

Aquabis(2,3-dimethyl-4-oxo-4*H*-pyrido-[1,2-*a*]pyrimidin-9-olato)nickel(II)

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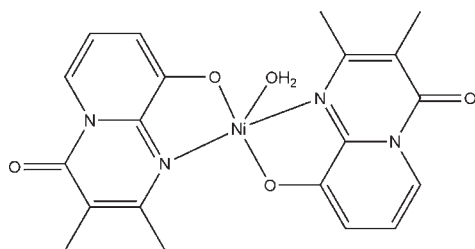
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Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.007$ Å; R factor = 0.049; wR factor = 0.132; data-to-parameter ratio = 13.0.

In the crystal structure of the mononuclear title complex, $[\text{Ni}(\text{C}_{10}\text{H}_9\text{N}_2\text{O}_2)_2(\text{H}_2\text{O})]$, the Ni^{II} ion is five-coordinated in a distorted square-pyramidal geometry by two N atoms and two O atoms from 2,3-dimethyl-4-oxopyrido[1,2-*a*]pyrimidin-9-olate ligands and one O atom from a water molecule. O—H...O hydrogen bonds between the coordinated water molecule and the ligand connect adjacent molecules, forming a ribbon parallel to the *b* axis.

Related literature

For the design and synthesis of self-assembling systems with organic ligands containing N and O donors, see: Wei *et al.* (2009); Sun *et al.* (2008); Bayot *et al.* (2006); Chen *et al.* (2007). For structures of quinolin-8-ol complexes, see: Wu *et al.* (2006).



Experimental

Crystal data

$[\text{Ni}(\text{C}_{10}\text{H}_9\text{N}_2\text{O}_2)_2(\text{H}_2\text{O})]$

$M_r = 455.11$

Monoclinic, $P2_1/c$

$a = 13.4032$ (14) Å

$b = 12.1313$ (12) Å

$c = 12.4631$ (11) Å

$\beta = 99.386$ (1)°

$V = 1999.3$ (3) Å³

$Z = 4$

Mo $K\alpha$ radiation

$\mu = 1.01$ mm⁻¹

$T = 298$ K

$0.30 \times 0.20 \times 0.12$ mm

Data collection

Rigaku SCXmini CCD area-

detector diffractometer

Absorption correction: multi-scan

(*CrystalClear*; Rigaku, 2005)

$T_{\text{min}} = 0.751$, $T_{\text{max}} = 0.888$

10283 measured reflections

3520 independent reflections

2242 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.045$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.049$

$wR(F^2) = 0.132$

$S = 1.03$

3520 reflections

271 parameters

H-atom parameters constrained

$\Delta\rho_{\text{max}} = 0.41$ e Å⁻³

$\Delta\rho_{\text{min}} = -0.41$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O5—H5A...O2 ⁱ	0.85	1.83	2.672 (5)	173
O5—H5B...O4 ⁱⁱ	0.85	1.85	2.669 (5)	162

Symmetry codes: (i) $-x + 1, -y + 1, -z$; (ii) $-x + 2, -y + 1, -z + 1$.

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; 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*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZQ2018).

References

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supplementary materials

Acta Cryst. (2010). E66, m5 [doi:10.1107/S1600536809051563]

Aquabis(2,3-dimethyl-4-oxo-4*H*-pyrido[1,2-*a*]pyrimidin-9-olato)nickel(II)

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Comment

Considerable attention has been paid to the design and synthesis of complexes with organic ligands containing N and O donors (Wei *et al.*, 2009; Sun *et al.*, 2008; Bayot *et al.*, 2006; Chen, *et al.*, 2007). Quinolin-8-ol is one such ligand and several crystal structures of complexes containing it have been reported (Wu *et al.*, 2006). We report here the synthesis and crystal structure of the title complex (I) (Fig. 1). In (I), the Ni atom is five-coordinated by two pyridine nitrogen atoms and two oxygen atoms from the hydroxy groups and one oxygen atom from a water molecule (Fig. 1). Intermolecular O—H...O hydrogen bonds (Fig.2 and Table 1) connecting the molecules of (I) define the crystal packing.

Experimental

All chemicals used (reagent grade) were commercially available. An aqueous solution (5 ml) of Ni(Ac)₂·4H₂O (24.9 mg, 0.1 mmol) was added to an ethanol solution (10 ml) containing 2,3-dimethyl-9-hydroxypyrido[1,2-*a*]pyrimidin-4-one (38.0 mg, 0.2 mmol) then filtered off. The resulting solution was continuously stirred for about 30 min and then filtered. The filtrate was slowly evaporated at room temperature over several days and colorless prism crystals suitable for X-ray analysis were obtained.

Refinement

The H atoms bound to carbon were placed in geometrical positions and refined using a riding model, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C) for aromatic H atoms, and with C—H = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms. The H atoms of the coordinated water were located from the Fourier difference map and refined with a distance restraint of O—H = 0.85 Å.

Figures

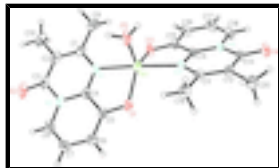


Fig. 1. The molecular structure of the title molecule and the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

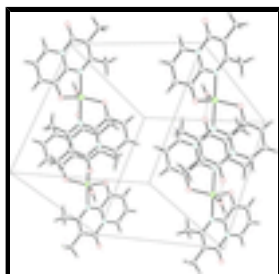


Fig. 2. Crystal packing of compound (I). Hydrogen bonds are shown as dashed lines.

Aquabis(2,3-dimethyl-4-oxo-4H-pyrido[1,2-a]pyrimidin-9-olato)nickel(II)

Crystal data

[Ni(C ₁₀ H ₉ N ₂ O ₂) ₂ (H ₂ O)]	$F(000) = 944$
$M_r = 455.11$	$D_x = 1.512 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
Hall symbol: -P 2ybc	Cell parameters from 2294 reflections
$a = 13.4032 (14) \text{ \AA}$	$\theta = 2.3\text{--}23.7^\circ$
$b = 12.1313 (12) \text{ \AA}$	$\mu = 1.01 \text{ mm}^{-1}$
$c = 12.4631 (11) \text{ \AA}$	$T = 298 \text{ K}$
$\beta = 99.3860 (10)^\circ$	Prism, colorless
$V = 1999.3 (3) \text{ \AA}^3$	$0.30 \times 0.20 \times 0.12 \text{ mm}$
$Z = 4$	

Data collection

Rigaku SCXmini CCD area-detector diffractometer	3520 independent reflections
Radiation source: fine-focus sealed tube graphite	2242 reflections with $I > 2\sigma(I)$
phi and ω scans	$R_{\text{int}} = 0.045$
Absorption correction: multi-scan (<i>CrystalClear</i> ; Rigaku, 200)	$\theta_{\text{max}} = 25.0^\circ$, $\theta_{\text{min}} = 1.5^\circ$
$T_{\text{min}} = 0.751$, $T_{\text{max}} = 0.888$	$h = -15 \rightarrow 15$
10283 measured reflections	$k = -13 \rightarrow 14$
	$l = -8 \rightarrow 14$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.049$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.132$	H-atom parameters constrained
$S = 1.03$	$w = 1/[\sigma^2(F_o^2) + (0.0496P)^2 + 2.7285P]$
3520 reflections	where $P = (F_o^2 + 2F_c^2)/3$
271 parameters	$(\Delta/\sigma)_{\text{max}} = 0.001$
0 restraints	$\Delta\rho_{\text{max}} = 0.41 \text{ e \AA}^{-3}$
	$\Delta\rho_{\text{min}} = -0.40 \text{ e \AA}^{-3}$

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	0.79535 (4)	0.41721 (5)	0.19800 (5)	0.0428 (2)
N1	0.6831 (2)	0.4337 (3)	0.0534 (3)	0.0351 (9)
N2	0.5489 (3)	0.3281 (3)	-0.0425 (3)	0.0413 (10)
N3	0.9220 (2)	0.3915 (3)	0.3261 (3)	0.0334 (8)
N4	1.0960 (3)	0.4366 (3)	0.3602 (3)	0.0348 (9)
O1	0.7277 (2)	0.2737 (3)	0.1993 (2)	0.0460 (8)
O2	0.4536 (3)	0.3929 (3)	-0.1970 (3)	0.0690 (12)
O3	0.9049 (2)	0.4701 (3)	0.1247 (2)	0.0460 (8)
O4	1.1941 (2)	0.3960 (3)	0.5228 (3)	0.0536 (9)
O5	0.7303 (2)	0.5312 (3)	0.2785 (3)	0.0679 (11)
H5A	0.6697	0.5514	0.2562	0.082*
H5B	0.7550	0.5674	0.3350	0.082*
C1	0.6639 (3)	0.5152 (4)	-0.0221 (4)	0.0404 (11)
C2	0.5870 (4)	0.5058 (4)	-0.1098 (4)	0.0475 (13)
C3	0.5254 (3)	0.4119 (5)	-0.1233 (4)	0.0479 (13)
C4	0.6274 (3)	0.3425 (4)	0.0416 (3)	0.0337 (10)
C5	0.6514 (3)	0.2575 (4)	0.1225 (4)	0.0373 (11)
C6	0.5915 (4)	0.1653 (4)	0.1126 (4)	0.0504 (13)
H6	0.6050	0.1089	0.1634	0.061*
C7	0.5104 (4)	0.1549 (5)	0.0275 (5)	0.0621 (15)
H7	0.4700	0.0922	0.0231	0.075*
C8	0.4899 (4)	0.2337 (5)	-0.0480 (5)	0.0586 (15)
H8	0.4358	0.2252	-0.1045	0.070*
C9	0.7298 (4)	0.6146 (4)	-0.0027 (4)	0.0582 (14)
H9A	0.7661	0.6130	0.0703	0.087*
H9B	0.6887	0.6798	-0.0130	0.087*
H9C	0.7769	0.6149	-0.0530	0.087*
C10	0.5654 (4)	0.5939 (5)	-0.1961 (4)	0.0653 (16)
H10A	0.5696	0.6652	-0.1622	0.098*
H10B	0.4987	0.5834	-0.2365	0.098*
H10C	0.6142	0.5891	-0.2445	0.098*
C11	0.9307 (3)	0.3468 (4)	0.4274 (3)	0.0352 (10)
C12	1.0208 (3)	0.3451 (4)	0.4981 (3)	0.0362 (10)
C13	1.1084 (3)	0.3907 (4)	0.4675 (4)	0.0378 (11)
C14	1.0038 (3)	0.4335 (3)	0.2942 (3)	0.0311 (10)
C15	0.9932 (3)	0.4783 (4)	0.1855 (3)	0.0360 (10)
C16	1.0767 (4)	0.5258 (4)	0.1534 (4)	0.0466 (12)
H16	1.0721	0.5558	0.0841	0.056*

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C17	1.1679 (4)	0.5290 (4)	0.2247 (4)	0.0527 (13)
H17	1.2234	0.5623	0.2021	0.063*
C18	1.1788 (3)	0.4855 (4)	0.3254 (4)	0.0480 (13)
H18	1.2410	0.4883	0.3711	0.058*
C19	0.8349 (3)	0.3004 (4)	0.4571 (4)	0.0484 (13)
H19A	0.8131	0.3456	0.5121	0.073*
H19B	0.8470	0.2268	0.4842	0.073*
H19C	0.7833	0.2993	0.3938	0.073*
C20	1.0318 (4)	0.2944 (4)	0.6096 (4)	0.0551 (14)
H20A	0.9703	0.3043	0.6384	0.083*
H20B	1.0866	0.3293	0.6566	0.083*
H20C	1.0457	0.2170	0.6048	0.083*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0354 (3)	0.0546 (4)	0.0368 (4)	-0.0007 (3)	0.0008 (3)	0.0014 (3)
N1	0.0296 (19)	0.045 (2)	0.029 (2)	0.0054 (17)	0.0013 (15)	-0.0004 (17)
N2	0.034 (2)	0.052 (3)	0.035 (2)	0.0108 (19)	-0.0008 (17)	-0.0133 (18)
N3	0.0277 (19)	0.043 (2)	0.029 (2)	-0.0016 (16)	0.0040 (15)	0.0005 (16)
N4	0.0308 (19)	0.042 (2)	0.030 (2)	-0.0009 (16)	0.0009 (16)	-0.0070 (16)
O1	0.0438 (19)	0.053 (2)	0.0376 (19)	0.0011 (15)	-0.0052 (15)	0.0100 (15)
O2	0.051 (2)	0.105 (3)	0.044 (2)	0.028 (2)	-0.0141 (18)	-0.015 (2)
O3	0.0358 (18)	0.067 (2)	0.0329 (18)	-0.0040 (16)	-0.0014 (14)	0.0100 (16)
O4	0.042 (2)	0.075 (3)	0.038 (2)	0.0039 (17)	-0.0102 (16)	-0.0068 (16)
O5	0.048 (2)	0.098 (3)	0.048 (2)	0.028 (2)	-0.0204 (16)	-0.032 (2)
C1	0.042 (3)	0.046 (3)	0.035 (3)	0.012 (2)	0.011 (2)	0.007 (2)
C2	0.052 (3)	0.057 (3)	0.034 (3)	0.024 (3)	0.009 (2)	0.005 (2)
C3	0.037 (3)	0.072 (4)	0.032 (3)	0.025 (3)	-0.004 (2)	-0.010 (3)
C4	0.028 (2)	0.043 (3)	0.029 (2)	0.004 (2)	0.0021 (19)	-0.006 (2)
C5	0.034 (3)	0.039 (3)	0.040 (3)	0.003 (2)	0.008 (2)	-0.002 (2)
C6	0.049 (3)	0.042 (3)	0.062 (4)	0.002 (2)	0.014 (3)	0.003 (2)
C7	0.049 (3)	0.043 (3)	0.092 (5)	-0.005 (3)	0.005 (3)	-0.017 (3)
C8	0.037 (3)	0.066 (4)	0.068 (4)	-0.004 (3)	-0.006 (3)	-0.031 (3)
C9	0.062 (3)	0.052 (3)	0.062 (4)	0.005 (3)	0.013 (3)	0.017 (3)
C10	0.071 (4)	0.078 (4)	0.046 (3)	0.034 (3)	0.006 (3)	0.018 (3)
C11	0.040 (3)	0.038 (3)	0.028 (3)	0.003 (2)	0.008 (2)	0.002 (2)
C12	0.047 (3)	0.035 (3)	0.026 (2)	0.004 (2)	0.002 (2)	-0.0003 (19)
C13	0.041 (3)	0.038 (3)	0.030 (3)	0.006 (2)	-0.004 (2)	-0.008 (2)
C14	0.029 (2)	0.037 (2)	0.027 (2)	0.0029 (19)	0.0013 (18)	-0.0050 (18)
C15	0.037 (3)	0.042 (3)	0.028 (3)	-0.001 (2)	0.004 (2)	-0.004 (2)
C16	0.050 (3)	0.060 (3)	0.031 (3)	-0.011 (2)	0.010 (2)	0.000 (2)
C17	0.047 (3)	0.067 (4)	0.046 (3)	-0.014 (3)	0.015 (3)	-0.007 (3)
C18	0.029 (3)	0.067 (3)	0.047 (3)	-0.010 (2)	0.005 (2)	-0.008 (3)
C19	0.046 (3)	0.061 (3)	0.040 (3)	-0.004 (2)	0.012 (2)	0.004 (2)
C20	0.064 (3)	0.060 (3)	0.037 (3)	0.002 (3)	-0.004 (3)	0.007 (2)

Geometric parameters (Å, °)

Ni1—O3	1.959 (3)	C6—H6	0.9300
Ni1—O1	1.964 (3)	C7—C8	1.338 (8)
Ni1—O5	1.991 (3)	C7—H7	0.9300
Ni1—N3	2.155 (3)	C8—H8	0.9300
Ni1—N1	2.160 (3)	C9—H9A	0.9600
N1—C4	1.329 (5)	C9—H9B	0.9600
N1—C1	1.360 (5)	C9—H9C	0.9600
N2—C4	1.370 (5)	C10—H10A	0.9600
N2—C8	1.387 (6)	C10—H10B	0.9600
N2—C3	1.429 (6)	C10—H10C	0.9600
N3—C14	1.327 (5)	C11—C12	1.374 (6)
N3—C11	1.361 (5)	C11—C19	1.503 (6)
N4—C14	1.368 (5)	C12—C13	1.406 (6)
N4—C18	1.389 (5)	C12—C20	1.505 (6)
N4—C13	1.433 (6)	C14—C15	1.445 (6)
O1—C5	1.297 (5)	C15—C16	1.374 (6)
O2—C3	1.239 (5)	C16—C17	1.390 (7)
O3—C15	1.301 (5)	C16—H16	0.9300
O4—C13	1.241 (5)	C17—C18	1.347 (7)
O5—H5A	0.8499	C17—H17	0.9300
O5—H5B	0.8499	C18—H18	0.9300
C1—C2	1.379 (6)	C19—H19A	0.9600
C1—C9	1.491 (7)	C19—H19B	0.9600
C2—C3	1.401 (7)	C19—H19C	0.9600
C2—C10	1.511 (7)	C20—H20A	0.9600
C4—C5	1.442 (6)	C20—H20B	0.9600
C5—C6	1.370 (6)	C20—H20C	0.9600
C6—C7	1.395 (7)		
O3—Ni1—O1	132.53 (14)	N2—C8—H8	119.8
O3—Ni1—O5	115.52 (16)	C1—C9—H9A	109.5
O1—Ni1—O5	111.75 (15)	C1—C9—H9B	109.5
O3—Ni1—N3	80.38 (12)	H9A—C9—H9B	109.5
O1—Ni1—N3	100.05 (13)	C1—C9—H9C	109.5
O5—Ni1—N3	94.82 (13)	H9A—C9—H9C	109.5
O3—Ni1—N1	93.07 (13)	H9B—C9—H9C	109.5
O1—Ni1—N1	80.18 (13)	C2—C10—H10A	109.5
O5—Ni1—N1	93.07 (13)	C2—C10—H10B	109.5
N3—Ni1—N1	171.37 (13)	H10A—C10—H10B	109.5
C4—N1—C1	119.3 (4)	C2—C10—H10C	109.5
C4—N1—Ni1	108.5 (3)	H10A—C10—H10C	109.5
C1—N1—Ni1	132.2 (3)	H10B—C10—H10C	109.5
C4—N2—C8	120.3 (4)	N3—C11—C12	122.3 (4)
C4—N2—C3	120.1 (4)	N3—C11—C19	115.5 (4)
C8—N2—C3	119.6 (4)	C12—C11—C19	122.2 (4)
C14—N3—C11	118.7 (3)	C11—C12—C13	120.4 (4)
C14—N3—Ni1	108.2 (3)	C11—C12—C20	122.8 (4)

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C11—N3—Ni1	133.0 (3)	C13—C12—C20	116.8 (4)
C14—N4—C18	120.9 (4)	O4—C13—C12	127.5 (4)
C14—N4—C13	120.4 (4)	O4—C13—N4	117.0 (4)
C18—N4—C13	118.7 (4)	C12—C13—N4	115.5 (4)
C5—O1—Ni1	116.0 (3)	N3—C14—N4	122.7 (4)
C15—O3—Ni1	115.7 (3)	N3—C14—C15	117.7 (4)
Ni1—O5—H5A	120.6	N4—C14—C15	119.6 (4)
Ni1—O5—H5B	129.2	O3—C15—C16	124.7 (4)
H5A—O5—H5B	110.1	O3—C15—C14	117.3 (4)
N1—C1—C2	121.4 (4)	C16—C15—C14	118.0 (4)
N1—C1—C9	115.8 (4)	C15—C16—C17	119.9 (4)
C2—C1—C9	122.8 (4)	C15—C16—H16	120.0
C1—C2—C3	120.8 (4)	C17—C16—H16	120.0
C1—C2—C10	122.5 (5)	C18—C17—C16	122.4 (5)
C3—C2—C10	116.7 (5)	C18—C17—H17	118.8
O2—C3—C2	127.7 (5)	C16—C17—H17	118.8
O2—C3—N2	116.4 (5)	C17—C18—N4	119.1 (4)
C2—C3—N2	115.9 (4)	C17—C18—H18	120.4
N1—C4—N2	122.6 (4)	N4—C18—H18	120.4
N1—C4—C5	117.4 (4)	C11—C19—H19A	109.5
N2—C4—C5	120.0 (4)	C11—C19—H19B	109.5
O1—C5—C6	124.8 (4)	H19A—C19—H19B	109.5
O1—C5—C4	117.8 (4)	C11—C19—H19C	109.5
C6—C5—C4	117.4 (4)	H19A—C19—H19C	109.5
C5—C6—C7	121.0 (5)	H19B—C19—H19C	109.5
C5—C6—H6	119.5	C12—C20—H20A	109.5
C7—C6—H6	119.5	C12—C20—H20B	109.5
C8—C7—C6	121.0 (5)	H20A—C20—H20B	109.5
C8—C7—H7	119.5	C12—C20—H20C	109.5
C6—C7—H7	119.5	H20A—C20—H20C	109.5
C7—C8—N2	120.3 (5)	H20B—C20—H20C	109.5
C7—C8—H8	119.8		
O3—Ni1—N1—C4	133.7 (3)	N1—C4—C5—O1	-2.3 (6)
O1—Ni1—N1—C4	1.0 (3)	N2—C4—C5—O1	178.5 (4)
O5—Ni1—N1—C4	-110.5 (3)	N1—C4—C5—C6	177.6 (4)
O3—Ni1—N1—C1	-44.8 (4)	N2—C4—C5—C6	-1.6 (6)
O1—Ni1—N1—C1	-177.5 (4)	O1—C5—C6—C7	179.7 (4)
O5—Ni1—N1—C1	71.0 (4)	C4—C5—C6—C7	-0.1 (7)
O3—Ni1—N3—C14	6.0 (3)	C5—C6—C7—C8	1.1 (8)
O1—Ni1—N3—C14	137.8 (3)	C6—C7—C8—N2	-0.4 (8)
O5—Ni1—N3—C14	-109.1 (3)	C4—N2—C8—C7	-1.4 (7)
O3—Ni1—N3—C11	-176.6 (4)	C3—N2—C8—C7	-179.5 (5)
O1—Ni1—N3—C11	-44.9 (4)	C14—N3—C11—C12	1.0 (6)
O5—Ni1—N3—C11	68.3 (4)	Ni1—N3—C11—C12	-176.2 (3)
O3—Ni1—O1—C5	-87.5 (3)	C14—N3—C11—C19	-179.6 (4)
O5—Ni1—O1—C5	87.0 (3)	Ni1—N3—C11—C19	3.3 (6)
N3—Ni1—O1—C5	-173.6 (3)	N3—C11—C12—C13	0.2 (7)
N1—Ni1—O1—C5	-2.4 (3)	C19—C11—C12—C13	-179.2 (4)
O1—Ni1—O3—C15	-102.8 (3)	N3—C11—C12—C20	-179.0 (4)

O5—Ni1—O3—C15	82.8 (3)	C19—C11—C12—C20	1.7 (7)
N3—Ni1—O3—C15	-8.0 (3)	C11—C12—C13—O4	179.3 (4)
N1—Ni1—O3—C15	177.7 (3)	C20—C12—C13—O4	-1.6 (7)
C4—N1—C1—C2	0.9 (6)	C11—C12—C13—N4	-0.3 (6)
Ni1—N1—C1—C2	179.3 (3)	C20—C12—C13—N4	178.9 (4)
C4—N1—C1—C9	179.9 (4)	C14—N4—C13—O4	179.8 (4)
Ni1—N1—C1—C9	-1.7 (6)	C18—N4—C13—O4	-1.2 (6)
N1—C1—C2—C3	0.5 (7)	C14—N4—C13—C12	-0.6 (6)
C9—C1—C2—C3	-178.4 (4)	C18—N4—C13—C12	178.4 (4)
N1—C1—C2—C10	-178.7 (4)	C11—N3—C14—N4	-2.0 (6)
C9—C1—C2—C10	2.4 (7)	Ni1—N3—C14—N4	175.8 (3)
C1—C2—C3—O2	179.4 (4)	C11—N3—C14—C15	178.7 (4)
C10—C2—C3—O2	-1.4 (7)	Ni1—N3—C14—C15	-3.5 (4)
C1—C2—C3—N2	-0.9 (6)	C18—N4—C14—N3	-177.2 (4)
C10—C2—C3—N2	178.3 (4)	C13—N4—C14—N3	1.8 (6)
C4—N2—C3—O2	179.7 (4)	C18—N4—C14—C15	2.2 (6)
C8—N2—C3—O2	-2.1 (6)	C13—N4—C14—C15	-178.8 (4)
C4—N2—C3—C2	0.0 (6)	Ni1—O3—C15—C16	-171.8 (4)
C8—N2—C3—C2	178.2 (4)	Ni1—O3—C15—C14	8.5 (5)
C1—N1—C4—N2	-1.9 (6)	N3—C14—C15—O3	-2.9 (6)
Ni1—N1—C4—N2	179.4 (3)	N4—C14—C15—O3	177.8 (4)
C1—N1—C4—C5	179.0 (4)	N3—C14—C15—C16	177.5 (4)
Ni1—N1—C4—C5	0.3 (4)	N4—C14—C15—C16	-1.9 (6)
C8—N2—C4—N1	-176.8 (4)	O3—C15—C16—C17	-179.2 (4)
C3—N2—C4—N1	1.4 (6)	C14—C15—C16—C17	0.4 (7)
C8—N2—C4—C5	2.3 (6)	C15—C16—C17—C18	0.8 (8)
C3—N2—C4—C5	-179.5 (4)	C16—C17—C18—N4	-0.6 (8)
Ni1—O1—C5—C6	-176.6 (3)	C14—N4—C18—C17	-0.9 (7)
Ni1—O1—C5—C4	3.3 (5)	C13—N4—C18—C17	-179.9 (4)

Hydrogen-bond geometry (Å, °)

<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>
O5—H5A \cdots O2 ⁱ	0.85	1.83	2.672 (5)	173
O5—H5B \cdots O4 ⁱⁱ	0.85	1.85	2.669 (5)	162

Symmetry codes: (i) $-x+1, -y+1, -z$; (ii) $-x+2, -y+1, -z+1$.

Fig. 1

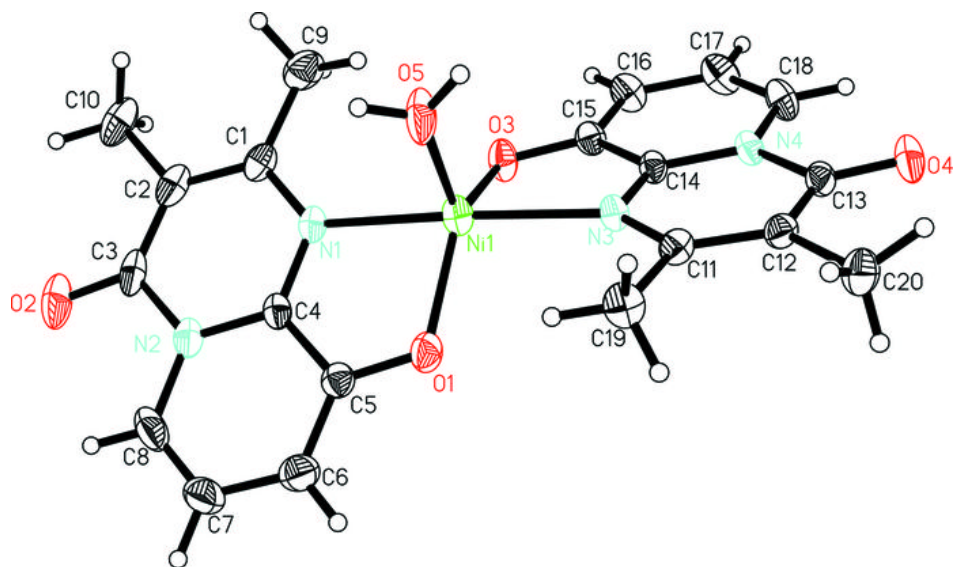


Fig. 2

