Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

catena-Poly[[bis(pyridine-κN)nickel(II)]-μ-oxalato-$\kappa^4O^1,O^2:O^{1'},O^{2'}$]

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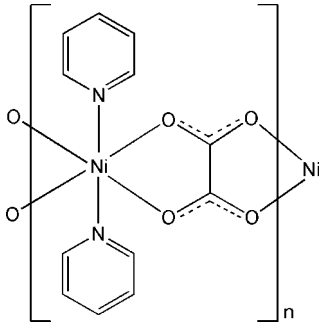
Received 6 July 2008; accepted 12 July 2008

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.042; wR factor = 0.103; data-to-parameter ratio = 17.5.

The title compound, $[Ni(C_2O_4)(C_5H_5N)_2]_n$, was synthesized under hydro(solvo)thermal conditions. The Ni^{II} atom, lying on a twofold rotation axis, has an octahedral coordination geometry involving two N atoms from two pyridine ligands and four O atoms from two oxalate ligands. The Ni atoms are connected by the tetradentate bridging oxalate ligands into a one-dimensional zigzag chain.

Related literature

For related literature, see: Lu *et al.* (1999); Vaidhyanathan *et al.* (2002); Wang *et al.* (2007); Yao *et al.* (2007).



Experimental

Crystal data

$[Ni(C_2O_4)(C_5H_5N)_2]$
M_r = 304.93
Monoclinic, $C2/c$
a = 14.357 (3) Å
b = 10.801 (2) Å
c = 8.6669 (17) Å
β = 91.52 (3)°
V = 1343.5 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.45 mm^{-1}
T = 293 (2) K
0.26 × 0.24 × 0.22 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.640, T_{max} = 0.726
6433 measured reflections
1519 independent reflections
1297 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.103
S = 1.04
1519 reflections
87 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.73 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ni1—O2^{i}	2.046 (2)	Ni1—N1	2.081 (2)
Ni1—O1	2.0716 (18)		
O2^{i}—Ni1—O2^{ii}	168.78 (10)	O2^{ii}—Ni1—N1	93.66 (9)
O2^{i}—Ni1—O1	89.88 (7)	O1—Ni1—N1	89.92 (9)
O2^{ii}—Ni1—O1	81.96 (7)	O1^{iii}—Ni1—N1	174.81 (8)
O1—Ni1—O1^{iii}	86.81 (11)	N1—Ni1—N1^{iii}	93.61 (13)
O2^{i}—Ni1—N1	94.02 (8)		

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

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-AUTO*; 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*.

The authors thank Yanbian University for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2144).

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supporting information

Acta Cryst. (2008). E**64**, m1040 [doi:10.1107/S1600536808021703]

catena-Poly[[bis(pyridine-κN)nickel(II)]-μ-oxalato-$\kappa^4O^1,O^2:O^{1'},O^{2'}$]

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S1. Comment

Much research work has been done on metal–oxalate compounds, in the context of studies of molecular-based magnets and open framework structures (Lu *et al.*, 1999; Yao *et al.*, 2007). The geometrical coordination mode and strength of this ligand provide both rigidity and preferred coordination specificity for metal centers (Vaidhyanathan *et al.*, 2002; Wang *et al.*, 2007). In this paper, we report the hydro(solvo)thermal synthesis and structure of a new one-dimensional nickelous oxalate coordination polymer.

The title compound consists of one Ni^{II} atom lying on a twofold rotation axis, an oxalate ligand and two coordinated pyridine molecules (Fig. 1). The Ni^{II} atom exhibits a distorted octahedral geometry, defined by four O atoms of two oxalate ligands and two pyridine N atoms in a *cis* arrangement. The Ni—O distances are 2.046 (2) and 2.0716 (18) Å, while the O—Ni—O angles show distortions particularly as a result of chelation (Table 1). The tetradentate oxalate ligands link adjacent Ni atoms into a one-dimensional zigzag chain.

S2. Experimental

A mixture of $K_2C_2O_4.H_2O$ (0.037 g, 0.2 mmol), H_3BO_3 (0.013 g, 0.2 mmol), $NiCl_2.2H_2O$ (0.033 g, 0.2 mmol), KOH (0.012 g, 0.2 mmol), pyridine (4 ml) and water (8 ml) in a 25 ml Teflon-lined stainless steel reactor was heated from 298 to 393 K in 2 h and maintained at 393 K for 72 h. After the mixture was cooled to 298 K, blue crystals of the title compound were obtained.

S3. Refinement

H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

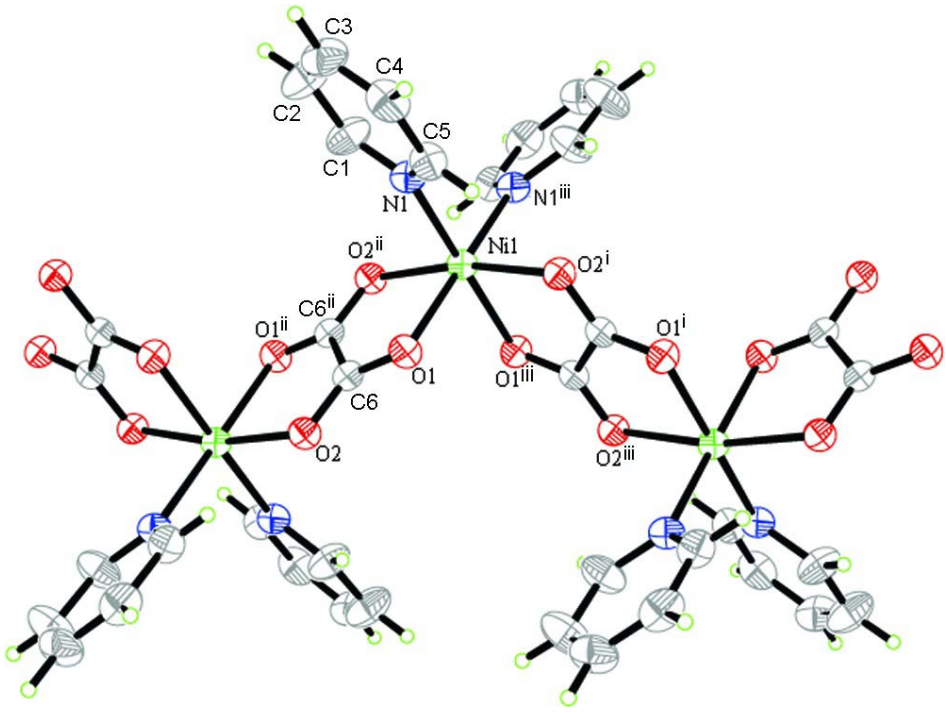

Figure 1

Part of the polymeric structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry codes: (i) x, 1-y, 1/2+z; (ii) 1-x, 1-y, -z; (iii) 1-x, y, 1/2-z.]

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Crystal data

$[Ni(C_2O_4)(C_5H_5N)_2]$
M_r = 304.93
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
a = 14.357 (3) Å
b = 10.801 (2) Å
c = 8.6669 (17) Å
β = 91.52 (3)°
V = 1343.5 (5) Å^3
Z = 4
F(000) = 624
D_x = 1.508 Mg m^{-3}
Mo *K*α radiation, λ = 0.71073 Å
Cell parameters from 1532 reflections
θ = 3.3–27.5°
μ = 1.45 mm^{-1}
T = 293 K
Block, blue
0.26 × 0.24 × 0.22 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Radiation source: rotating anode
Graphite monochromator
Detector resolution: 10.0 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.640, T_{max} = 0.726
6433 measured reflections
1519 independent reflections
1297 reflections with $I > 2\sigma(I)$
R_{int} = 0.041
θ_{max} = 27.5°, θ_{min} = 3.3°
h = −18→18
k = −13→13
l = −11→10

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.103$
$S = 1.04$
1519 reflections
87 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
$w = 1/[\sigma^2(F_o^2) + (0.0487P)^2 + 1.5041P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.73$ e Å^{-3}
$\Delta\rho_{min} = -0.30$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ni1	0.5000	0.35667 (4)	0.2500	0.04167 (19)
O1	0.57949 (11)	0.49601 (17)	0.1553 (2)	0.0468 (4)
O2	0.57299 (12)	0.62481 (16)	−0.0453 (2)	0.0465 (4)
N1	0.59041 (14)	0.2248 (2)	0.1633 (3)	0.0491 (5)
C1	0.5679 (2)	0.1569 (3)	0.0391 (5)	0.0726 (10)
H1	0.5088	0.1664	−0.0059	0.090*
C2	0.6274 (3)	0.0743 (4)	−0.0251 (6)	0.0911 (13)
H2	0.6085	0.0290	−0.1116	0.090*
C3	0.7145 (3)	0.0584 (3)	0.0378 (5)	0.0790 (11)
H3	0.7558	0.0019	−0.0040	0.090*
C4	0.7395 (2)	0.1274 (4)	0.1630 (5)	0.0725 (10)
H4	0.7986	0.1190	0.2083	0.090*
C5	0.6764 (2)	0.2103 (3)	0.2231 (4)	0.0592 (8)
H5	0.6946	0.2577	0.3083	0.090*
C6	0.54390 (16)	0.5345 (2)	0.0324 (3)	0.0405 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0290 (2)	0.0460 (3)	0.0499 (3)	0.000	−0.00167 (18)	0.000
O1	0.0341 (9)	0.0554 (11)	0.0503 (11)	−0.0087 (7)	−0.0082 (8)	0.0032 (8)
O2	0.0358 (9)	0.0508 (10)	0.0527 (11)	−0.0083 (7)	−0.0047 (8)	0.0002 (8)
N1	0.0351 (11)	0.0486 (12)	0.0637 (15)	0.0030 (9)	0.0034 (10)	0.0006 (10)
C1	0.0480 (17)	0.074 (2)	0.096 (3)	0.0063 (15)	−0.0007 (17)	−0.0296 (19)
C2	0.067 (2)	0.089 (3)	0.118 (3)	0.007 (2)	0.011 (2)	−0.043 (3)
C3	0.060 (2)	0.068 (2)	0.110 (3)	0.0157 (17)	0.025 (2)	−0.009 (2)
C4	0.0438 (16)	0.086 (2)	0.088 (3)	0.0185 (15)	0.0097 (16)	0.021 (2)
C5	0.0401 (14)	0.070 (2)	0.067 (2)	0.0114 (13)	0.0028 (13)	0.0074 (15)
C6	0.0293 (11)	0.0451 (13)	0.0470 (14)	−0.0015 (10)	0.0014 (10)	−0.0054 (11)

Geometric parameters (Å, º)

Ni1—O2^{i}	2.046 (2)	C1—C2	1.364 (5)
Ni1—O2^{ii}	2.046 (2)	C1—H1	0.9300

Ni1—O1	2.0716 (18)	C2—C3	1.362 (6)
Ni1—O1^{iii}	2.0716 (18)	C2—H2	0.9300
Ni1—N1	2.081 (2)	C3—C4	1.357 (6)
Ni1—N1^{iii}	2.081 (2)	C3—H3	0.9300
O1—C6	1.240 (3)	C4—C5	1.385 (5)
O2—C6	1.263 (3)	C4—H4	0.9300
O2—Ni1^{ii}	2.046 (2)	C5—H5	0.9300
N1—C1	1.335 (4)	C6—C6^{ii}	1.556 (4)
N1—C5	1.336 (3)		

O2^{i}—Ni1—O2^{ii}	168.78 (10)	C5—N1—Ni1	121.3 (2)
O2^{i}—Ni1—O1	89.88 (7)	N1—C1—C2	123.1 (3)
O2^{ii}—Ni1—O1	81.96 (7)	N1—C1—H1	118.4
O2^{i}—Ni1—O1^{iii}	81.96 (7)	C2—C1—H1	118.4
O2^{ii}—Ni1—O1^{iii}	89.88 (7)	C3—C2—C1	119.9 (4)
O1—Ni1—O1^{iii}	86.81 (11)	C3—C2—H2	120.1
O2^{i}—Ni1—N1	94.02 (8)	C1—C2—H2	120.1
O2^{ii}—Ni1—N1	93.66 (9)	C4—C3—C2	118.1 (3)
O1—Ni1—N1	89.92 (9)	C4—C3—H3	121.0
O1^{iii}—Ni1—N1	174.81 (8)	C2—C3—H3	121.0
O2^{i}—Ni1—N1^{iii}	93.66 (9)	C3—C4—C5	119.7 (3)
O2^{ii}—Ni1—N1^{iii}	94.02 (8)	C3—C4—H4	120.2
O1—Ni1—N1^{iii}	174.81 (8)	C5—C4—H4	120.2
O1^{iii}—Ni1—N1^{iii}	89.92 (9)	N1—C5—C4	122.4 (3)
N1—Ni1—N1^{iii}	93.61 (13)	N1—C5—H5	118.8
C6—O1—Ni1	111.39 (15)	C4—C5—H5	118.8
C6—O2—Ni1^{ii}	111.64 (15)	O1—C6—O2	125.6 (2)
C1—N1—C5	116.8 (3)	O1—C6—C6^{ii}	117.5 (3)
C1—N1—Ni1	121.8 (2)	O2—C6—C6^{ii}	116.9 (3)

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