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A one-dimensional nickel(II) coordination polymer with pyridine and isophthalate

Yong Wang, Zhong-Min Su,* Xiang-Rong Hao, Kui-Zhan Shao and Ya-Hui Zhao

Institute of Functional Material Chemistry, Department of Chemistry, Northeast Normal University, Changchun 130024, People's Republic of China

Correspondence e-mail: zmsu@nenu.edu.cn

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.038
wR factor = 0.071
Data-to-parameter ratio = 18.2

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

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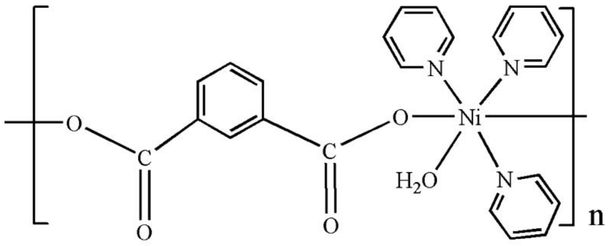
A nickel(II) coordination polymer, *catena*-poly[[aquatripyridinenickel(II)]-μ-isophthalato], $[Ni(C_8H_4O_4)(C_5H_5N)_3(H_2O)]_n$, obtained by reaction of *m*-bda, pyridine and $Ni(NO_3)_2\cdot 6H_2O$ under hydrothermal conditions, where *m*-bda is isophthalic acid, was characterized by single-crystal X-ray diffraction. The Ni^{II} atom is six-coordinate and lies at the centre of a distorted octahedron, coordinated by two carboxylate O atoms from two *m*-bda ligands, three N atoms from three pyridine molecules and one water molecule. The carboxylate groups of *m*-bda link the Ni^{II} atoms, forming an extended one-dimensional zigzag chain. The chains are then knitted together, forming a two-dimensional supramolecular arrangement, *via* C—H···O hydrogen bonds between the H atoms of pyridine rings and the coordinated carboxylate O atoms of *m*-bda.

Comment

In recent years, research on coordination polymers has expanded rapidly because of their fascinating structural diversity and potential application as functional materials (Moulton & Zaworotko, 2001; Batten & Robson, 1998). Multifunctional carboxylates and related species provide an effective means of designing novel hybrid structures with porous structures and other interesting properties (Kitagawa *et al.*, 2004; Yaghi *et al.*, 2003). Owing to their bridging ability, rigid carboxylate ligands are very important in the construction of coordination polymers (Eddaoudi *et al.*, 2002; Li *et al.*, 1999). To date, a number of one-, two- and three-dimensional infinite frameworks have been generated with isophthalic acid (*m*-bda, also called ipa) (De Bettencourt-Dias, 2005; Ma *et al.*, 2005; Shen *et al.*, 2005; Zhou *et al.*, 2004). Much of the work has so far been focused on coordination polymers co-operating with N-donor chelating or bridging ligands, such as 2,2′-bipyridine (2,2′-bpy), 4,4′-bipyridine (4,4′-bpy), and 1,10-phenanthroline (phen) and its analogues (Shen *et al.*, 2005; Ma *et al.*, 2004; Chen & Liu, 2002). However, structure reports on pyridine acting as the secondary monodentate N-donor ligand are not common. In this paper, we report the preparation and crystal structure of the title one-dimensional coordination polymer, formulated as $[Ni(m\text{-bda})(py)_3(H_2O)]_n$ (py is pyridine), (I).

The structure of (I) was revealed by single-crystal X-ray diffraction analysis. The asymmetric unit contains one independent Ni atom, which is octahedrally coordinated by two carboxylate O atoms of two *m*-bda molecules, one water molecule and three N atoms of three pyridine molecules. The bond lengths and angles involving Ni—O(carboxylate) are similar to those of other nickel–carboxylate coordination polymers (Baca *et al.*, 2005), with the Ni center displaying the typical distorted octahedral coordination (Table 1). The two *trans* pyridine ligands coordinated to Ni are almost perpendicular. The other pyridine ligand and the water ligand are also *trans* to each other (Fig. 1). The isophthalate dianion acts as a bridging ligand, linking two adjacent metal ions and forming a one-dimensional zigzag chain (Fig. 2). In each chain, the planes of every other *m*-bda benzene ring are coplanar, and adjacent rings exhibit only a small dihedral angle [12.3 (2)°].



(I)

The water molecule and carboxylate groups form extensive hydrogen-bonding interactions (Table 2). The hydrogen-bonding interactions can be divided into two types according to the different donors. One interaction is between the carboxylate O atoms and the coordinated water molecule [O5*W*—H···O2 and O5*W*–H···O4^{i}; symmetry code: (i) $-\frac{1}{2}+x, \frac{1}{2}-y, \frac{1}{2}+z$]. The other interactions are between pyridine C—H groups and carboxylate O atoms [C3—H···O2^{ii} and C8—H···O2^{iii}; symmetry codes: (ii) $-1+x, y, z$; (iii) $\frac{1}{2}+x, \frac{1}{2}-y, \frac{1}{2}+z$]. The C···O bond lengths are in the range 3.2–3.4 Å, which is similar to previous reports (Desiraju, 1996; Steed & Atwood, 2000). Weak C—H···O interactions of the *para*-H of the pyridine molecules and the carboxylate O atoms link adjacent one-dimensional chains, which associate with each other in a parallel manner, forming a two-dimensional supramolecular layer, as shown in Fig. 3.

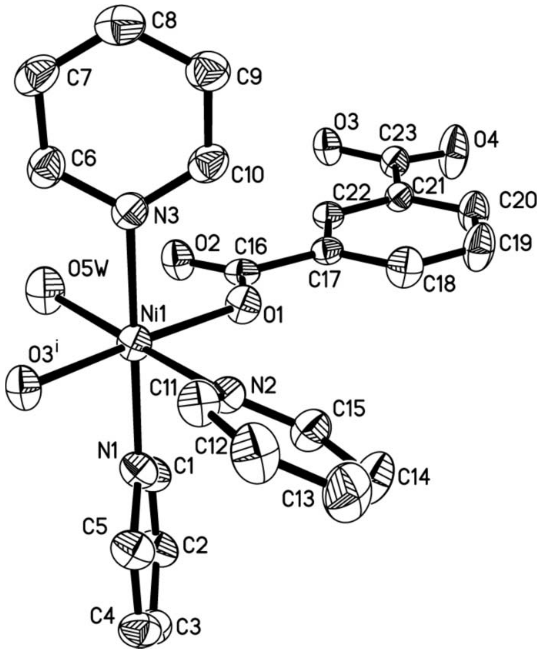


Figure 1
View of the local coordination of Ni^{II} with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted. [Symmetry code: (i) $-\frac{1}{2}+x, \frac{1}{2}-y, \frac{1}{2}+z$.]

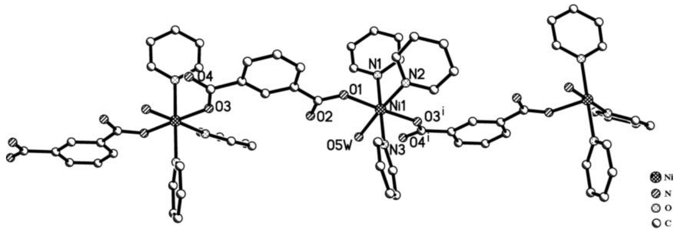


Figure 2
The one-dimensional chain-like fragment of (I). H atoms have been omitted. [Symmetry code: (i) $-\frac{1}{2}+x, \frac{1}{2}-y, \frac{1}{2}+z$.]

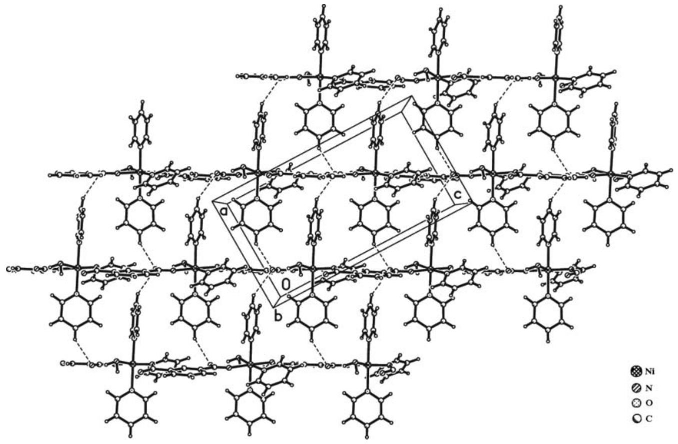


Figure 3
A packing diagram for the two-dimensional supramolecular hydrogen-bonding framework *via* C—H···O interactions. The view shows a layer parallel to the *ac* plane; the view direction is parallel to the *b* axis. Hydrogen bonds are indicated by dashed lines.

Experimental

A mixture of $Ni(NO_3)_2 \cdot 6H_2O$ (0.0872 g), H_2bda (0.0498 g), NaOH (0.0210 g), pyridine (1 ml) and water (10 ml) was stirred for 20 min in air. The mixture was then transferred to a 23 ml Teflon reactor and kept at 438 K for 3 d under autogenous pressure, then cooled to room temperature at a rate of 5 K h^{-1}. Blue block-shaped crystals of (I) were obtained; these were washed with distilled water and dried at room temperature (yield *ca* 60% based on Ni). Elemental analysis found: C 57.64, H 4.49, N 8.87%; calculated: C 57.78, H 4.43, N 8.79%.

Crystal data

$[Ni(C_8H_4O_4)(C_5H_5N)_3(H_2O)]$
$M_r = 478.14$
Monoclinic, $P2_1/n$
$a = 9.0723$ (5) Å
$b = 15.1897$ (8) Å
$c = 16.6524$ (9) Å
$\beta = 91.886$ (1)°
$V = 2293.5$ (2) Å^3
$Z = 4$
$D_x = 1.385$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 13853 reflections
$\theta = 1.8$–28.2°
$\mu = 0.88$ mm^{-1}
$T = 293$ (2) K
Block, blue
0.35 × 0.29 × 0.23 mm

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Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{\min} = 0.751$, $T_{\max} = 0.814$
14005 measured reflections
5392 independent reflections
2787 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.042$
$\theta_{\max} = 28.3°$
$h = -12 \rightarrow 11$
$k = -19 \rightarrow 20$
$l = -22 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.071$
$S = 1.00$
5392 reflections
297 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0201P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.29$ e Å^{-3}
$\Delta\rho_{\min} = -0.39$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

N1—Ni1	2.1372 (19)	Ni1—O3$^{\rm i}$	2.0280 (13)
N2—Ni1	2.1110 (17)	Ni1—O1	2.0446 (13)
N3—Ni1	2.102 (2)	Ni1—O5*W*	2.0727 (17)
O3$^{\rm i}$—Ni1—O1	176.88 (6)	O5*W*—Ni1—N2	175.67 (8)
O3$^{\rm i}$—Ni1—O5*W*	89.24 (7)	N3—Ni1—N2	90.06 (7)
O1—Ni1—O5*W*	93.85 (7)	O3$^{\rm i}$—Ni1—N1	89.74 (6)
O3$^{\rm i}$—Ni1—N3	89.93 (7)	O1—Ni1—N1	89.57 (6)
O1—Ni1—N3	90.73 (6)	O5*W*—Ni1—N1	93.84 (8)
O5*W*—Ni1—N3	86.56 (8)	N3—Ni1—N1	179.48 (7)
O3$^{\rm i}$—Ni1—N2	88.05 (6)	N2—Ni1—N1	89.52 (7)
O1—Ni1—N2	88.90 (6)		

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

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

D—H$\cdots$*A*	*D*—H	H$\cdots$*A*	*D*$\cdots$*A*	*D*—H$\cdots$*A*
O5*W*—H5*B*$\cdots$O2	0.94 (4)	1.81 (4)	2.647 (3)	146 (4)
O5*W*—H5*A*$\cdots$O4$^{\rm i}$	0.87 (3)	2.18 (3)	2.664 (3)	115 (2)
C3—H3$\cdots$O2$^{\rm ii}$	0.93	2.51	3.315 (4)	145
C8—H8$\cdots$O2$^{\rm iii}$	0.93	2.60	3.378 (3)	141

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

All H atoms on C atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 Å and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C). O-bound atoms H5*A* and H5*B* were located in an electron-density difference map and were refined freely.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL97*.

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References

Baca, S. G., Filippova, I. G., Franz, P., Arnbrus, C., Gdaniec, M., Stoeckli-Evans, H., Simonov, Y. A., Gherco, O. A., Bejan, T., Gerbeleu, N. & Decurtins, S. (2005). *Inorg. Chim. Acta*, **358**, 1762–1770.

Batten, S. R. & Robson, R. (1998). *Angew. Chem. Int. Ed.* **37**, 1460–1494.

Chen, X. M. & Liu, G. F. (2002). *Chem. Eur. J.* **8**, 4811–4817.

De Bettencourt-Dias, A. (2005). *Inorg. Chem.* **44**, 2734–2741.

Desiraju, G. R. (1996). *Acc. Chem. Res.* **29**, 441–449.

Eddaoudi, M., Kim, J., Nathaniel, R., Vodak, D., Joseph, W., O'Keeffe, M. & Yaghi, O. M. (2002). *Science*, **295**, 469–472.

Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.

Kitagawa, S., Kitaura, R. & Noro, S. (2004). *Angew. Chem. Int. Ed.* **43**, 2334–2375.

Li, H., Eddaoudi, M., O'Keeffe, M. & Yaghi, O. M. (1999). *Nature (London)*, **402**, 276–279.

Ma, C. B., Chen, C. N., Liu, Q. T., Chen, F., Liao, D. Z., Li, L. C. & Sun, L. H. (2004). *Eur. J. Inorg. Chem.* pp. 3316–3325.

Ma, C. B., Hu, M. Q., Chen, C. N. & Liu, Q. T. (2005). *Inorg. Chem. Commun.* **8**, 219–221.

Moulton, B. & Zaworotko, M. J. (2001). *Chem. Rev.* **101**, 1629–1658.

Rigaku (1998). *PROCESS-AUTO*. Rigaku Corporation, Tokyo, Japan.

Sheldrick, G. M. (1990). *SHELXTL-Plus*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

Shen, W. Z., Chen, X. Y., Cheng, P., Yan. S. P., Zhai. B., Liao. D. Z. & Jiang, Z. H. (2005). *Eur. J. Inorg. Chem.* pp. 2297–2305.

Steed, J. W. & Atwood, J. L. (2000). *Supramolecular Chemistry*, p. 26. Chichester: John Wiley & Son.

Yaghi, O. M., O'Keeffe, M., Ockwig, N. W., Chae, H. K., Eddaoudi, M. & Kim, J. (2003). *Nature (London)*, **423**, 705–714.

Zhou, Y. F., Jiang, F. L., Yuan, D. Q., Wu, B. L., Wang, R. H., Lin, Z. Z. & Hong, M. C. (2004). *Angew. Chem. Int. Ed.* **43**, 5665–5668.

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