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Aqua[1-(pyrazin-2-yl)ethanone oximato-κ^2N,N'][1-(pyrazin-2-yl)ethanone oxime-κ^2N,N'](thiocyanato-κN)nickel(II)

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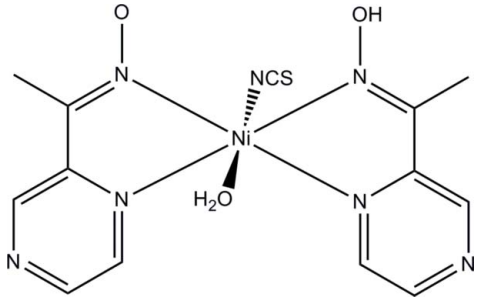
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.004 Å; R factor = 0.020; wR factor = 0.045; data-to-parameter ratio = 11.8.

In the title complex, $[Ni(C_6H_6N_3O)(NCS)(C_6H_7N_3O)(H_2O)]$ or [Ni(mpko)(SCN)(mpkoH)(H_2O)] [where mpkoH = 1-(pyrazin-2-yl)ethanone oxime], the Ni^{II} cation is in a slightly distorted octahedral geometry, being coordinated in the equatorial plane by four N atoms from two different mpkoH ligands, one of which is deprotonated, and by one N atom from a thiocyanate anion and one O atom from a water molecule in the axial positions. There is an intramolecular O—H···O hydrogen bond involving the oxime units of the two ligands. In the crystal, a three-dimensional supramolecular architecture is formed by O—H···O and O—H···N hydrogen bonds.

Related literature

For magnetic properties of related oxime complexes, see: Escuer *et al.* (2010); Radek *et al.* (1999, 2001); Spini (1973).



Experimental

Crystal data

$[Ni(C_6H_6N_3O)(NCS)(C_6H_7N_3O)(H_2O)]$
M_r = 408.09
Monoclinic, *Cc*
a = 11.917 (8) Å
b = 11.899 (8) Å
c = 12.354 (8) Å
β = 108.220 (5)°
V = 1664.1 (19) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.32 mm^{-1}
T = 296 K
0.36 × 0.32 × 0.29 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.648, T_{max} = 0.701
5816 measured reflections
2809 independent reflections
2700 reflections with $I > 2\sigma(I)$
R_{int} = 0.017

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.020
$wR(F^2)$ = 0.045
S = 1.05
2809 reflections
238 parameters
5 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}
Absolute structure: Flack (1983), 1258 Friedel pairs
Flack parameter: 0.079 (9)

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H1*O*···O3	0.89 (4)	1.63 (4)	2.505 (3)	167 (5)
O1—H1*W*···N2^{i}	0.82	2.14	2.941 (4)	166
O1—H2*W*···O3^{ii}	0.89 (2)	1.84 (2)	2.690 (3)	161 (2)

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

Data collection: *APEX2* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SU2441).

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supplementary materials

Acta Cryst. (2012). E**68**, m883 [doi:10.1107/S1600536812024622]

Aqua[1-(pyrazin-2-yl)ethanone oximato-κ^2N,N'][1-(pyrazin-2-yl)ethanone oxime-κ^2N,N'](thiocyanato-κN)nickel(II)

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Comment

In the past decades, much attention has been paid to the design and synthesis of oximes complexes. Oximes can be feasibly synthesized by the Schiff base condensation of an aldehyde or ketone with hydroxylamine. To date, various oximate ligands as bridging ligands have been extensively explored for their great ability to form homo- and heterometallic polynuclear complexes, which can transmit magnetic exchange efficiently (Radek *et al.* 1999, 2001). Among oximate bridging ligands, *R*-substituted-pyridyloximes, (py)C(*R*)NOH, salycylaldoximes and *R*-saoH_2 play an outstanding role to generate a great variety of polynuclear complexes which not only have aesthetically pleasing structures, but also possess interesting magnetic properties of single molecule magnet (SMM) and single chain magnet (SCM) behavior (Escuer *et al.*, 2010; Spini, 1973).

The title compound, Fig. 1, is a new nickel complex obtained by the reaction of nickel chloride hexahydrate with mpkoH (methyl pyrazine-2-yl ketoxime) in CH_3OH solution. The Ni^{II} cation is in a slightly distorted octahedral geometry. The equatorial plane is defined by four N atoms from two mpkoH ligands - one of which is deprotonated, while the axial positions are occupied by one N atom from a SCN^- anion and one water O atom. There is an intramolecular O-H···O hydrogen bond (Table 1) involving the the oxime moieties of the two ligands.

In the crystal a three-dimensional supramolecular architecture is formed by O—H···O and O—H···N hydrogen bonds (Fig. 2 and Table 1).

Experimental

The title complex was prepared by the addition of nickel chloride hexahydrate (23.9 mg, 0.1 mmol) to a CH_3OH solution of methyl pyrazine-2-yl ketoxime (28 mg, 0.2 mmol); the pH was adjusted to 8 with 1*M* KSCN. Slow evaporation of the solvent gave red block-like crystals of the title compound, suitable for X-ray analysis, after several days at room temperature [Yield 31 mg, 77%]. Anal. Calc. for $C_{13}H_{15}N_7NiO_3S$: C, 38.26; H, 3.71; N, 24.03. Found: C, 36.93; H, 3.4; N, 25.1%.

Refinement

The OH and water H atoms were located in a difference Fourier map. All except one of the water H atoms [H1W; constrained to be 0.82 Å with $U_{iso}(H) = 1.5U_{eq}(O)$], were freely refined. The C-bound H atoms were placed in calculated positions and refined as riding atoms: C—H = 0.93 and 0.96Å for CH and CH_3 H atoms, respectively, with $U_{iso}(H) = k \times U_{eq}(C)$, where k = 1.5 for CH_3 H atoms and = 1.2 for other H atoms.

Computing details

Data collection: *APEX2* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT* (Bruker, 2000); 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* (Sheldrick, 2008).

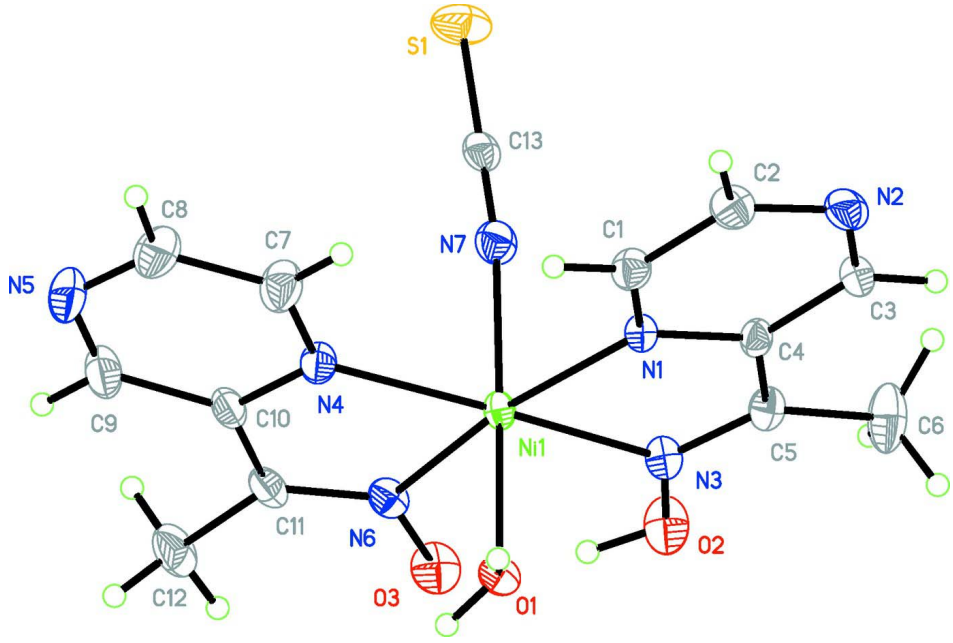

Figure 1

A view of the molecular structure of the title compound with the atom numbering. Displacement ellipsoids are drawn at the 30% probability level.

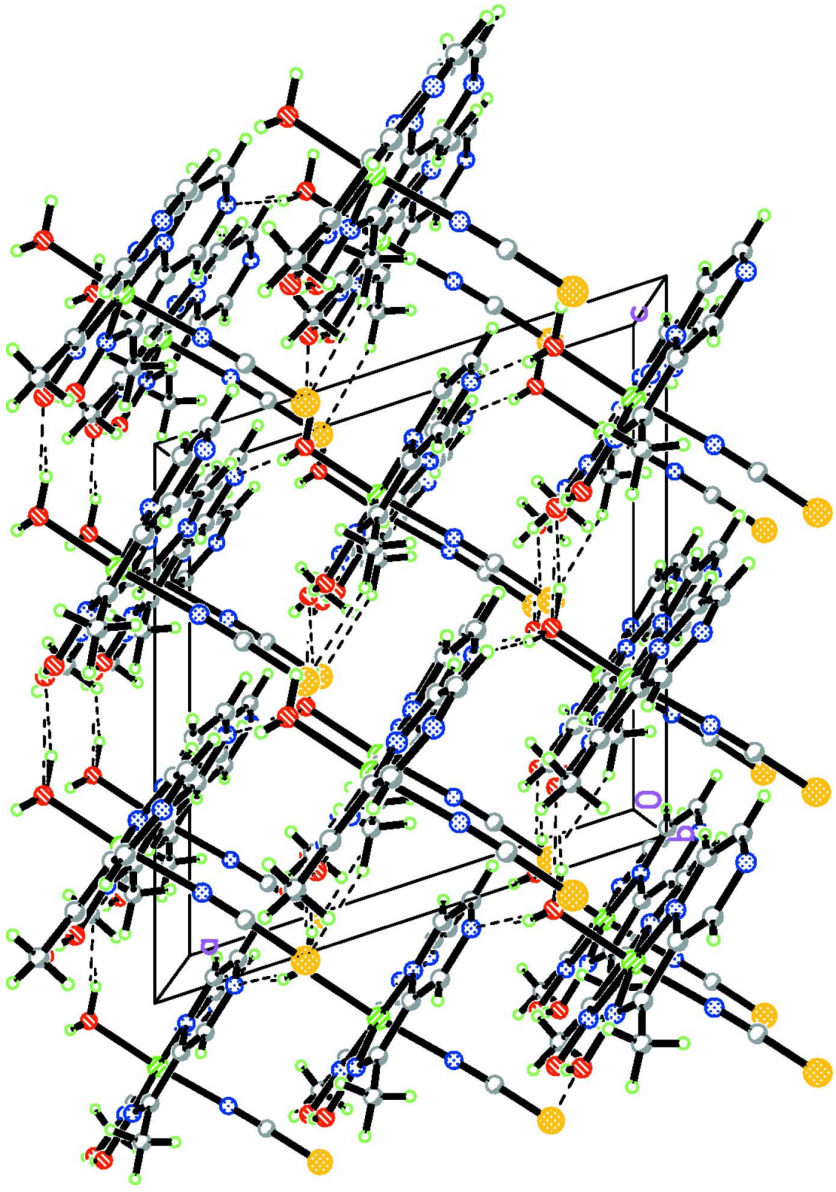

Figure 2

The crystal packing of the title compound, viewed along the *b* axis. The O-H···O and O-H···N hydrogen bonds are shown as dashed lines (see Table 1 for details).

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Crystal data

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Monoclinic, *Cc*
Hall symbol: C -2yc
$a = 11.917$ (8) Å
$b = 11.899$ (8) Å
$c = 12.354$ (8) Å
$\beta = 108.220$ (5)°
$V = 1664.1$ (19) Å^3
$Z = 4$
$F(000) = 840$
$D_x = 1.629$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4663 reflections

θ = 2.5–28.9°
μ = 1.32 mm^{-1}
T = 296 K

Block, red
0.36 × 0.32 × 0.29 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.648, T_{max} = 0.701

5816 measured reflections
2809 independent reflections
2700 reflections with $I > 2\sigma(I)$
R_{int} = 0.017
θ_{max} = 25.5°, θ_{min} = 2.5°
h = −13→14
k = −14→14
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.020
$wR(F^2)$ = 0.045
S = 1.05
2809 reflections
238 parameters
5 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
$w = 1/[\sigma^2(F_o^2) + (0.0195P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0035 (2)
Absolute structure: Flack (1983), 1258 Friedel pairs
Flack parameter: 0.079 (9)

Special details

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

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	0.06769 (2)	0.04643 (2)	0.79647 (2)	0.0232 (1)
S1	−0.29404 (7)	0.01219 (7)	0.48705 (6)	0.0505 (3)
O1	0.22258 (19)	0.04631 (13)	0.93718 (17)	0.0297 (6)
O2	0.1754 (2)	0.19519 (17)	0.65847 (17)	0.0455 (7)
O3	0.21552 (17)	−0.01069 (15)	0.64998 (15)	0.0416 (6)
N1	−0.00488 (18)	0.17283 (15)	0.87702 (17)	0.0243 (6)
N2	−0.12050 (19)	0.35594 (17)	0.93569 (18)	0.0389 (7)
N3	0.11228 (18)	0.19306 (17)	0.73314 (18)	0.0291 (7)
N4	0.02311 (18)	−0.11543 (16)	0.83966 (17)	0.0308 (7)
N5	−0.0404 (2)	−0.33939 (18)	0.8492 (3)	0.0609 (10)
N6	0.14984 (18)	−0.05268 (16)	0.71043 (16)	0.0294 (6)

N7	−0.0897 (2)	0.04323 (17)	0.6682 (2)	0.0364 (9)
C1	−0.0646 (2)	0.1639 (2)	0.9510 (2)	0.0324 (8)
C2	−0.1229 (2)	0.2544 (2)	0.9789 (2)	0.0376 (8)
C3	−0.0582 (2)	0.36562 (18)	0.8631 (2)	0.0338 (8)
C4	−0.0003 (2)	0.27569 (18)	0.83197 (19)	0.0262 (7)
C5	0.0660 (2)	0.28514 (19)	0.7509 (2)	0.0309 (7)
C6	0.0749 (3)	0.3925 (2)	0.6917 (2)	0.0552 (12)
C7	−0.0488 (3)	−0.1484 (2)	0.8961 (2)	0.0452 (10)
C8	−0.0807 (3)	−0.2595 (3)	0.8998 (3)	0.0552 (11)
C9	0.0317 (3)	−0.3073 (2)	0.7932 (3)	0.0508 (10)
C10	0.0655 (3)	−0.19532 (16)	0.7858 (3)	0.0332 (7)
C11	0.1399 (2)	−0.1601 (2)	0.7182 (2)	0.0321 (8)
C12	0.1990 (3)	−0.2437 (2)	0.6627 (3)	0.0485 (10)
C13	−0.1750 (2)	0.03029 (18)	0.5946 (2)	0.0290 (8)
H1	−0.06730	0.09470	0.98520	0.0390*
H1O	0.200 (4)	0.125 (3)	0.654 (3)	0.092 (14)*
H1W	0.26870	−0.00070	0.92730	0.0450*
H2	−0.16540	0.24360	1.02960	0.0450*
H2W	0.207 (2)	0.0450 (19)	1.0028 (13)	0.053 (9)*
H3	−0.05340	0.43590	0.83190	0.0410*
H6A	0.13750	0.43750	0.74000	0.0830*
H6B	0.00160	0.43270	0.67490	0.0830*
H6C	0.09130	0.37630	0.62200	0.0830*
H7	−0.07890	−0.09500	0.93470	0.0540*
H8	−0.13260	−0.27820	0.93960	0.0660*
H9	0.06190	−0.36210	0.75640	0.0610*
H12A	0.14020	−0.28170	0.60260	0.0730*
H12B	0.24150	−0.29750	0.71840	0.0730*
H12C	0.25290	−0.20530	0.63180	0.0730*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0290 (2)	0.0193 (1)	0.0225 (1)	0.0021 (2)	0.0098 (1)	−0.0009 (2)
S1	0.0319 (4)	0.0722 (5)	0.0404 (4)	0.0037 (3)	0.0012 (3)	−0.0099 (3)
O1	0.0305 (11)	0.0341 (11)	0.0258 (11)	0.0046 (7)	0.0106 (9)	−0.0009 (7)
O2	0.0666 (14)	0.0386 (11)	0.0455 (12)	0.0003 (10)	0.0382 (11)	0.0025 (9)
O3	0.0520 (11)	0.0481 (10)	0.0342 (10)	0.0031 (9)	0.0270 (9)	−0.0049 (8)
N1	0.0280 (11)	0.0209 (10)	0.0245 (10)	0.0003 (8)	0.0089 (9)	0.0004 (8)
N2	0.0336 (12)	0.0374 (11)	0.0453 (13)	0.0056 (9)	0.0119 (10)	−0.0114 (10)
N3	0.0369 (13)	0.0269 (11)	0.0259 (10)	0.0019 (9)	0.0135 (9)	0.0008 (8)
N4	0.0342 (12)	0.0252 (11)	0.0340 (11)	−0.0011 (9)	0.0122 (9)	−0.0011 (9)
N5	0.0601 (17)	0.0271 (12)	0.088 (2)	−0.0061 (12)	0.0124 (16)	0.0101 (13)
N6	0.0315 (11)	0.0319 (10)	0.0236 (10)	0.0050 (9)	0.0071 (9)	−0.0050 (8)
N7	0.0376 (18)	0.0334 (14)	0.0363 (16)	0.0025 (9)	0.0087 (13)	−0.0069 (9)
C1	0.0346 (14)	0.0312 (13)	0.0341 (14)	−0.0014 (11)	0.0145 (12)	0.0001 (11)
C2	0.0380 (15)	0.0403 (14)	0.0385 (14)	0.0008 (11)	0.0178 (12)	−0.0066 (11)
C3	0.0327 (14)	0.0237 (12)	0.0423 (14)	0.0036 (10)	0.0080 (11)	0.0003 (10)
C4	0.0294 (13)	0.0204 (11)	0.0245 (12)	−0.0015 (10)	0.0024 (10)	−0.0019 (9)
C5	0.0380 (14)	0.0262 (12)	0.0284 (12)	−0.0024 (11)	0.0104 (11)	0.0008 (9)

C6	0.096 (3)	0.0296 (13)	0.0501 (18)	−0.0041 (14)	0.0375 (18)	0.0044 (12)
C7	0.0537 (19)	0.0355 (15)	0.0549 (18)	−0.0051 (13)	0.0291 (16)	0.0012 (12)
C8	0.053 (2)	0.0441 (18)	0.072 (2)	−0.0113 (16)	0.0244 (18)	0.0159 (16)
C9	0.055 (2)	0.0264 (12)	0.0639 (18)	0.0060 (11)	0.0084 (18)	−0.0039 (14)
C10	0.0328 (13)	0.0239 (10)	0.0367 (14)	0.0079 (14)	0.0019 (10)	−0.0015 (13)
C11	0.0321 (14)	0.0296 (13)	0.0293 (13)	0.0109 (11)	0.0021 (11)	−0.0053 (10)
C12	0.055 (2)	0.0380 (16)	0.0482 (17)	0.0155 (14)	0.0098 (15)	−0.0156 (13)
C13	0.0308 (15)	0.0275 (12)	0.0317 (13)	0.0049 (10)	0.0141 (12)	−0.0034 (9)

Geometric parameters (Å, º)

Ni1—O1	2.103 (3)	N7—C13	1.143 (3)
Ni1—N1	2.130 (2)	C1—C2	1.382 (4)
Ni1—N3	2.049 (2)	C3—C4	1.391 (3)
Ni1—N4	2.110 (2)	C4—C5	1.461 (4)
Ni1—N6	2.032 (2)	C5—C6	1.492 (4)
Ni1—N7	2.043 (3)	C7—C8	1.380 (4)
S1—C13	1.627 (3)	C9—C10	1.403 (3)
O2—N3	1.361 (3)	C10—C11	1.457 (4)
O3—N6	1.336 (3)	C11—C12	1.503 (4)
O1—H1W	0.8200	C1—H1	0.9300
O1—H2W	0.887 (18)	C2—H2	0.9300
O2—H1O	0.89 (4)	C3—H3	0.9300
N1—C1	1.327 (3)	C6—H6A	0.9600
N1—C4	1.353 (3)	C6—H6B	0.9600
N2—C2	1.325 (3)	C6—H6C	0.9600
N2—C3	1.336 (3)	C7—H7	0.9300
N3—C5	1.276 (3)	C8—H8	0.9300
N4—C10	1.346 (4)	C9—H9	0.9300
N4—C7	1.322 (4)	C12—H12A	0.9600
N5—C9	1.317 (5)	C12—H12B	0.9600
N5—C8	1.309 (5)	C12—H12C	0.9600
N6—C11	1.290 (3)		
O1—Ni1—N1	89.65 (8)	C3—C4—C5	123.5 (2)
O1—Ni1—N3	92.91 (8)	C4—C5—C6	122.6 (2)
O1—Ni1—N4	90.90 (7)	N3—C5—C4	114.0 (2)
O1—Ni1—N6	89.43 (8)	N3—C5—C6	123.4 (2)
O1—Ni1—N7	175.60 (9)	N4—C7—C8	122.2 (3)
N1—Ni1—N3	76.64 (8)	N5—C8—C7	122.3 (3)
N1—Ni1—N4	110.80 (8)	N5—C9—C10	123.9 (3)
N1—Ni1—N6	170.52 (8)	N4—C10—C9	118.6 (3)
N1—Ni1—N7	88.12 (9)	N4—C10—C11	118.0 (2)
N3—Ni1—N4	171.68 (8)	C9—C10—C11	123.3 (3)
N3—Ni1—N6	93.99 (8)	N6—C11—C12	123.7 (2)
N3—Ni1—N7	90.26 (9)	C10—C11—C12	121.8 (2)
N4—Ni1—N6	78.65 (8)	N6—C11—C10	114.5 (2)
N4—Ni1—N7	86.36 (8)	S1—C13—N7	178.2 (2)
N6—Ni1—N7	93.39 (9)	N1—C1—H1	119.00
Ni1—O1—H1W	109.00	C2—C1—H1	119.00

Ni1—O1—H2W	112.0 (15)	N2—C2—H2	119.00
H1W—O1—H2W	118.00	C1—C2—H2	119.00
N3—O2—H1O	107 (3)	N2—C3—H3	118.00
Ni1—N1—C4	111.85 (16)	C4—C3—H3	118.00
C1—N1—C4	117.1 (2)	C5—C6—H6A	109.00
Ni1—N1—C1	130.46 (15)	C5—C6—H6B	109.00
C2—N2—C3	115.8 (2)	C5—C6—H6C	109.00
O2—N3—C5	117.4 (2)	H6A—C6—H6B	110.00
Ni1—N3—C5	119.20 (18)	H6A—C6—H6C	109.00
Ni1—N3—O2	122.62 (15)	H6B—C6—H6C	109.00
Ni1—N4—C10	110.89 (18)	N4—C7—H7	119.00
C7—N4—C10	117.2 (2)	C8—C7—H7	119.00
Ni1—N4—C7	131.30 (17)	N5—C8—H8	119.00
C8—N5—C9	115.9 (3)	C7—C8—H8	119.00
Ni1—N6—O3	122.51 (14)	N5—C9—H9	118.00
Ni1—N6—C11	117.75 (17)	C10—C9—H9	118.00
O3—N6—C11	119.7 (2)	C11—C12—H12A	109.00
Ni1—N7—C13	173.0 (2)	C11—C12—H12B	109.00
N1—C1—C2	122.0 (2)	C11—C12—H12C	110.00
N2—C2—C1	122.3 (2)	H12A—C12—H12B	110.00
N2—C3—C4	123.2 (2)	H12A—C12—H12C	110.00
N1—C4—C3	119.7 (2)	H12B—C12—H12C	110.00
N1—C4—C5	116.9 (2)		

O1—Ni1—N1—C1	−86.7 (2)	C1—N1—C4—C5	179.8 (2)
N3—Ni1—N1—C1	−179.7 (2)	Ni1—N1—C4—C3	171.17 (18)
N4—Ni1—N1—C1	4.2 (2)	C1—N1—C4—C3	−0.8 (3)
N7—Ni1—N1—C1	89.6 (2)	C2—N2—C3—C4	1.0 (4)
O1—Ni1—N1—C4	102.77 (17)	C3—N2—C2—C1	0.1 (4)
N3—Ni1—N1—C4	9.69 (16)	Ni1—N3—C5—C6	−168.53 (19)
N4—Ni1—N1—C4	−166.41 (16)	O2—N3—C5—C6	1.9 (4)
N7—Ni1—N1—C4	−81.03 (17)	Ni1—N3—C5—C4	9.5 (3)
O1—Ni1—N3—O2	90.31 (19)	O2—N3—C5—C4	179.9 (2)
N1—Ni1—N3—O2	179.3 (2)	C10—N4—C7—C8	−0.5 (4)
N6—Ni1—N3—O2	0.7 (2)	Ni1—N4—C10—C11	5.1 (3)
N7—Ni1—N3—O2	−92.7 (2)	C7—N4—C10—C11	176.8 (3)
O1—Ni1—N3—C5	−99.8 (2)	C7—N4—C10—C9	−0.3 (4)
N1—Ni1—N3—C5	−10.86 (19)	Ni1—N4—C7—C8	169.3 (2)
N6—Ni1—N3—C5	170.6 (2)	Ni1—N4—C10—C9	−172.1 (3)
N7—Ni1—N3—C5	77.2 (2)	C8—N5—C9—C10	−0.1 (5)
O1—Ni1—N4—C7	97.6 (2)	C9—N5—C8—C7	−0.7 (5)
N1—Ni1—N4—C7	7.7 (3)	Ni1—N6—C11—C12	−177.9 (2)
N6—Ni1—N4—C7	−173.1 (2)	O3—N6—C11—C10	−179.7 (2)
N7—Ni1—N4—C7	−78.9 (2)	O3—N6—C11—C12	0.2 (4)
O1—Ni1—N4—C10	−92.1 (2)	Ni1—N6—C11—C10	2.3 (3)
N1—Ni1—N4—C10	177.9 (2)	N1—C1—C2—N2	−1.6 (4)
N6—Ni1—N4—C10	−2.9 (2)	N2—C3—C4—N1	−0.7 (4)
N7—Ni1—N4—C10	91.3 (2)	N2—C3—C4—C5	178.7 (2)
O1—Ni1—N6—O3	−86.70 (18)	N1—C4—C5—N3	−0.2 (3)

N3—Ni1—N6—O3	6.18 (18)	N1—C4—C5—C6	177.9 (2)
N4—Ni1—N6—O3	−177.73 (19)	C3—C4—C5—C6	−1.6 (4)
N7—Ni1—N6—O3	96.68 (18)	C3—C4—C5—N3	−179.7 (2)
O1—Ni1—N6—C11	91.28 (18)	N4—C7—C8—N5	1.1 (5)
N3—Ni1—N6—C11	−175.84 (19)	N5—C9—C10—C11	−176.4 (3)
N4—Ni1—N6—C11	0.25 (18)	N5—C9—C10—N4	0.6 (5)
N7—Ni1—N6—C11	−85.35 (19)	N4—C10—C11—C12	175.1 (3)
Ni1—N1—C1—C2	−168.28 (18)	C9—C10—C11—N6	171.9 (3)
C4—N1—C1—C2	1.9 (4)	C9—C10—C11—C12	−7.9 (5)
Ni1—N1—C4—C5	−8.3 (3)	N4—C10—C11—N6	−5.1 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H1*O*···O3	0.89 (4)	1.63 (4)	2.505 (3)	167 (5)
O1—H1*W*···N2^{i}	0.82	2.14	2.941 (4)	166
O1—H2*W*···O3^{ii}	0.89 (2)	1.84 (2)	2.690 (3)	161 (2)

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