

Poly[[diaqua- μ_2 -4,4'-bipyridyl- μ_2 -o-phthalato-nickel(II)] dihydrate]

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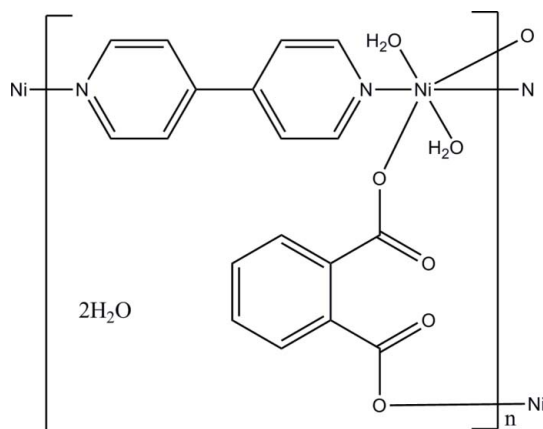
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Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.030; wR factor = 0.091; data-to-parameter ratio = 14.4.

In the title layer complex, $\{[\text{Ni}(\text{C}_8\text{H}_4\text{O}_4)(\text{C}_{10}\text{H}_8\text{N}_2)(\text{H}_2\text{O})_2] \cdot 2\text{H}_2\text{O}\}_n$, the Ni atom has a distorted octahedral environment, defined by the phthalate and 4,4'-bipyridyl ligands which link the Ni atoms, forming a square lattice in the bc plane. This extends into a three-dimensional supramolecular network through $\text{O}-\text{H} \cdots \text{O}$ hydrogen-bonding interactions. The Ni atom lies on, and both ligands are bisected by, a crystallographic twofold axis.

Related literature

For related literature, see: Burrows *et al.* (2000); Hagrman *et al.* (1999); Ma *et al.* (2003); Zheng *et al.* (1999).



Experimental

Crystal data

$[\text{Ni}(\text{C}_8\text{H}_4\text{O}_4)(\text{C}_{10}\text{H}_8\text{N}_2)(\text{H}_2\text{O})_2] \cdot 2\text{H}_2\text{O}$
 $M_r = 451.07$
 Monoclinic, $P2_1/c$
 $a = 7.6160$ (15) Å
 $b = 11.372$ (2) Å
 $c = 12.954$ (4) Å
 $\beta = 123.63$ (2)°
 $V = 934.2$ (4) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 1.09$ mm⁻¹
 $T = 298$ (2) K
 $0.55 \times 0.35 \times 0.25$ mm

Data collection

Rigaku R-Axis RAPID diffractometer
 Absorption correction: multi-scan (ABSCOR; Higashi, 1995)
 $T_{\min} = 0.58$, $T_{\max} = 0.76$
 8992 measured reflections
 2142 independent reflections
 1968 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.020$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.030$
 $wR(F^2) = 0.091$
 $S = 1.12$
 2142 reflections
 149 parameters
 6 restraints
 H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\max} = 0.53$ e Å⁻³
 $\Delta\rho_{\min} = -0.25$ e Å⁻³

Table 1

Selected bond lengths (Å).

Ni1—O1W	2.1244 (14)	Ni1—O1	2.1383 (15)
Ni1—N1 ⁱ	2.135 (2)	Ni1—N2	2.152 (2)

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

Table 2

Hydrogen-bond geometry (Å, °).

$D-\text{H} \cdots A$	$D-\text{H}$	$\text{H} \cdots A$	$D \cdots A$	$D-\text{H} \cdots A$
O2W—H2WA ⁱ ⋯O1	0.84 (3)	2.056 (16)	2.809 (2)	149 (3)
O1W—H1WA ⁱⁱ ⋯O2W ⁱⁱ	0.84 (3)	1.906 (11)	2.716 (2)	163 (2)
O1W—H1WB ⁱⁱⁱ ⋯O2 ⁱⁱⁱ	0.83 (3)	1.874 (10)	2.703 (2)	174 (2)
O2W—H2WB ^{iv} ⋯O2 ^{iv}	0.84 (2)	2.009 (11)	2.834 (2)	169 (3)

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BG2157).

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supporting information

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Poly[[diaqua- μ_2 -4,4'-bipyridyl- μ_2 -o-phthalato-nickel(II)] dihydrate]**Xiao Zhang, ZhiHui Yi, Wujiong Xia, Chao Yang and Bing Li****S1. Comment**

The construction of novel metal coordination polymers, based on the interaction between metal ions and organic ligands has attracted widespread interest among chemists owing to their potential applications and intriguing variety of architectures and topologies. (Hagman *et al.*, 1999). In the design of coordination polymers with different dimensions, Pht, 4,4'-bipy, and some other ligands have proved promising (Ma *et al.*, 2003, Burrows *et al.*, 2000). Among these, the bridging coordination modes of Pht have revealed as favouring the formation of polymeric structures. We report here the synthesis and structure of the title compound containing two-dimensional polymeric layers of $[\text{Ni}(\text{Pht})(4,4'\text{-bipy})(\text{H}_2\text{O})_2]_n$ in which the metal atoms are connected by bridging Pht and 4,4'-bipy ligands.

The Pht and 4,4'-bipy ligands have C_2 intrinsic symmetry with a two fold axis that passes through the midpoints of the C7–C7ⁱⁱⁱ and C9–C9ⁱⁱⁱ bonds in Pht and through the N1 and N2 atoms in 4,4'-bipy, thus determining their geometry (Fig. 1). The two pyridyl rings in the 4,4'-bipy group are not coplanar, the dihedral angle subtended being 54.0°. The cation also lies on the two fold axis and is coordinated by two N atoms from the 4,4'-bipy molecules, two O atoms from the Pht residue, and two O atoms of the H₂O molecules forming a distorted octahedral environment. The Ni atoms form a square lattice in the *bc* plane, one side being directed along the *a* axis due to the 1, 6-bridging function of the Pht residue [the Ni–Ni distance is 7.616 (2) Å], and the other side being stretched along the *b* axis owing to the *endo*-bidentate function of the 4,4'-bipy molecule [the Ni–Ni distance is 11.372 (2) Å] (Fig. 2). The formation of lattices of this type is encountered rather often when the bridging bidentate 4,4'-bipy ligand is combined with another bridging ligand, such as $[\text{Co}(\text{C}_2\text{O}_4)(4,4'\text{-bipy})]_n$ (Zheng *et al.*, 1999). The layers are united into a three-dimensional framework along *c* axis by H-bonds involving coordinated (O1W), uncoordinated (O2W) water molecules and a carboxyl oxygen atom (Fig. 3 and Table 2). The distance between neighboring layers is 5.39 (1) Å.

S2. Experimental

All reagents were of analytical grade and were used without further purification. A mixture of NiCl₂·6H₂O (0.25 g, 1.05 mmol), H₂Pht (0.2 g, 1.20 mmol), 4,4'-bipy (0.2 g, 1.04 mmol) and distilled water (12 ml) was neutralized to pH = 5.5 with sodium hydroxide aqueous solution under stirring for 1 h and sealed in a 20 ml Teflon-lined stainless steel reactor, then heated at 170 °C for 3 days. After cooling to room temperature, the green block crystals were isolated, washed with distilled water, and dried at ambient temperature. Yield: 0.17 g (36% based on Ni).

S3. Refinement

All H atoms attached to C atoms and unambiguously defined by stereochemistry were placed in calculated positions (H–C = 0.93 Å) and allowed to ride, with $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$. H atoms attached to O atoms were located in late-stage difference maps and refined with restrained distances of O–H = 0.85 (1) Å, H···H = 1.35 (2) Å and free $U_{\text{iso}}(\text{H})$.

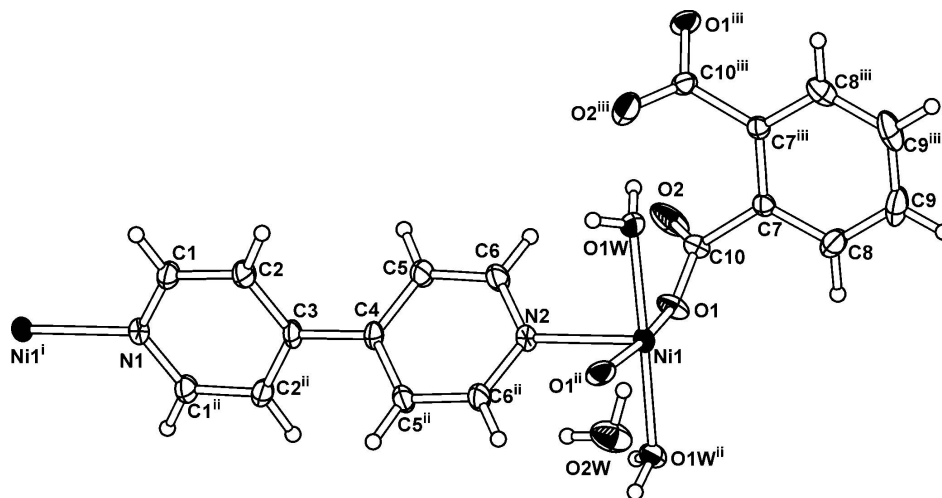


Figure 1

View of the title compound, with displacement ellipsoids drawn at the 50% probability level [Symmetry codes: (i) $x, y - 1, z$; (ii) $-x, y, -z + 1/2$; (iii) $-x + 1, y, -z + 1/2$].

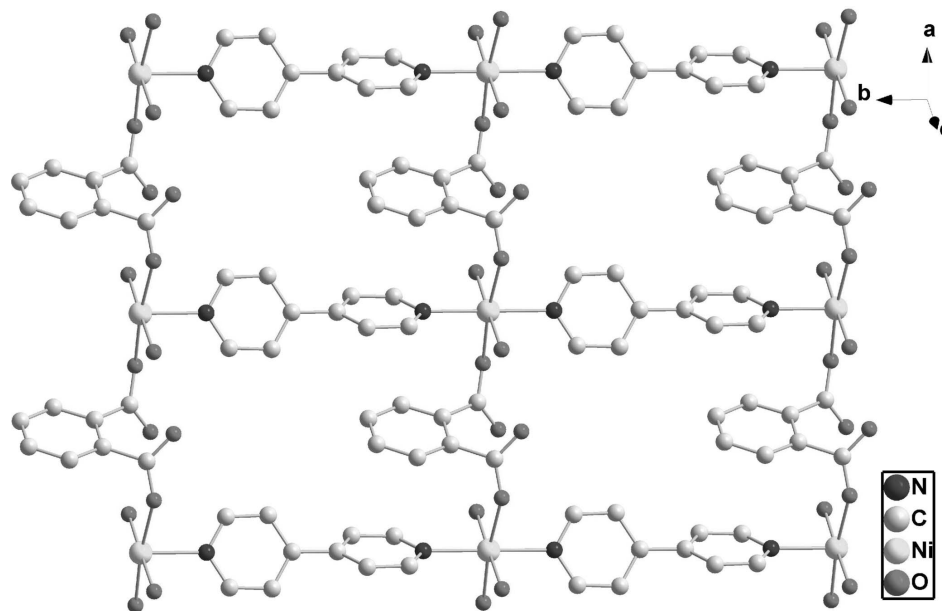
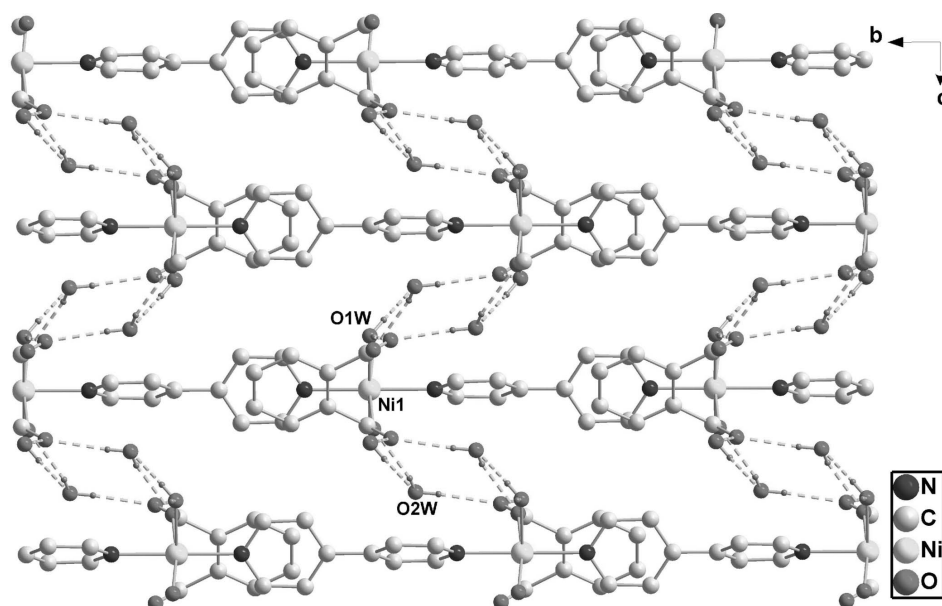


Figure 2

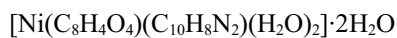
Polymer layer in the title compound. (The uncoordinated waters have been omitted for clarity).

**Figure 3**

Formation of a three-dimensional framework in the title compound (dashed lines show hydrogen bonds).

Poly[[diaqua- μ_2 -4,4'-bipyridyl- μ_2 -o-phthalato-nickel(II)] dihydrate]

Crystal data



$M_r = 451.07$

Monoclinic, $P2_1/c$

Hall symbol: $-P\ 2_1/c$

$a = 7.6160$ (15) Å

$b = 11.372$ (2) Å

$c = 12.954$ (4) Å

$\beta = 123.63$ (2)°

$V = 934.2$ (4) Å³

$Z = 2$

$F(000) = 468$

$D_x = 1.604$ Mg m⁻³

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

Cell parameters from 8171 reflections

$\theta = 3.2\text{--}27.5^\circ$

$\mu = 1.09$ mm⁻¹

$T = 298$ K

Block, green

$0.55 \times 0.35 \times 0.25$ mm

Data collection

Rigaku R-AXIS RAPID

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: 10 pixels mm⁻¹

ω scans

Absorption correction: empirical (using intensity measurements)

(*ABSCOR*; Higashi, 1995)

$T_{\min} = 0.58$, $T_{\max} = 0.76$

8992 measured reflections

2142 independent reflections

1968 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.020$

$\theta_{\max} = 27.5^\circ$, $\theta_{\min} = 3.2^\circ$

$h = -9 \rightarrow 8$

$k = -14 \rightarrow 14$

$l = -16 \rightarrow 16$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.030$

$wR(F^2) = 0.091$

$S = 1.12$

2142 reflections

149 parameters

6 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

$$w = 1/[\sigma^2(F_o^2) + (0.0548P)^2 + 0.4267P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.53 \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{\min} = -0.25 \text{ e } \text{Å}^{-3}$

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 (Å²)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Ni1	0.0000	0.72030 (2)	0.2500	0.01769 (12)
O1	0.3358 (2)	0.70882 (11)	0.37051 (13)	0.0245 (3)
O2	0.6416 (2)	0.65853 (13)	0.39977 (15)	0.0373 (4)
N1	0.0000	-0.09196 (17)	0.2500	0.0177 (4)
N2	0.0000	0.53103 (17)	0.2500	0.0207 (4)
C1	-0.0330 (3)	-0.03021 (15)	0.15229 (16)	0.0223 (4)
H1	-0.0574	-0.0713	0.0834	0.027*
C2	-0.0327 (3)	0.09169 (15)	0.14895 (16)	0.0228 (4)
H2	-0.0542	0.1307	0.0797	0.027*
C3	0.0000	0.1551 (2)	0.2500	0.0191 (5)
C4	0.0000	0.28534 (19)	0.2500	0.0197 (5)
C5	0.1289 (3)	0.34832 (15)	0.22487 (18)	0.0244 (4)
H5	0.2156	0.3093	0.2064	0.029*
C6	0.1261 (3)	0.47013 (15)	0.22773 (19)	0.0244 (4)
H6	0.2161	0.5115	0.2135	0.029*
C7	0.4933 (2)	0.84072 (14)	0.30166 (14)	0.0160 (3)
C8	0.4914 (3)	0.94753 (17)	0.35359 (18)	0.0259 (4)
H8	0.4854	0.9479	0.4234	0.031*
C9	0.4982 (3)	1.05329 (17)	0.3028 (2)	0.0340 (5)
H9	0.5003	1.1240	0.3396	0.041*
C10	0.4895 (3)	0.72697 (14)	0.36067 (16)	0.0190 (3)
O1W	0.0029 (2)	0.71811 (10)	0.08697 (12)	0.0216 (3)
O2W	0.3483 (3)	0.58768 (15)	0.56342 (15)	0.0392 (4)
H2WA	0.385 (5)	0.608 (2)	0.516 (2)	0.059*
H1WA	-0.091 (3)	0.673 (2)	0.034 (2)	0.048 (8)*
H1WB	0.113 (2)	0.705 (2)	0.090 (2)	0.032 (6)*
H2WB	0.362 (5)	0.5147 (9)	0.571 (3)	0.060 (10)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.01990 (18)	0.01195 (17)	0.02568 (19)	0.000	0.01542 (14)	0.000
O1	0.0194 (6)	0.0303 (7)	0.0295 (7)	0.0009 (5)	0.0170 (5)	0.0078 (5)
O2	0.0295 (7)	0.0349 (8)	0.0598 (10)	0.0140 (6)	0.0324 (7)	0.0256 (7)
N1	0.0185 (9)	0.0120 (9)	0.0227 (9)	0.000	0.0114 (8)	0.000
N2	0.0248 (10)	0.0118 (9)	0.0321 (11)	0.000	0.0198 (9)	0.000
C1	0.0291 (9)	0.0149 (8)	0.0235 (8)	0.0001 (7)	0.0150 (7)	-0.0013 (6)
C2	0.0321 (9)	0.0146 (8)	0.0236 (8)	0.0013 (7)	0.0166 (7)	0.0030 (6)
C3	0.0201 (11)	0.0096 (10)	0.0275 (12)	0.000	0.0131 (10)	0.000
C4	0.0252 (12)	0.0099 (10)	0.0244 (11)	0.000	0.0141 (10)	0.000
C5	0.0296 (9)	0.0142 (7)	0.0389 (10)	0.0027 (7)	0.0249 (8)	0.0006 (7)
C6	0.0283 (9)	0.0146 (8)	0.0404 (10)	0.0007 (7)	0.0253 (8)	0.0018 (7)
C7	0.0138 (7)	0.0157 (7)	0.0199 (7)	-0.0003 (6)	0.0102 (6)	-0.0001 (6)
C8	0.0241 (9)	0.0256 (9)	0.0307 (9)	-0.0027 (7)	0.0170 (8)	-0.0102 (7)
C9	0.0275 (10)	0.0166 (8)	0.0555 (13)	-0.0019 (7)	0.0214 (10)	-0.0107 (8)
C10	0.0189 (8)	0.0211 (8)	0.0199 (8)	-0.0004 (6)	0.0126 (7)	0.0024 (6)
O1W	0.0231 (6)	0.0197 (6)	0.0284 (7)	-0.0027 (5)	0.0182 (6)	-0.0048 (5)
O2W	0.0393 (8)	0.0440 (9)	0.0432 (9)	0.0144 (7)	0.0283 (7)	0.0197 (7)

Geometric parameters (\AA , $^\circ$)

Ni1—O1W	2.1244 (14)	C3—C4	1.481 (3)
Ni1—O1W ⁱ	2.1244 (14)	C4—C5	1.392 (2)
Ni1—N1 ⁱⁱ	2.135 (2)	C4—C5 ⁱ	1.392 (2)
Ni1—O1	2.1383 (15)	C5—C6	1.386 (2)
Ni1—O1 ⁱ	2.1383 (15)	C5—H5	0.9300
Ni1—N2	2.152 (2)	C6—H6	0.9300
O1—C10	1.263 (2)	C7—C8	1.393 (2)
O2—C10	1.247 (2)	C7—C7 ^{iv}	1.397 (3)
N1—C1	1.344 (2)	C7—C10	1.511 (2)
N1—C1 ⁱ	1.344 (2)	C8—C9	1.385 (3)
N1—Ni1 ⁱⁱⁱ	2.135 (2)	C8—H8	0.9300
N2—C6	1.339 (2)	C9—C9 ^{iv}	1.384 (5)
N2—C6 ⁱ	1.339 (2)	C9—H9	0.9300
C1—C2	1.387 (2)	O1W—H1WA	0.84 (3)
C1—H1	0.9300	O1W—H1WB	0.83 (3)
C2—C3	1.391 (2)	O2W—H2WA	0.84 (3)
C2—H2	0.9300	O2W—H2WB	0.84 (2)
C3—C2 ⁱ	1.391 (2)		
O1W—Ni1—O1W ⁱ	178.66 (6)	C2—C3—C2 ⁱ	117.6 (2)
O1W—Ni1—N1 ⁱⁱ	90.67 (3)	C2—C3—C4	121.22 (11)
O1W ⁱ —Ni1—N1 ⁱⁱ	90.67 (3)	C2 ⁱ —C3—C4	121.22 (11)
O1W—Ni1—O1	93.34 (6)	C5—C4—C5 ⁱ	118.0 (2)
O1W ⁱ —Ni1—O1	86.58 (6)	C5—C4—C3	120.98 (10)
N1 ⁱⁱ —Ni1—O1	93.50 (4)	C5 ⁱ —C4—C3	120.98 (11)

O1W—Ni1—O1 ⁱ	86.58 (6)	C6—C5—C4	119.00 (17)
O1W ⁱ —Ni1—O1 ⁱ	93.34 (6)	C6—C5—H5	120.5
N1 ⁱⁱ —Ni1—O1 ⁱ	93.50 (4)	C4—C5—H5	120.5
O1—Ni1—O1 ⁱ	173.00 (7)	N2—C6—C5	123.11 (17)
O1W—Ni1—N2	89.33 (3)	N2—C6—H6	118.4
O1W ⁱ —Ni1—N2	89.33 (3)	C5—C6—H6	118.4
N1 ⁱⁱ —Ni1—N2	180.0	C8—C7—C7 ^{iv}	119.25 (11)
O1—Ni1—N2	86.50 (4)	C8—C7—C10	119.60 (16)
O1 ⁱ —Ni1—N2	86.50 (4)	C7 ^{iv} —C7—C10	121.10 (9)
C10—O1—Ni1	135.82 (12)	C9—C8—C7	120.97 (19)
C1—N1—C1 ⁱ	117.0 (2)	C9—C8—H8	119.5
C1—N1—Ni1 ⁱⁱⁱ	121.51 (10)	C7—C8—H8	119.5
C1 ⁱ —N1—Ni1 ⁱⁱⁱ	121.51 (10)	C9 ^{iv} —C9—C8	119.73 (12)
C6—N2—C6 ⁱ	117.7 (2)	C9 ^{iv} —C9—H9	120.1
C6—N2—Ni1	121.15 (10)	C8—C9—H9	120.1
C6 ⁱ —N2—Ni1	121.15 (10)	O2—C10—O1	124.17 (16)
N1—C1—C2	123.31 (16)	O2—C10—C7	117.79 (15)
N1—C1—H1	118.3	O1—C10—C7	118.01 (15)
C2—C1—H1	118.3	Ni1—O1W—H1WA	109.8 (19)
C1—C2—C3	119.41 (16)	Ni1—O1W—H1WB	121.7 (17)
C1—C2—H2	120.3	H1WA—O1W—H1WB	108.2 (19)
C3—C2—H2	120.3	H2WA—O2W—H2WB	106 (2)
O1W—Ni1—O1—C10	18.21 (17)	C2 ⁱ —C3—C4—C5	126.71 (13)
O1W ⁱ —Ni1—O1—C10	-163.14 (17)	C2—C3—C4—C5 ⁱ	126.71 (13)
N1 ⁱⁱ —Ni1—O1—C10	-72.67 (17)	C2 ⁱ —C3—C4—C5 ⁱ	-53.29 (13)
N2—Ni1—O1—C10	107.33 (17)	C5 ⁱ —C4—C5—C6	0.97 (13)
O1W—Ni1—N2—C6	43.77 (11)	C3—C4—C5—C6	-179.03 (13)
O1W ⁱ —Ni1—N2—C6	-136.23 (11)	C6 ⁱ —N2—C6—C5	1.05 (14)
O1—Ni1—N2—C6	-49.62 (11)	Ni1—N2—C6—C5	-178.95 (14)
O1 ⁱ —Ni1—N2—C6	130.38 (11)	C4—C5—C6—N2	-2.1 (3)
O1W—Ni1—N2—C6 ⁱ	-136.23 (11)	C7 ^{iv} —C7—C8—C9	1.3 (3)
O1W ⁱ —Ni1—N2—C6 ⁱ	43.77 (11)	C10—C7—C8—C9	178.96 (17)
O1—Ni1—N2—C6 ⁱ	130.38 (11)	C7—C8—C9—C9 ^{iv}	1.6 (4)
O1 ⁱ —Ni1—N2—C6 ⁱ	-49.62 (11)	Ni1—O1—C10—O2	-133.71 (17)
Ni1 ⁱⁱⁱ —N1—C1—C2	-179.49 (13)	Ni1—O1—C10—C7	48.5 (2)
N1—C1—C2—C3	-1.0 (3)	C8—C7—C10—O2	-119.1 (2)
C1—C2—C3—C2 ⁱ	0.47 (12)	C7 ^{iv} —C7—C10—O2	58.5 (3)
C1—C2—C3—C4	-179.53 (12)	C8—C7—C10—O1	58.9 (2)
C2—C3—C4—C5	-53.29 (13)	C7 ^{iv} —C7—C10—O1	-123.5 (2)

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O2W—H2WA \cdots O1	0.84 (3)	2.06 (2)	2.809 (2)	149 (3)
O1W—H1WA \cdots O2W [†]	0.84 (3)	1.91 (1)	2.716 (2)	163 (2)

O1 <i>W</i> —H1 <i>WB</i> ···O2 ^{iv}	0.83 (3)	1.87 (1)	2.703 (2)	174 (2)
O2 <i>W</i> —H2 <i>WB</i> ···O2 ^v	0.84 (2)	2.01 (1)	2.834 (2)	169 (3)

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