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## Structure Reports

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# catena-Poly[[*(2,2'*-bipyridine- $\kappa^2N,N'$ )-nickel(II)]- $\mu$ -oxalato- $\kappa^4O^1,O^2:O^1',O^2'$ ]

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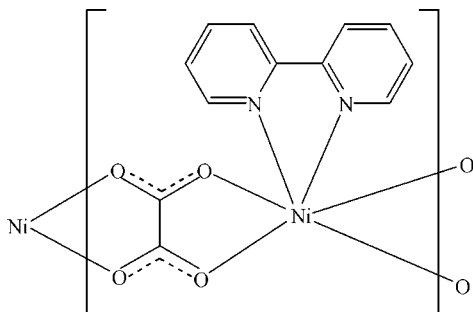
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Key indicators: single-crystal X-ray study;  $T = 296$  K; mean  $\sigma(C-C) = 0.010$  Å;  $R$  factor = 0.048;  $wR$  factor = 0.155; data-to-parameter ratio = 12.2.

The title compound,  $[Ni(C_2O_4)(C_{10}H_8N_2)]_n$ , is isostructural with its  $Mn^{II}$ ,  $Fe^{II}$ ,  $Cu^{II}$  and  $Zn^{II}$  analogues. Each  $Ni^{II}$  atom is chelated by two oxalate ligands and one 2,2'-bipyridine, forming a slightly distorted octahedral geometry. Oxalate acts as a bridge to link neighbouring pairs of  $Ni^{II}$  cations, forming a one-dimensional wave-like chain. The crystal showed partial inversion twinning.

## Related literature

For related literature, see: Hong & Do (1997); Eddaoudi *et al.* (2001); Liang *et al.* (2004); Shi *et al.* (2005). For the isostructural  $Mn^{II}$ ,  $Fe^{II}$ ,  $Cu^{II}$  and  $Zn^{II}$  complexes, see: Li *et al.* (2006); Deguenon *et al.* (1990); Fun *et al.* (1999); Luo *et al.* (2001); Yu *et al.* (2006); Lin *et al.* (2006).



## Experimental

## Crystal data

$[Ni(C_2O_4)(C_{10}H_8N_2)]$   
 $M_r = 302.91$   
 Orthorhombic,  $Pna2_1$   
 $a = 9.6486$  (14) Å  
 $b = 9.2627$  (14) Å  
 $c = 13.883$  (2) Å

$V = 1240.7$  (3) Å<sup>3</sup>  
 $Z = 4$   
 Mo  $K\alpha$  radiation  
 $\mu = 1.57$  mm<sup>-1</sup>  
 $T = 296$  (2) K  
 $0.12 \times 0.10 \times 0.06$  mm

## Data collection

Bruker APEXII CCD area-detector diffractometer  
 Absorption correction: multi-scan (SADABS; Bruker, 2001)  
 $T_{min} = 0.834$ ,  $T_{max} = 0.912$

6146 measured reflections  
 2114 independent reflections  
 1810 reflections with  $I > 2\sigma(I)$   
 $R_{int} = 0.030$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.047$   
 $wR(F^2) = 0.154$   
 $S = 1.00$   
 2114 reflections  
 173 parameters  
 1 restraint

H-atom parameters constrained  
 $\Delta\rho_{max} = 0.44$  e Å<sup>-3</sup>  
 $\Delta\rho_{min} = -0.43$  e Å<sup>-3</sup>  
 Absolute structure: Flack (1983),  
 971 Friedel pairs  
 Flack parameter: 0.20 (3)

Data collection: APEX2 (Bruker, 2004); cell refinement: SAINT-Plus (Bruker, 2001); data reduction: SAINT-Plus; 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: SHELXTL.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CF2213).

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**supplementary materials**

*Acta Cryst.* (2008). E64, m1258 [ doi:10.1107/S1600536808028389 ]

***catena*-Poly[[*(2,2'*-bipyridine- $\kappa^2$ N,N')nickel(II)]- $\mu$ -oxalato- $\kappa^4$ O<sup>1</sup>,O<sup>2</sup>:O<sup>1'</sup>,O<sup>2'</sup>]**

**S. Li, X.-L. Yan, S.-B. Wang and Y.-F. Ma**

### Comment

The design of coordination compounds has attracted long-lasting research interest not only because of their appealing structural and topological novelty but also due to their unusual optical, electronic, magnetic and catalytic properties, and their further potential medical value derived from their antiviral properties and the inhibition of angiogenesis. To date, much of the work has been focused on coordination polymers with organic acid ligands (Hong *et al.* 1997; Eddaoudi *et al.* 2001; Liang *et al.* 2004; Shi *et al.* 2005).

Here we report the synthesis and X-ray crystal structure analysis of the title compound, (I), with a bridging oxalate ligand. It is isostructural with its Mn<sup>II</sup>, Fe<sup>II</sup>, Cu<sup>II</sup>, and Zn<sup>II</sup> analogues (Li *et al.*, 2006; Deguenon *et al.*, 1990; Fun *et al.*, 1999; Luo *et al.*, 2001; Yu *et al.*, 2006; Lin *et al.*, 2006).

As shown in Fig. 1, the Ni(II) atom is chelated by two oxalates and one 2,2'-bipyridine, forming a slightly distorted octahedral geometry. Oxalate acts as a bridge to link neighboring pairs of Ni(II) cations, forming a one-dimensional wave-like chain (Fig. 2). The Ni—N and Ni—O bond lengths are in the ranges 2.239 (5)–2.243 (5) and 2.161 (4)–2.166 (4) Å, respectively.

### Experimental

A mixture of nickel(II) nitrate hexahydrate (0.1 mmol), oxalic acid (0.2 mmol), 2,2'-bipyridine (0.1 mmol), and water (16 ml) in a 25 ml Teflon-lined stainless steel autoclave was kept at 473 K for three days. Green crystals were obtained after cooling to room temperature, with a yield of 6%. Anal. Calc. for C<sub>12</sub>H<sub>8</sub>N<sub>2</sub>NiO<sub>4</sub>: C 47.54, H 2.64, N 9.24%; Found: C 47.51, H 2.58, N 9.16%.

### Refinement

All H atoms were placed in calculated positions with C—H = 0.93 Å and refined as riding with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

### Figures

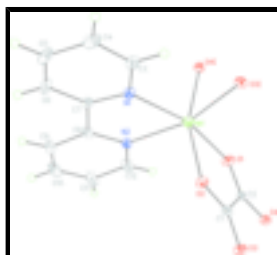


Fig. 1. The coordination of the Ni atom in the title structure, drawn with 30% probability displacement ellipsoids. [Symmetry code: (I) 1/2+x, 1/2-y, z.]

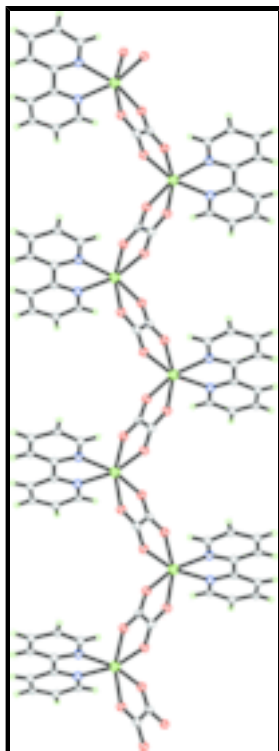


Fig. 2. The chain of the title compound, viewed along the [010] direction.

**catena-Poly[[*(2,2'*-bipyridine- $\kappa^2N,N'$ )nickel(II)]- $\mu$ -oxalato- $\kappa^4O^1,O^2:O^1',O^2'$ ]**

*Crystal data*

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

*M<sub>r</sub>* = 302.91

Orthorhombic, *Pna*2<sub>1</sub>

Hall symbol: P 2c -2n

*a* = 9.6486 (14) Å

*b* = 9.2627 (14) Å

*c* = 13.883 (2) Å

*V* = 1240.7 (3) Å<sup>3</sup>

*Z* = 4

*F*<sub>000</sub> = 616

*D<sub>x</sub>* = 1.622 Mg m<sup>-3</sup>

Mo *K*α radiation

$\lambda$  = 0.71073 Å

Cell parameters from 1779 reflections

$\theta$  = 2.6–21.5°

$\mu$  = 1.57 mm<sup>-1</sup>

*T* = 296 (2) K

Block, green

0.12 × 0.10 × 0.06 mm

*Data collection*

Bruker APEXII CCD area-detector  
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

*T* = 296(2) K

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan  
(SADABS; Bruker, 2001)

2114 independent reflections

1810 reflections with *I* > 2σ(*I*)

*R*<sub>int</sub> = 0.030

$\theta_{\max}$  = 25.1°

$\theta_{\min}$  = 2.6°

*h* = -11→5

$T_{\min} = 0.834$ ,  $T_{\max} = 0.912$   
6146 measured reflections

$k = -11 \rightarrow 11$   
 $l = -16 \rightarrow 16$

### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.047$

$wR(F^2) = 0.154$

$S = 1.00$

2114 reflections

173 parameters

1 restraint

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

$$w = 1/[\sigma^2(F_o^2) + (0.118P)^2]$$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.44 \text{ e } \text{\AA}^{-3}$

$\Delta\rho_{\min} = -0.43 \text{ e } \text{\AA}^{-3}$

Extinction correction: none

Absolute structure: Flack (1983), 971 Friedel pairs

Flack parameter: 0.20 (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 ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Ni1	0.88396 (7)	1.09402 (7)	0.25107 (8)	0.04352 (14)
O1	1.0093 (4)	1.2363 (5)	0.1613 (3)	0.0503 (11)
O2	1.0673 (4)	1.1297 (4)	0.3368 (3)	0.0415 (9)
O3	0.7686 (4)	1.2511 (5)	0.3347 (3)	0.0452 (10)
O4	0.7033 (4)	1.1389 (4)	0.1640 (3)	0.0416 (9)
N1	0.8006 (5)	0.9059 (5)	0.3352 (4)	0.0401 (11)
N2	0.9510 (5)	0.8925 (5)	0.1747 (4)	0.0395 (11)
C1	1.1555 (6)	1.2124 (6)	0.3004 (4)	0.0380 (12)
C2	1.1199 (4)	1.2745 (6)	0.1993 (4)	0.0305 (12)
C3	0.7196 (8)	0.9174 (8)	0.4115 (5)	0.0535 (17)
H3	0.6964	1.0099	0.4320	0.064*
C4	0.6668 (8)	0.8030 (10)	0.4630 (5)	0.070 (2)
H4	0.6106	0.8163	0.5168	0.084*
C5	0.7033 (9)	0.6629 (9)	0.4291 (6)	0.073 (2)

## supplementary materials

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H5	0.6728	0.5809	0.4613	0.087*
C6	0.7820 (8)	0.6507 (7)	0.3504 (6)	0.0633 (19)
H6	0.8054	0.5598	0.3269	0.076*
C7	0.8286 (6)	0.7736 (6)	0.3038 (4)	0.0405 (13)
C8	0.9159 (6)	0.7661 (7)	0.2154 (4)	0.0408 (13)
C9	0.9646 (9)	0.6356 (7)	0.1766 (6)	0.0627 (19)
H9	0.9447	0.5484	0.2067	0.075*
C10	1.0418 (10)	0.6383 (10)	0.0936 (7)	0.081 (3)
H10	1.0713	0.5519	0.0663	0.097*
C11	1.0758 (8)	0.7647 (9)	0.0510 (5)	0.066 (2)
H11	1.1292	0.7669	-0.0048	0.080*
C12	1.0277 (8)	0.8924 (8)	0.0937 (5)	0.0601 (19)
H12	1.0495	0.9802	0.0651	0.072*

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Ni1	0.0387 (2)	0.0456 (2)	0.0463 (2)	0.0000 (2)	-0.0004 (3)	0.0045 (3)
O1	0.042 (2)	0.065 (3)	0.044 (3)	-0.012 (2)	-0.0101 (19)	0.022 (2)
O2	0.0384 (19)	0.052 (2)	0.034 (2)	-0.0078 (19)	-0.0056 (16)	0.0150 (18)
O3	0.039 (2)	0.061 (2)	0.036 (2)	0.0098 (19)	-0.0144 (18)	-0.0128 (19)
O4	0.042 (2)	0.048 (2)	0.035 (2)	-0.0017 (18)	-0.0036 (17)	-0.0095 (18)
N1	0.043 (3)	0.045 (3)	0.032 (2)	-0.0063 (18)	0.006 (2)	-0.0005 (19)
N2	0.045 (3)	0.038 (2)	0.036 (3)	0.0049 (19)	0.008 (2)	0.002 (2)
C1	0.038 (3)	0.036 (3)	0.040 (3)	0.007 (3)	-0.004 (3)	0.004 (3)
C2	0.028 (3)	0.034 (3)	0.029 (3)	-0.002 (2)	-0.0031 (19)	0.005 (2)
C3	0.062 (4)	0.058 (4)	0.041 (4)	-0.005 (3)	0.016 (3)	0.005 (3)
C4	0.068 (4)	0.098 (6)	0.043 (4)	-0.024 (5)	0.015 (4)	0.011 (4)
C5	0.087 (5)	0.071 (5)	0.060 (4)	-0.034 (4)	0.011 (4)	0.021 (4)
C6	0.088 (5)	0.039 (3)	0.063 (4)	-0.022 (3)	0.004 (4)	-0.002 (3)
C7	0.040 (3)	0.045 (3)	0.037 (3)	-0.008 (3)	0.000 (3)	0.005 (2)
C8	0.045 (3)	0.046 (3)	0.031 (3)	0.008 (3)	0.000 (3)	-0.005 (2)
C9	0.089 (5)	0.041 (3)	0.058 (4)	0.012 (3)	-0.002 (4)	0.005 (3)
C10	0.096 (7)	0.073 (5)	0.073 (5)	0.040 (5)	0.009 (5)	-0.017 (5)
C11	0.091 (5)	0.070 (5)	0.037 (4)	0.028 (4)	0.012 (4)	0.003 (3)
C12	0.069 (5)	0.064 (4)	0.047 (4)	0.023 (3)	0.014 (3)	0.012 (3)

### Geometric parameters ( $\text{\AA}$ , $^\circ$ )

Ni1—O4	2.162 (4)	C3—C4	1.376 (10)
Ni1—O2	2.157 (4)	C3—H3	0.930
Ni1—O1	2.180 (4)	C4—C5	1.425 (13)
Ni1—O3	2.169 (4)	C4—H4	0.930
Ni1—N2	2.242 (5)	C5—C6	1.335 (12)
Ni1—N1	2.246 (5)	C5—H5	0.930
O1—C2	1.242 (6)	C6—C7	1.385 (9)
O2—C1	1.251 (7)	C6—H6	0.930
O3—C1 <sup>i</sup>	1.238 (6)	C7—C8	1.491 (8)

O4—C2 <sup>i</sup>	1.237 (6)	C8—C9	1.404 (9)
N1—C3	1.322 (8)	C9—C10	1.372 (12)
N1—C7	1.328 (7)	C9—H9	0.930
N2—C8	1.343 (8)	C10—C11	1.353 (13)
N2—C12	1.346 (9)	C10—H10	0.930
C1—O3 <sup>ii</sup>	1.238 (6)	C11—C12	1.402 (10)
C1—C2	1.554 (6)	C11—H11	0.930
C2—O4 <sup>ii</sup>	1.237 (6)	C12—H12	0.930
O4—Ni1—O2	160.07 (14)	N1—C3—C4	125.0 (7)
O4—Ni1—O1	90.65 (14)	N1—C3—H3	117.5
O2—Ni1—O1	76.55 (13)	C4—C3—H3	117.5
O4—Ni1—O3	75.90 (14)	C3—C4—C5	115.9 (7)
O2—Ni1—O3	91.31 (15)	C3—C4—H4	122.0
O1—Ni1—O3	100.66 (17)	C5—C4—H4	122.0
O4—Ni1—N2	97.39 (17)	C6—C5—C4	119.3 (7)
O2—Ni1—N2	98.72 (18)	C6—C5—H5	120.4
O1—Ni1—N2	94.20 (18)	C4—C5—H5	120.4
O3—Ni1—N2	163.69 (17)	C5—C6—C7	119.8 (7)
O4—Ni1—N1	98.71 (17)	C5—C6—H6	120.1
O2—Ni1—N1	97.23 (17)	C7—C6—H6	120.1
O1—Ni1—N1	164.72 (18)	N1—C7—C6	122.7 (6)
O3—Ni1—N1	93.35 (18)	N1—C7—C8	115.3 (5)
N2—Ni1—N1	72.74 (17)	C6—C7—C8	122.0 (6)
C2—O1—Ni1	114.0 (3)	N2—C8—C9	120.3 (6)
C1—O2—Ni1	115.4 (4)	N2—C8—C7	116.6 (5)
C1 <sup>i</sup> —O3—Ni1	115.4 (3)	C9—C8—C7	123.0 (6)
C2 <sup>i</sup> —O4—Ni1	115.3 (3)	C8—C9—C10	119.2 (7)
C3—N1—C7	117.2 (5)	C8—C9—H9	120.4
C3—N1—Ni1	124.5 (4)	C10—C9—H9	120.4
C7—N1—Ni1	118.2 (4)	C11—C10—C9	121.0 (7)
C8—N2—C12	119.3 (5)	C11—C10—H10	119.5
C8—N2—Ni1	117.0 (4)	C9—C10—H10	119.5
C12—N2—Ni1	123.7 (4)	C10—C11—C12	117.7 (7)
O2—C1—O3 <sup>ii</sup>	127.7 (5)	C10—C11—H11	121.2
O2—C1—C2	116.2 (5)	C12—C11—H11	121.2
O3 <sup>ii</sup> —C1—C2	116.2 (5)	N2—C12—C11	122.4 (7)
O4 <sup>ii</sup> —C2—O1	125.1 (5)	N2—C12—H12	118.8
O4 <sup>ii</sup> —C2—C1	117.0 (4)	C11—C12—H12	118.8
O1—C2—C1	117.8 (4)		
O4—Ni1—O1—C2	162.4 (4)	O1—Ni1—N2—C12	-7.8 (6)
O2—Ni1—O1—C2	-2.1 (4)	O3—Ni1—N2—C12	147.8 (6)
O3—Ni1—O1—C2	86.7 (4)	N1—Ni1—N2—C12	-179.8 (6)
N2—Ni1—O1—C2	-100.1 (4)	Ni1—O2—C1—O3 <sup>ii</sup>	-179.5 (5)
N1—Ni1—O1—C2	-69.5 (8)	Ni1—O2—C1—C2	-0.7 (6)
O4—Ni1—O2—C1	-49.9 (7)	Ni1—O1—C2—O4 <sup>ii</sup>	-175.8 (5)
O1—Ni1—O2—C1	1.4 (4)	Ni1—O1—C2—C1	2.5 (6)

## supplementary materials

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O3—Ni1—O2—C1	-99.2 (4)	O2—C1—C2—O4 <sup>ii</sup>	177.1 (6)
N2—Ni1—O2—C1	93.7 (4)	O3 <sup>ii</sup> —C1—C2—O4 <sup>ii</sup>	-3.9 (7)
N1—Ni1—O2—C1	167.2 (4)	O2—C1—C2—O1	-1.3 (7)
O4—Ni1—O3—C1 <sup>i</sup>	3.6 (4)	O3 <sup>ii</sup> —C1—C2—O1	177.7 (6)
O2—Ni1—O3—C1 <sup>i</sup>	168.2 (4)	C7—N1—C3—C4	2.7 (11)
O1—Ni1—O3—C1 <sup>i</sup>	91.6 (4)	Ni1—N1—C3—C4	179.3 (6)
N2—Ni1—O3—C1 <sup>i</sup>	-63.7 (8)	N1—C3—C4—C5	-0.5 (11)
N1—Ni1—O3—C1 <sup>i</sup>	-94.5 (4)	C3—C4—C5—C6	-1.4 (12)
O2—Ni1—O4—C2 <sup>i</sup>	-52.8 (7)	C4—C5—C6—C7	1.0 (12)
O1—Ni1—O4—C2 <sup>i</sup>	-102.2 (4)	C3—N1—C7—C6	-3.1 (9)
O3—Ni1—O4—C2 <sup>i</sup>	-1.3 (4)	Ni1—N1—C7—C6	-179.9 (5)
N2—Ni1—O4—C2 <sup>i</sup>	163.5 (4)	C3—N1—C7—C8	177.8 (6)
N1—Ni1—O4—C2 <sup>i</sup>	89.9 (4)	Ni1—N1—C7—C8	0.9 (6)
O4—Ni1—N1—C3	-80.8 (6)	C5—C6—C7—N1	1.3 (11)
O2—Ni1—N1—C3	87.1 (6)	C5—C6—C7—C8	-179.6 (7)
O1—Ni1—N1—C3	152.0 (6)	C12—N2—C8—C9	3.2 (9)
O3—Ni1—N1—C3	-4.6 (6)	Ni1—N2—C8—C9	-174.3 (5)
N2—Ni1—N1—C3	-175.9 (6)	C12—N2—C8—C7	-178.8 (6)
O4—Ni1—N1—C7	95.7 (4)	Ni1—N2—C8—C7	3.6 (7)
O2—Ni1—N1—C7	-96.3 (4)	N1—C7—C8—N2	-3.0 (7)
O1—Ni1—N1—C7	-31.5 (9)	C6—C7—C8—N2	177.8 (6)
O3—Ni1—N1—C7	171.9 (4)	N1—C7—C8—C9	174.9 (6)
N2—Ni1—N1—C7	0.6 (4)	C6—C7—C8—C9	-4.3 (9)
O4—Ni1—N2—C8	-99.2 (5)	N2—C8—C9—C10	-3.7 (11)
O2—Ni1—N2—C8	92.6 (4)	C7—C8—C9—C10	178.5 (7)
O1—Ni1—N2—C8	169.6 (4)	C8—C9—C10—C11	2.4 (13)
O3—Ni1—N2—C8	-34.7 (9)	C9—C10—C11—C12	-0.9 (13)
N1—Ni1—N2—C8	-2.3 (4)	C8—N2—C12—C11	-1.7 (11)
O4—Ni1—N2—C12	83.4 (6)	Ni1—N2—C12—C11	175.7 (6)
O2—Ni1—N2—C12	-84.9 (6)	C10—C11—C12—N2	0.4 (12)

Symmetry codes: (i)  $x-1/2, -y+5/2, z$ ; (ii)  $x+1/2, -y+5/2, z$ .

Fig. 1

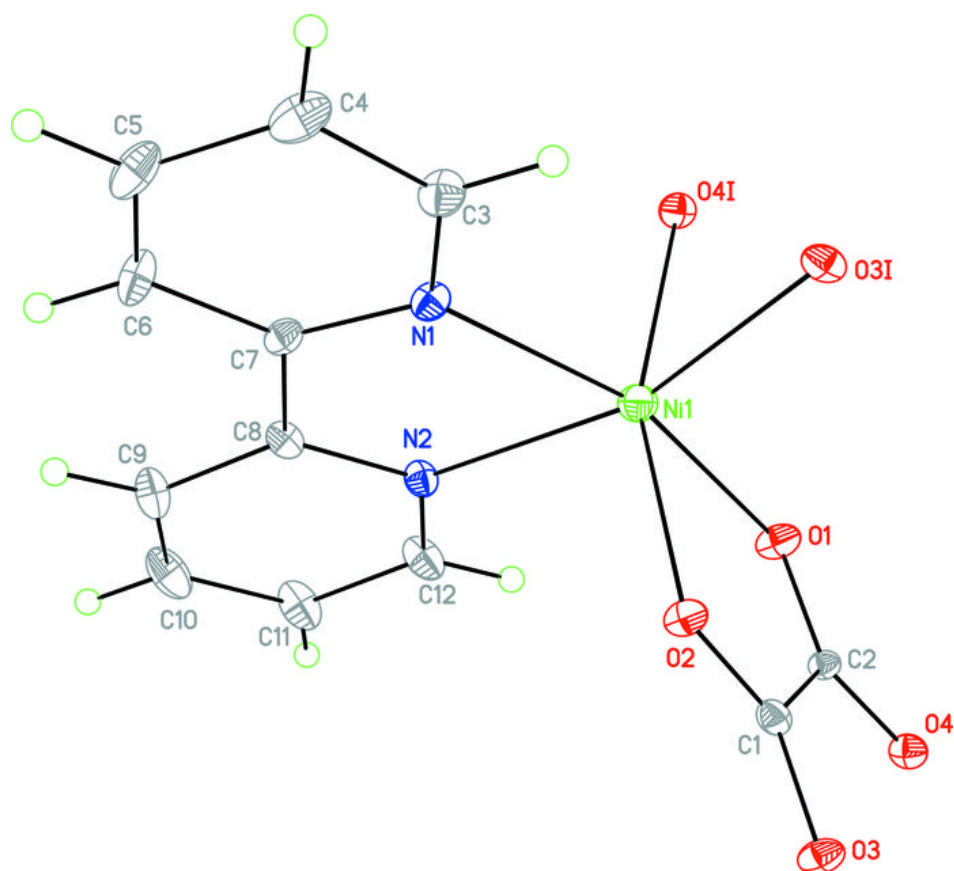


Fig. 2

