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Diaquabis[5-(pyrimidin-2-yl-κN)tetrazolato-κN^1]nickel(II)

Y.-E Qiu

Department of Chemistry, Dezhou University, Dezhou 253011, People's Republic of China
Correspondence e-mail: zyzh20060601@126.com

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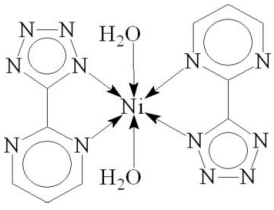
Key indicators: single-crystal X-ray study; T = 113 K; mean σ(C–C) = 0.009 Å; R factor = 0.079; wR factor = 0.189; data-to-parameter ratio = 10.7.

In the title complex, $[Ni(C_5H_3N_6)_2(H_2O)_2]$, the Ni^{II} atom is located in a general position and is coordinated by four N atoms from two 5-(pyrimidin-2-yl)tetrazolate ligands and O atoms of two water molecules in a distorted octahedral geometry. The bond distances and angles around the metal center lie in the ranges 2.051 (5)–2.097 (5) Å and 78.88 (19)–101.22 (19)°, respectively. The title complex is isostructural with its Mn^{II} and Cu^{II} analogues; it is, however, structurally different from an Ni^{II} complex obtained by direct reaction of 2-(1*H*-tetrazol-5-yl)pyrimidine with an Ni^{II} salt under hydrothermal conditions. In the crystal structure, molecules are linked together by O—H···N hydrogen bonds, forming a two-dimensional network parallel to the (001) plane.

Related literature

For related literature, see: Jin *et al.* (2007); Liu & Fan (2007*a*,*b*); Rodríguez *et al.* (2005, 2006, 2007); Zhang *et al.* (2007).



Experimental

Crystal data

$[Ni(C_5H_3N_6)_2(H_2O)_2]$
M_r = 389.01
Monoclinic, $P2_1/c$
a = 7.1271 (14) Å
b = 12.707 (3) Å
c = 16.401 (4) Å
β = 106.95 (3)°
V = 1420.8 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.41 mm^{-1}
T = 113 (2) K
0.20 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.766, T_{max} = 1.000
(expected range = 0.595–0.777)
8530 measured reflections
2556 independent reflections
2113 reflections with $I > 2\sigma(I)$
R_{int} = 0.086

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.079
$wR(F^2)$ = 0.189
S = 1.00
2556 reflections
238 parameters
30 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.55 e Å^{-3}
$\Delta\rho_{min}$ = −0.66 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ni1—N1	2.057 (5)	Ni1—N11	2.092 (5)
Ni1—N5	2.096 (5)	Ni1—O1*W*	2.087 (5)
Ni1—N7	2.051 (5)	Ni1—O2*W*	2.097 (5)
N1—Ni1—N5	78.88 (19)	N7—Ni1—O1*W*	90.45 (19)
N1—Ni1—N11	100.25 (19)	N7—Ni1—O2*W*	89.63 (19)
N1—Ni1—O1*W*	90.80 (19)	N11—Ni1—N5	179.0 (2)
N1—Ni1—O2*W*	89.12 (19)	N11—Ni1—O2*W*	88.52 (18)
N5—Ni1—O2*W*	90.91 (18)	O1*W*—Ni1—N11	91.29 (19)
N7—Ni1—N1	178.7 (2)	O1*W*—Ni1—N5	89.28 (18)
N7—Ni1—N5	101.22 (19)	O1*W*—Ni1—O2*W*	179.78 (18)
N7—Ni1—N11	79.63 (19)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*WA*···N10^{i}	0.85 (2)	1.97 (2)	2.788 (7)	162 (6)
O1*W*—H1*WB*···N3^{ii}	0.84 (2)	1.97 (3)	2.804 (7)	167 (6)
O2*W*—H2*WA*···N9^{iii}	0.84 (2)	1.97 (2)	2.798 (6)	170 (6)
O2*W*—H2*WB*···N4^{iv}	0.85 (2)	1.97 (3)	2.776 (7)	160 (6)

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); 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: CI2479).

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supplementary materials

Acta Cryst. (2007). E**63**, m2872-m2873 [**doi:10.1107/S1600536807053998**]

Diaquabis[5-(pyrimidin-2-yl-κN)tetrazolato-κN^1]nickel(II)

Y.-E. Qiu

Comment

The syntheses and crystal structures of Na^{II}, Mn^{II}, Fe^{II}, Co^{II}, Ni^{II}, Cu^{II} and Zn^{II} complexes with 5-(pyrimidin-2-yl)tetrazolate group have been reported (Jin et al., 2007; Liu & Fan, 2007a,b; Rodríguez et al., 2005, 2006, 2007; Zhang et al., 2007). Such complexes were obtained by different methods and the ligand performed several coordination modes. Except the Mn^{II} and Cu^{II} complexes, which are mononuclear being similar to the title complex, other complexes have an extended structure. It is interesting to note that the two Ni^{II} complexes of this ligand obtained by different synthesis methods, the direct reaction of 2-(1H-tetrazol-5-yl)pyrimidine and the in situ reaction (this report) from pyrimidine-2-carbonitrile in the presence of NaN_3 with nickel(II) salt under the hydrothermal condition, have different structures, indicating the influence of synthesis method on the formation of complexes and the coordination diversity of the ligand.

The title complex has a mononuclear structure (Fig. 1). The Ni^{II} atom, located in a general position, is coordinated by two ligands using pyrimidine and tetrazole N atoms in the 1-position and two water molecules in the trans positions. The coordination bond distances and angles are normal (Table 1). In the crystal structure, the complex molecules are linked via O_w—H···N hydrogen bonds, forming a two-dimensional network parallel to the (0 0 1) plane (Fig. 2). The hydrogen bond parameters are listed in Table 2.

Experimental

A mixture of $NiCl_2{\cdot}6H_2O$ (24 mg, 0.1 mmol), NaN_3 (26 mg, 0.4 mmol) and pyrimidine-2-carbonitrile (21 mg, 0.2 mmol) in water (8 ml) was placed in a Teflon-lined stainless-steel Parr bomb that was heated at 393 K for 48 h. Pale purple crystals of the title compound were collected after the bomb was subsequently allowed to cool to room temperature (yield 10%). Caution: Azide and tetrazole derivatives are potentially explosive. Although we have met no problems in this work, only a small amount of them should be prepared and handled with great caution.

Refinement

H atoms of water molecules were located in a difference map and refined with bond restraints O—H = 0.85 (2) Å, and with U_{iso}(H) = 1.5U_{eq}(O). The remaining H atoms were included in calculated positions and treated in the subsequent refinement as riding atoms, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C).

Figures

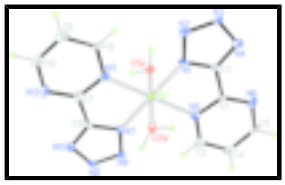

Fig. 1. The molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level.

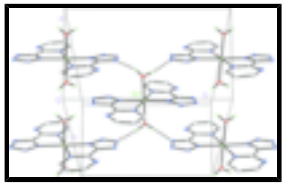

Fig. 2. Part of a hydrogen-bonded (dashed lines) two-dimensional network in the title compound.

Diaquabis[5-(pyrimidin-2-yl-κN)tetrazolato-κN^1]nickel(II)

Crystal data

$[Ni(C_5H_3N_6)_2(H_2O)_2]$	F_{000} = 792
M_r = 389.01	D_x = 1.819 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 3850 reflections
a = 7.1271 (14) Å	θ = 2.1–27.9º
b = 12.707 (3) Å	μ = 1.41 mm^{-1}
c = 16.401 (4) Å	T = 113 (2) K
β = 106.95 (3)º	Block, pink
V = 1420.8 (6) Å^3	0.20 × 0.20 × 0.18 mm
Z = 4	

Data collection

Bruker Smart CCD area-detector diffractometer	2556 independent reflections
Radiation source: fine-focus sealed tube	2113 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.086
T = 113(2) K	θ_{max} = 25.3º
φ and ω scans	θ_{min} = 2.1º
Absorption correction: multi-scan (SADABS; Bruker, 1998)	h = −8→8
T_{min} = 0.766, T_{max} = 1.000	k = −15→15
8530 measured reflections	l = −19→13

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites

$R[F^2 > 2\sigma(F^2)] = 0.079$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.189$	$w = 1/[\sigma^2(F_o^2) + (0.086P)^2 + 8.6013P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{max} = 0.001$
2556 reflections	$\Delta\rho_{max} = 0.55$ e Å^{-3}
238 parameters	$\Delta\rho_{min} = -0.66$ e Å^{-3}
30 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}
Ni1	0.25242 (11)	0.47686 (6)	0.24666 (5)	0.0118 (3)
N1	0.2788 (7)	0.3174 (4)	0.2683 (3)	0.0132 (11)
N2	0.3804 (7)	0.2494 (4)	0.3253 (3)	0.0152 (11)
N3	0.3235 (7)	0.1528 (4)	0.2983 (3)	0.0143 (11)
N4	0.1851 (7)	0.1586 (4)	0.2219 (3)	0.0157 (11)
N5	0.0297 (7)	0.4194 (4)	0.1424 (3)	0.0126 (11)
N6	−0.0996 (7)	0.2598 (4)	0.0717 (3)	0.0194 (12)
N7	0.2223 (7)	0.6361 (4)	0.2268 (3)	0.0155 (12)
N8	0.1181 (7)	0.7071 (4)	0.1701 (3)	0.0150 (11)
N9	0.1716 (8)	0.8014 (4)	0.2017 (3)	0.0162 (11)
N10	0.3094 (7)	0.7949 (4)	0.2779 (3)	0.0139 (11)
N11	0.4738 (7)	0.5319 (4)	0.3520 (3)	0.0141 (11)
N12	0.5935 (8)	0.6925 (4)	0.4264 (3)	0.0176 (12)
C1	0.0196 (8)	0.3148 (5)	0.1342 (4)	0.0124 (13)
C2	0.1624 (9)	0.2607 (5)	0.2061 (4)	0.0135 (13)
C3	−0.1014 (10)	0.4764 (5)	0.0838 (4)	0.0201 (14)
H3A	−0.1006	0.5510	0.0880	0.024*
C4	−0.2378 (9)	0.4268 (6)	0.0170 (4)	0.0215 (15)
H4A	−0.3338	0.4658	−0.0243	0.026*
C5	−0.2285 (9)	0.3175 (5)	0.0131 (4)	0.0180 (14)
H5A	−0.3177	0.2823	−0.0334	0.022*
C6	0.3364 (9)	0.6922 (4)	0.2920 (4)	0.0127 (13)

C7	0.4767 (9)	0.6372 (5)	0.3631 (4)	0.0165 (14)
C8	0.6065 (9)	0.4777 (5)	0.4115 (4)	0.0159 (13)
H8A	0.6117	0.4033	0.4066	0.019*
C9	0.7352 (10)	0.5264 (5)	0.4795 (4)	0.0227 (15)
H9A	0.8302	0.4872	0.5211	0.027*
C10	0.7228 (9)	0.6333 (6)	0.4856 (4)	0.0227 (15)
H10A	0.8088	0.6677	0.5335	0.027*
O1W	0.4472 (6)	0.4697 (3)	0.1733 (3)	0.0163 (10)
H1WA	0.539 (6)	0.425 (3)	0.185 (4)	0.024*
H1WB	0.499 (8)	0.530 (2)	0.179 (4)	0.024*
O2W	0.0576 (6)	0.4839 (3)	0.3208 (3)	0.0150 (9)
H2WA	−0.021 (7)	0.433 (3)	0.316 (4)	0.022*
H2WB	−0.004 (8)	0.541 (2)	0.320 (4)	0.022*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0069 (4)	0.0118 (5)	0.0172 (5)	0.0002 (3)	0.0041 (3)	0.0011 (3)
N1	0.009 (3)	0.010 (3)	0.022 (3)	0.0056 (19)	0.008 (2)	0.009 (2)
N2	0.008 (3)	0.018 (3)	0.022 (3)	0.003 (2)	0.009 (2)	0.001 (2)
N3	0.007 (3)	0.014 (3)	0.020 (3)	−0.001 (2)	0.001 (2)	0.001 (2)
N4	0.011 (3)	0.018 (3)	0.021 (3)	0.003 (2)	0.009 (2)	−0.003 (2)
N5	0.008 (2)	0.017 (3)	0.013 (3)	0.001 (2)	0.0042 (19)	0.003 (2)
N6	0.010 (3)	0.027 (3)	0.022 (3)	−0.006 (2)	0.007 (2)	−0.003 (2)
N7	0.014 (3)	0.010 (3)	0.023 (3)	−0.001 (2)	0.007 (2)	−0.006 (2)
N8	0.010 (3)	0.008 (2)	0.025 (3)	0.002 (2)	0.003 (2)	0.007 (2)
N9	0.020 (3)	0.010 (2)	0.027 (3)	0.003 (2)	0.020 (2)	0.000 (2)
N10	0.013 (3)	0.013 (3)	0.016 (3)	−0.001 (2)	0.005 (2)	−0.001 (2)
N11	0.007 (3)	0.016 (3)	0.019 (3)	−0.001 (2)	0.003 (2)	0.000 (2)
N12	0.015 (3)	0.023 (3)	0.017 (3)	−0.007 (2)	0.007 (2)	−0.009 (2)
C1	0.006 (3)	0.013 (3)	0.021 (3)	−0.004 (2)	0.009 (2)	−0.002 (2)
C2	0.014 (3)	0.013 (3)	0.017 (3)	0.004 (2)	0.009 (2)	0.004 (2)
C3	0.016 (3)	0.023 (4)	0.022 (3)	0.001 (3)	0.007 (3)	0.001 (3)
C4	0.008 (3)	0.032 (4)	0.024 (3)	0.003 (3)	0.004 (2)	0.006 (3)
C5	0.006 (3)	0.030 (4)	0.019 (3)	−0.006 (2)	0.006 (2)	−0.004 (3)
C6	0.014 (3)	0.006 (3)	0.026 (3)	−0.003 (2)	0.017 (3)	−0.002 (2)
C7	0.013 (3)	0.026 (4)	0.014 (3)	−0.004 (3)	0.008 (2)	−0.003 (3)
C8	0.005 (3)	0.020 (3)	0.024 (3)	0.002 (2)	0.007 (2)	0.002 (2)
C9	0.011 (3)	0.033 (4)	0.026 (4)	0.005 (3)	0.008 (3)	0.004 (3)
C10	0.012 (3)	0.037 (4)	0.017 (3)	−0.004 (3)	0.002 (2)	−0.006 (3)
O1W	0.013 (2)	0.015 (2)	0.020 (2)	−0.0012 (17)	0.0040 (18)	0.0015 (18)
O2W	0.011 (2)	0.009 (2)	0.024 (2)	−0.0030 (16)	0.0043 (18)	−0.0013 (17)

Geometric parameters (Å, °)

Ni1—N1	2.057 (5)	N11—C8	1.336 (8)
Ni1—N5	2.096 (5)	N11—C7	1.349 (8)
Ni1—N7	2.051 (5)	N12—C7	1.327 (7)
Ni1—N11	2.092 (5)	N12—C10	1.355 (8)

Ni1—O1W	2.087 (5)	C1—C2	1.482 (8)
Ni1—O2W	2.097 (5)	C3—C4	1.386 (9)
N1—N2	1.323 (7)	C3—H3A	0.95
N1—C2	1.324 (8)	C4—C5	1.394 (9)
N2—N3	1.327 (7)	C4—H4A	0.95
N3—N4	1.351 (7)	C5—H5A	0.95
N4—C2	1.324 (8)	C6—C7	1.473 (8)
N5—C1	1.337 (8)	C8—C9	1.368 (9)
N5—C3	1.341 (8)	C8—H8A	0.95
N6—C1	1.324 (7)	C9—C10	1.366 (10)
N6—C5	1.339 (8)	C9—H9A	0.95
N7—C6	1.344 (8)	C10—H10A	0.95
N7—N8	1.351 (7)	O1W—H1WA	0.85 (2)
N8—N9	1.318 (7)	O1W—H1WB	0.84 (2)
N9—N10	1.348 (7)	O2W—H2WA	0.84 (2)
N10—C6	1.329 (7)	O2W—H2WB	0.85 (2)
N1—Ni1—N5	78.88 (19)	N6—C1—C2	120.5 (5)
N1—Ni1—N11	100.25 (19)	N5—C1—C2	112.1 (5)
N1—Ni1—O1W	90.80 (19)	N4—C2—N1	111.6 (5)
N1—Ni1—O2W	89.12 (19)	N4—C2—C1	128.8 (5)
N5—Ni1—O2W	90.91 (18)	N1—C2—C1	119.5 (5)
N7—Ni1—N1	178.7 (2)	N5—C3—C4	120.2 (6)
N7—Ni1—N5	101.22 (19)	N5—C3—H3A	119.9
N7—Ni1—N11	79.63 (19)	C4—C3—H3A	119.9
N7—Ni1—O1W	90.45 (19)	C3—C4—C5	117.3 (6)
N7—Ni1—O2W	89.63 (19)	C3—C4—H4A	121.4
N11—Ni1—N5	179.0 (2)	C5—C4—H4A	121.4
N11—Ni1—O2W	88.52 (18)	N6—C5—C4	123.0 (6)
O1W—Ni1—N11	91.29 (19)	N6—C5—H5A	118.5
O1W—Ni1—N5	89.28 (18)	C4—C5—H5A	118.5
O1W—Ni1—O2W	179.78 (18)	N10—C6—N7	111.0 (5)
N2—N1—C2	106.3 (5)	N10—C6—C7	129.4 (5)
N2—N1—Ni1	140.3 (4)	N7—C6—C7	119.5 (5)
C2—N1—Ni1	113.4 (4)	N12—C7—N11	127.7 (6)
N1—N2—N3	108.4 (5)	N12—C7—C6	119.6 (6)
N2—N3—N4	109.2 (5)	N11—C7—C6	112.6 (5)
C2—N4—N3	104.5 (5)	N11—C8—C9	121.7 (6)
C1—N5—C3	117.4 (5)	N11—C8—H8A	119.1
C1—N5—Ni1	115.7 (4)	C9—C8—H8A	119.1
C3—N5—Ni1	126.9 (4)	C10—C9—C8	117.9 (6)
C1—N6—C5	114.7 (6)	C10—C9—H9A	121.1
C6—N7—N8	106.1 (5)	C8—C9—H9A	121.1
C6—N7—Ni1	112.7 (4)	N12—C10—C9	123.0 (6)
N8—N7—Ni1	141.1 (4)	N12—C10—H10A	118.5
N9—N8—N7	107.4 (5)	C9—C10—H10A	118.5
N8—N9—N10	110.9 (5)	Ni1—O1W—H1WA	120 (5)
C6—N10—N9	104.6 (5)	Ni1—O1W—H1WB	104 (5)
C8—N11—C7	115.7 (5)	H1WA—O1W—H1WB	108 (3)
C8—N11—Ni1	129.4 (4)	Ni1—O2W—H2WA	117 (4)

C7—N11—Ni1	114.9 (4)	Ni1—O2W—H2WB	117 (4)
C7—N12—C10	114.0 (6)	H2WA—O2W—H2WB	109 (3)
N6—C1—N5	127.4 (5)		
O1W—Ni1—N1—N2	94.4 (6)	C5—N6—C1—C2	176.6 (5)
N11—Ni1—N1—N2	3.0 (7)	C3—N5—C1—N6	3.8 (9)
N5—Ni1—N1—N2	−176.5 (7)	Ni1—N5—C1—N6	−176.0 (5)
O2W—Ni1—N1—N2	−85.4 (6)	C3—N5—C1—C2	−175.9 (5)
O1W—Ni1—N1—C2	−83.7 (4)	Ni1—N5—C1—C2	4.4 (6)
N11—Ni1—N1—C2	−175.1 (4)	N3—N4—C2—N1	0.0 (7)
N5—Ni1—N1—C2	5.4 (4)	N3—N4—C2—C1	−175.3 (6)
O2W—Ni1—N1—C2	96.5 (4)	N2—N1—C2—N4	0.6 (7)
C2—N1—N2—N3	−0.9 (7)	Ni1—N1—C2—N4	179.3 (4)
Ni1—N1—N2—N3	−179.1 (5)	N2—N1—C2—C1	176.3 (5)
N1—N2—N3—N4	0.9 (6)	Ni1—N1—C2—C1	−5.0 (7)
N2—N3—N4—C2	−0.5 (6)	N6—C1—C2—N4	−4.4 (10)
N7—Ni1—N5—C1	175.8 (4)	N5—C1—C2—N4	175.3 (6)
N1—Ni1—N5—C1	−5.5 (4)	N6—C1—C2—N1	−179.3 (6)
O1W—Ni1—N5—C1	85.5 (4)	N5—C1—C2—N1	0.4 (8)
O2W—Ni1—N5—C1	−94.4 (4)	C1—N5—C3—C4	−1.2 (9)
N7—Ni1—N5—C3	−3.9 (6)	Ni1—N5—C3—C4	178.5 (5)
N1—Ni1—N5—C3	174.8 (6)	N5—C3—C4—C5	−1.6 (10)
O1W—Ni1—N5—C3	−94.2 (5)	C1—N6—C5—C4	−0.2 (9)
O2W—Ni1—N5—C3	85.9 (5)	C3—C4—C5—N6	2.3 (10)
O1W—Ni1—N7—C6	−98.0 (4)	N9—N10—C6—N7	0.9 (7)
N11—Ni1—N7—C6	−6.8 (4)	N9—N10—C6—C7	176.5 (6)
N5—Ni1—N7—C6	172.6 (4)	N8—N7—C6—N10	−0.7 (7)
O2W—Ni1—N7—C6	81.7 (4)	Ni1—N7—C6—N10	−178.4 (4)
O1W—Ni1—N7—N8	85.5 (7)	N8—N7—C6—C7	−176.9 (5)
N11—Ni1—N7—N8	176.7 (7)	Ni1—N7—C6—C7	5.4 (7)
N5—Ni1—N7—N8	−3.9 (7)	C10—N12—C7—N11	0.0 (9)
O2W—Ni1—N7—N8	−94.7 (7)	C10—N12—C7—C6	−176.7 (6)
C6—N7—N8—N9	0.3 (6)	C8—N11—C7—N12	−1.0 (9)
Ni1—N7—N8—N9	176.9 (5)	Ni1—N11—C7—N12	176.2 (5)
N7—N8—N9—N10	0.3 (6)	C8—N11—C7—C6	175.9 (5)
N8—N9—N10—C6	−0.7 (6)	Ni1—N11—C7—C6	−6.9 (6)
N7—Ni1—N11—C8	−175.5 (6)	N10—C6—C7—N12	2.8 (10)
N1—Ni1—N11—C8	5.8 (6)	N7—C6—C7—N12	178.1 (6)
O1W—Ni1—N11—C8	−85.3 (5)	N10—C6—C7—N11	−174.3 (6)
O2W—Ni1—N11—C8	94.6 (5)	N7—C6—C7—N11	1.0 (8)
N7—Ni1—N11—C7	7.7 (4)	C7—N11—C8—C9	0.5 (9)
N1—Ni1—N11—C7	−171.0 (4)	Ni1—N11—C8—C9	−176.2 (5)
O1W—Ni1—N11—C7	97.9 (4)	N11—C8—C9—C10	0.8 (10)
O2W—Ni1—N11—C7	−82.2 (4)	C7—N12—C10—C9	1.5 (9)
C5—N6—C1—N5	−3.0 (9)	C8—C9—C10—N12	−1.9 (10)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H1WA···N10^{i}	0.85 (2)	1.97 (2)	2.788 (7)	162 (6)

O1W—H1WB···N3^{ii}	0.84 (2)	1.97 (3)	2.804 (7)	167 (6)
O2W—H2WA···N9^{iii}	0.84 (2)	1.97 (2)	2.798 (6)	170 (6)
O2W—H2WB···N4^{iv}	0.85 (2)	1.97 (3)	2.776 (7)	160 (6)

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

Fig. 1

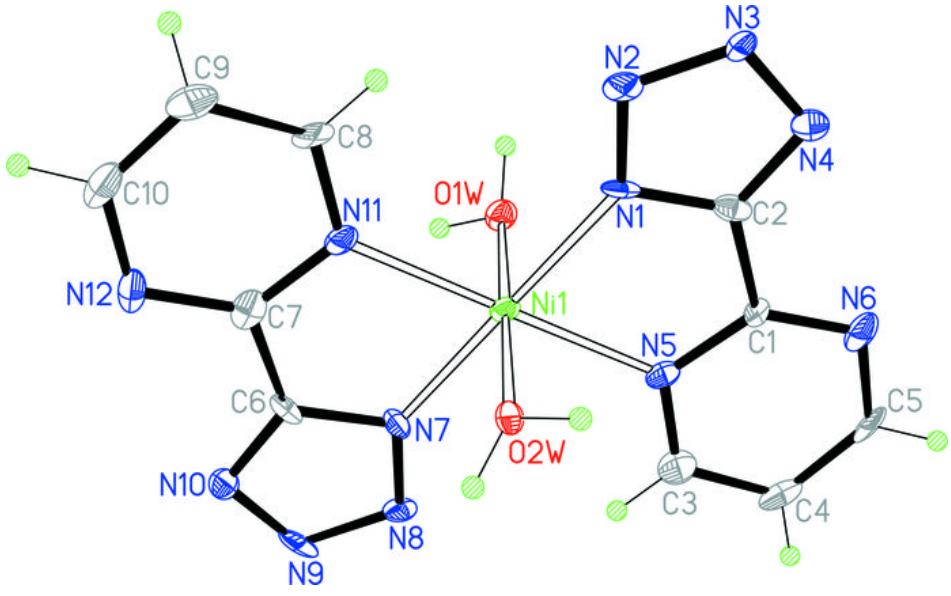
N3
N2
C9
C8
N4
C10
O1W
N1
C2
N11
N12
Ni1
N6
C7
N5
C1
C6
C5
N7
O2W
N10
C3
C4
N8
N9

Fig. 2