow 9$
5649 measured reflections	$k = -13 \rightarrow 11$
	$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.043$	Hydrogen site location: difmap and geom
$wR(F^2) = 0.122$	H atoms treated by a mixture of independent and constrained refinement
$S = 1.00$	$w = 1/[\sigma^2(F_o^2) + (0.071P)^2 + 0.9983P]$
3823 reflections	where $P = (F_o^2 + 2F_c^2)/3$
314 parameters	$(\Delta/\sigma)_{\text{max}} < 0.001$
12 restraints	$\Delta\rho_{\text{max}} = 0.99 \text{ e \AA}^{-3}$
	$\Delta\rho_{\text{min}} = -0.73 \text{ e \AA}^{-3}$

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	0.72908 (5)	-0.02881 (3)	0.78571 (3)	0.02430 (16)
C1	0.8232 (5)	-0.3096 (3)	0.8659 (2)	0.0303 (7)
H1	0.7701	-0.2738	0.9296	0.036*
C2	0.8972 (5)	-0.4404 (3)	0.8591 (3)	0.0371 (8)
H2	0.8903	-0.4931	0.9163	0.044*
C3	0.9816 (5)	-0.4922 (3)	0.7667 (3)	0.0385 (8)
H3	1.0368	-0.5807	0.7612	0.046*
C4	0.9848 (5)	-0.4139 (3)	0.6820 (3)	0.0321 (7)
H4	1.0424	-0.4480	0.6187	0.038*
C5	0.9009 (4)	-0.2836 (3)	0.6926 (2)	0.0227 (6)
C6	0.8764 (4)	-0.1940 (3)	0.6036 (2)	0.0254 (6)
C7	0.7338 (5)	0.0090 (3)	0.5475 (3)	0.0360 (8)
H7	0.6633	0.0927	0.5628	0.043*
C8	0.7884 (6)	-0.0224 (4)	0.4454 (3)	0.0476 (9)
H8	0.7524	0.0376	0.3922	0.057*
C9	0.8975 (7)	-0.1445 (4)	0.4233 (3)	0.0532 (11)
H9	0.9406	-0.1680	0.3551	0.064*
C10	0.9418 (6)	-0.2309 (4)	0.5028 (3)	0.0429 (9)
H10	1.0157	-0.3141	0.4893	0.052*
C11	0.5174 (4)	0.2464 (3)	0.8072 (3)	0.0296 (7)
C12	0.4966 (4)	0.3864 (3)	0.7871 (2)	0.0245 (6)
C13	0.4091 (4)	0.4774 (3)	0.8608 (2)	0.0244 (6)
H13	0.3675	0.4506	0.9243	0.029*
C14	0.3821 (4)	0.6079 (3)	0.8421 (2)	0.0218 (6)
C15	0.2887 (4)	0.7042 (3)	0.9250 (2)	0.0229 (6)
C16	0.4381 (4)	0.6470 (3)	0.7464 (2)	0.0242 (6)
H16	0.4168	0.7345	0.7311	0.029*
C17	0.5258 (4)	0.5548 (3)	0.6739 (2)	0.0237 (6)
C18	0.5605 (4)	0.4251 (3)	0.6923 (2)	0.0267 (6)
H18	0.6250	0.3647	0.6429	0.032*
H1W	0.394 (6)	0.0433 (19)	0.814 (4)	0.080*
H2W	0.430 (7)	-0.089 (3)	0.824 (3)	0.080*
H3W	1.002 (7)	0.0536 (18)	0.815 (4)	0.080*
H4W	1.071 (6)	-0.077 (3)	0.827 (3)	0.080*
H5W	0.784 (5)	-0.065 (3)	0.979 (4)	0.080*
H6W	0.696 (6)	0.062 (2)	0.980 (4)	0.080*
H7W	0.857 (4)	0.785 (5)	0.129 (4)	0.080*
H8W	1.005 (6)	0.792 (5)	0.064 (2)	0.080*

supplementary materials

N1	0.5843 (4)	0.5975 (3)	0.5725 (2)	0.0317 (6)
N2	0.7764 (3)	-0.0739 (2)	0.62575 (19)	0.0254 (5)
N3	0.8242 (3)	-0.2316 (2)	0.78473 (18)	0.0236 (5)
O1	0.6531 (3)	0.16736 (19)	0.76279 (17)	0.0296 (5)
O2	0.3983 (4)	0.2176 (2)	0.8663 (3)	0.0569 (8)
O3	0.2273 (3)	0.6637 (2)	1.00532 (18)	0.0380 (6)
O4	0.2779 (3)	0.82113 (19)	0.90681 (17)	0.0294 (5)
O5	0.5189 (4)	0.7083 (2)	0.54771 (19)	0.0495 (7)
O6	0.6974 (4)	0.5196 (2)	0.51729 (18)	0.0413 (6)
O1W	0.4496 (3)	-0.0279 (2)	0.79179 (19)	0.0316 (5)
O2W	1.0016 (3)	-0.0185 (2)	0.79477 (19)	0.0318 (5)
O3W	0.7027 (4)	-0.0088 (2)	0.95279 (18)	0.0391 (6)
O4W	0.9500 (5)	0.8091 (4)	0.1199 (5)	0.115 (2)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0280 (2)	0.0187 (2)	0.0255 (2)	-0.00530 (16)	0.00210 (15)	-0.00138 (14)
C1	0.0380 (18)	0.0296 (16)	0.0247 (15)	-0.0118 (14)	-0.0005 (13)	0.0040 (12)
C2	0.043 (2)	0.0311 (18)	0.0399 (19)	-0.0143 (15)	-0.0094 (15)	0.0133 (14)
C3	0.043 (2)	0.0190 (15)	0.051 (2)	-0.0035 (14)	-0.0063 (16)	0.0027 (14)
C4	0.0348 (17)	0.0220 (15)	0.0365 (17)	-0.0031 (13)	0.0035 (14)	-0.0048 (13)
C5	0.0252 (15)	0.0196 (14)	0.0234 (14)	-0.0059 (11)	0.0000 (11)	-0.0005 (11)
C6	0.0297 (16)	0.0206 (14)	0.0260 (15)	-0.0072 (12)	0.0024 (12)	-0.0012 (11)
C7	0.046 (2)	0.0288 (17)	0.0308 (17)	-0.0059 (15)	-0.0046 (14)	0.0077 (13)
C8	0.072 (3)	0.043 (2)	0.0282 (18)	-0.016 (2)	-0.0062 (17)	0.0108 (15)
C9	0.086 (3)	0.051 (2)	0.0237 (17)	-0.023 (2)	0.0098 (18)	-0.0020 (16)
C10	0.064 (2)	0.0338 (18)	0.0284 (17)	-0.0100 (17)	0.0155 (16)	-0.0061 (14)
C11	0.0266 (16)	0.0163 (14)	0.0451 (18)	-0.0048 (12)	0.0056 (14)	-0.0013 (13)
C12	0.0228 (14)	0.0147 (13)	0.0349 (16)	-0.0032 (11)	0.0015 (12)	0.0003 (11)
C13	0.0242 (15)	0.0192 (14)	0.0292 (15)	-0.0053 (11)	0.0028 (12)	0.0023 (11)
C14	0.0218 (14)	0.0180 (14)	0.0256 (14)	-0.0053 (11)	-0.0004 (11)	0.0000 (11)
C15	0.0230 (14)	0.0168 (13)	0.0276 (15)	-0.0030 (11)	-0.0022 (11)	0.0005 (11)
C16	0.0289 (15)	0.0158 (13)	0.0284 (15)	-0.0069 (11)	-0.0034 (12)	0.0014 (11)
C17	0.0274 (15)	0.0230 (14)	0.0210 (14)	-0.0069 (12)	-0.0013 (11)	-0.0001 (11)
C18	0.0287 (15)	0.0210 (14)	0.0296 (15)	-0.0053 (12)	0.0009 (12)	-0.0049 (12)
N1	0.0414 (16)	0.0322 (15)	0.0241 (13)	-0.0147 (12)	-0.0001 (11)	-0.0007 (11)
N2	0.0306 (13)	0.0224 (12)	0.0237 (12)	-0.0079 (10)	-0.0006 (10)	0.0018 (10)
N3	0.0288 (13)	0.0186 (12)	0.0234 (12)	-0.0066 (10)	-0.0006 (10)	-0.0007 (9)
O1	0.0319 (12)	0.0136 (10)	0.0401 (12)	-0.0018 (8)	0.0103 (10)	-0.0012 (8)
O2	0.0483 (16)	0.0202 (12)	0.100 (2)	-0.0103 (11)	0.0408 (16)	-0.0044 (13)
O3	0.0522 (15)	0.0225 (11)	0.0353 (12)	-0.0055 (10)	0.0178 (11)	0.0009 (9)
O4	0.0399 (12)	0.0151 (10)	0.0314 (11)	-0.0049 (9)	0.0044 (9)	-0.0014 (8)
O5	0.080 (2)	0.0305 (14)	0.0337 (13)	-0.0095 (13)	0.0069 (13)	0.0105 (10)
O6	0.0484 (15)	0.0429 (14)	0.0293 (12)	-0.0085 (12)	0.0131 (11)	-0.0061 (10)
O1W	0.0281 (12)	0.0221 (11)	0.0443 (13)	-0.0073 (9)	0.0061 (10)	0.0013 (10)
O2W	0.0297 (12)	0.0237 (11)	0.0424 (13)	-0.0070 (9)	-0.0075 (10)	0.0023 (10)
O3W	0.0660 (18)	0.0267 (12)	0.0248 (11)	-0.0132 (12)	0.0003 (11)	-0.0043 (9)

O4W 0.0426 (19) 0.079 (3) 0.227 (6) -0.0297 (18) 0.054 (3) -0.107 (3)

Geometric parameters (Å, °)

Ni1—O1	2.051 (2)	C11—O2	1.246 (4)
Ni1—O2W	2.079 (2)	C11—O1	1.256 (4)
Ni1—O1W	2.088 (2)	C11—C12	1.490 (4)
Ni1—O3W	2.142 (2)	C12—C13	1.375 (4)
Ni1—N2	2.097 (2)	C12—C18	1.387 (4)
Ni1—N3	2.100 (2)	C13—C14	1.380 (4)
C1—N3	1.331 (4)	C13—H13	0.9300
C1—C2	1.365 (5)	C14—C16	1.377 (4)
C1—H1	0.9300	C14—C15	1.499 (4)
C2—C3	1.366 (5)	C15—O3	1.232 (4)
C2—H2	0.9300	C15—O4	1.256 (3)
C3—C4	1.371 (5)	C16—C17	1.372 (4)
C3—H3	0.9300	C16—H16	0.9300
C4—C5	1.376 (4)	C17—C18	1.366 (4)
C4—H4	0.9300	C17—N1	1.463 (4)
C5—N3	1.345 (4)	C18—H18	0.9300
C5—C6	1.471 (4)	N1—O5	1.205 (4)
C6—N2	1.331 (4)	N1—O6	1.224 (3)
C6—C10	1.382 (4)	O1W—H1W	0.81 (3)
C7—N2	1.326 (4)	O1W—H2W	0.82 (4)
C7—C8	1.369 (5)	O2W—H3W	0.82 (3)
C7—H7	0.9300	O2W—H4W	0.82 (4)
C8—C9	1.371 (6)	O3W—H5W	0.82 (4)
C8—H8	0.9300	O3W—H6W	0.82 (3)
C9—C10	1.361 (5)	O4W—H7W	0.81 (4)
C9—H9	0.9300	O4W—H8W	0.81 (3)
C10—H10	0.9300		
O1—Ni1—O2W	88.23 (9)	O2—C11—O1	125.6 (3)
O1—Ni1—O1W	89.39 (9)	O2—C11—C12	117.3 (3)
O2W—Ni1—O1W	173.81 (9)	O1—C11—C12	117.1 (3)
O1—Ni1—N2	94.35 (9)	C13—C12—C18	120.0 (3)
O2W—Ni1—N2	89.63 (10)	C13—C12—C11	120.1 (3)
O1W—Ni1—N2	96.25 (10)	C18—C12—C11	119.9 (3)
O1—Ni1—N3	170.92 (9)	C14—C13—C12	121.1 (3)
O2W—Ni1—N3	89.18 (9)	C14—C13—H13	119.5
O1W—Ni1—N3	94.02 (9)	C12—C13—H13	119.5
N2—Ni1—N3	76.92 (9)	C13—C14—C16	119.1 (3)
O1—Ni1—O3W	93.00 (9)	C13—C14—C15	119.5 (3)
O2W—Ni1—O3W	88.23 (10)	C16—C14—C15	121.3 (3)
O1W—Ni1—O3W	86.19 (10)	O3—C15—O4	124.8 (3)
N2—Ni1—O3W	172.27 (9)	O3—C15—C14	118.2 (2)
N3—Ni1—O3W	95.62 (9)	O4—C15—C14	117.1 (3)
N3—C1—C2	122.5 (3)	C17—C16—C14	119.0 (3)
N3—C1—H1	118.8	C17—C16—H16	120.5
C2—C1—H1	118.8	C14—C16—H16	120.5

supplementary materials

C1—C2—C3	118.7 (3)	C18—C17—C16	122.9 (3)
C1—C2—H2	120.7	C18—C17—N1	118.6 (3)
C3—C2—H2	120.6	C16—C17—N1	118.5 (3)
C2—C3—C4	120.0 (3)	C17—C18—C12	117.8 (3)
C2—C3—H3	120.0	C17—C18—H18	121.1
C4—C3—H3	120.0	C12—C18—H18	121.1
C3—C4—C5	118.5 (3)	O5—N1—O6	123.2 (3)
C3—C4—H4	120.8	O5—N1—C17	118.1 (3)
C5—C4—H4	120.8	O6—N1—C17	118.7 (3)
N3—C5—C4	121.7 (3)	C7—N2—C6	118.3 (3)
N3—C5—C6	115.5 (2)	C7—N2—Ni1	125.9 (2)
C4—C5—C6	122.7 (3)	C6—N2—Ni1	115.4 (2)
N2—C6—C10	121.4 (3)	C1—N3—C5	118.7 (3)
N2—C6—C5	114.9 (3)	C1—N3—Ni1	126.6 (2)
C10—C6—C5	123.5 (3)	C5—N3—Ni1	114.67 (18)
N2—C7—C8	123.3 (3)	C11—O1—Ni1	125.67 (19)
N2—C7—H7	118.4	Ni1—O1W—H1W	105 (4)
C8—C7—H7	118.4	Ni1—O1W—H2W	113 (4)
C9—C8—C7	118.3 (3)	H1W—O1W—H2W	116 (3)
C9—C8—H8	120.8	Ni1—O2W—H3W	109 (3)
C7—C8—H8	120.8	Ni1—O2W—H4W	116 (4)
C10—C9—C8	119.0 (3)	H3W—O2W—H4W	113 (3)
C10—C9—H9	120.5	Ni1—O3W—H5W	109 (3)
C8—C9—H9	120.5	Ni1—O3W—H6W	120 (4)
C9—C10—C6	119.6 (3)	H5W—O3W—H6W	111 (3)
C9—C10—H10	120.2	H7W—O4W—H8W	116 (3)
C6—C10—H10	120.2		

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1W—H1W \cdots O2	0.81 (3)	2.00 (3)	2.727 (3)	150 (5)
O1W—H2W \cdots O4 ⁱ	0.82 (4)	1.96 (5)	2.715 (3)	154 (4)
O2W—H3W \cdots O4W ⁱⁱ	0.82 (3)	1.82 (4)	2.614 (4)	166 (4)
O2W—H4W \cdots O4 ⁱⁱⁱ	0.82 (4)	1.96 (4)	2.757 (3)	164 (4)
O3W—H5W \cdots O4W ^{iv}	0.82 (4)	2.42 (2)	3.185 (7)	156 (5)
O3W—H6W \cdots O4 ^v	0.82 (3)	1.97 (2)	2.735 (3)	155 (4)
O4W—H7W \cdots O2 ^{vi}	0.81 (4)	1.91 (2)	2.697 (4)	161 (5)
O4W—H8W \cdots O3 ^{vii}	0.81 (3)	1.98 (4)	2.639 (4)	138 (5)

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

Fig. 1

