metal-organic compounds

Poly[diaqua[μ-1,4-bis(1*H*-imidazol-1-yl)-benzene-κ^2N^3:$N^{3'}$](μ-fumarato-κ^2O^1:O^4)-nickel(II)]

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In the title compound, $[Ni(C_4H_2O_4)(C_{12}H_{10}N_4)(H_2O)_2]_n$, the Ni^{II} ion has a distorted octahedral coordination geometry. The asymmetric unit is composed of an Ni^{2+} ion, located on a twofold rotation axis, one half of a 1,4-bis(1*H*-imidazol-1-yl)benzene (BIMB) ligand and one half of a fumarte (fum^{2-}) dianion, both ligands being located about inversion centers, and a coordinating water molecule. The Ni^{II} ions are linked by two BIMB ligands and two fum^{2-} dianions, forming a four-connected layered structure parallel to (010) with a 4^4-sql topology. Within each layer, there are rhombic grids with dimensions of *ca* 13.5 × 9.0 Å and approximate angles of 109 and 70°. The crystal packing features a two-dimensional → two-dimensional parallel/parallel interpenetration in which one undulating layer is catenated to another equivalent one, forming a new bilayer. Moreover, the entangled two-dimensional layers are connected by O—H···O and C—H···O hydrogen bonds, generating a three-dimensional structure.

Related literature

For multi-dimensional coordination polymers and their applications, see: Batten & Robson (1998); Carlucci *et al.* (2003*a*,*b*); Moulton & Zaworotko (2001); Sun *et al.* (2006); Wu *et al.* (2011); Bu *et al.* (2004). For their potential applications in electron transfer and drug delivery, see: Harriman & Sauvage (1996); Raymo & Sauvage (1999). For the structures of some related compounds, see: Chen *et al.* (2010); Li *et al.* (2012); Bu *et al.* (2004).
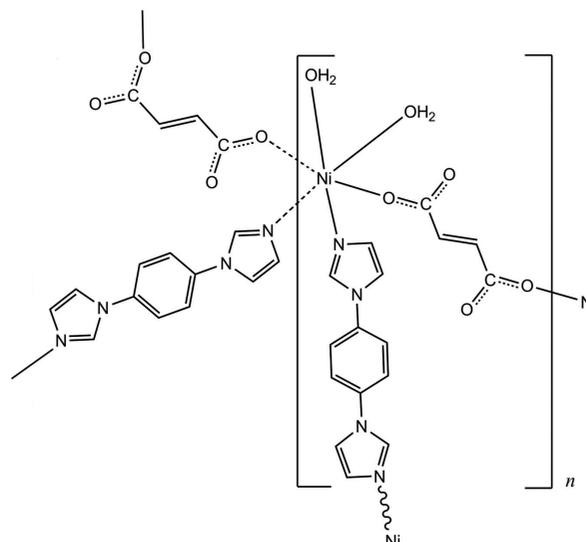
Experimental

Crystal data

$[Ni(C_4H_2O_4)(C_{12}H_{10}N_4)(H_2O)_2]$	V = 1666.67 (11) Å^3
M_r = 419.04	Z = 4
Orthorhombic, $Pbcn$	Mo $K\alpha$ radiation
a = 11.2806 (4) Å	μ = 1.21 mm^{-1}
b = 16.3703 (7) Å	T = 296 K
c = 9.0253 (3) Å	0.23 × 0.22 × 0.20 mm

Data collection

Bruke APEXII CCD area-dector diffractometer	8512 measured reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	2108 independent reflections
T_{min} = 0.768, T_{max} = 0.794	1827 reflections with $I > 2\sigma(I)$
	R_{int} = 0.019

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030	2 restraints
$wR(F^2)$ = 0.093	H-atom parameters constrained
S = 1.08	$\Delta\rho_{max}$ = 0.36 e Å^{-3}
2108 reflections	$\Delta\rho_{min}$ = −0.48 e Å^{-3}
123 parameters	

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3Y···O2^i	0.85	1.96	2.7033 (18)	146
O3—H3X···O2^{ii}	0.85	2.03	2.8361 (18)	159
C3—H3···O2^{ii}	0.93	2.49	3.360 (2)	155

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2003); 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) and *DIAMOND* (Brandenburg, 2010); software used to prepare material for publication: *SHELXTL* and *publCIF* (Westrip, 2010).

Normal University) and the Ministry of Education of Gansu (No. 1101–05).

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supporting information

Poly[diaqua[*μ*-1,4-bis(1*H*-imidazol-1-yl)benzene-*κ²N³:N³′*](*μ*-fumarato-*κ²O¹:O⁴*)nickel(II)]

Chang-Xin Bian, Xiao-Qiang Yao and Yu-Min Song

S1. Comment

Entanglement, one of the ubiquitous phenomena in nature, has received considerable attention due to their intrinsic aesthetic architectures (Bu *et al.*, 2004; Carlucci *et al.*, 2003*a*; Wu *et al.*, 2011) and potential applications (Sun *et al.*, 2006; Moulton & Zaworotko, 2001). Many structurally interesting entangled structures, such as polyrotaxane, polycatenation, polythreading, have been discussed in detail by (Batten *et al.*, 1998; Carlucci *et al.*, 2003*b*). Polycatenation as a type of interesting networks of entangled systems has attracted much attention for their potential application in energy of electron transfer and drug delivery (Harriman & Sauvage, 1996; Raymo & Sauvage, 1999). Herein, we report on the crystal structure of a Ni^{II} coordination polymer built from linear BIMB and fum^{2-} ligands, which features a two-dimensional → two-dimensional parallel/parallel polycatenation network.

The asymmetric unit of the title compound contains half a Ni^{II} ion located on a two-fold rotation axis, half a fum^{2-} dianion and half a BIMB ligand both located about inversion centers, and a coordinated water molecule. Each Ni^{II} ion is coordinated by two water molecules, two different carboxylate O atoms from two different fum^{2-} dianions and by two N atoms from two different BIMB ligands, and has a distorted octahedral geometry (Fig. 1).

It is interesting to note that the maleic acid (hydrolysis product of maleic anhydride) is converted into fumaric acid on the self-assembly of the title compound. This is probably because *trans*-fumaric has a higher thermal stability than *cis*-maleic acid.

In the crystal, each Ni^{II} ion is connected by two BIMB ligands and two fum^{2-} ligands to form an infinite two-dimensional puckered sheet with rhombic grids (Fig. 2). Within each layer, the rhombic grids have dimensions of ca. 13.5 Å × 9.0 Å with angles of of ca. 109.60 and 70.40° (defined by Ni···Ni distances and Ni···Ni···Ni angles). The large size of the grids in two adjacent layers allow a two-dimensional → two-dimensional parallel/parallel polycatenation to occur (Fig. 3). From a topological perspective, each Ni^{II} ion can be regarded as a four-connected node, thus this two-dimensional network can be assigned to the 4⁴-**sql** topology.

Moreover, the entangled two-dimensional layers are further connected by O–H···O hydrogen bonds to generate a three-dimensional structure (Fig. 4).

The structure of a similar Ni^{II} coordination polymer assembled by BIMB ligand and adipic acid has been described by (Chen *et al.*, 2010). However, compared with the title compound, the adipic acid is a longer spacer length and more flexible, and crystallizes in the lower symmetry triclinic space group $P\bar{1}$ rather than orthorhombic space group *Pbcn* for the title compound with the short fumarate spacer.

Another relevant example reported by (Bu *et al.*, 2004) is a Zn^{II} coordination polymer (Li *et al.* 2012). Like the title complex, it is also built from BIMB and fum^{2-} ligands. However, the difference in the metal center results in an interesting 5-fold interpenetrated three-dimensional framework based on a diamondoid topology.

In summary, we have synthesized a Ni^{II} coordination polymer by the hydrothermal reaction of Ni(NO$_3$)$_2$ with H$_2$fum and BIMB ligands, which features a two-dimensional → two-dimensional parallel/parallel polycatenation network. On comparing with two relevant complexes based on the BIMB ligand, we found that the coordination geometry of the central metal ions and the flexibility of the auxiliary carboxylate ligands indeed have a significant effect on the architecture of the target complexes.

S2. Experimental

A mixture of 1,4-Bis(1-imidazolyl)benzene (BIMB) (0.032 g, 0.15 mmol), maleic anydride (0.015 g, 0.15 mmol) and Ni(NO$_3$)$_2$ (0.045 g, 0.25 mmol) in N,N'-dimethylformamide (DMF) (4 ml) and H$_2$O (2 ml) was placed in a Teflon-lined stainless steel vessel and heated at 363 K for 3 days. On cooling to room temperature green block-like single crystals suitable for X-ray diffraction were obtained [70% yield (based on BIMB ligand)]. Anal. Calcd for C$_{16}$H$_{16}$N$_4$O$_6$Ni: C, 45.86; H, 3.85; N, 13.37%. Found: C, 45.93; H, 3.87; N, 13.41%. Spectroscopic data for the title compound are given in the archived CIF.

S3. Refinement

The water H atoms were located in a difference Fourier map and included as riding atoms, with O—H = 0.85 and U_{iso}(H) = 1.5Ueq(O). The C-bound H atoms were placed in calculated positions and treated as riding: C—H = 0.93 Å with U_{iso}(H) = 1.2U$_{eq}$(C).
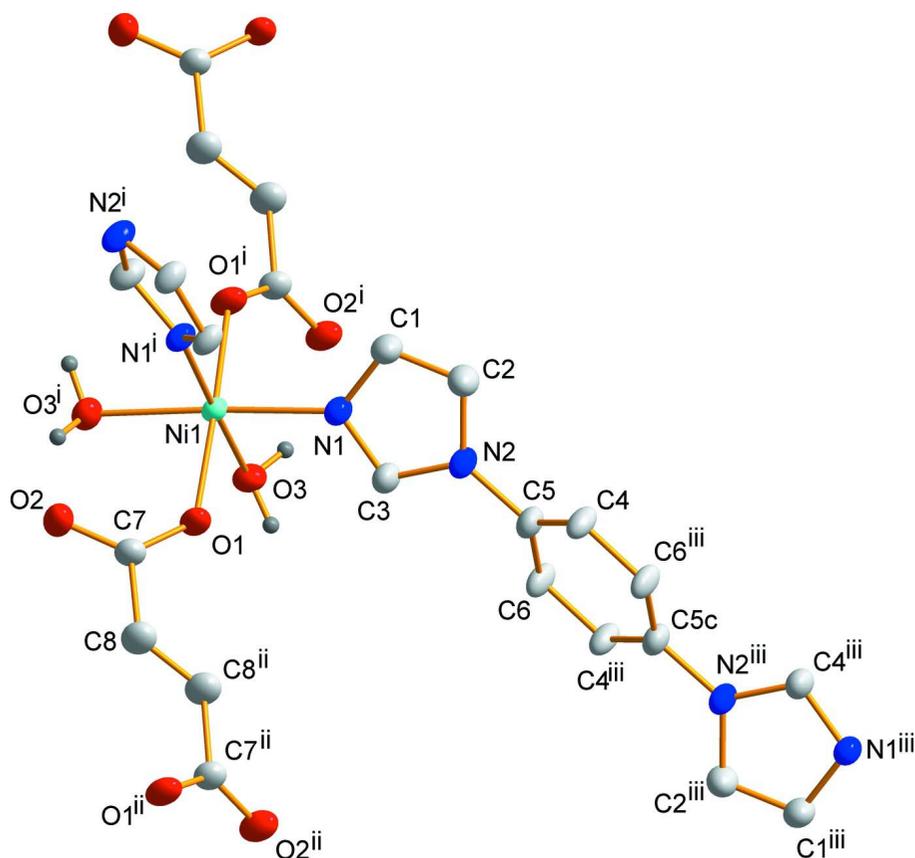
Figure 1

The molecular structure of the title compound, with atom numbering. The displacement ellipsoids are drawn at the 50%
probability level [H atoms have been omitted for clarity; symmetry codes: (i) $1 - x$, y, $0.5 - z$; (ii) $1 - x$, y, $-0.5 - z$; (iii) $2 - x$, $-y$, $-z$].
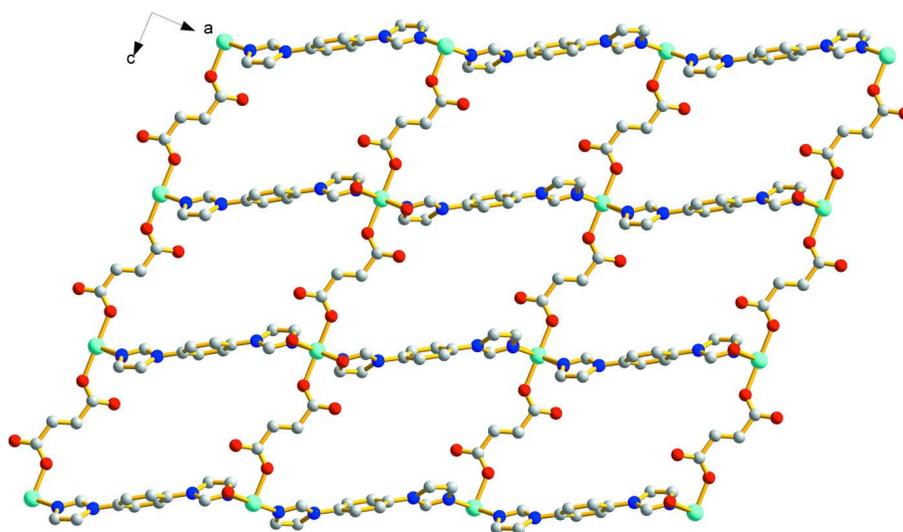
Figure 2

A view of the two-dimensional undulated 4^4-**sql** layer of the title compound.
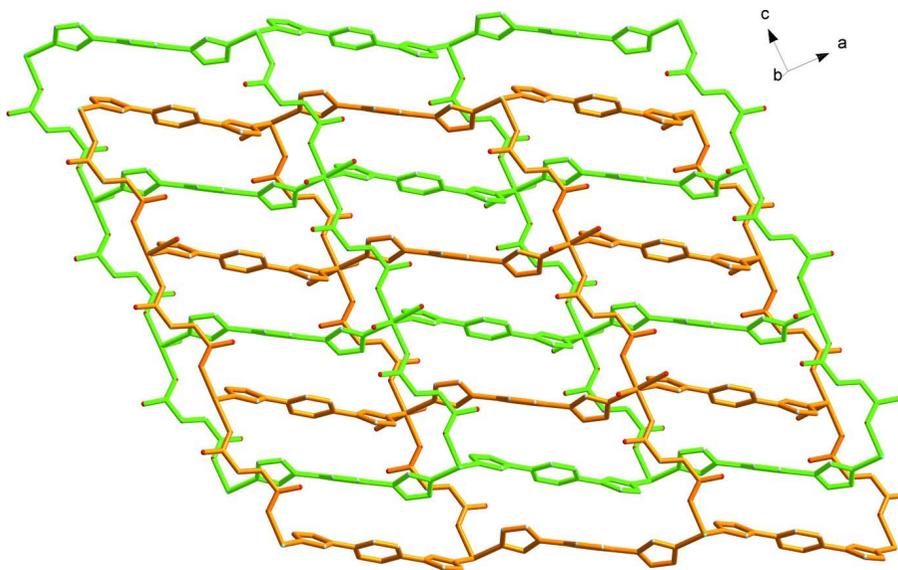
Figure 3

A view of the two-fold parallel polycatenation of the two-dimensional layers in the crystal structure of the title compound.
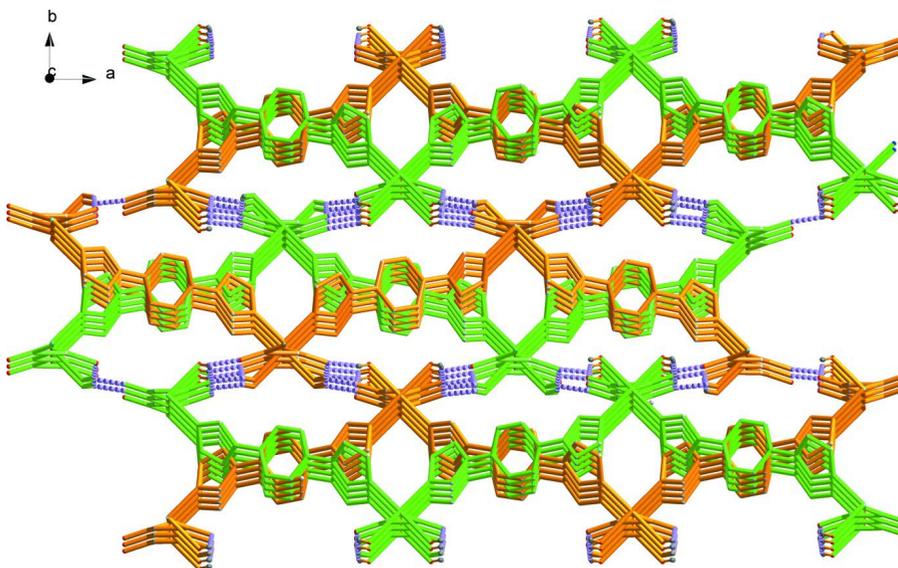
Figure 4

A view of the entangled two-dimensional layers that extended to a three-dimensional structure *via* O–H⋯O hydrogen bonds in the crystal structure of the title compound.

Poly[diaqua[µ-1,4-bis(1*H*-imidazol-1-yl)benzene- κ^2N^3:$N^{3'}$](µ-fumarato- κ^2O^1:O^4)nickel(II)]

Crystal data

[Ni(C$_4$H$_2$O$_4$)(C$_{12}$H$_{10}$N$_4$)(H$_2$O)$_2$]	b = 16.3703 (7) Å
M_r = 419.04	c = 9.0253 (3) Å
Orthorhombic, *Pbcn*	V = 1666.67 (11) Å^3
Hall symbol: -P 2n 2ab	Z = 4
a = 11.2806 (4) Å	F(000) = 864

$D_x = 1.670$ Mg m^{-3}

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 4217 reflections

$\theta = 2.5$–$28.4°$

$\mu = 1.21$ mm^{-1}

$T = 296$ K

Block, green

$0.23 \times 0.22 \times 0.20$ mm

Data collection

Bruke APEXII CCD area-dector diffractometer	8512 measured reflections
Radiation source: fine-focus sealed tube	2108 independent reflections
Graphite monochromator	1827 reflections with $I > 2\sigma(I)$
CCD rotation images, thin slices scans	$R_{int} = 0.019$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$\theta_{max} = 28.5°$, $\theta_{min} = 2.2°$
	$h = -13 \rightarrow 15$
$T_{min} = 0.768$, $T_{max} = 0.794$	$k = -18 \rightarrow 21$
	$l = -12 \rightarrow 12$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.030$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.093$	
$S = 1.08$	H-atom parameters constrained
2108 reflections	$w = 1/[\sigma^2(F_o^2) + (0.047P)^2 + 1.0911P]$ where $P = (F_o^2 + 2F_c^2)/3$
123 parameters	
2 restraints	$(\Delta/\sigma)_{max} < 0.001$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{max} = 0.36$ e Å^{-3}
	$\Delta\rho_{min} = -0.48$ e Å^{-3}

Special details

Experimental. Spectroscopic data for the title compound :

IR (KBr, cm^{-1}): 3380m, 3133m, 1564s, 1533s, 1385s, 1307w, 1269w, 1130w, 1195w, 1074m, 970w, 880w, 829m, 751m, 682w, 656w, 534w, 495w.

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}
C1	0.85967 (16)	0.48653 (12)	0.8087 (2)	0.0337 (4)
H1	0.9127	0.5069	0.8785	0.040*
C2	0.76108 (18)	0.52549 (13)	0.7609 (2)	0.0353 (4)
H2	0.7344	0.5768	0.7899	0.042*
C3	0.77741 (16)	0.40688 (11)	0.6505 (2)	0.0294 (4)
H3	0.7616	0.3627	0.5889	0.035*
C4	0.57558 (18)	0.56487 (12)	0.5293 (3)	0.0409 (5)
H4	0.6266	0.6082	0.5487	0.049*
C5	0.60153 (15)	0.48748 (11)	0.5802 (2)	0.0290 (4)

C6	0.52718 (19)	0.42289 (12)	0.5509 (3)	0.0408 (5)
H6	0.5461	0.3709	0.5851	0.049*
C7	1.08521 (15)	0.29993 (11)	0.43626 (19)	0.0266 (3)
C8	1.05530 (18)	0.30159 (14)	0.2748 (2)	0.0348 (4)
H8	1.1169	0.3027	0.2064	0.042*
N1	0.86960 (13)	0.41195 (10)	0.73829 (16)	0.0261 (3)
N2	0.70833 (13)	0.47384 (9)	0.66080 (18)	0.0288 (3)
Ni1	1.0000	0.323481 (18)	0.7500	0.01981 (12)
O1	1.00329 (10)	0.31848 (9)	0.52371 (16)	0.0310 (3)
O2	1.18776 (11)	0.27709 (9)	0.47076 (14)	0.0347 (3)
O3	0.86671 (12)	0.23178 (8)	0.74938 (13)	0.0291 (3)
H3Y	0.8214	0.2383	0.8237	0.044*
H3X	0.8264	0.2356	0.6701	0.044*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0277 (8)	0.0378 (10)	0.0358 (10)	0.0029 (7)	−0.0078 (8)	−0.0101 (8)
C2	0.0317 (9)	0.0328 (9)	0.0414 (11)	0.0050 (8)	−0.0073 (8)	−0.0121 (8)
C3	0.0260 (8)	0.0294 (9)	0.0327 (9)	0.0065 (7)	−0.0078 (7)	−0.0043 (7)
C4	0.0341 (10)	0.0268 (9)	0.0617 (14)	0.0004 (7)	−0.0200 (10)	−0.0014 (9)
C5	0.0221 (8)	0.0304 (9)	0.0344 (9)	0.0059 (6)	−0.0081 (7)	−0.0022 (7)
C6	0.0358 (10)	0.0244 (8)	0.0621 (14)	0.0050 (7)	−0.0197 (10)	0.0031 (9)
C7	0.0272 (8)	0.0337 (9)	0.0189 (7)	0.0008 (7)	−0.0008 (6)	−0.0015 (7)
C8	0.0321 (10)	0.0489 (11)	0.0233 (8)	0.0010 (9)	0.0014 (7)	0.0001 (8)
N1	0.0212 (7)	0.0307 (8)	0.0266 (7)	0.0027 (6)	−0.0046 (5)	−0.0025 (6)
N2	0.0230 (7)	0.0287 (7)	0.0346 (8)	0.0049 (6)	−0.0086 (6)	−0.0031 (6)
Ni1	0.01593 (17)	0.02772 (18)	0.01579 (17)	0.000	−0.00177 (9)	0.000
O1	0.0255 (6)	0.0512 (9)	0.0164 (6)	0.0054 (5)	−0.0009 (4)	−0.0025 (5)
O2	0.0270 (6)	0.0532 (8)	0.0238 (6)	0.0093 (6)	0.0004 (5)	−0.0013 (6)
O3	0.0263 (6)	0.0357 (7)	0.0253 (7)	−0.0042 (5)	−0.0021 (5)	−0.0035 (5)

Geometric parameters (Å, º)

C1—C2	1.353 (3)	C6—H6	0.9300
C1—N1	1.381 (2)	C7—O1	1.253 (2)
C1—H1	0.9300	C7—O2	1.255 (2)
C2—N2	1.373 (2)	C7—C8	1.496 (3)
C2—H2	0.9300	C8—C8^{ii}	1.326 (4)
C3—N1	1.310 (2)	C8—H8	0.9300
C3—N2	1.348 (2)	N1—Ni1	2.0670 (15)
C3—H3	0.9300	Ni1—O1	2.0443 (15)
C4—C5	1.379 (3)	Ni1—O1^{iii}	2.0443 (15)
C4—C6^{i}	1.381 (3)	Ni1—N1^{iii}	2.0671 (15)
C4—H4	0.9300	Ni1—O3^{iii}	2.1247 (13)
C5—C6	1.375 (3)	Ni1—O3	2.1247 (13)
C5—N2	1.425 (2)	O3—H3Y	0.8500
C6—C4^{i}	1.381 (3)	O3—H3X	0.8501

C2—C1—N1	109.66 (16)	C3—N1—Ni1	123.47 (13)
C2—C1—H1	125.2	C1—N1—Ni1	130.81 (12)
N1—C1—H1	125.2	C3—N2—C2	107.19 (15)
C1—C2—N2	106.02 (17)	C3—N2—C5	125.53 (15)
C1—C2—H2	127.0	C2—N2—C5	127.28 (15)
N2—C2—H2	127.0	O1—Ni1—O1ⁱⁱⁱ	175.41 (8)
N1—C3—N2	111.46 (16)	O1—Ni1—N1	89.42 (5)
N1—C3—H3	124.3	O1ⁱⁱⁱ—Ni1—N1	93.80 (5)
N2—C3—H3	124.3	O1—Ni1—N1ⁱⁱⁱ	93.79 (5)
C5—C4—C6ⁱ	119.07 (18)	O1ⁱⁱⁱ—Ni1—N1ⁱⁱⁱ	89.42 (5)
C5—C4—H4	120.5	N1—Ni1—N1ⁱⁱⁱ	91.04 (9)
C6ⁱ—C4—H4	120.5	O1—Ni1—O3ⁱⁱⁱ	87.80 (5)
C6—C5—C4	120.85 (16)	O1ⁱⁱⁱ—Ni1—O3ⁱⁱⁱ	88.96 (5)
C6—C5—N2	119.55 (16)	N1—Ni1—O3ⁱⁱⁱ	177.19 (5)
C4—C5—N2	119.57 (16)	N1ⁱⁱⁱ—Ni1—O3ⁱⁱⁱ	89.51 (6)
C5—C6—C4ⁱ	120.07 (18)	O1—Ni1—O3	88.96 (5)
C5—C6—H6	120.0	O1ⁱⁱⁱ—Ni1—O3	87.79 (5)
C4ⁱ—C6—H6	120.0	N1—Ni1—O3	89.50 (6)
O1—C7—O2	126.58 (16)	N1ⁱⁱⁱ—Ni1—O3	177.19 (5)
O1—C7—C8	116.29 (16)	O3ⁱⁱⁱ—Ni1—O3	90.09 (8)
O2—C7—C8	117.06 (16)	C7—O1—Ni1	130.74 (12)
C8ⁱⁱ—C8—C7	122.8 (2)	Ni1—O3—H3Y	109.6
C8ⁱⁱ—C8—H8	118.6	Ni1—O3—H3X	109.3
C7—C8—H8	118.6	H3Y—O3—H3X	109.5
C3—N1—C1	105.67 (15)		

N1—C1—C2—N2	0.8 (2)	C4—C5—N2—C2	36.9 (3)
C6ⁱ—C4—C5—C6	0.6 (4)	C3—N1—Ni1—O1	45.30 (16)
C6ⁱ—C4—C5—N2	178.9 (2)	C1—N1—Ni1—O1	−131.70 (17)
C4—C5—C6—C4ⁱ	−0.6 (4)	C3—N1—Ni1—O1ⁱⁱⁱ	−131.42 (15)
N2—C5—C6—C4ⁱ	−178.9 (2)	C1—N1—Ni1—O1ⁱⁱⁱ	51.58 (17)
O1—C7—C8—C8ⁱⁱ	−16.9 (2)	C3—N1—Ni1—N1ⁱⁱⁱ	139.09 (17)
O2—C7—C8—C8ⁱⁱ	160.34 (12)	C1—N1—Ni1—N1ⁱⁱⁱ	−37.91 (15)
N2—C3—N1—C1	−0.2 (2)	C3—N1—Ni1—O3ⁱⁱⁱ	38.0 (12)
N2—C3—N1—Ni1	−177.88 (12)	C1—N1—Ni1—O3ⁱⁱⁱ	−139.0 (10)
C2—C1—N1—C3	−0.4 (2)	C3—N1—Ni1—O3	−43.66 (15)
C2—C1—N1—Ni1	177.04 (15)	C1—N1—Ni1—O3	139.33 (17)
N1—C3—N2—C2	0.7 (2)	O2—C7—O1—Ni1	2.1 (3)
N1—C3—N2—C5	−179.97 (17)	C8—C7—O1—Ni1	179.05 (13)
C1—C2—N2—C3	−0.9 (2)	O1ⁱⁱⁱ—Ni1—O1—C7	−73.40 (17)
C1—C2—N2—C5	179.80 (19)	N1—Ni1—O1—C7	152.04 (17)
C6—C5—N2—C3	36.0 (3)	N1ⁱⁱⁱ—Ni1—O1—C7	61.04 (17)
C4—C5—N2—C3	−142.3 (2)	O3ⁱⁱⁱ—Ni1—O1—C7	−28.32 (17)
C6—C5—N2—C2	−144.8 (2)	O3—Ni1—O1—C7	−118.44 (17)

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) −*x*+2, *y*, −*z*+1/2; (iii) −*x*+2, *y*, −*z*+3/2.

Hydrogen-bond geometry (Å, º)

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O3—H3$Y$$\cdots$O2[iii]	0.85	1.96	2.7033 (18)	146
O3—H3$X$$\cdots$O2[iv]	0.85	2.03	2.8361 (18)	159
C3—H3$\cdots$O2[iv]	0.93	2.49	3.360 (2)	155

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