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Poly[[aqua(2,2′-bipyridine)(μ_3-pyridine-3,4-dicarboxylato)nickel(II)] monohydrate]

Zhongfang Li,* Suwen Wang, Qian Zhang and Xianjin Yu

College of Chemical Engineering, Shandong University of Technology, Zibo 255049, People's Republic of China
Correspondence e-mail: zhfli_sdut@yahoo.com.cn

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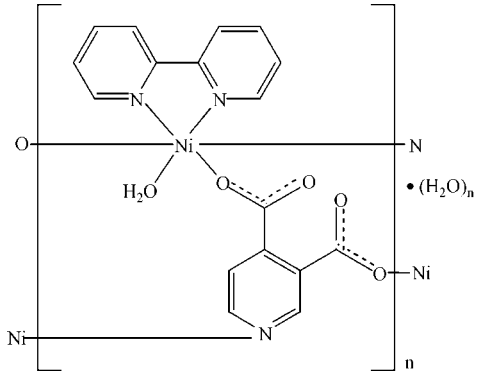
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.050; wR factor = 0.157; data-to-parameter ratio = 11.4.

The asymmetric unit of the title compound, $\{[Ni(C_7H_3NO_4)(C_{10}H_8N_2)(H_2O)]\cdot H_2O\}_n$, contains one nickel cation chelated by a 2,2′-bipyridine ligand and further coordinated by two monodentate carboxylate groups belonging to two independent pyridine-3,4-dicarboxylate ligands and one water molecule. The Ni^{II} atom is six-coordinate, exhibiting octahedral geometry with three N and three O atoms. Each pair of neighbouring Ni^{II} cations is bridged by two independent pyridine-3,4-dicarboxylate ligands, which are coordinated to two further Ni^{II} cations through pyridine N atoms to give corrugated layers parallel to the (110) plane. The coordinated and uncoordinated water molecules act as donors in O—H···O hydrogen bonds.

Related literature

For related literature, see: An *et al.* (2000); Baroni *et al.* (1996); Go *et al.* (2004); Hundal *et al.* (2002); Li *et al.* (1993).



Experimental

Crystal data

$[Ni(C_7H_3NO_4)(C_{10}H_8N_2)(H_2O)]\cdot H_2O$
M_r = 416.01
Orthorhombic, *Pbca*
a = 15.590 (2) Å
b = 12.3716 (18) Å
c = 17.012 (3) Å
V = 3281.1 (8) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 1.23 mm^{-1}
T = 293 (2) K
0.38 × 0.24 × 0.18 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.653, T_{max} = 0.810
24372 measured reflections
2924 independent reflections
2351 reflections with $I > 2\sigma(I)$
R_{int} = 0.071

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.158
S = 1.00
2924 reflections
256 parameters
6 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.57 e Å^{-3}
$\Delta\rho_{min}$ = −0.95 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O5—H1W···O6^{i}	0.798 (19)	2.03 (2)	2.824 (4)	173 (5)
O5—H2W···O2^{ii}	0.807 (19)	1.863 (19)	2.648 (3)	164 (4)
O6—H3W···O4^{iii}	0.82 (4)	1.97 (4)	2.786 (4)	177 (5)
O6—H4W···O2^{iv}	0.81 (4)	2.04 (2)	2.835 (4)	168 (4)

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CF2139).

References

An, J., Chen, Z. D., Bian, J., Chen, J. T., Wang, S. X., Gao, S. & Xu, G. X. (2000). *Inorg. Chim. Acta*, **299**, 28–30.
Baroni, T. E., Heppert, J. A., Hodel, R. R., Kingsborough, R. P., Morton, M. D., Pheingold, A. L. & Yap, G. P. A. (1996). *Organometallics*, **15**, 4872–4874.
Bruker (2001). *SADABS*, *SAINT-Plus* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2004). *APEX2*. Bruker AXS Inc., Madison, Wisconsin, USA.
Go, Y. B., Wang, X. Q. & Anokhina, E. V. (2004). *Inorg. Chem.* **43**, 5360–5364.
Hundal, G., Hundal, M. S., Obrai, S., Poonia, N. S. & Kumar, S. (2002). *Inorg. Chem.* **41**, 2077–2086.
Li, M. X., Xu, Z. & You, X. Z. (1993). *Polyhedron*, **12**, 921–923.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

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supplementary materials

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Poly[[aqua(2,2'-bipyridine)(μ_3-pyridine-3,4-dicarboxylato)nickel(II)] monohydrate]

Z. Li, S. Wang, Q. Zhang and X. Yu

Comment

Complexes containing carboxylic acids have been the interest of chemists due to their potential applications, such as in catalysis, optics, information storage, medicine, molecular electrochemistry, biochemistry and biological pharmaceutics (Li *et al.*, 1993; Go *et al.*, 2004). Thus far, N-containing aromatic carboxylic acids have been widely used in dye intermediates, organic synthesis, sensitization materials, functional pigments, adipiodone and acetrizoic acid (An *et al.*, 2000). Pyridine-carboxylic acids are also good ligands in coordination chemistry due to their strong coordination ability and versatile co-ordination modes, so much attention has been paid to them in recent decades (Baroni *et al.*, 1996; Hundal *et al.*, 2002). Here we report the new title nickel complex.

The asymmetric unit of the title compound contains one nickel cation chelated by a 2,2'-bipyridine ligand and further coordinated by two monodentate carboxylate groups belonging to two independent pyridine-3,4-dicarboxylate ligands and one water molecule (Fig. 1). Ni^{II} is six-coordinate, exhibiting octahedral geometry with three N and three O atoms. Each pair of neighboring Ni^{II} cations is bridged by two independent pyridine-3,4-dicarboxylate ligands, which are coordinated to two further Ni^{II} cations through pyridine N atoms to give corrugated layers parallel to the (110) plane (Fig. 2). The coordinated and uncoordinated water molecules act as donors in O—H···O hydrogen bonds.

Experimental

A mixture of nickel(II) chloride (1 mmol), pyridine-3,4-dicarboxylic acid (1 mmol), and 2,2-bipyridine (2 mmol) in a mixed 1:1 solvent of H_2O and ehanol in a 25 ml Teflon-lined stainless steel autoclave was kept at 473 K for ten days. Green crystals were obtained after cooling to room temperature, with a yield of 22%. Anal. Calc. for $C_{17}H_{15}NiN_3O_6$: C 49.04, H 3.61, N 10.12%; Found: C 48.89, H 3.41, N 10.06%.

Refinement

The H atoms of the water molecules were located in a difference density map and were refined with distance restraints H···H = 1.38 (2) Å and O—H = 0.88 (2) Å, and with a fixed U_{iso}(H) of 0.80 Å^2. All other H atoms were placed in calculated positions with a C—H bond distance of 0.93%A and U_{iso}(H) = 1.2U_{eq}(C).

Figures

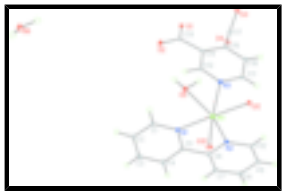

Fig. 1. The asymmetric unit of the title compound, with additional atoms to complete the co-ordination of the Ni atom, drawn with 30% probability displacement ellipsoids. Atoms with the suffix I are at the symmetry positions ($x - 1/2, -y + 1/2, -z$).

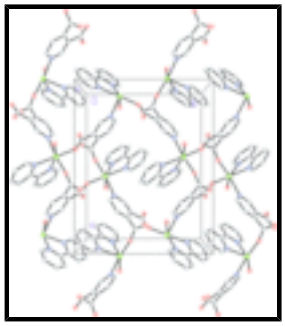

Fig. 2. A view of a corrugated layer parallel to the (110) plane. Hydrogen bonds are not shown.

Poly[[aqua(2,2'-bipyridine)(μ$_3$-pyridine-3,4-dicarboxylato)nickel(II)] monohydrate]

Crystal data

$[Ni(C_7H_3NO_4)(C_{10}H_8N_2)(H_2O)]\cdot H_2O$	F_{000} = 1712
M_r = 416.01	D_x = 1.684 Mg m^{-3}
Orthorhombic, *Pbca*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 2924 reflections
a = 15.590 (2) Å	θ = 2.4–25.2º
b = 12.3716 (18) Å	μ = 1.23 mm^{-1}
c = 17.012 (3) Å	*T* = 293 (2) K
V = 3281.1 (8) Å^3	Block, green
Z = 8	0.38 × 0.24 × 0.18 mm

Data collection

Bruker APEXII CCD area-detector diffractometer	2924 independent reflections
Radiation source: fine-focus sealed tube	2351 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.071
T = 293(2) K	θ_{max} = 25.2º
φ and ω scans	θ_{min} = 2.4º
Absorption correction: multi-scan (SADABS; Bruker, 2001)	*h* = −18→18
T_{min} = 0.653, T_{max} = 0.810	*k* = −14→14
24372 measured reflections	*l* = −20→20

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.050$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.158$	$w = 1/[\sigma^2(F_o^2) + (0.121P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{max} < 0.001$
2924 reflections	$\Delta\rho_{max} = 0.57$ e Å^{-3}
256 parameters	$\Delta\rho_{min} = -0.95$ e Å^{-3}
6 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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)

	x	*y*	*z*	U_{iso}*/U_{eq}
C5	−0.0540 (2)	0.3914 (3)	0.0593 (2)	0.0205 (7)
C6	−0.06399 (19)	0.3397 (3)	−0.0191 (2)	0.0192 (7)
C7	−0.1189 (2)	0.3808 (3)	−0.0778 (2)	0.0289 (8)
H7	−0.1516	0.4422	−0.0681	0.035*
C11	0.2092 (2)	0.2351 (3)	−0.0664 (2)	0.0265 (8)
H11	0.1814	0.1784	−0.0918	0.032*
C1	0.0212 (2)	0.4004 (3)	0.1760 (2)	0.0277 (8)
H1	0.0653	0.3744	0.2075	0.033*
C12	0.2256 (2)	0.3423 (3)	0.0407 (2)	0.0199 (7)
H12	0.2090	0.3618	0.0912	0.024*
C10	−0.0239 (2)	0.2004 (3)	−0.1025 (2)	0.0277 (8)
H10	0.0084	0.1383	−0.1111	0.033*
C2	−0.0275 (3)	0.4853 (3)	0.2044 (2)	0.0308 (8)
H2	−0.0165	0.5161	0.2532	0.037*
C9	−0.0766 (3)	0.2378 (3)	−0.1628 (2)	0.0355 (9)
H9	−0.0796	0.2015	−0.2105	0.043*

C8	−0.1239 (3)	0.3293 (3)	−0.1499 (2)	0.0372 (9)
H8	−0.1591	0.3567	−0.1893	0.045*
C4	−0.1062 (3)	0.4747 (3)	0.0845 (2)	0.0366 (10)
H4	−0.1506	0.4990	0.0526	0.044*
C3	−0.0925 (3)	0.5220 (3)	0.1572 (3)	0.0397 (10)
H3	−0.1274	0.5785	0.1740	0.048*
Ni1	0.06160 (3)	0.18951 (4)	0.06873 (3)	0.0286 (2)
N1	0.00879 (17)	0.3532 (2)	0.10608 (17)	0.0208 (6)
N2	−0.01779 (17)	0.2501 (2)	−0.03261 (17)	0.0198 (6)
N3	0.18294 (17)	0.2623 (2)	0.00577 (17)	0.0239 (7)
O5	0.13690 (16)	0.18750 (19)	0.18060 (16)	0.0266 (6)
O6	0.23546 (18)	0.1385 (2)	0.73885 (16)	0.0318 (6)
C14	0.29352 (19)	0.3989 (2)	0.00638 (19)	0.0173 (7)
C16	0.2761 (2)	0.2873 (3)	−0.1057 (2)	0.0256 (8)
H16	0.2920	0.2650	−0.1558	0.031*
C15	0.3183 (2)	0.3715 (3)	−0.07012 (19)	0.0190 (7)
C17	0.3845 (2)	0.4315 (3)	−0.11961 (19)	0.0209 (7)
O4	0.35850 (17)	0.5084 (2)	−0.15887 (16)	0.0342 (7)
C13	0.3335 (2)	0.4879 (3)	0.0545 (2)	0.0181 (7)
O1	0.38974 (14)	0.54323 (18)	0.02138 (14)	0.0233 (5)
O2	0.30669 (18)	0.5012 (2)	0.12400 (15)	0.0314 (6)
O3	0.45914 (15)	0.3942 (2)	−0.12202 (16)	0.0307 (6)
H1W	0.166 (2)	0.238 (2)	0.193 (3)	0.046*
H2W	0.163 (2)	0.136 (2)	0.164 (3)	0.046*
H3W	0.209 (3)	0.101 (3)	0.770 (2)	0.046*
H4W	0.260 (3)	0.106 (3)	0.7045 (19)	0.046*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C5	0.0195 (16)	0.0157 (17)	0.0263 (19)	0.0025 (13)	0.0007 (13)	0.0031 (13)
C6	0.0169 (16)	0.0190 (17)	0.0217 (17)	−0.0011 (13)	0.0002 (12)	0.0031 (14)
C7	0.0282 (19)	0.0268 (19)	0.032 (2)	0.0093 (15)	−0.0060 (16)	0.0011 (15)
C11	0.0243 (18)	0.0212 (19)	0.034 (2)	−0.0075 (14)	−0.0007 (14)	−0.0084 (14)
C1	0.0286 (18)	0.0267 (19)	0.0277 (19)	0.0051 (15)	−0.0034 (15)	−0.0007 (15)
C12	0.0230 (16)	0.0167 (16)	0.0201 (16)	−0.0012 (13)	−0.0003 (13)	−0.0010 (13)
C10	0.0249 (18)	0.026 (2)	0.032 (2)	0.0021 (14)	0.0026 (16)	−0.0074 (15)
C2	0.038 (2)	0.027 (2)	0.027 (2)	0.0034 (16)	0.0016 (16)	−0.0073 (15)
C9	0.038 (2)	0.039 (2)	0.029 (2)	−0.0015 (18)	−0.0037 (17)	−0.0121 (17)
C8	0.032 (2)	0.043 (2)	0.036 (2)	0.0029 (18)	−0.0118 (17)	0.0003 (18)
C4	0.037 (2)	0.038 (2)	0.035 (2)	0.0220 (18)	−0.0076 (18)	−0.0056 (17)
C3	0.047 (2)	0.034 (2)	0.038 (2)	0.0216 (19)	0.0013 (19)	−0.0055 (17)
Ni1	0.0280 (3)	0.0231 (3)	0.0347 (4)	0.00224 (18)	−0.00148 (19)	0.00007 (18)
N1	0.0196 (14)	0.0184 (15)	0.0242 (15)	0.0021 (11)	0.0004 (11)	−0.0021 (12)
N2	0.0181 (13)	0.0185 (14)	0.0227 (15)	0.0013 (11)	0.0004 (11)	0.0009 (11)
N3	0.0194 (14)	0.0220 (15)	0.0303 (17)	−0.0044 (12)	0.0006 (12)	−0.0010 (12)
O5	0.0304 (14)	0.0200 (13)	0.0295 (14)	0.0032 (10)	−0.0039 (11)	−0.0012 (10)
O6	0.0420 (16)	0.0262 (14)	0.0272 (14)	−0.0015 (12)	0.0072 (12)	0.0000 (11)

C14	0.0163 (15)	0.0113 (15)	0.0242 (17)	0.0002 (12)	−0.0033 (13)	0.0021 (13)
C16	0.0281 (18)	0.0243 (18)	0.0244 (19)	−0.0001 (14)	0.0028 (15)	−0.0051 (14)
C15	0.0160 (15)	0.0174 (17)	0.0236 (18)	0.0057 (13)	−0.0040 (13)	0.0024 (12)
C17	0.0235 (17)	0.0221 (17)	0.0170 (17)	0.0005 (14)	−0.0015 (13)	−0.0035 (13)
O4	0.0383 (15)	0.0289 (14)	0.0353 (16)	0.0098 (12)	0.0018 (12)	0.0149 (12)
C13	0.0172 (15)	0.0103 (15)	0.0268 (18)	0.0013 (12)	−0.0021 (13)	−0.0004 (13)
O1	0.0242 (12)	0.0163 (12)	0.0293 (13)	−0.0060 (10)	0.0007 (10)	−0.0023 (9)
O2	0.0433 (15)	0.0251 (13)	0.0257 (14)	−0.0136 (11)	0.0068 (11)	−0.0072 (11)
O3	0.0191 (12)	0.0354 (15)	0.0377 (16)	0.0098 (11)	0.0039 (11)	0.0108 (12)

Geometric parameters (Å, °)

C5—N1	1.347 (4)	C4—C3	1.386 (6)
C5—C4	1.381 (5)	C4—H4	0.930
C5—C6	1.488 (5)	C3—H3	0.930
C6—N2	1.342 (4)	Ni1—O3^{i}	2.108 (2)
C6—C7	1.410 (5)	Ni1—O1^{ii}	2.121 (2)
C7—C8	1.385 (6)	Ni1—O5	2.236 (3)
C7—H7	0.930	Ni1—N2	2.251 (3)
C11—N3	1.337 (5)	Ni1—N1	2.277 (3)
C11—C16	1.398 (5)	Ni1—N3	2.353 (3)
C11—H11	0.930	O5—H1W	0.798 (19)
C1—N1	1.339 (5)	O5—H2W	0.807 (19)
C1—C2	1.383 (5)	O6—H3W	0.82 (4)
C1—H1	0.930	O6—H4W	0.81 (4)
C12—N3	1.332 (4)	C14—C15	1.399 (5)
C12—C14	1.397 (5)	C14—C13	1.507 (4)
C12—H12	0.930	C16—C15	1.374 (5)
C10—N2	1.343 (5)	C16—H16	0.930
C10—C9	1.392 (6)	C15—C17	1.524 (5)
C10—H10	0.930	C17—O4	1.231 (4)
C2—C3	1.370 (6)	C17—O3	1.253 (4)
C2—H2	0.930	C13—O1	1.248 (4)
C9—C8	1.369 (6)	C13—O2	1.264 (4)
C9—H9	0.930	O1—Ni1^{iii}	2.121 (2)
C8—H8	0.930	O3—Ni1^{iv}	2.108 (2)
N1—C5—C4	120.5 (3)	O5—Ni1—N2	160.79 (9)
N1—C5—C6	117.1 (3)	O3^{i}—Ni1—N1	92.46 (10)
C4—C5—C6	122.5 (3)	O1^{ii}—Ni1—N1	173.86 (10)
N2—C6—C7	120.1 (3)	O5—Ni1—N1	87.84 (9)
N2—C6—C5	116.9 (3)	N2—Ni1—N1	73.66 (10)
C7—C6—C5	122.9 (3)	O3^{i}—Ni1—N3	173.10 (11)
C8—C7—C6	119.8 (3)	O1^{ii}—Ni1—N3	82.32 (10)
C8—C7—H7	120.1	O5—Ni1—N3	88.26 (10)
C6—C7—H7	120.1	N2—Ni1—N3	88.05 (10)
N3—C11—C16	123.5 (3)	N1—Ni1—N3	94.42 (10)
N3—C11—H11	118.3	C1—N1—C5	118.5 (3)

C16—C11—H11	118.3	C1—N1—Ni1	125.7 (2)
N1—C1—C2	124.2 (3)	C5—N1—Ni1	114.2 (2)
N1—C1—H1	117.9	C6—N2—C10	119.5 (3)
C2—C1—H1	117.9	C6—N2—Ni1	116.0 (2)
N3—C12—C14	124.4 (3)	C10—N2—Ni1	124.4 (2)
N3—C12—H12	117.8	C12—N3—C11	116.4 (3)
C14—C12—H12	117.8	C12—N3—Ni1	118.9 (2)
N2—C10—C9	122.8 (3)	C11—N3—Ni1	124.6 (2)
N2—C10—H10	118.6	Ni1—O5—H1W	121 (4)
C9—C10—H10	118.6	Ni1—O5—H2W	88 (3)
C3—C2—C1	116.9 (4)	H1W—O5—H2W	115 (3)
C3—C2—H2	121.5	H3W—O6—H4W	115 (3)
C1—C2—H2	121.5	C12—C14—C15	118.4 (3)
C8—C9—C10	118.4 (4)	C12—C14—C13	116.9 (3)
C8—C9—H9	120.8	C15—C14—C13	124.6 (3)
C10—C9—H9	120.8	C15—C16—C11	119.8 (3)
C9—C8—C7	119.4 (4)	C15—C16—H16	120.1
C9—C8—H8	120.3	C11—C16—H16	120.1
C7—C8—H8	120.3	C16—C15—C14	117.5 (3)
C5—C4—C3	120.1 (4)	C16—C15—C17	116.7 (3)
C5—C4—H4	119.9	C14—C15—C17	125.7 (3)
C3—C4—H4	119.9	O4—C17—O3	124.9 (3)
C2—C3—C4	119.8 (4)	O4—C17—C15	117.0 (3)
C2—C3—H3	120.1	O3—C17—C15	117.9 (3)
C4—C3—H3	120.1	O1—C13—O2	125.7 (3)
$O3^{i}$—Ni1—$O1^{ii}$	90.88 (10)	O1—C13—C14	116.5 (3)
$O3^{i}$—Ni1—O5	91.50 (10)	O2—C13—C14	117.8 (3)
$O1^{ii}$—Ni1—O5	97.24 (9)	C13—O1—$Ni1^{iii}$	123.2 (2)
$O3^{i}$—Ni1—N2	94.37 (10)	C17—O3—$Ni1^{iv}$	150.5 (2)
$O1^{ii}$—Ni1—N2	100.94 (10)		

Symmetry codes: (i) *x*−1/2, −*y*+1/2, −*z*; (ii) −*x*+1/2, *y*−1/2, *z*; (iii) −*x*+1/2, *y*+1/2, *z*; (iv) *x*+1/2, −*y*+1/2, −*z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H1W···$O6^{v}$	0.798 (19)	2.03 (2)	2.824 (4)	173 (5)
O5—H2W···$O2^{ii}$	0.807 (19)	1.863 (19)	2.648 (3)	164 (4)
O6—H3W···$O4^{vi}$	0.82 (4)	1.97 (4)	2.786 (4)	177 (5)
O6—H4W···$O2^{vii}$	0.81 (4)	2.04 (2)	2.835 (4)	168 (4)

Symmetry codes: (v) *x*, −*y*+1/2, *z*−1/2; (ii) −*x*+1/2, *y*−1/2, *z*; (vi) −*x*+1/2, *y*−1/2, *z*+1; (vii) *x*, −*y*+1/2, *z*+1/2.

Fig. 1

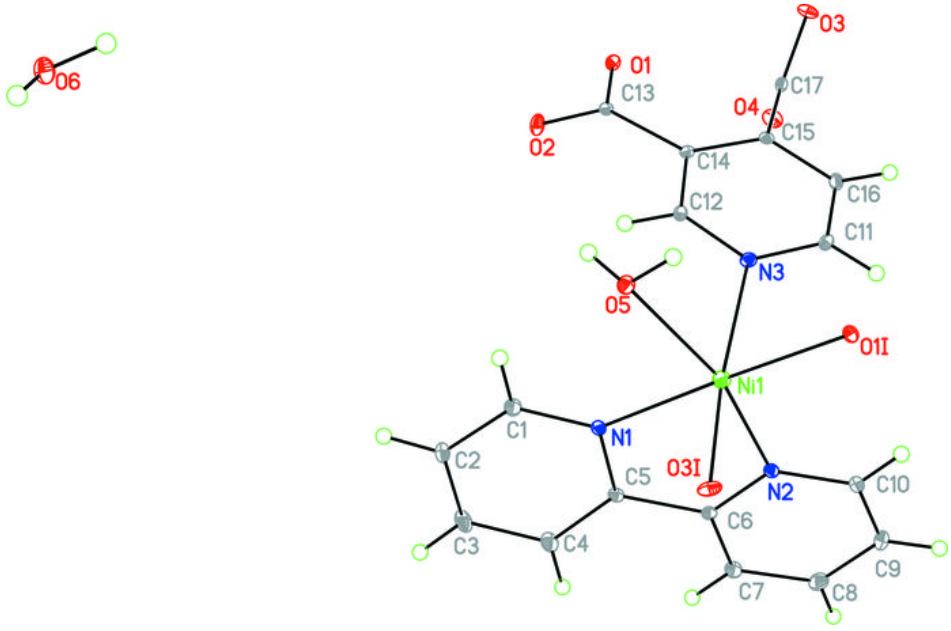
O6
O3
O1
C13
C17
O4
O2
C15
C14
C16
C12
C11
N3
O5
O1I
Ni1
C1
N1
C2
C5
O3I
N2
C10
C6
C3
C4
C9
C7
C8

Fig. 2