

## Bis(3-aminopyrazine-2-carboxylato- $\kappa^2N^1,O$ )diaquanickel(II) dihydrate

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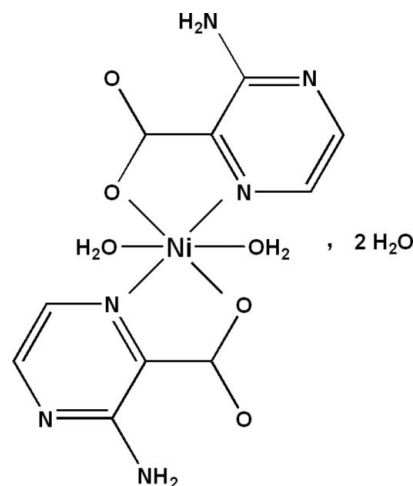
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Key indicators: single-crystal X-ray study;  $T = 150$  K; mean  $\sigma(C-C) = 0.004$  Å;  $R$  factor = 0.028;  $wR$  factor = 0.073; data-to-parameter ratio = 10.4.

In the title compound,  $[Ni(C_5H_4N_3O_2)_2(H_2O)_2] \cdot 2H_2O$ , the  $Ni^{II}$  ion lies on an inversion center and is coordinated in an slightly distorted octahedral environment by two N,O-chelating 3-aminopyrazine-2-carboxylate (APZC) ligands in the equatorial plane and two *trans*-axial aqua ligands. In the crystal,  $O-H \cdots O$ ,  $N-H \cdots O$  and  $O-H \cdots N$  hydrogen bonds involving the solvent water molecules, aqua and APZC ligands form layers parallel to (010). These layers are linked further *via*  $O-H \cdots O$ ,  $N-H \cdots O$  and  $C-H \cdots O$  hydrogen bonds involving the axial aqua ligands, amino groups and the carboxylate groups of the APZC ligands, forming a three-dimensional network.

### Related literature

For background to hybrid compounds, see: Bouchene *et al.* (2013); Bouacida *et al.* (2007, 2009). For the structure of the non-hydrated analogue, see: Ptasiwicz-Bak & Leciejewicz (1999). For 3-aminopyrazine-2-carboxylate-metal ( $M$ ) complexes, see: Bouchene *et al.* (2013) [ $M = Co(II)$ ]; Leciejewicz *et al.* (1997) [ $M = Ca(II)$ ]; Leciejewicz *et al.* (1998) [ $M = Sr(II)$ ]; Ptasiwicz-Bak & Leciejewicz (1997) [ $M = Mg(II)$ ]; Tayebbe *et al.* (2008) [ $M = Na(I)$ ]; Ptasiwicz-Bak & Leciejewicz (1999). For properties and applications of pyrazine-2-carboxylic acid, see: Zhang & Mitchison (2003); Manju & Chaudhary, (2010); Chanda & Sangeetika (2004).



### Experimental

#### Crystal data

$[Ni(C_5H_4N_3O_2)_2(H_2O)_2] \cdot 2H_2O$   
 $M_r = 406.98$   
 Monoclinic,  $P2_1/c$   
 $a = 9.7939$  (15) Å  
 $b = 5.1123$  (9) Å  
 $c = 16.776$  (3) Å  
 $\beta = 115.838$  (11)°

$V = 756.0$  (2) Å<sup>3</sup>  
 $Z = 2$   
 Mo  $K\alpha$  radiation  
 $\mu = 1.34$  mm<sup>-1</sup>  
 $T = 150$  K  
 $0.18 \times 0.16 \times 0.15$  mm

#### Data collection

Bruker APEXII CCD  
 diffractometer  
 6200 measured reflections

1326 independent reflections  
 1121 reflections with  $I > 2\sigma(I)$   
 $R_{int} = 0.051$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.028$   
 $wR(F^2) = 0.073$   
 $S = 1.04$   
 1326 reflections  
 127 parameters

H atoms treated by a mixture of independent and constrained refinement  
 $\Delta\rho_{max} = 0.36$  e Å<sup>-3</sup>  
 $\Delta\rho_{min} = -0.59$  e Å<sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$O1W-H1A \cdots O2W^i$	0.83 (3)	1.97 (3)	2.789 (3)	169 (3)
$O1W-H1B \cdots O1^{ii}$	0.75 (3)	1.94 (3)	2.690 (3)	176 (4)
$N3-H1N \cdots O2W^{iii}$	0.86	2.27	3.117 (3)	168
$O2W-H2A \cdots O2W^{iv}$	0.77 (3)	2.12 (3)	2.867 (3)	164 (4)
$O2W-H2B \cdots N2^v$	0.78 (3)	2.03 (3)	2.792 (3)	168 (3)
$N3-H2N \cdots O2$	0.86	2.10	2.733 (3)	130
$N3-H2N \cdots O2^{vi}$	0.86	2.20	2.871 (3)	135
$C5-H5 \cdots O1W^{vii}$	0.93	2.54	3.377 (4)	150

Symmetry codes: (i)  $-x+1, -y+1, -z+2$ ; (ii)  $-x+1, -y, -z+2$ ; (iii)  $-x, -y+1, -z+2$ ; (iv)  $-x, y-\frac{1}{2}, -z+\frac{3}{2}$ ; (v)  $x, -y+\frac{3}{2}, z-\frac{1}{2}$ ; (vi)  $-x, -y, -z+2$ ; (vii)  $x, y+1, z$ .

Data collection: APEX2 (Bruker, 2011); cell refinement: SAINT (Bruker, 2011); data reduction: SAINT; program(s) used to solve structure: SIR2002 (Burla *et al.*, 2005); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 for Windows (Farrugia, 2012) and DIAMOND (Brandenburg & Berndt, 2001); software used to prepare material for publication: WinGX (Farrugia, 2012).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5610).

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## References

- Bouacida, S., Belhouas, R., Kechout, H., Merazig, H. & Bénard-Rocherullé, P. (2009). *Acta Cryst.* **E65**, o628–o629.
- Bouacida, S., Merazig, H., Benard-Rocherulle, P. & Rizzoli, C. (2007). *Acta Cryst.* **E63**, m379–m381.
- Bouchene, R., Bouacida, S., Berrah, F., Belhouas, R. & Merazig, H. (2013). *Acta Cryst.* **E69**, m129–m130.
- Brandenburg, K. & Berndt, M. (2001). *DIAMOND*. Crystal Impact, Bonn, Germany.
- Bruker (2011). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Burla, M. C., Caliandro, R., Camalli, M., Carrozzini, B., Cascarano, G. L., De Caro, L., Giacovazzo, C., Polidori, G. & Spagna, R. (2005). *J. Appl. Cryst.* **38**, 381–388.
- Chanda, S. & Sangeetika, J. (2004). *J. Indian Chem. Soc.* **81**, 203–206.
- Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
- Leciejewicz, J., Ptasiwicz-Bak, H. & Paluchowska, B. (1997). *Pol. J. Chem.* **71**, 1339–1364.
- Leciejewicz, J., Ptasiwicz-Bak, H. & Zachara, J. (1998). *Pol. J. Chem.* **72**, 1994–1998.
- Manju, A. & Chaudhary, D. (2010). *Asian J. Chem. Environ. Res.* **3**, 13–17.
- Ptasiwicz-Bak, H. & Leciejewicz, J. (1997). *Pol. J. Chem.* **71**, 1350–1358.
- Ptasiwicz-Bak, H. & Leciejewicz, J. (1999). *Pol. J. Chem.* **73**, 717–725.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Tayebce, R., Amani, V. & Khavasi, H. P. (2008). *Chin. J. Chem.* **26**, 500–504.
- Zhang, Y. & Mitchison, D. A. (2003). *Int. J. Tuberc. Lung Dis.* **7**, 6–21.

## supporting information

*Acta Cryst.* (2013). E69, m309–m310 [doi:10.1107/S1600536813012208]

**Bis(3-aminopyrazine-2-carboxylato- $\kappa^2N^1,O$ )diaquanickel(II) dihydrate**

**Rafika Bouchene, Amina Khadri, Sofiane Bouacida, Fadila Berrah and Hocine Merazig**

**S1. Comment**

The pyrazine-2-carboxylic acid bridging ligand, owing to its ability to act in acidic environments (Zhang & Mitchison, 2003), has been extensively studied for biological applications, such as anti-tubercular (Manju *et al.*, 2010), antipyretic, antitumor, and anticancer (Chanda *et al.*, 2004). An additional amino substitution on 3-amino-2-pyrazine carboxylic acid could be expected to enhance crystal packing through extensive hydrogen bonding. APZC has a large variety of coordination geometries in metal complexes (Leciejewicz *et al.*, 1997, 1998; Ptasiwicz-Bak & Leciejewicz, 1997; Tayebbe *et al.*, 2008).

In continuation of our search to enrich the variety of such kinds of hybrid compounds and to investigate the influence of hydrogen bonds on the structural features (Bouacida *et al.*, 2007, 2009), we report here the synthesis and crystal structure of the title compound, (I), as an extension of our earlier work on N,O chelated ligands (Bouchene *et al.* 2013) which can be involved in covalent interactions in metal coordination chemistry.

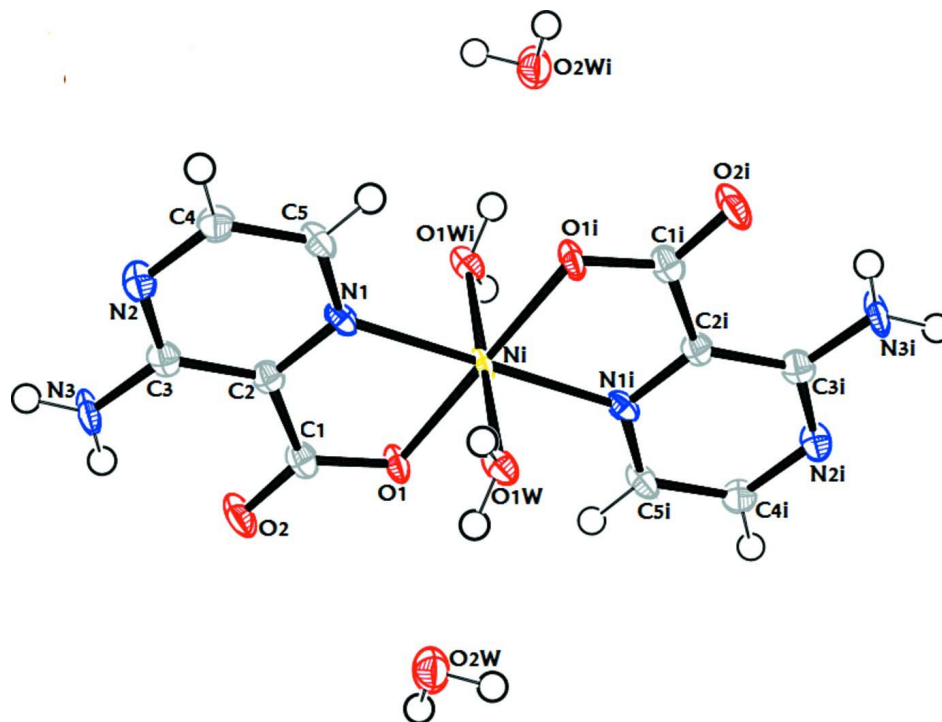
The asymmetric unit of (I) consists of one-half of the molecule, with the other half generated by a crystallographic inversion center. The molecular structure is shown in Fig. 1. The Ni<sup>II</sup> ion is coordinated by two 3-amino-2-pyrazine carboxylate ligands *via* N,O-chelating groups in the equatorial plane and two aqua O atoms in the axial sites forming a slightly distorted octahedral coordination environment. The Ni—N, Ni—O and Ni—O<sub>aqua</sub> distances are consistent with the reported data for the anhydrous Ni(II)(APZC)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub> complex (Ptasiwicz-Bak & Leciejewicz, 1999). In the crystal, the solvent water molecules and complex molecules are involved in intermolecular O—H $\cdots$ O, O—H $\cdots$ N and N—H $\cdots$ O hydrogen bonds forming two-dimensional layers parallel to (010) (Fig.2). Further O—H $\cdots$ O hydrogen bonds (Fig.3) involving the aqua ligands, N—H $\cdots$ O hydrogen bonds the carboxylate groups of the APZC ligands form a three-dimensional network.

**S2. Experimental**

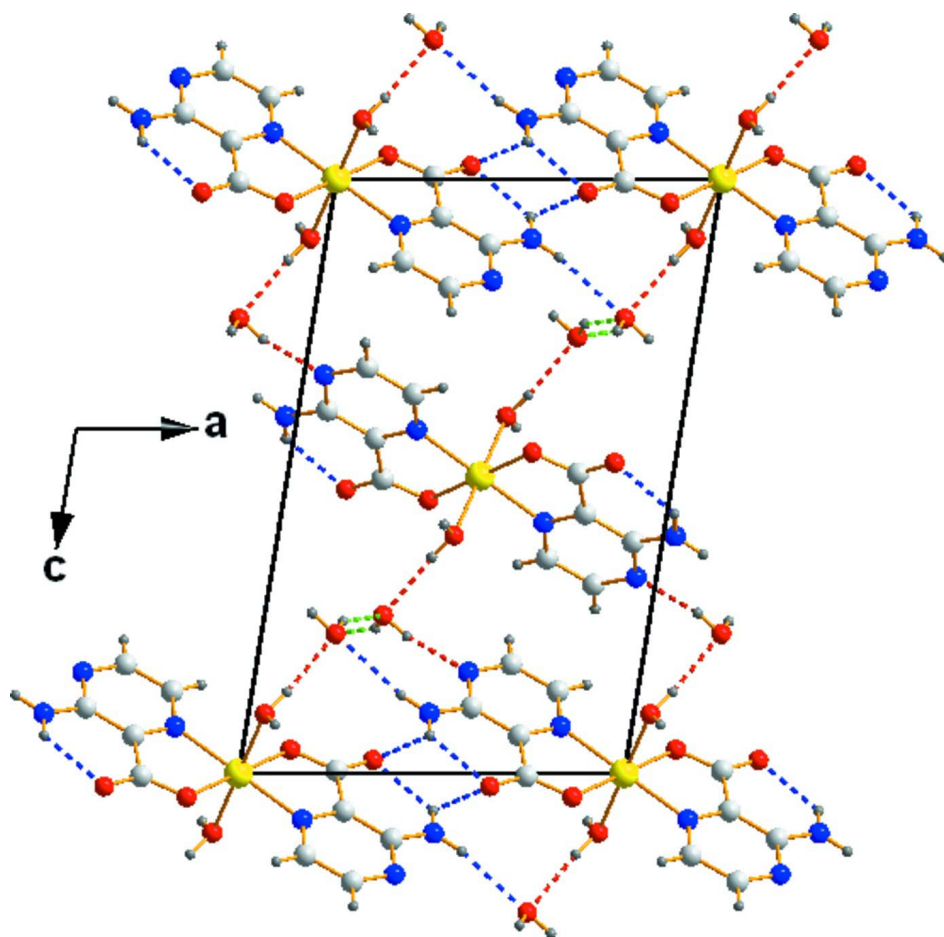
Nickel dichloride hexahydrate (0.2 mmol) and 3-aminopyrazine-2-carboxylic acid (0.02 mmol) were dissolved in acidified water with concentrated hydrogen chloride acid (37%). Light green crystals, suitable for X-ray diffraction study, were obtained from evaporation of obtained solution for three days.

**S3. Refinement**

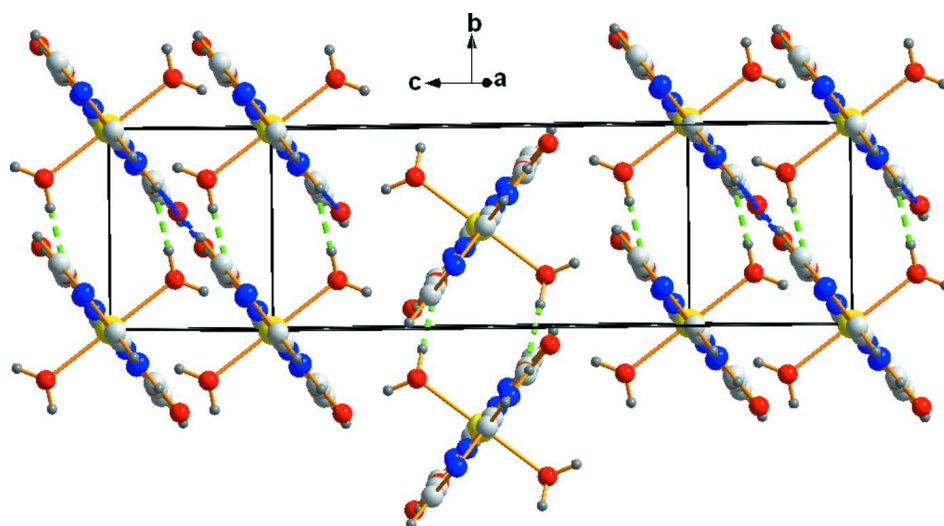
The H atoms bonded to C and N were located in difference Fourier maps but subsequently introduced in calculated positions and treated as riding on their parent atoms (C or N) with C—H = 0.93 Å and N—H = 0.86 Å with  $U_{iso}(H) = 1.2U_{eq}(C \text{ or } N)$ . Atoms H1W and H2W were located in a difference Fourier map and refined isotropically with  $U_{iso}(H) = 1.5U_{eq}(O)$ .

**Figure 1**

The molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented as small spheres of arbitrary radii. Symmetry code: (i)  $-x+1, -y+1, -z+2$ .

**Figure 2**

Partial packing plot viewed along the *b* axis showing the hydrogen bonds (dashed lines) forming layers.

**Figure 3**

Partial packing of (I) showing only the O—H...O hydrogen bonds which connect the layers in Fig. 2 into a three-dimensional network.

**Bis(3-aminopyrazine-2-carboxylato- $\kappa^2N^1,O$ )diaquanickel(II) dihydrate***Crystal data*[Ni(C<sub>5</sub>H<sub>4</sub>N<sub>3</sub>O<sub>2</sub>)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>] $\cdot$ 2H<sub>2</sub>O $M_r = 406.98$ Monoclinic,  $P2_1/c$  $a = 9.7939$  (15) Å $b = 5.1123$  (9) Å $c = 16.776$  (3) Å $\beta = 115.838$  (11)° $V = 756.0$  (2) Å<sup>3</sup> $Z = 2$  $F(000) = 420$  $D_x = 1.788$  Mg m<sup>-3</sup>Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 2285 reflections

 $\theta = 2.7$ – $25^\circ$  $\mu = 1.34$  mm<sup>-1</sup> $T = 150$  K

Cube, white

 $0.18 \times 0.16 \times 0.15$  mm*Data collection*Bruker APEXII CCD  
diffractometer

Radiation source: sealed tube

Graphite monochromator

 $\varphi$  and  $\omega$  scans

6200 measured reflections

1326 independent reflections

1121 reflections with  $I > 2\sigma(I)$  $R_{\text{int}} = 0.051$  $\theta_{\text{max}} = 25.1^\circ$ ,  $\theta_{\text{min}} = 2.7^\circ$  $h = -11 \rightarrow 11$  $k = -6 \rightarrow 6$  $l = -19 \rightarrow 19$ *Refinement*Refinement on  $F^2$ 

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.028$  $wR(F^2) = 0.073$  $S = 1.04$ 

1326 reflections

127 parameters

0 restraints

Primary atom site location: structure-invariant  
direct methodsSecondary atom site location: difference Fourier  
mapHydrogen site location: inferred from  
neighbouring sitesH atoms treated by a mixture of independent  
and constrained refinement $w = 1/[\sigma^2(F_o^2) + (0.0363P)^2 + 0.4886P]$ where  $P = (F_o^2 + 2F_c^2)/3$  $(\Delta/\sigma)_{\text{max}} < 0.001$  $\Delta\rho_{\text{max}} = 0.36$  e Å<sup>-3</sup> $\Delta\rho_{\text{min}} = -0.59$  e Å<sup>-3</sup>*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<sup>2</sup>)*

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.2428 (3)	0.2367 (5)	0.99519 (16)	0.0089 (5)
C2	0.2750 (3)	0.4494 (4)	1.06347 (15)	0.0079 (5)
C3	0.1864 (3)	0.4915 (5)	1.11094 (15)	0.0090 (5)
C4	0.3430 (3)	0.8353 (5)	1.18295 (16)	0.0098 (5)
H4	0.3692	0.9711	1.2239	0.012*

C5	0.4304 (3)	0.7942 (5)	1.13805 (15)	0.0097 (5)
H5	0.5141	0.8999	1.1492	0.012*
N1	0.3937 (2)	0.6010 (4)	1.07831 (13)	0.0074 (4)
N2	0.2227 (2)	0.6890 (4)	1.17019 (13)	0.0102 (4)
N3	0.0696 (2)	0.3396 (4)	1.10092 (14)	0.0125 (5)
H1N	0.0202	0.3689	1.1316	0.015*
H2N	0.0436	0.2122	1.0637	0.015*
O1	0.33555 (17)	0.2240 (3)	0.96010 (11)	0.0090 (4)
O2	0.13487 (18)	0.0885 (3)	0.97784 (12)	0.0137 (4)
O1W	0.6426 (2)	0.2542 (4)	1.10017 (12)	0.0102 (4)
H1A	0.726 (3)	0.312 (6)	1.1356 (19)	0.015*
H1B	0.652 (3)	0.124 (6)	1.083 (2)	0.015*
O2W	0.0735 (2)	0.6137 (4)	0.76616 (12)	0.0133 (4)
H2A	0.046 (4)	0.472 (6)	0.754 (2)	0.02*
H2B	0.104 (3)	0.663 (6)	0.733 (2)	0.02*
Ni1	0.5	0.5	1	0.00664 (16)

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.0073 (11)	0.0071 (12)	0.0116 (12)	0.0010 (9)	0.0036 (10)	0.0014 (10)
C2	0.0067 (12)	0.0078 (12)	0.0087 (11)	0.0002 (9)	0.0029 (10)	0.0009 (9)
C3	0.0078 (11)	0.0088 (12)	0.0098 (11)	0.0029 (10)	0.0031 (9)	0.0029 (11)
C4	0.0114 (12)	0.0077 (12)	0.0105 (12)	-0.0014 (9)	0.0050 (10)	-0.0024 (10)
C5	0.0068 (12)	0.0089 (12)	0.0137 (13)	-0.0011 (9)	0.0048 (10)	-0.0017 (10)
N1	0.0040 (10)	0.0067 (10)	0.0102 (10)	0.0004 (8)	0.0019 (8)	0.0009 (8)
N2	0.0097 (10)	0.0101 (11)	0.0123 (10)	-0.0008 (8)	0.0061 (9)	0.0001 (8)
N3	0.0094 (10)	0.0139 (11)	0.0195 (11)	-0.0052 (9)	0.0113 (9)	-0.0056 (9)
O1	0.0069 (8)	0.0093 (8)	0.0137 (9)	-0.0018 (7)	0.0073 (7)	-0.0032 (7)
O2	0.0092 (9)	0.0135 (9)	0.0213 (10)	-0.0055 (7)	0.0092 (8)	-0.0059 (8)
O1W	0.0077 (9)	0.0081 (9)	0.0147 (9)	-0.0015 (7)	0.0046 (8)	-0.0030 (8)
O2W	0.0148 (10)	0.0129 (9)	0.0169 (10)	-0.0035 (8)	0.0115 (8)	-0.0018 (8)
Ni1	0.0049 (2)	0.0062 (2)	0.0106 (2)	-0.00089 (17)	0.00506 (18)	-0.00108 (18)

*Geometric parameters (Å, °)*

C1—O2	1.228 (3)	N1—Ni1	2.0657 (19)
C1—O1	1.281 (3)	N3—H1N	0.86
C1—C2	1.510 (3)	N3—H2N	0.86
C2—N1	1.327 (3)	O1—Ni1	2.0233 (16)
C2—C3	1.427 (3)	O1W—Ni1	2.0755 (18)
C3—N3	1.331 (3)	O1W—H1A	0.83 (3)
C3—N2	1.351 (3)	O1W—H1B	0.74 (3)
C4—N2	1.332 (3)	O2W—H2A	0.77 (3)
C4—C5	1.381 (3)	O2W—H2B	0.78 (3)
C4—H4	0.93	Ni1—O1 <sup>i</sup>	2.0233 (16)
C5—N1	1.340 (3)	Ni1—N1 <sup>i</sup>	2.066 (2)
C5—H5	0.93	Ni1—O1W <sup>i</sup>	2.0755 (18)

O2—C1—O1	124.7 (2)	H1N—N3—H2N	120
O2—C1—C2	119.8 (2)	C1—O1—Ni1	115.72 (15)
O1—C1—C2	115.5 (2)	Ni1—O1W—H1A	118 (2)
N1—C2—C3	120.2 (2)	Ni1—O1W—H1B	113 (2)
N1—C2—C1	116.0 (2)	H1A—O1W—H1B	110 (3)
C3—C2—C1	123.7 (2)	H2A—O2W—H2B	108 (3)
N3—C3—N2	117.7 (2)	O1—Ni1—O1 <sup>i</sup>	180
N3—C3—C2	122.7 (2)	O1—Ni1—N1	80.54 (7)
N2—C3—C2	119.6 (2)	O1 <sup>i</sup> —Ni1—N1	99.46 (7)
N2—C4—C5	122.8 (2)	O1—Ni1—N1 <sup>i</sup>	99.46 (7)
N2—C4—H4	118.6	O1 <sup>i</sup> —Ni1—N1 <sup>i</sup>	80.54 (7)
C5—C4—H4	118.6	N1—Ni1—N1 <sup>i</sup>	180.0000 (10)
N1—C5—C4	119.5 (2)	O1—Ni1—O1W <sup>i</sup>	89.81 (7)
N1—C5—H5	120.3	O1 <sup>i</sup> —Ni1—O1W <sup>i</sup>	90.19 (7)
C4—C5—H5	120.3	N1—Ni1—O1W <sup>i</sup>	90.92 (7)
C2—N1—C5	119.9 (2)	N1 <sup>i</sup> —Ni1—O1W <sup>i</sup>	89.08 (7)
C2—N1—Ni1	112.20 (15)	O1—Ni1—O1W	90.19 (7)
C5—N1—Ni1	127.92 (16)	O1 <sup>i</sup> —Ni1—O1W	89.81 (7)
C4—N2—C3	117.9 (2)	N1—Ni1—O1W	89.08 (7)
C3—N3—H1N	120	N1 <sup>i</sup> —Ni1—O1W	90.92 (7)
C3—N3—H2N	120	O1W <sup>i</sup> —Ni1—O1W	180.00 (9)
O2—C1—C2—N1	180.0 (2)	N3—C3—N2—C4	177.5 (2)
O1—C1—C2—N1	1.0 (3)	C2—C3—N2—C4	-1.1 (3)
O2—C1—C2—C3	0.2 (4)	O2—C1—O1—Ni1	178.74 (18)
O1—C1—C2—C3	-178.8 (2)	C2—C1—O1—Ni1	-2.3 (3)
N1—C2—C3—N3	-177.5 (2)	C1—O1—Ni1—N1	2.15 (16)
C1—C2—C3—N3	2.3 (4)	C1—O1—Ni1—N1 <sup>i</sup>	-177.85 (16)
N1—C2—C3—N2	1.0 (3)	C1—O1—Ni1—O1W <sup>i</sup>	-88.81 (16)
C1—C2—C3—N2	-179.2 (2)	C1—O1—Ni1—O1W	91.19 (16)
N2—C4—C5—N1	0.5 (4)	C2—N1—Ni1—O1	-1.50 (15)
C3—C2—N1—C5	0.0 (3)	C5—N1—Ni1—O1	179.2 (2)
C1—C2—N1—C5	-179.9 (2)	C2—N1—Ni1—O1 <sup>i</sup>	178.50 (15)
C3—C2—N1—Ni1	-179.41 (17)	C5—N1—Ni1—O1 <sup>i</sup>	-0.8 (2)
C1—C2—N1—Ni1	0.8 (2)	C2—N1—Ni1—O1W <sup>i</sup>	88.16 (16)
C4—C5—N1—C2	-0.7 (3)	C5—N1—Ni1—O1W <sup>i</sup>	-91.1 (2)
C4—C5—N1—Ni1	178.57 (17)	C2—N1—Ni1—O1W	-91.84 (16)
C5—C4—N2—C3	0.4 (3)	C5—N1—Ni1—O1W	88.9 (2)

Symmetry code: (i)  $-x+1, -y+1, -z+2$ .

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$O1W-H1A\cdots O2W^i$	0.83 (3)	1.97 (3)	2.789 (3)	169 (3)
$O1W-H1B\cdots O1^{ii}$	0.75 (3)	1.94 (3)	2.690 (3)	176 (4)
$N3-H1N\cdots O2W^{iii}$	0.86	2.27	3.117 (3)	168



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O2 <i>W</i> —H2 <i>A</i> ···O2 <i>W</i> <sup>iv</sup>	0.77 (3)	2.12 (3)	2.867 (3)	164 (4)
O2 <i>W</i> —H2 <i>B</i> ···N2 <sup>v</sup>	0.78 (3)	2.03 (3)	2.792 (3)	168 (3)
N3—H2 <i>N</i> ···O2	0.86	2.10	2.733 (3)	130
N3—H2 <i>N</i> ···O2 <sup>vi</sup>	0.86	2.20	2.871 (3)	135
C5—H5···O1 <i>W</i> <sup>ii</sup>	0.93	2.54	3.377 (4)	150

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Symmetry codes: (i)  $-x+1, -y+1, -z+2$ ; (ii)  $-x+1, -y, -z+2$ ; (iii)  $-x, -y+1, -z+2$ ; (iv)  $-x, y-1/2, -z+3/2$ ; (v)  $x, -y+3/2, z-1/2$ ; (vi)  $-x, -y, -z+2$ ; (vii)  $x, y+1, z$ .