Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

catena-Poly[[diaquabis(formato-κO)-nickel(II)]-μ-2,4,6-tris(4-pyridyl)-1,3,5-triazine-κ^2N^2:N^4]

Miao Feng,[a] Hui-Juan Tian,[a] Huai-Feng Mi[a]* and Tong-Liang Hu[b]

[a]Biochemical Section of Key Laboratory of Functional Polymer Materials, The Ministry of Education of China, Chemical School of Nankai University, 300071 Tianjin, People's Republic of China, and [b]Department of Chemistry, Nankai University, Tianjin 300071, People's Republic of China
Correspondence e-mail: hfmi@nankai.edu.cn

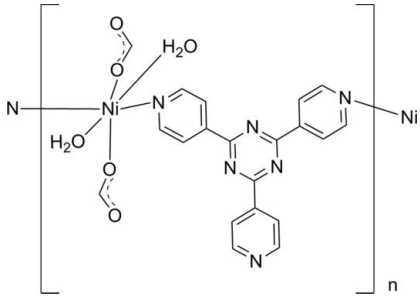
Received 19 March 2011; accepted 2 April 2011

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.034; wR factor = 0.078; data-to-parameter ratio = 15.0.

In the title compound, $[Ni(CHO_2)_2(C_{18}H_{12}N_6)(H_2O)_2]_n$, the Ni^{II} ion, lying on a crystallographic inversion center, has a distorted octahedral coordination comprising two water ligands, two O-atom donors from formate ligands and two N-atom donors from the 2,4,6-tris(4-pyridyl)-1,3,5-triazine ligands. These ligands bridge the Ni^{II} complex units, forming zigzag chains along the c axis. Adjacent chains are linked by O—H···O hydrogen bonds, forming a three-dimensional supramolecular network.

Related literature

For the structures and properties of coordination compounds with 2,4,6-tris(4-pyridyl)-1,3,5-triazine as a ligand, see: Abrahams *et al.* (1999); Barrios *et al.* (2007); Batten *et al.* (1995); Dybtsev *et al.* (2004). 2~2~O ligand should bind through the O atom



Experimental

Crystal data

$[Ni(CHO_2)_2(C_{18}H_{12}N_6)(H_2O)_2]$
M_r = 497.11
Monoclinic, $C2/c$
a = 24.725 (5) Å
b = 10.969 (2) Å
c = 7.4196 (15) Å
β = 90.23 (3)°
V = 2012.2 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.02 mm^{-1}
T = 293 K
0.15 × 0.10 × 0.10 mm

Data collection

Rigaku SCX-mini diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.836, T_{max} = 1.000
10365 measured reflections
2302 independent reflections
1937 reflections with $I > 2\sigma(I)$
R_{int} = 0.040

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.078
S = 1.05
2302 reflections
153 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H6···O2^{i}	0.86	1.96	2.818 (2)	177
O3—H7···O2^{ii}	0.83	1.95	2.777 (2)	174

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

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); 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: *publCIF* (Westrip, 2010).

This work was supported by the National Natural Science Foundation of China [project approval No. 20974053].

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BQ2289).

References

Abrahams, B. F., Batten, S. R., Grannas, M. J., Hamit, H., Hoskins, B. F. & Robson, R. (1999). *Angew. Chem. Int. Ed.* **38**, 1475–1477.
Barrios, L. A., Ribas, J. & Aromi, G. (2007). *Inorg. Chem.* **46**, 7154–7162.
Batten, S. R., Hoskins, B. F. & Robson, R. (1995). *Angew. Chem. Int. Ed.* **34**, 820–822.
Dybtsev, D. N., Chun, H. & Kim, K. (2004). *Chem. Commun.* pp. 1594–1595.
Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Rigaku (1998). *PROCESS-AUTO*. Rigaku Corporation, Tokyo, Japan.
Rigaku/MSC (2002). *CrystalStructure*. Rigaku/MSC, The Woodlands, Texas, USA.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

supporting information

Acta Cryst. (2011). E**67**, m563 [doi:10.1107/S1600536811012281]

catena-Poly[[diaquabis(formato-κO)nickel(II)]-μ-2,4,6-tris(4-pyridyl)-1,3,5-triazine-$\kappa^2N^2:N^4$]

Miao Feng, Hui-Juan Tian, Huai-Feng Mi and Tong-Liang Hu

S1. Comment

As an interesting polydentate nitrogen donor ligand, 2,4,6-tris(4-pyridyl)-1,3,5-triazine has attracted increasing attention in the synthesis of novel transition metal complexes with novel topology and properties (Abrahams *et al.*, 1999; Dybtsev *et al.*, 2004; Barrios *et al.*, 2007; Batten *et al.*, 1995). Our interest in 2,4,6-tris(4-pyridyl)-1,3,5-triazine transition metal complexes prompts us to report the title compound (I).

As shown in Fig. 1, in the title compound, [Ni($C_{18}H_{12}N_6$)(H_2O)$_2$($HCOO$)$_2$]n, the Ni^{II} ion, lying on a crystallographic inversion center, has a distorted octahedral coordination sphere comprising two water ligands, two O-atom donors from formate ligands and two N-atom donors from the 2,4,6-tris(4-pyridyl)-1,3,5-triazine ligands. These ligands bridge the Ni^{II} complex units to form zigzag chains along *c* axis (Fig. 2). Adjacent chains are linked by O—H···O hydrogen bonds (Table 1), forming a three-dimensional supramolecular network (Fig. 3).

S2. Experimental

A mixture of Ni($HCOO$)$_2$.2H_2O (0.15 mmol), 2,4,6-tris(4-pyridyl)-1,3,5-triazine (0.05 mmol), and 10 ml H_2O were put in a 23-ml Teflon liner reactor and heated at 413 K in oven for 72 h. The resulting solution was slowly cooled to room temperature to yield single crystals of the title compound.

S3. Refinement

All H atoms were positioned geometrically (C—H = 0.93 Å) and allowed to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(parent atom). The H atoms of the water molecules were located in Fourier difference maps and refined isotropically.

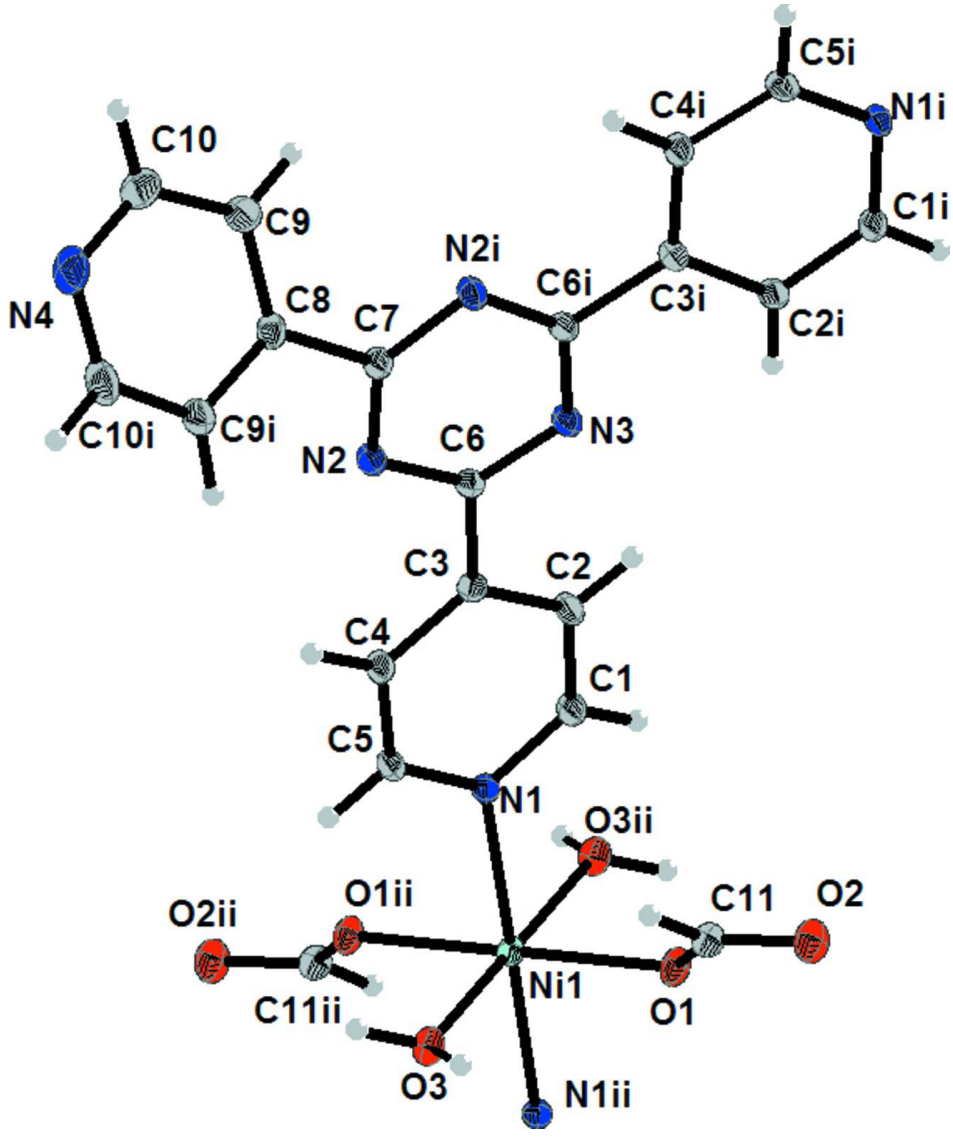


Figure 1

A fragment of the title compound showing the atom numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Symmetry codes: (i) (-*x*, -*y*, -*z* + 1.5); (ii) (-*x* + 1/2, -*y* + 1.5, -*z* + 2).

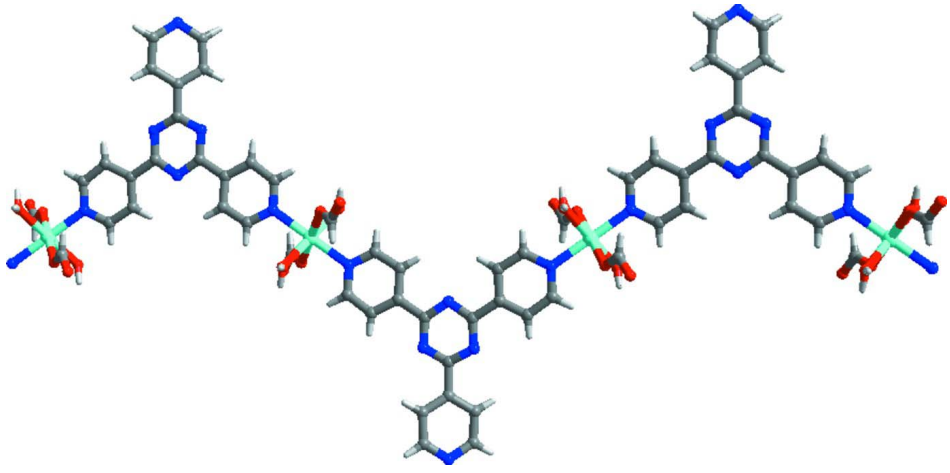


Figure 2

A view of the title structure along the *c* axis, showing the zigzag chain.

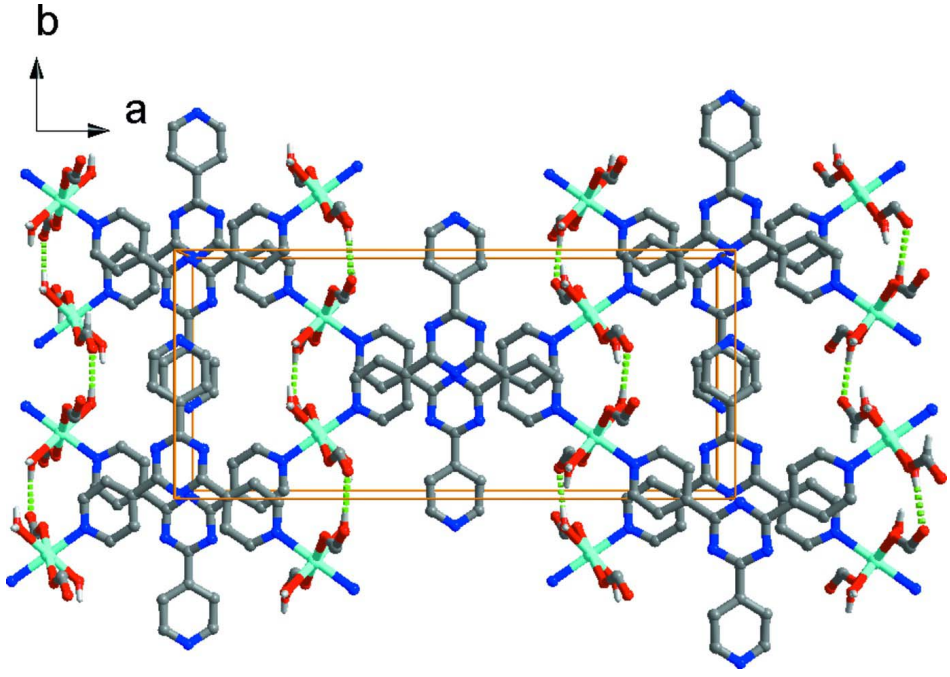


Figure 3

The crystal packing of the title compound. O—H···O hydrogen bonds are shown as dashed lines.

***catena*-Poly[[diaquabis(formato-κO)nickel(II)]-μ- 2,4,6-tris(4-pyridyl)-1,3,5-triazine-$\kappa^2N^2:N^4$]**

Crystal data

$[Ni(CHO_2)_2(C_{18}H_{12}N_6)(H_2O)_2]$
$M_r = 497.11$
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
$a = 24.725$ (5) Å
$b = 10.969$ (2) Å
$c = 7.4196$ (15) Å
$\beta = 90.23$ (3)°
$V = 2012.2$ (7) Å^3
$Z = 4$
$F(000) = 1024$
$D_x = 1.641$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9569 reflections
$\theta = 3.1$–27.5°
$\mu = 1.02$ mm^{-1}

T = 293 K
Block, green

0.15 × 0.10 × 0.10 mm

Data collection

Rigaku SCX-mini diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.836, T_{max} = 1.000

10365 measured reflections
2302 independent reflections
1937 reflections with $I > 2\sigma(I)$
R_{int} = 0.040
θ_{max} = 27.5°, θ_{min} = 3.1°
h = −31→32
k = −14→14
l = −9→9

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.078
S = 1.05
2302 reflections
153 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0334P)^2 + 2.3183P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Ni1	0.2500	0.7500	1.0000	0.01798 (11)
O1	0.22888 (6)	0.64439 (12)	0.78618 (18)	0.0263 (3)
O2	0.19168 (7)	0.61015 (14)	0.5190 (2)	0.0337 (4)
O3	0.29896 (6)	0.86926 (12)	0.85264 (19)	0.0263 (3)
H6	0.3027	0.9430	0.8884	0.039*
H7	0.3001	0.8711	0.7403	0.039*
N1	0.18044 (6)	0.86186 (14)	0.9633 (2)	0.0204 (4)
N2	0.04510 (7)	1.19452 (15)	0.8071 (2)	0.0251 (4)
N3	0.0000	1.0076 (2)	0.7500	0.0245 (5)
N4	0.0000	1.6408 (2)	0.7500	0.0428 (7)
C1	0.13264 (8)	0.81007 (18)	0.9265 (3)	0.0241 (4)
H1	0.1299	0.7257	0.9355	0.029*
C2	0.08733 (8)	0.87491 (18)	0.8760 (3)	0.0248 (4)
H2	0.0551	0.8349	0.8495	0.030*

C3	0.09060 (8)	1.00126 (18)	0.8654 (3)	0.0210 (4)
C4	0.13930 (8)	1.05662 (18)	0.9086 (3)	0.0239 (4)
H4	0.1427	1.1410	0.9053	0.029*
C5	0.18282 (8)	0.98373 (18)	0.9569 (3)	0.0240 (4)
H5	0.2154	1.0215	0.9864	0.029*
C6	0.04255 (8)	1.07256 (18)	0.8045 (3)	0.0208 (4)
C7	0.0000	1.2503 (3)	0.7500	0.0229 (6)
C8	0.0000	1.3860 (3)	0.7500	0.0252 (6)
C9	−0.04675 (9)	1.4505 (2)	0.7877 (3)	0.0327 (5)
H9	−0.0791	1.4101	0.8097	0.039*
C10	−0.04418 (10)	1.5768 (2)	0.7918 (4)	0.0400 (6)
H10	−0.0750	1.6194	0.8257	0.048*
C11	0.20837 (8)	0.67816 (19)	0.6412 (3)	0.0246 (4)
H11	0.2052	0.7617	0.6226	0.029*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.01931 (18)	0.01621 (18)	0.01840 (18)	0.00276 (15)	−0.00433 (12)	−0.00092 (15)
O1	0.0344 (8)	0.0217 (7)	0.0227 (7)	0.0047 (6)	−0.0086 (6)	−0.0032 (6)
O2	0.0428 (9)	0.0349 (9)	0.0233 (8)	0.0010 (7)	−0.0093 (7)	−0.0037 (7)
O3	0.0350 (8)	0.0216 (7)	0.0224 (7)	−0.0013 (6)	0.0005 (6)	0.0019 (6)
N1	0.0188 (8)	0.0193 (8)	0.0231 (8)	0.0024 (7)	−0.0044 (6)	0.0001 (7)
N2	0.0212 (9)	0.0180 (8)	0.0362 (10)	0.0011 (7)	−0.0062 (7)	−0.0005 (7)
N3	0.0193 (12)	0.0187 (12)	0.0353 (14)	0.000	−0.0059 (10)	0.000
N4	0.0506 (19)	0.0189 (14)	0.059 (2)	0.000	−0.0079 (15)	0.000
C1	0.0238 (10)	0.0154 (10)	0.0332 (11)	−0.0003 (8)	−0.0034 (8)	0.0014 (8)
C2	0.0191 (10)	0.0196 (10)	0.0357 (12)	−0.0029 (8)	−0.0057 (8)	0.0002 (9)
C3	0.0192 (9)	0.0210 (10)	0.0226 (10)	0.0023 (8)	−0.0023 (8)	−0.0013 (8)
C4	0.0228 (10)	0.0159 (9)	0.0330 (11)	0.0000 (8)	−0.0052 (8)	−0.0007 (8)
C5	0.0181 (10)	0.0222 (10)	0.0316 (11)	−0.0020 (8)	−0.0050 (8)	−0.0036 (9)
C6	0.0178 (9)	0.0196 (10)	0.0249 (10)	0.0007 (8)	−0.0012 (8)	−0.0009 (8)
C7	0.0224 (13)	0.0167 (13)	0.0297 (14)	0.000	−0.0021 (11)	0.000
C8	0.0285 (15)	0.0185 (14)	0.0284 (15)	0.000	−0.0066 (12)	0.000
C9	0.0278 (11)	0.0236 (11)	0.0466 (14)	0.0024 (9)	−0.0025 (10)	0.0023 (10)
C10	0.0407 (14)	0.0256 (12)	0.0536 (16)	0.0108 (11)	−0.0052 (12)	−0.0010 (11)
C11	0.0275 (11)	0.0234 (10)	0.0228 (10)	0.0023 (8)	−0.0015 (8)	0.0002 (8)

Geometric parameters (Å, º)

Ni1—O1^{i}	2.0309 (14)	C1—C2	1.378 (3)
Ni1—O1	2.0309 (14)	C1—H1	0.9300
Ni1—O3^{i}	2.0934 (14)	C2—C3	1.391 (3)
Ni1—O3	2.0935 (14)	C2—H2	0.9300
Ni1—N1	2.1293 (16)	C3—C4	1.385 (3)
Ni1—N1^{i}	2.1294 (16)	C3—C6	1.491 (3)
O1—C11	1.244 (2)	C4—C5	1.387 (3)
O2—C11	1.244 (2)	C4—H4	0.9300

O3—H6	0.8557	C5—H5	0.9300
O3—H7	0.8343	C7—N2^{ii}	1.339 (2)
N1—C1	1.338 (3)	C7—C8	1.489 (4)
N1—C5	1.339 (3)	C8—C9^{ii}	1.385 (3)
N2—C7	1.339 (2)	C8—C9	1.385 (3)
N2—C6	1.339 (3)	C9—C10	1.387 (3)
N3—C6^{ii}	1.332 (2)	C9—H9	0.9300
N3—C6	1.332 (2)	C10—H10	0.9300
N4—C10	1.336 (3)	C11—H11	0.9300
N4—C10^{ii}	1.336 (3)		

O1^{i}—Ni1—O1	180.0	C1—C2—H2	120.6
O1^{i}—Ni1—O3^{i}	95.50 (6)	C3—C2—H2	120.6
O1—Ni1—O3^{i}	84.50 (6)	C4—C3—C2	118.34 (18)
O1^{i}—Ni1—O3	84.50 (6)	C4—C3—C6	122.08 (18)
O1—Ni1—O3	95.50 (6)	C2—C3—C6	119.57 (18)
O3^{i}—Ni1—O3	180.0	C3—C4—C5	118.69 (18)
O1^{i}—Ni1—N1	88.64 (6)	C3—C4—H4	120.7
O1—Ni1—N1	91.36 (6)	C5—C4—H4	120.7
O3^{i}—Ni1—N1	87.62 (6)	N1—C5—C4	123.41 (18)
O3—Ni1—N1	92.38 (6)	N1—C5—H5	118.3
O1^{i}—Ni1—N1^{i}	91.36 (6)	C4—C5—H5	118.3
O1—Ni1—N1^{i}	88.64 (6)	N3—C6—N2	125.14 (19)
O3^{i}—Ni1—N1^{i}	92.39 (6)	N3—C6—C3	116.04 (18)
O3—Ni1—N1^{i}	87.61 (6)	N2—C6—C3	118.82 (17)
N1—Ni1—N1^{i}	180.0	N2^{ii}—C7—N2	125.7 (3)
C11—O1—Ni1	127.47 (13)	N2^{ii}—C7—C8	117.17 (13)
Ni1—O3—H6	119.3	N2—C7—C8	117.17 (13)
Ni1—O3—H7	124.0	C9^{ii}—C8—C9	118.5 (3)
H6—O3—H7	106.4	C9^{ii}—C8—C7	120.74 (14)
C1—N1—C5	117.10 (16)	C9—C8—C7	120.74 (14)
C1—N1—Ni1	119.57 (13)	C8—C9—C10	118.5 (2)
C5—N1—Ni1	122.98 (13)	C8—C9—H9	120.8
C7—N2—C6	114.35 (18)	C10—C9—H9	120.8
C6^{ii}—N3—C6	115.4 (2)	N4—C10—C9	123.8 (2)
C10—N4—C10^{ii}	116.6 (3)	N4—C10—H10	118.1
N1—C1—C2	123.56 (18)	C9—C10—H10	118.1
N1—C1—H1	118.2	O2—C11—O1	125.8 (2)
C2—C1—H1	118.2	O2—C11—H11	117.1
C1—C2—C3	118.84 (18)	O1—C11—H11	117.1

O3^{i}—Ni1—O1—C11	125.73 (18)	C3—C4—C5—N1	0.3 (3)
O3—Ni1—O1—C11	−54.27 (18)	C6^{ii}—N3—C6—N2	−0.22 (15)
N1—Ni1—O1—C11	38.26 (18)	C6^{ii}—N3—C6—C3	−179.8 (2)
N1^{i}—Ni1—O1—C11	−141.74 (18)	C7—N2—C6—N3	0.4 (3)
O1^{i}—Ni1—N1—C1	−137.13 (16)	C7—N2—C6—C3	180.00 (15)
O1—Ni1—N1—C1	42.87 (16)	C4—C3—C6—N3	173.55 (17)
O3^{i}—Ni1—N1—C1	−41.57 (15)	C2—C3—C6—N3	−5.0 (3)

O3—Ni1—N1—C1	138.43 (15)	C4—C3—C6—N2	−6.1 (3)
O1^{i}—Ni1—N1—C5	49.91 (16)	C2—C3—C6—N2	175.33 (19)
O1—Ni1—N1—C5	−130.09 (16)	C6—N2—C7—N2^{ii}	−0.19 (13)
O3^{i}—Ni1—N1—C5	145.47 (16)	C6—N2—C7—C8	179.82 (13)
O3—Ni1—N1—C5	−34.53 (16)	N2^{ii}—C7—C8—C9^{ii}	−145.57 (15)
C5—N1—C1—C2	2.8 (3)	N2—C7—C8—C9^{ii}	34.43 (15)
Ni1—N1—C1—C2	−170.57 (17)	N2^{ii}—C7—C8—C9	34.43 (15)
N1—C1—C2—C3	−1.2 (3)	N2—C7—C8—C9	−145.57 (15)
C1—C2—C3—C4	−0.9 (3)	C9^{ii}—C8—C9—C10	−2.10 (17)
C1—C2—C3—C6	177.77 (19)	C7—C8—C9—C10	177.90 (17)
C2—C3—C4—C5	1.3 (3)	C10^{ii}—N4—C10—C9	−2.33 (18)
C6—C3—C4—C5	−177.31 (19)	C8—C9—C10—N4	4.5 (4)
C1—N1—C5—C4	−2.3 (3)	Ni1—O1—C11—O2	−173.47 (16)
Ni1—N1—C5—C4	170.79 (16)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H6···O2^{iii}	0.86	1.96	2.818 (2)	177
O3—H7···O2^{iv}	0.83	1.95	2.777 (2)	174

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