Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

catena-Poly[[[(1,10-phenanthroline)nickel(II)]-μ-4,4′-oxydibenzoato] 0.25-hydrate]

Hong-Ping Xiao,* Jia-Guo Wang, Xin-Hua Li, Mao-Lin Hu and Wei-Bing Zhang

School of Chemistry and Materials Science,
Wenzhou Normal College, Zhejiang Wenzhou
325027, People's Republic of China

Correspondence e-mail: hp_xiao@wznc.zj.cn

Received 23 December 2004
Accepted 4 January 2005
Online 8 January 2005

In the title compound, $\{[Ni(C_{14}H_8O_5)(C_{12}H_8N_2)]\cdot0.25H_2O\}_n$, the Ni atom displays a distorted octahedral geometry defined by four carboxy O atoms from two 4,4′-oxydibenzoate (oba) dianions and two N atoms from a 1,10-phenanthroline molecule. The V-shaped oba anion acts as a bridge between two Ni atoms in a tris-bidentate coordination mode, forming a zigzag coordination polymer.

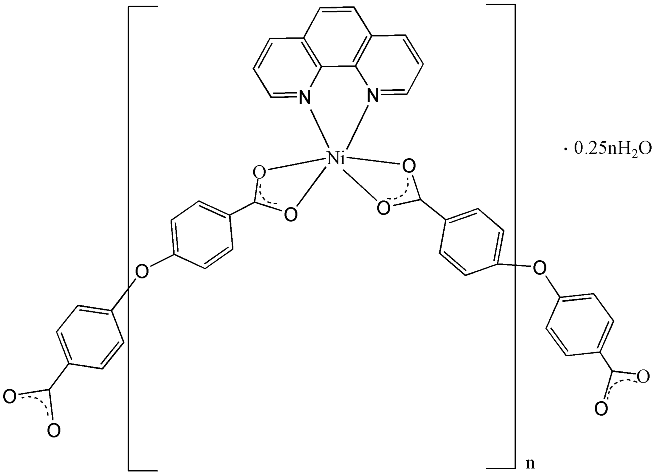
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.005 Å
H-atom completeness 97%
Disorder in solvent or counterion
R factor = 0.050
wR factor = 0.127
Data-to-parameter ratio = 15.1

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

In the construction of coordination polymers, numerous terephthalate complexes have been extensively studied because of their potential application as functional materials and the considerable interest arising from the variety of framework topologies they adopt (Sun *et al.*, 2003; Xiao & Zhu, 2003; Yaghi *et al.*, 1998). In contrast to the extensively studied rigid terephthalic acid, the flexible V-shaped H_2oba ligand (oba is 4,4′-oxydibenzoate) shows versatility as manifested by the interesting two- and three-dimensional polymeric structures (Liu *et al*, 2002; Wang *et al.*, 2004). Recently, we used the flexible H_2oba ligand and the Ni^{II} ion to construct a new coordination polymer, namely $\{[Ni(phen)(oba)]_n\cdot0.25nH_2O\}$ (phen is 1,10-phenanthroline), (I). We report here the crystal structure of (I).



(I)

In (I), the Ni^{II} atom is coordinated by four O atoms from two bidentate oba ligands and two N atoms from a chelate phen ligand to furnish a highly distorted octahedral coordination environment (Fig. 1). The Ni—O bond lengths are in the range 2.0492 (18)–2.1469 (19) Å. The *trans* angles of the octahedron are 159.55 (9), 159.78 (8) and 163.88 (8)°, and the other angles are in the range 63.12 (7)–103.57 (7)° (Table 1).

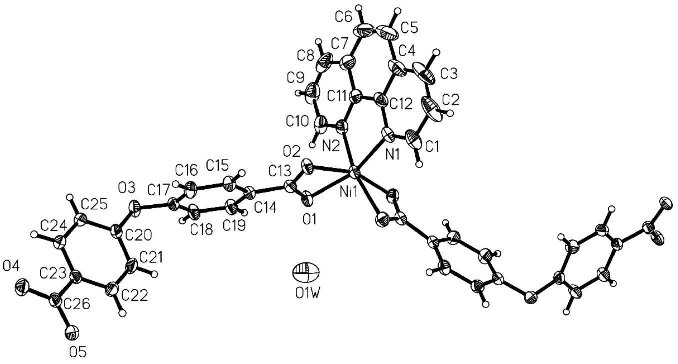


Figure 1
The coordination environment of atom Ni1 in (I). Displacement ellipsoids are drawn at the 30% probability level. Only the contents of the asymmetric unit are numbered. Water atom O1*W* has a partial occupancy of 0.25.

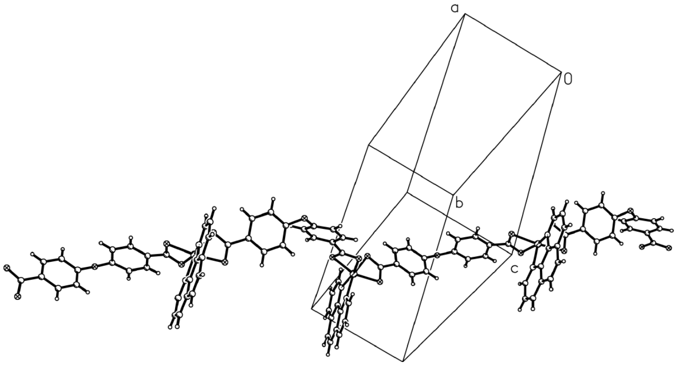


Figure 2
The zigzag chain structure of (I). The water molecules have been omitted.

In the crystal structure, the Ni^{II} atoms are linked by the oba ligands to form zigzag chains running along [101]. The phen ligands protrude on both sides of the zigzag chain (Fig. 2). The dihedral angle between the planes of the two benzene rings of the oba dianion is 81.2 (1)°. The mean plane through the phen ligand forms dihedral angles of 86.6 (1) and 88.5 (1)°, respectively, with the C14–C19 and C20–C25 benzene rings, indicating that the phen plane is perpendicular to the two benzene rings of the oba ligand. Weak C—H···O hydrogen bonds involving two benzene ring C atoms (C15 and C22) and weakly coordinated carboxy O atoms (O2 and O5) represent additional attractions between neighboring zigzag chains (Table 2). These C—H···O hydrogen bonds connect the zigzag chains into a two-dimensional network structure.

Experimental

The title compound was synthesized by a hydrothermal method from a mixture of 4,4′-oxybis(benzoic acid) (0.5 mmol), $Ni(CH_3COO)_2\cdot 4H_2O$ (0.5 mmol), 1,10-phenanthroline (0.5 mmol) and water (18.0 ml) in a 30.0 ml Teflon-lined stainless steel reactor. The solution was heated at 423 K for four days. After the completion of the reaction, the system was slowly cooled to room temperature and green crystals were collected.

Crystal data

$[Ni(C_{14}H_8O_5)(C_{12}H_8N_2)]\cdot 0.25H_2O$
$M_r = 499.62$
Monoclinic, $P2_1/n$
$a = 7.7115\ (7)$ Å
$b = 18.8101\ (16)$ Å
$c = 15.2619\ (13)$ Å
$\beta = 97.023\ (1)°$
$V = 2197.2\ (3)$ Å^3
$Z = 4$

$D_x = 1.510$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2851 reflections
$\theta = 2.6–23.1°$
$\mu = 0.93$ mm^{-1}
$T = 298\ (2)$ K
Block, green
0.29 × 0.22 × 0.18 mm

Data collection

Bruker SMART APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{min} = 0.775$, $T_{max} = 0.851$
13 101 measured reflections

4766 independent reflections
3602 reflections with $I > 2\sigma(I)$
$R_{int} = 0.035$
$\theta_{max} = 27.0°$
$h = -9 \rightarrow 8$
$k = -12 \rightarrow 24$
$l = -19 \rightarrow 19$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.050$
$wR(F^2) = 0.127$
$S = 1.02$
4766 reflections
316 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0693P)^2 + 0.1832P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.0001$
$\Delta\rho_{max} = 0.66$ e Å^{-3}
$\Delta\rho_{min} = -0.26$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ni1—N2	2.049 (2)	Ni1—O2	2.0889 (19)
Ni1—O5^i	2.0492 (18)	Ni1—O1	2.1041 (18)
Ni1—N1	2.061 (2)	Ni1—O4^i	2.1469 (19)
N2—Ni1—O5^i	102.64 (9)	N1—Ni1—O1	159.55 (9)
N2—Ni1—N1	80.80 (9)	O2—Ni1—O1	63.12 (7)
O5^i—Ni1—N1	98.23 (9)	N2—Ni1—O4^i	163.88 (8)
N2—Ni1—O2	92.18 (8)	O5^i—Ni1—O4^i	63.04 (7)
O5^i—Ni1—O2	159.78 (8)	N1—Ni1—O4^i	93.49 (9)
N1—Ni1—O2	97.66 (8)	O2—Ni1—O4^i	103.57 (7)
N2—Ni1—O1	92.43 (9)	O1—Ni1—O4^i	97.73 (8)
O5^i—Ni1—O1	102.09 (7)		

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

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C15—H15···O5^{ii}	0.93	2.49	3.389 (3)	163
C22—H22···O2^{iii}	0.93	2.46	3.289 (3)	149

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

H atoms attached to C atoms were placed in calculated positions, with C—H distances of 0.93 Å, and were included in the refinement in the riding-model approximation, with $U_{iso}(H) = 1.2U_{eq}(C)$. At this stage, the maximum difference density of 1.18 e Å^{-3} indicated the presence of a possible atom site. This peak was found near atom O1, at a hydrogen-bonding distance of 2.73 Å. Attempts to refine this peak as a water O atom (O1*W*) with full occupancy resulted in a high U_{iso} value, and hence it was refined with partial occupancy. The occupancy factor of O1*W* was initially refined to 0.26 (1) and later fixed at 0.25. The H atoms of the water molecule were not located in the difference map.

m258 Xiao *et al.* • $[Ni(C_{14}H_8O_5)(C_{12}H_8N_2)]\cdot 0.25H_2O$ *Acta Cryst.* (2005). E**61**, m257–m259

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2002); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

The authors acknowledge financial support by the Zhejiang Provincial Natural Science Foundation (No. Y404294) and the Wenzhou Science and Technology Project of China (No. S2003A008).

References

Bruker (2002). *SMART* (Version 5.618), *SAINT* (Version 6.02a), *SADABS* (Version 2.03) and *SHELXTL* (Version 5.03). Bruker AXS Inc., Madison, Wisconsin, USA.

Liu, G. F., Qiao, Z. P., Wang, H. Z., Chen, X. M. & Yang, G. (2002). *New J. Chem.* **26**, 791–795.

Sun, D. F., Cao, R., Sun, Y. Q., Bi, W. H., Yuan, D. Q., Shi, Q. & Li, X. (2003). *Chem. Commun.* pp. 1528–1529.

Wang, Y. B., Wang, Z. M., Yan, C. H. & Jin, L. P. (2004). *J. Mol. Struct.* **692**, 177–186.

Xiao, H. P. & Zhu, L. G. (2003). *Chin. J. Inorg. Chem.* **19**, 1179–1183.

Yaghi, O. M., Li, H., Davis, C., Richardson, D. & Groy, T. (1998). *Acc. Chem. Res.* **31**, 474–484.

Acta Cryst. (2005). E**61**, m257–m259 Xiao *et al.* • $[Ni(C_{14}H_8O_5)(C_{12}H_8N_2)]\cdot 0.25H_2O$ **m259**