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Poly[[diaquanickel(II)]-μ_2-4,4′-bipyridine-κ^2N:N'-μ-*p*-phenylenedioxydiacetato-κ^2O:O']

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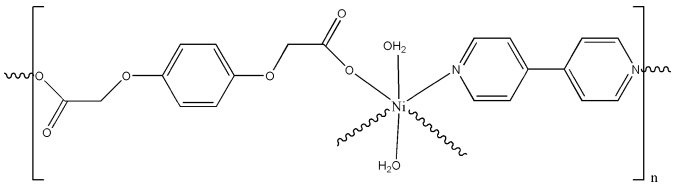
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.034; wR factor = 0.086; data-to-parameter ratio = 13.7.

The title coordination polymer, $[Ni(C_{10}H_8O_6)(C_{10}H_8N_2)(H_2O)_2]_n$, was obtained by the hydrothermal reaction of nickel(II) sulfate, benzene-1,4-dioxydiacetic acid (*p*-phenylenedioxydiacetic acid) and 4,4′-bipyridine (4,4′-bpy) in alkaline aqueous solution. Each Ni^{II} atom is coordinated by two O atoms from two benzene-1,4-dioxydiacetate ligands, two N atoms from two 4,4′-bpy ligands and two water molecules, and displays a distorted octahedral geometry. The Ni^{II} atom and benzene-1,4-dioxydiacetate and 4,4′-bpy moieties lie on inversion centres. The benzene-1,4-dioxydiacetate ligands bridge the Ni^{II} atoms to form infinite zigzag chains, which are further interconnected by 4,4′-bpy ligands to form a grid-like layer parallel to the $(0\bar{1}1)$ plane. Moreover, there are O—H···O hydrogen-bonding interactions within the grid-like layer between the coordinated water molecules and the carboxylate O atoms.

Related literature

For related literature, see: Gao *et al.* (2005); Hong *et al.* (2006); Qiu *et al.* (2006, 2007).



Experimental

Crystal data

$[Ni(C_{10}H_8O_6)(C_{10}H_8N_2)(H_2O)_2]$
M_r = 475.09
Triclinic, $P\bar{1}$
a = 5.7541 (1) Å
b = 8.1704 (1) Å
c = 10.6437 (2) Å
α = 106.157 (1)°
β = 96.818 (1)°
γ = 97.341 (1)°
V = 470.40 (1) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 1.09 mm^{-1}
T = 293 (2) K
0.26 × 0.23 × 0.19 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.765, T_{max} = 0.820
6907 measured reflections
1952 independent reflections
1769 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.086
S = 1.08
1952 reflections
142 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

Table 1
Selected bond lengths (Å).

N1—Ni1	2.1735 (18)	Ni1—O1*W*	2.1245 (16)
Ni1—O1	2.0869 (15)		
O1—Ni1—O1*W*	87.83 (6)	O1*W*—Ni1—N1	91.96 (7)
O1—Ni1—N1	89.77 (7)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*···O2^{i}	0.82	1.81	2.605 (2)	163
O1*W*—H2*W*···O1^{ii}	0.81	2.21	2.962 (2)	155

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003) and *CAMERON* (Watkin *et al.*, 1993); software used to prepare material for publication: *SHELXL97*.

The authors thank South China Normal University for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2287).

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Acta Cryst. (2008). E**64**, m57 [https://doi.org/10.1107/S1600536807062794]

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S1. Comment

Benzene-1,4-dioxydiacetic acid is an important biologically active compound that has been commonly used in herbicides and plant-growth agents. The two phenoxyacetate groups have versatile bonding modes to metal ions and easily forms complexes (Gao *et al.*, 2005; Hong *et al.*, 2006; Qiu *et al.*, 2006; Qiu *et al.*, 2007). Recently, we obtained the title nickel polymer (I), its crystal structure is reported here.

In the structure of (I) each Ni^{II} atom is coordinated by two O atoms from two benzene-1,4-dioxydiacetate ligands, two N atom from two 4,4′-bpy ligands, and displays a distorted octahedral geometry. The Ni atom lies on an inversion center and benzene-1,4-dioxydiacetate and 4,4′-bpy moieties lie other inversion centers. The benzene-1,4-dioxydiacetate ligands bridge nickel ions to form infinite zigzag chains, which are further interconnected by 4,4′-bpy ligands to form a grid-like layer parallel to the (0 - 1 1) plane (Fig. 2). Moreover, there are O—H···O hydrogen bonding interactions within the grid-like layer between the coordinated water molecules and the carboxylate O atoms (Table 1).

S2. Experimental

A mixture of $NiSO_4$ (0.5 mmol), benzene-1,4-dioxydiacetic acid (0.5 mmol), 4,4′-bipyridine (0.5 mmol), NaOH (1 mmol) and H_2O (12 ml) was placed in a 23 ml Teflon reactor, which was heated at 433 K for three days and then cooled to room temperature at a rate of 5 K h^{-1}. Single crystals were obtained after washing with water and drying in air.

S3. Refinement

All H atoms attached to C atoms were fixed geometrically and treated as riding with C—H = 0.93 Å (aromatic) or 0.97 Å (methylene and U_{iso}(H) = 1.2U_{eq}(C). H atoms of water molecule were located in difference Fourier maps and included in the subsequent refinement using restraints (O—H = 0.82 (1) Å and H···H = 1.34 (2) Å) with U_{iso}(H) = 1.5U_{eq}(O). In the last stage of refinement, they were treated as riding on their parent O atoms.

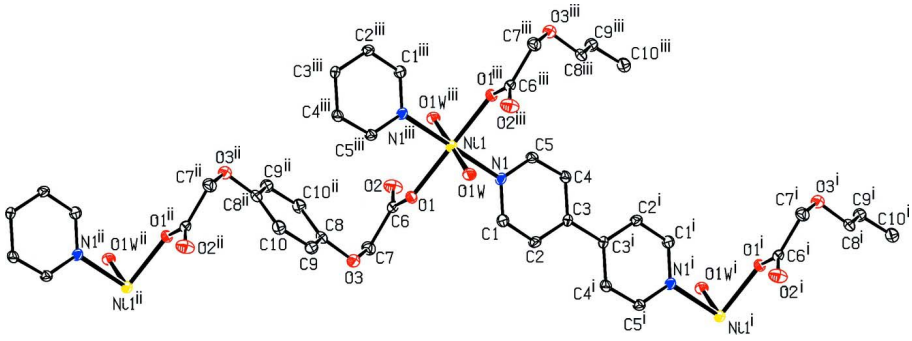

Figure 1

The structure of (I), showing the atom-numbering scheme and displacement ellipsoids drawn at the 30% probability level. H atoms have been omitted for clarity. [Symmetry codes: (i) -*x*, -*y* + 1, -*z* + 1; (ii) -*x* + 1, -*y* + 2, -*z* + 3; (iii) -*x*, -*y* + 2, -*z* + 2]]

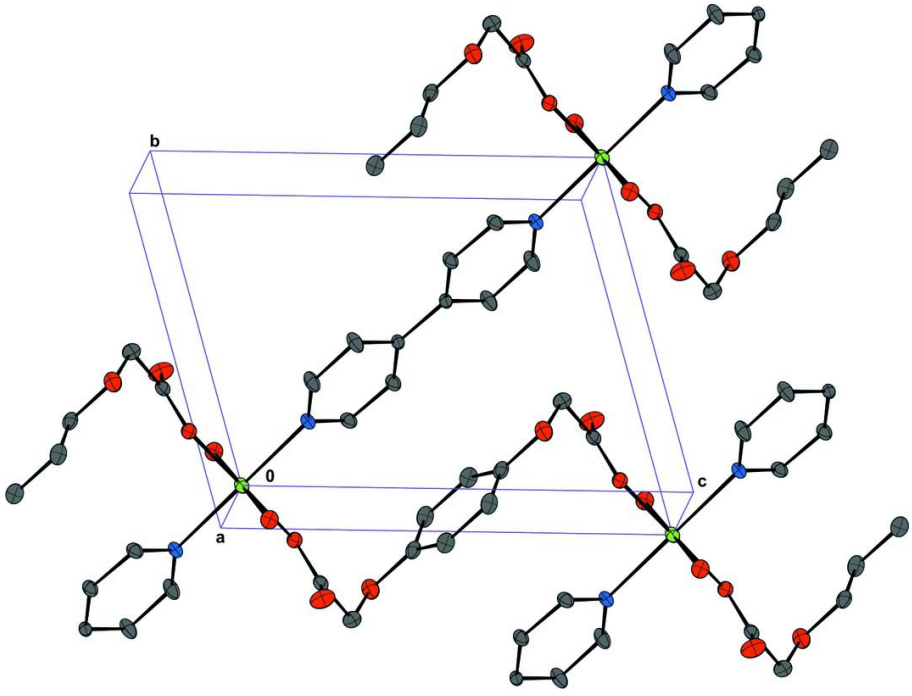

Figure 2

The two-dimensional layer structure of the title compound, viewed along the *a* axis.

Poly[[diaquanickel(II)]-μ_2-4,4′-bipyridine-κ^2N:N'- μ-*p*-phenylenedioxydiacetato-κ^2O:O']

Crystal data

$[Ni(C_{10}H_8O_6)(C_{10}H_8N_2)(H_2O)_2]$
M_r = 475.09
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 5.7541 (1) Å
b = 8.1704 (1) Å
c = 10.6437 (2) Å
α = 106.157 (1)°
β = 96.818 (1)°
γ = 97.341 (1)°
V = 470.40 (1) Å^3
Z = 1
F(000) = 246
D_x = 1.677 Mg m^{-3}
Mo *K*α radiation, λ = 0.71073 Å
Cell parameters from 1800 reflections
θ = 1.4–28.0°
μ = 1.09 mm^{-1}

T = 293 K
Block, green

0.26 × 0.23 × 0.19 mm

Data collection

Bruker APEXII area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.765, T_{max} = 0.820

6907 measured reflections
1952 independent reflections
1769 reflections with $I > 2\sigma(I)$
R_{int} = 0.026
θ_{max} = 26.5°, θ_{min} = 2.0°
$h = -7 \rightarrow 7$
$k = -8 \rightarrow 10$
$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.086
S = 1.08
1952 reflections
142 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
$w = 1/[\sigma^2(F_o^2) + (0.0346P)^2 + 0.4701P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 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 (Å²)

	x	y	z	U_{iso}*/U_{eq}
C1	0.1666 (4)	0.7074 (3)	0.7930 (2)	0.0318 (6)
H1	0.2876	0.7217	0.8633	0.038*
C2	0.1734 (4)	0.5879 (3)	0.6736 (2)	0.0314 (6)
H2	0.2965	0.5240	0.6655	0.038*
C3	−0.0019 (4)	0.5624 (3)	0.5655 (2)	0.0201 (5)
C4	−0.1819 (4)	0.6612 (3)	0.5876 (2)	0.0262 (5)
H4	−0.3058	0.6487	0.5192	0.031*
C5	−0.1772 (4)	0.7772 (3)	0.7101 (2)	0.0264 (5)
H5	−0.3005	0.8405	0.7218	0.032*
C6	0.1281 (4)	0.7277 (3)	1.1257 (2)	0.0253 (5)
C7	0.3161 (5)	0.6440 (3)	1.1868 (3)	0.0327 (6)
H7A	0.2457	0.5854	1.2444	0.039*
H7B	0.3633	0.5572	1.1163	0.039*
C8	0.5001 (4)	0.8782 (3)	1.3782 (2)	0.0273 (5)

C9	0.6973 (4)	1.0042 (3)	1.4391 (3)	0.0315 (6)
H9	0.8307	1.0079	1.3978	0.038*
C10	0.6996 (4)	1.1242 (3)	1.5598 (3)	0.0315 (6)
H10	0.8344	1.2067	1.5997	0.038*
N1	−0.0044 (3)	0.8038 (2)	0.81332 (18)	0.0227 (4)
Ni1	0.0000	1.0000	1.0000	0.02315 (14)
O1	0.2019 (3)	0.8651 (2)	1.09891 (15)	0.0251 (4)
O2	−0.0799 (3)	0.6527 (2)	1.1047 (2)	0.0427 (5)
O3	0.5228 (3)	0.7621 (2)	1.26119 (17)	0.0332 (4)
O1W	0.3239 (3)	1.1425 (2)	0.98244 (16)	0.0289 (4)
H1W	0.2733	1.2183	0.9556	0.043*
H2W	0.4307	1.1122	0.9424	0.043*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0272 (12)	0.0431 (15)	0.0187 (12)	0.0114 (11)	−0.0037 (9)	−0.0003 (11)
C2	0.0272 (12)	0.0421 (15)	0.0207 (12)	0.0160 (11)	0.0006 (9)	−0.0009 (11)
C3	0.0237 (11)	0.0198 (11)	0.0155 (11)	0.0018 (9)	0.0034 (9)	0.0040 (9)
C4	0.0279 (12)	0.0282 (12)	0.0186 (11)	0.0084 (9)	−0.0033 (9)	0.0019 (9)
C5	0.0281 (12)	0.0257 (12)	0.0233 (12)	0.0104 (9)	0.0010 (9)	0.0025 (10)
C6	0.0307 (12)	0.0254 (12)	0.0201 (11)	0.0100 (10)	0.0063 (9)	0.0040 (9)
C7	0.0391 (14)	0.0283 (13)	0.0327 (14)	0.0099 (11)	0.0040 (11)	0.0111 (11)
C8	0.0275 (11)	0.0332 (13)	0.0256 (12)	0.0098 (10)	0.0017 (9)	0.0145 (10)
C9	0.0228 (11)	0.0448 (15)	0.0318 (14)	0.0072 (10)	0.0079 (10)	0.0175 (12)
C10	0.0246 (11)	0.0379 (14)	0.0326 (14)	0.0008 (10)	0.0026 (10)	0.0142 (11)
N1	0.0247 (9)	0.0231 (10)	0.0175 (9)	0.0040 (8)	0.0035 (8)	0.0014 (8)
Ni1	0.0242 (2)	0.0247 (2)	0.0187 (2)	0.00564 (16)	0.00278 (16)	0.00319 (17)
O1	0.0280 (8)	0.0250 (9)	0.0221 (8)	0.0067 (7)	0.0013 (7)	0.0070 (7)
O2	0.0309 (10)	0.0373 (11)	0.0653 (14)	0.0067 (8)	0.0079 (9)	0.0234 (10)
O3	0.0301 (9)	0.0409 (11)	0.0281 (9)	0.0112 (8)	0.0036 (7)	0.0077 (8)
O1W	0.0231 (8)	0.0335 (9)	0.0317 (9)	0.0058 (7)	0.0060 (7)	0.0110 (8)

Geometric parameters (Å, º)

C1—N1	1.338 (3)	C7—H7B	0.9700
C1—C2	1.379 (3)	C8—O3	1.372 (3)
C1—H1	0.9300	C8—C9	1.387 (3)
C2—C3	1.386 (3)	C8—C10^{ii}	1.392 (3)
C2—H2	0.9300	C9—C10	1.380 (4)
C3—C4	1.395 (3)	C9—H9	0.9300
C3—C3^{i}	1.486 (4)	C10—C8^{ii}	1.392 (3)
C4—C5	1.377 (3)	C10—H10	0.9300
C4—H4	0.9300	N1—Ni1	2.1735 (18)
C5—N1	1.340 (3)	Ni1—O1	2.0869 (15)
C5—H5	0.9300	Ni1—O1^{iii}	2.0869 (15)
C6—O2	1.237 (3)	Ni1—O1W^{iii}	2.1245 (16)
C6—O1	1.268 (3)	Ni1—O1W	2.1245 (16)

C6—C7	1.526 (3)	Ni1—N1^{iii}	2.1735 (18)
C7—O3	1.425 (3)	O1W—H1W	0.8206
C7—H7A	0.9700	O1W—H2W	0.8144
N1—C1—C2	123.6 (2)	C10—C9—H9	119.3
N1—C1—H1	118.2	C8—C9—H9	119.3
C2—C1—H1	118.2	C9—C10—C8^{ii}	119.9 (2)
C1—C2—C3	120.4 (2)	C9—C10—H10	120.0
C1—C2—H2	119.8	C8^{ii}—C10—H10	120.0
C3—C2—H2	119.8	C1—N1—C5	116.27 (19)
C2—C3—C4	115.8 (2)	C1—N1—Ni1	122.60 (15)
C2—C3—C3^{i}	122.1 (2)	C5—N1—Ni1	121.09 (15)
C4—C3—C3^{i}	122.1 (2)	O1—Ni1—O1^{iii}	180.000 (1)
C5—C4—C3	120.3 (2)	O1—Ni1—O1W^{iii}	92.17 (6)
C5—C4—H4	119.8	O1^{iii}—Ni1—O1W^{iii}	87.83 (6)
C3—C4—H4	119.8	O1—Ni1—O1W	87.83 (6)
N1—C5—C4	123.5 (2)	O1^{iii}—Ni1—O1W	92.17 (6)
N1—C5—H5	118.3	O1W^{iii}—Ni1—O1W	180.0
C4—C5—H5	118.3	O1—Ni1—N1^{iii}	90.23 (7)
O2—C6—O1	126.6 (2)	O1^{iii}—Ni1—N1^{iii}	89.77 (7)
O2—C6—C7	116.8 (2)	O1W^{iii}—Ni1—N1^{iii}	91.96 (7)
O1—C6—C7	116.6 (2)	O1W—Ni1—N1^{iii}	88.04 (7)
O3—C7—C6	114.3 (2)	O1—Ni1—N1	89.77 (7)
O3—C7—H7A	108.7	O1^{iii}—Ni1—N1	90.23 (7)
C6—C7—H7A	108.7	O1W^{iii}—Ni1—N1	88.04 (7)
O3—C7—H7B	108.7	O1W—Ni1—N1	91.96 (7)
C6—C7—H7B	108.7	N1^{iii}—Ni1—N1	180.000 (1)
H7A—C7—H7B	107.6	C6—O1—Ni1	126.73 (15)
O3—C8—C9	115.9 (2)	C8—O3—C7	117.78 (19)
O3—C8—C10^{ii}	125.3 (2)	Ni1—O1W—H1W	100.2
C9—C8—C10^{ii}	118.8 (2)	Ni1—O1W—H2W	131.1
C10—C9—C8	121.3 (2)	H1W—O1W—H2W	108.2

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
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O1*W*—H2*W*···O1^{iv}	0.81	2.21	2.962 (2)	155

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