

**catena-Poly[[tetraaquanickel(II)]- $\mu$ -(9,10-dioxo-9,10-dihydroanthracene-1,4,5,8-tetracarboxylato)- $\kappa^2$ O<sup>1</sup>:O<sup>8</sup>]-[tetraaquanickel(II)]- $\mu$ -4,4'-bipyridine- $\kappa^2$ N:N']**

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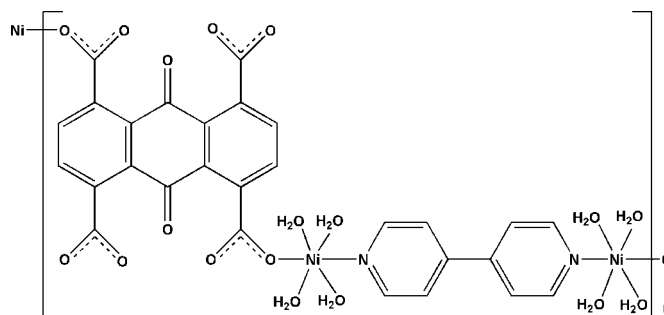
Received 8 June 2012; accepted 18 June 2012

Key indicators: single-crystal X-ray study;  $T = 291$  K; mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å;  $R$  factor = 0.048;  $wR$  factor = 0.102; data-to-parameter ratio = 13.8.

In the crystal of the title polymeric complex,  $[\text{Ni}_2(\text{C}_{18}\text{H}_4\text{O}_{10})(\text{C}_{10}\text{H}_8\text{N}_2)(\text{H}_2\text{O})_8]_n$ , each  $\text{Ni}^{\text{II}}$  cation is coordinated by four water molecules in the equatorial plane, and is further bridged by an 9,10-dioxo-9,10-dihydroanthracene-1,4,5,8-tetracarboxylate anion and a 4,4'-bipyridine ligand in the axial directions, forming a distorted octahedral geometry. The 9,10-dioxo-9,10-dihydroanthracene-1,4,5,8-tetracarboxylate anion is centrosymmetric with the centroid of the quinone ring located about an inversion center; the 4,4'-bipyridine ligand is also centrosymmetric with the mid-point of the C—C bond linking two pyridine rings located about another inversion center. The 9,10-dioxo-9,10-dihydroanthracene-1,4,5,8-tetracarboxylate anion and bipyridine ligand bridge the  $\text{Ni}^{\text{II}}$  cations, forming a polymeric chain along the  $b$  axis.  $\pi$ - $\pi$  stacking is observed between pyridine and benzene rings [centroid-centroid distance =  $3.705(2)$  Å]. All of the coordinating water molecules are involved in O—H...O hydrogen bonding.

## Related literature

For the synthesis, see: Liu *et al.* (2010).



## Experimental

### Crystal data

$[\text{Ni}_2(\text{C}_{18}\text{H}_4\text{O}_{10})(\text{C}_{10}\text{H}_8\text{N}_2)(\text{H}_2\text{O})_8]$   
 $M_r = 797.94$   
 Monoclinic,  $P2_1/n$   
 $a = 8.6359(16)$  Å  
 $b = 21.2426(12)$  Å  
 $c = 8.6416(13)$  Å  
 $\beta = 92.789(3)^\circ$

$V = 1583.4(4)$  Å<sup>3</sup>  
 $Z = 2$   
 Mo  $K\alpha$  radiation  
 $\mu = 1.28$  mm<sup>-1</sup>  
 $T = 291$  K  
 $0.28 \times 0.24 \times 0.22$  mm

### Data collection

Bruker SMART APEXII CCD diffractometer  
 Absorption correction: multi-scan (SADABS; Bruker, 2001)  
 $T_{\text{min}} = 0.716$ ,  $T_{\text{max}} = 0.767$

8595 measured reflections  
 3111 independent reflections  
 2297 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.056$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.048$   
 $wR(F^2) = 0.102$   
 $S = 1.00$   
 3111 reflections

226 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.86$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.49$  e Å<sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O6—H6X...O4	0.85	2.14	2.642 (4)	118
O6—H6Y...O1 <sup>i</sup>	0.85	2.16	2.630 (3)	115
O7—H7Y...O2 <sup>i</sup>	0.85	1.82	2.618 (3)	155
O7—H7X...O4 <sup>ii</sup>	0.85	1.88	2.717 (4)	168
O8—H8X...O6 <sup>ii</sup>	0.85	2.42	3.243 (4)	164
O8—H8Y...O7 <sup>iii</sup>	0.85	2.50	3.330 (4)	167
O9—H9X...O7 <sup>iii</sup>	0.85	2.17	2.973 (3)	158
O9—H9Y...O3	0.85	2.26	3.099 (3)	170

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

Data collection: APEX2 (Bruker, 2007); cell refinement: SAINT (Bruker, 2007); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 2008); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL.

This work was supported financially by the Science and Technology Project of the State General Administration of Quality Supervision, Inspection and Quarantine, China (2011QK121, 2011QK122).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5560).

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## References

Bruker (2001). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.

Bruker (2007). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.

Liu, Y.-M., He, R., Wang, F.-M., Lu, C.-S. & Meng, Q.-J. (2010). *Inorg. Chem. Commun.* **13**, 1375–1379.

Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.

## supplementary materials

*Acta Cryst.* (2012). E68, m960–m961 [doi:10.1107/S1600536812027493]

***catena*-Poly[[tetraaquanickel(II)]- $\mu$ -(9,10-dioxo-9,10-dihydroanthracene-1,4,5,8-tetracarboxylato)- $\kappa^2 O^1:O^8$ -[tetraaquanickel(II)]- $\mu$ -4,4'-bipyridine- $\kappa^2 N:N'$ ]**

**Yang-Mei Liu, Kai Cao and Feng-Lin Wang**

### Comment

The molecular structure of the title complex (I) is showing in Fig. 1. The asymmetric unit of I contains one independent nickel(II) ion, a half 9,10-dioxo-9,10-dihydroanthracene-1,4,5,8-tetracarboxylic acid ligand, a half 4,4-bipyridine ligand, four coordinating water molecules.

The nickel atom is in a normal octahedral geometry with O atoms which from the coordinating water molecules on the equatorial plane and O atom from the carboxylate group, N atom from the 4,4-bipyridine in the axial position. Every nickel atom is coordinated with one 9,10-dioxo-9,10-dihydroanthracene-1,4,5,8-tetracarboxylate ligand and one 4,4-bipyridine ligand. And every 9,10-dioxo-9,10-dihydroanthracene-1,4,5,8-tetracarboxylic acid ligand coordinates with two nickel atoms and they form a one-dimensional nickel chain along *b* axis. There are two nickel chains which cross each other in the crystal structure.

### Experimental

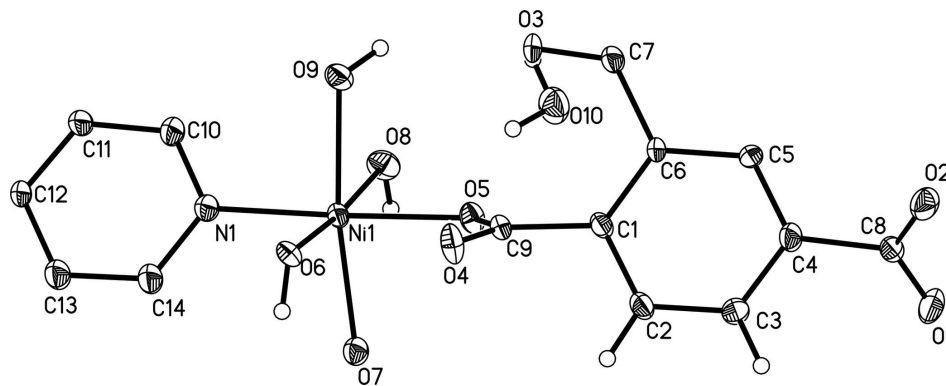
The title compound was obtained unintentionally as the product of an attempted synthesis of a polymeric network Ni complex with 9,10-dioxo-9,10-dihydroanthracene-1,4,5,8-tetracarboxylic acid and 4,4-bipyridine (Liu *et al.*, 2010), the pH value of the mixture was adjusted to 8.0 with NaOH solution, and then solution was heated at 393 K for 3 d. After the mixture was slowly cooled to room temperature, green crystals of the title compound were obtained.

### Refinement

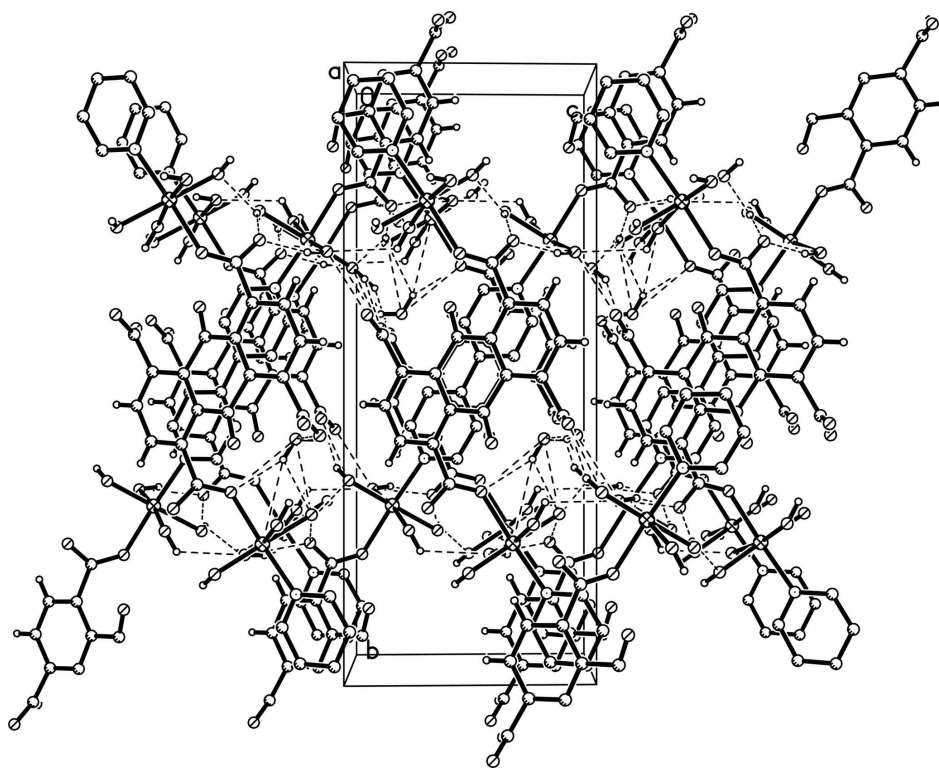
Water H atoms were located in a difference map and refined with distance restraints of O—H = 0.85 Å, other H atoms were placed in calculated positions with C—H = 0.93 Å and refined in riding mode.  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C}, \text{O})$ .

### Computing details

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINTE* (Bruker, 2007); data reduction: *SAINTE* (Bruker, 2007); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).


**Figure 1**

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


**Figure 2**

The packing of (I), viewed down the *a* axis.

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*Crystal data*

[Ni<sub>2</sub>(C<sub>18</sub>H<sub>4</sub>O<sub>10</sub>)(C<sub>10</sub>H<sub>8</sub>N<sub>2</sub>)(H<sub>2</sub>O)<sub>8</sub>]

*M<sub>r</sub>* = 797.94

Monoclinic, *P*2<sub>1</sub>/*n*

Hall symbol: -*P* 2<sub>1</sub>*n*

*a* = 8.6359 (16) Å

*b* = 21.2426 (12) Å

*c* = 8.6416 (13) Å

$\beta$  = 92.789 (3)°

*V* = 1583.4 (4) Å<sup>3</sup>

*Z* = 2

*F*(000) = 820

*D<sub>x</sub>* = 1.674 Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073 \text{ \AA}$   
 Cell parameters from 1207 reflections  
 $\theta = 2.5\text{--}21.8^\circ$   
 $\mu = 1.28 \text{ mm}^{-1}$

$T = 291 \text{ K}$   
 Block, green  
 $0.28 \times 0.24 \times 0.22 \text{ mm}$

*Data collection*

Bruker SMART APEXII CCD  
 diffractometer  
 Radiation source: sealed tube  
 Graphite monochromator  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan  
 (SADABS; Bruker, 2001)  
 $T_{\min} = 0.716$ ,  $T_{\max} = 0.767$

8595 measured reflections  
 3111 independent reflections  
 2297 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.056$   
 $\theta_{\max} = 26.0^\circ$ ,  $\theta_{\min} = 1.9^\circ$   
 $h = -9 \rightarrow 10$   
 $k = -26 \rightarrow 25$   
 $l = -7 \rightarrow 10$

*Refinement*

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.048$   
 $wR(F^2) = 0.102$   
 $S = 1.00$   
 3111 reflections  
 226 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  
 $w = 1/[\sigma^2(F_o^2) + (0.04P)^2 + 1.66P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.86 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\min} = -0.49 \text{ e \AA}^{-3}$

*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 ( $\text{\AA}^2$ )*

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.1039 (5)	0.38729 (17)	0.6495 (5)	0.0279 (9)
C2	0.2016 (4)	0.39108 (17)	0.7843 (4)	0.0231 (8)
H2	0.2351	0.3543	0.8334	0.028*
C3	0.2482 (4)	0.44891 (17)	0.8487 (4)	0.0219 (8)
H3	0.3128	0.4499	0.9380	0.026*
C4	0.1983 (5)	0.50468 (18)	0.7798 (4)	0.0253 (8)
C5	0.1014 (4)	0.50163 (17)	0.6407 (4)	0.0197 (7)
C6	0.0513 (4)	0.44257 (18)	0.5757 (4)	0.0243 (8)
C7	-0.0636 (4)	0.43979 (16)	0.4486 (4)	0.0177 (7)
C8	0.2460 (5)	0.56481 (18)	0.8562 (4)	0.0254 (8)
C9	0.0736 (4)	0.32135 (17)	0.5866 (4)	0.0225 (8)
C10	0.0110 (4)	0.14286 (18)	0.0564 (4)	0.0228 (8)
H10	-0.0205	0.1805	0.0100	0.027*

C11	-0.0207 (4)	0.08759 (16)	-0.0196 (4)	0.0222 (8)
H11	-0.0731	0.0895	-0.1161	0.027*
C12	0.0200 (4)	0.02965 (17)	0.0378 (4)	0.0223 (8)
C13	0.1022 (4)	0.03075 (17)	0.1803 (4)	0.0226 (8)
H13	0.1327	-0.0067	0.2285	0.027*
C14	0.1388 (5)	0.08895 (17)	0.2511 (4)	0.0265 (8)
H14	0.2024	0.0894	0.3411	0.032*
N1	0.0841 (3)	0.14441 (14)	0.1922 (4)	0.0229 (7)
Ni1	0.10940 (5)	0.22477 (2)	0.33004 (5)	0.02030 (14)
O1	0.3792 (3)	0.57569 (12)	0.8713 (3)	0.0307 (7)
O2	0.1359 (3)	0.59770 (12)	0.9128 (3)	0.0290 (6)
O3	-0.1319 (3)	0.39084 (11)	0.4195 (3)	0.0222 (6)
O4	0.0032 (3)	0.28515 (12)	0.6693 (3)	0.0293 (6)
O5	0.1290 (3)	0.30879 (11)	0.4574 (3)	0.0242 (6)
O6	0.0040 (3)	0.17982 (11)	0.5068 (3)	0.0214 (5)
H6X	0.0512	0.1923	0.5898	0.026*
H6Y	-0.0052	0.1415	0.4795	0.026*
O7	0.3310 (3)	0.20054 (11)	0.4219 (3)	0.0204 (5)
H7X	0.3965	0.2055	0.3525	0.024*
H7Y	0.3314	0.1623	0.4510	0.024*
O8	0.1681 (3)	0.27455 (12)	0.1160 (3)	0.0289 (6)
H8X	0.2466	0.2873	0.0692	0.035*
H8Y	0.0907	0.2797	0.0526	0.035*
O9	-0.1130 (3)	0.26235 (12)	0.2516 (3)	0.0269 (6)
H9X	-0.1200	0.2630	0.1531	0.032*
H9Y	-0.1223	0.2996	0.2861	0.032*

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.038 (2)	0.0167 (19)	0.029 (2)	-0.0067 (17)	0.0048 (17)	0.0011 (16)
C2	0.030 (2)	0.0183 (18)	0.0221 (19)	0.0004 (15)	0.0091 (15)	0.0003 (14)
C3	0.0259 (19)	0.0222 (19)	0.0173 (18)	-0.0010 (15)	-0.0017 (14)	-0.0068 (14)
C4	0.032 (2)	0.0183 (18)	0.026 (2)	-0.0035 (16)	0.0039 (16)	-0.0004 (15)
C5	0.0205 (18)	0.0158 (17)	0.0234 (19)	0.0034 (14)	0.0068 (14)	-0.0014 (14)
C6	0.0250 (19)	0.028 (2)	0.0190 (19)	0.0009 (16)	-0.0060 (15)	-0.0030 (15)
C7	0.0182 (16)	0.0215 (19)	0.0129 (17)	-0.0045 (14)	-0.0039 (13)	-0.0033 (13)
C8	0.032 (2)	0.027 (2)	0.0173 (18)	-0.0026 (17)	-0.0018 (15)	-0.0035 (15)
C9	0.0210 (18)	0.0227 (19)	0.025 (2)	0.0110 (15)	0.0092 (15)	0.0008 (15)
C10	0.034 (2)	0.0190 (18)	0.0156 (18)	0.0016 (16)	0.0027 (15)	-0.0020 (14)
C11	0.034 (2)	0.0181 (18)	0.0145 (18)	-0.0110 (16)	-0.0041 (14)	-0.0021 (14)
C12	0.0266 (19)	0.0186 (19)	0.0213 (19)	-0.0064 (15)	-0.0029 (14)	-0.0054 (15)
C13	0.0229 (19)	0.0194 (18)	0.026 (2)	0.0073 (15)	0.0082 (15)	0.0004 (15)
C14	0.034 (2)	0.0195 (19)	0.025 (2)	-0.0061 (16)	-0.0079 (16)	0.0010 (15)
N1	0.0224 (15)	0.0182 (15)	0.0271 (17)	0.0018 (13)	-0.0096 (13)	-0.0073 (13)
Ni1	0.0171 (2)	0.0217 (2)	0.0218 (2)	0.0006 (2)	-0.00221 (16)	-0.0025 (2)
O1	0.0302 (16)	0.0160 (13)	0.0459 (18)	-0.0110 (12)	0.0011 (13)	-0.0077 (12)
O2	0.0299 (15)	0.0217 (14)	0.0342 (16)	0.0048 (11)	-0.0101 (12)	-0.0123 (11)
O3	0.0311 (14)	0.0136 (13)	0.0200 (13)	0.0032 (10)	-0.0177 (11)	-0.0030 (10)
O4	0.0465 (17)	0.0224 (14)	0.0193 (13)	-0.0118 (12)	0.0035 (12)	-0.0132 (11)

O5	0.0356 (15)	0.0155 (13)	0.0219 (13)	0.0004 (11)	0.0049 (11)	0.0015 (10)
O6	0.0235 (13)	0.0210 (13)	0.0193 (13)	0.0063 (11)	-0.0032 (10)	0.0017 (10)
O7	0.0194 (12)	0.0205 (13)	0.0206 (13)	-0.0057 (10)	-0.0064 (10)	0.0019 (10)
O8	0.0405 (16)	0.0186 (13)	0.0279 (15)	-0.0069 (12)	0.0047 (12)	0.0000 (11)
O9	0.0299 (14)	0.0215 (14)	0.0286 (14)	0.0075 (11)	-0.0054 (11)	0.0006 (11)

*Geometric parameters (Å, °)*

C1—C6	1.401 (5)	C11—H11	0.9300
C1—C2	1.407 (6)	C12—C13	1.391 (5)
C1—C9	1.521 (5)	C12—C12 <sup>ii</sup>	1.453 (7)
C2—C3	1.400 (5)	C13—C14	1.409 (5)
C2—H2	0.9298	C13—H13	0.9300
C3—C4	1.385 (5)	C14—N1	1.359 (5)
C3—H3	0.9300	C14—H14	0.9300
C4—C5	1.432 (5)	N1—Ni1	2.087 (3)
C4—C8	1.487 (5)	Ni1—O6	2.051 (2)
C5—C6	1.433 (5)	Ni1—O5	2.099 (3)
C5—C7 <sup>i</sup>	1.492 (5)	Ni1—O7	2.100 (2)
C6—C7	1.445 (5)	Ni1—O9	2.159 (3)
C7—O3	1.215 (4)	Ni1—O8	2.211 (3)
C7—C5 <sup>i</sup>	1.492 (5)	O6—H6X	0.8500
C8—O1	1.174 (5)	O6—H6Y	0.8500
C8—O2	1.295 (5)	O7—H7X	0.8500
C9—O4	1.230 (4)	O7—H7Y	0.8500
C9—O5	1.265 (4)	O8—H8X	0.8505
C10—N1	1.305 (5)	O8—H8Y	0.8498
C10—C11	1.366 (5)	O9—H9X	0.8500
C10—H10	0.9300	O9—H9Y	0.8499
C11—C12	1.367 (5)		
C6—C1—C2	119.8 (3)	C12—C13—H13	120.2
C6—C1—C9	124.3 (4)	C14—C13—H13	120.2
C2—C1—C9	115.7 (3)	N1—C14—C13	122.1 (3)
C3—C2—C1	121.9 (3)	N1—C14—H14	119.0
C3—C2—H2	118.6	C13—C14—H14	119.0
C1—C2—H2	119.4	C10—N1—C14	117.3 (3)
C4—C3—C2	120.1 (3)	C10—N1—Ni1	124.5 (3)
C4—C3—H3	119.9	C14—N1—Ni1	118.0 (2)
C2—C3—H3	119.9	O6—Ni1—N1	90.37 (12)
C3—C4—C5	118.6 (3)	O6—Ni1—O5	91.88 (10)
C3—C4—C8	118.0 (3)	N1—Ni1—O5	176.51 (11)
C5—C4—C8	123.3 (3)	O6—Ni1—O7	91.93 (10)
C4—C5—C6	121.4 (3)	N1—Ni1—O7	94.80 (10)
C4—C5—C7 <sup>i</sup>	120.0 (3)	O5—Ni1—O7	87.80 (10)
C6—C5—C7 <sup>i</sup>	118.3 (3)	O6—Ni1—O9	89.18 (10)
C1—C6—C5	118.1 (3)	N1—Ni1—O9	93.22 (11)
C1—C6—C7	120.5 (3)	O5—Ni1—O9	84.14 (10)
C5—C6—C7	121.1 (3)	O7—Ni1—O9	171.90 (10)
O3—C7—C6	120.0 (3)	O6—Ni1—O8	166.82 (10)

O3—C7—C5 <sup>i</sup>	121.0 (3)	N1—Ni1—O8	86.30 (11)
C6—C7—C5 <sup>i</sup>	118.9 (3)	O5—Ni1—O8	90.92 (9)
O1—C8—O2	125.8 (4)	O7—Ni1—O8	101.05 (10)
O1—C8—C4	117.9 (4)	O9—Ni1—O8	78.29 (11)
O2—C8—C4	116.0 (3)	C9—O5—Ni1	128.2 (2)
O4—C9—O5	126.9 (4)	Ni1—O6—H6X	105.7
O4—C9—C1	116.7 (3)	Ni1—O6—H6Y	106.1
O5—C9—C1	116.3 (3)	H6X—O6—H6Y	124.6
N1—C10—C11	122.0 (4)	Ni1—O7—H7X	109.2
N1—C10—H10	119.0	Ni1—O7—H7Y	109.6
C11—C10—H10	119.0	H7X—O7—H7Y	109.5
C10—C11—C12	123.9 (3)	Ni1—O8—H8X	140.4
C10—C11—H11	118.1	Ni1—O8—H8Y	113.3
C12—C11—H11	118.1	H8X—O8—H8Y	105.8
C11—C12—C13	114.7 (3)	Ni1—O9—H9X	109.8
C11—C12—C12 <sup>ii</sup>	124.5 (4)	Ni1—O9—H9Y	109.3
C13—C12—C12 <sup>ii</sup>	120.8 (4)	H9X—O9—H9Y	109.5
C12—C13—C14	119.6 (3)		
C6—C1—C2—C3	0.3 (6)	C2—C1—C9—O4	64.4 (5)
C9—C1—C2—C3	175.5 (3)	C6—C1—C9—O5	62.1 (5)
C1—C2—C3—C4	0.0 (6)	C2—C1—C9—O5	-112.8 (4)
C2—C3—C4—C5	-1.2 (6)	N1—C10—C11—C12	0.1 (6)
C2—C3—C4—C8	177.6 (4)	C10—C11—C12—C13	-1.9 (6)
C3—C4—C5—C6	2.3 (5)	C10—C11—C12—C12 <sup>ii</sup>	176.5 (5)
C8—C4—C5—C6	-176.5 (4)	C11—C12—C13—C14	-1.2 (5)
C3—C4—C5—C7 <sup>i</sup>	-171.5 (3)	C12 <sup>ii</sup> —C12—C13—C14	-179.7 (4)
C8—C4—C5—C7 <sup>i</sup>	9.7 (6)	C12—C13—C14—N1	6.3 (6)
C2—C1—C6—C5	0.7 (6)	C11—C10—N1—C14	4.9 (6)
C9—C1—C6—C5	-174.0 (3)	C11—C10—N1—Ni1	-170.8 (3)
C2—C1—C6—C7	-172.5 (3)	C13—C14—N1—C10	-8.1 (6)
C9—C1—C6—C7	12.8 (6)	C13—C14—N1—Ni1	167.9 (3)
C4—C5—C6—C1	-2.0 (6)	C10—N1—Ni1—O6	122.4 (3)
C7 <sup>i</sup> —C5—C6—C1	171.9 (3)	C14—N1—Ni1—O6	-53.4 (3)
C4—C5—C6—C7	171.1 (3)	C10—N1—Ni1—O7	-145.7 (3)
C7 <sup>i</sup> —C5—C6—C7	-15.0 (6)	C14—N1—Ni1—O7	38.6 (3)
C1—C6—C7—O3	10.8 (6)	C10—N1—Ni1—O9	33.2 (3)
C5—C6—C7—O3	-162.2 (3)	C14—N1—Ni1—O9	-142.6 (3)
C1—C6—C7—C5 <sup>i</sup>	-171.9 (3)	C10—N1—Ni1—O8	-44.9 (3)
C5—C6—C7—C5 <sup>i</sup>	15.1 (6)	C14—N1—Ni1—O8	139.4 (3)
C3—C4—C8—O1	60.7 (5)	O4—C9—O5—Ni1	4.4 (6)
C5—C4—C8—O1	-120.5 (4)	C1—C9—O5—Ni1	-178.6 (2)
C3—C4—C8—O2	-113.1 (4)	O6—Ni1—O5—C9	-6.8 (3)
C5—C4—C8—O2	65.7 (5)	O9—Ni1—O5—C9	82.2 (3)
C6—C1—C9—O4	-120.6 (4)	O8—Ni1—O5—C9	160.3 (3)

Symmetry codes: (i)  $-x, -y+1, -z+1$ ; (ii)  $-x, -y, -z$ .



Hydrogen-bond geometry (Å, °)

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
O6—H6X···O4	0.85	2.14	2.642 (4)	118
O6—H6Y···O1 <sup>iii</sup>	0.85	2.16	2.630 (3)	115
O7—H7Y···O2 <sup>iii</sup>	0.85	1.82	2.618 (3)	155
O7—H7X···O4 <sup>iv</sup>	0.85	1.88	2.717 (4)	168
O8—H8X···O6 <sup>iv</sup>	0.85	2.42	3.243 (4)	164
O8—H8Y···O7 <sup>v</sup>	0.85	2.50	3.330 (4)	167
O9—H9X···O7 <sup>v</sup>	0.85	2.17	2.973 (3)	158
O9—H9Y···O3	0.85	2.26	3.099 (3)	170

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