

Xue-Hua Sun

Chemistry and Chemical Engineering College,
State Key Laboratory of Chemical Engineering,
Yanán University, Yanán 716000, People's
Republic of China

Correspondence e-mail: xuehuasun@xdz.com

Key indicators

Single-crystal X-ray study

T = 293 K

Mean $\sigma(\text{C}-\text{C}) = 0.003 \text{ \AA}$

R factor = 0.027

wR factor = 0.073

Data-to-parameter ratio = 13.6

For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.*catena*-Poly[[triaquanickel(II)]- μ -5-hydroxyisophthalato]

The title compound, $[\text{Ni}(\text{C}_8\text{H}_{10}\text{O}_8)(\text{H}_2\text{O})_3]_n$, a one-dimensional chain complex of 5-hydroxyisophthalate with Ni^{2+} , was prepared by a hydrothermal reaction. The coordination geometry around the Ni atom is distorted octahedral with the central Ni atom bound to three O atoms of two 5-hydroxyisophthalate ligands, which act as bidentate and monodentate ligands, positioned in the equatorial plane. The three remaining coordination sites are occupied by water molecules. In the crystal structure, an extensive hydrogen-bonding network is formed, which involves the coordinated water molecules and the ligand substituents.

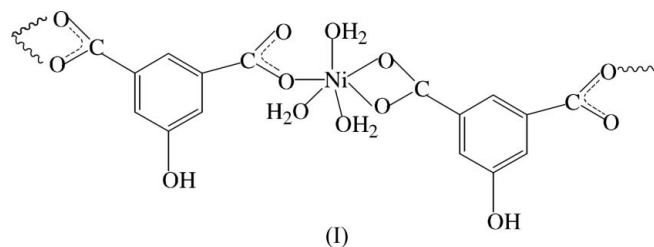
Received 20 June 2005

Accepted 26 July 2005

Online 12 October 2005

Comment

It is well known that organic ligands play important roles in the rational design and construction of novel metal-organic frameworks (Plater *et al.*, 2001; Li, Cao, Sun *et al.*, 2004). Benzenedicarboxylates and their derivatives have been extensively employed to link metal ions in the synthesis of one-, two- or three-dimensional structures. They often act as bridging or chelating ligands (Xiao *et al.*, 2004; Li & Chi, 2004; Cao *et al.*, 2004*a,b*). A new three-dimensional coordination polymer, namely *catena*-poly[[triaquanickel(II)]- μ -5-hydroxyisophthalato], (I), built from a infinite coordination chain through hydrogen bonding, has been synthesized and structurally characterized.



The structure of the asymmetric unit of (I) is shown in Fig. 1. Selected bond lengths and angles are given in Table 1 and details of the hydrogen bonding are given in Table 2. The infinite coordination chain of (I) is shown in Fig. 2 and the three-dimensional hydrogen-bonded network is illustrated in Fig. 3.

Experimental

The title compound, (I), was obtained as the main phase from the hydrothermal reaction of nickel(II) nitrate hexahydrate and 5-hydroxyisophthalic acid, with the molar ratio 1:1, which was placed in a Teflon-lined stainless steel Parr bomb at 393 K for one week. After cooling to room temperature, green single crystals were obtained.

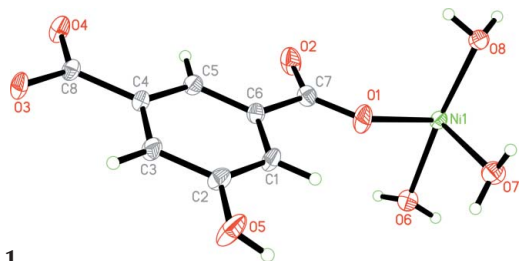


Figure 1
The asymmetric unit of (I) with the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.

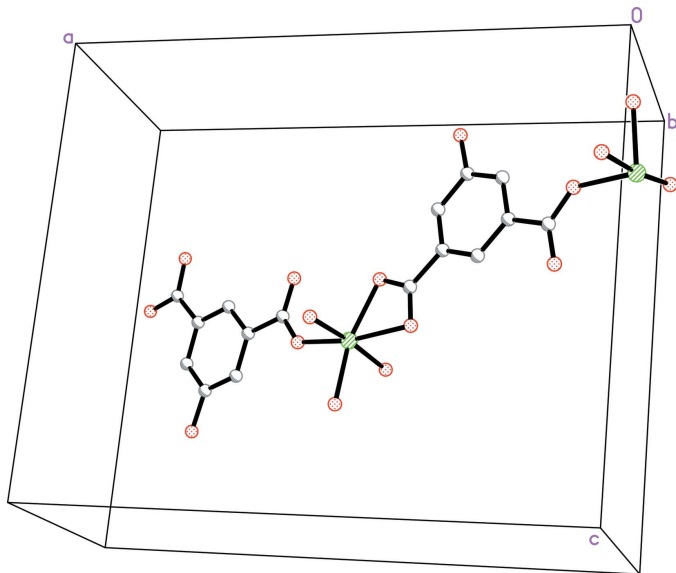


Figure 2
A view of the one-dimensional chain structure of (I).

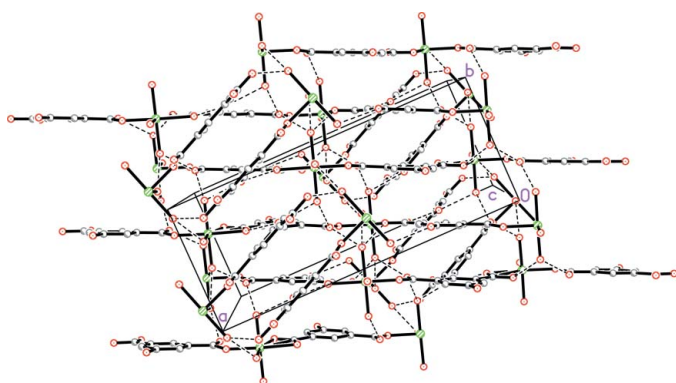


Figure 3
A view of the crystal packing in (I) and the three-dimensional hydrogen-bonding network. H atoms have been omitted for clarity and O...O contacts are shown as dashed lines. Further details are given in Table 2.

Crystal data

[Ni(C₈H₄O₅)(H₂O)₃]
M_r = 292.87
 Orthorhombic, *Pccn*
a = 17.932 (4) Å
b = 7.4244 (15) Å
c = 15.067 (3) Å
V = 2005.9 (7) Å³
Z = 8
D_x = 1.940 Mg m⁻³

Mo Kα radiation
 Cell parameters from 117 reflections
 $\theta = 2.8\text{--}25^\circ$
 $\mu = 1.97\text{ mm}^{-1}$
T = 293 (2) K
 Block, green
 0.22 × 0.15 × 0.11 mm

Data collection

Bruker SMART APEX CCD diffractometer
 φ and ω scans
 Absorption correction: ψ scan; North *et al.*, 1968
 $T_{\min} = 0.671$, $T_{\max} = 0.807$
 9342 measured reflections
 2432 independent reflections
 1951 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.029$
 $\theta_{\text{max}} = 28.1^\circ$
 $h = -13 \rightarrow 23$
 $k = -9 \rightarrow 8$
 $l = -19 \rightarrow 17$
 2 standard reflections every 150 reflections
 intensity decay: none

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.027$
 $wR(F^2) = 0.073$
 $S = 1.08$
 2432 reflections
 179 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0392P)^2 + 0.3505P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.33\text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.50\text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (Å, °).

Ni1—O1	2.0174 (15)	O1—C7	1.264 (2)
Ni1—O6	2.0435 (15)	O2—C7	1.253 (2)
Ni1—O7	2.0433 (16)	O3—C8	1.271 (2)
Ni1—O8	2.0527 (14)	O4—C8	1.266 (2)
Ni1—O3 ⁱ	2.0745 (13)	O5—C2	1.370 (2)
Ni1—O4 ⁱ	2.2299 (15)		
O1—Ni1—O6	88.55 (6)	O3 ⁱ —Ni1—O4 ⁱ	60.61 (5)
O1—Ni1—O7	91.18 (6)	O3 ⁱ —Ni1—C8 ⁱ	30.37 (5)
O1—Ni1—O8	92.70 (6)	O4 ⁱ —Ni1—C8 ⁱ	30.27 (5)
O1—Ni1—O3 ⁱ	108.44 (5)	Ni1—O1—C7	134.71 (13)
O1—Ni1—O4 ⁱ	169.03 (5)	Ni1 ⁱⁱ —O3—C8	94.06 (10)
O1—Ni1—C8 ⁱ	138.79 (6)	Ni1 ⁱⁱ —O4—C8	87.13 (11)
O6—Ni1—O7	86.77 (6)	O5—C2—C3	117.58 (17)
O6—Ni1—O8	173.70 (6)	O5—C2—C1	122.03 (17)
O3 ⁱ —Ni1—O6	94.76 (6)	O1—C7—O2	125.27 (17)
O4 ⁱ —Ni1—O6	91.86 (6)	O2—C7—C6	117.98 (16)
O6—Ni1—C8 ⁱ	94.83 (6)	O1—C7—C6	116.74 (17)
O7—Ni1—O8	87.04 (5)	Ni1 ⁱⁱ —C8—O3	55.58 (9)
O3 ⁱ —Ni1—O7	160.34 (6)	O3—C8—C4	119.01 (15)
O4 ⁱ —Ni1—O7	99.78 (6)	Ni1 ⁱⁱ —C8—C4	173.31 (13)
O7—Ni1—C8 ⁱ	129.98 (6)	O4—C8—C4	122.89 (17)
O3 ⁱ —Ni1—O8	90.70 (5)	Ni1 ⁱⁱ —C8—O4	62.60 (10)
O4 ⁱ —Ni1—O8	88.09 (6)	O3—C8—O4	118.10 (16)
O8—Ni1—C8 ⁱ	88.30 (6)		

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

Table 2

Hydrogen-bond geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O5—H5A...O4 ⁱⁱⁱ	0.82	1.84	2.656 (2)	170
O6—H6B...O5 ^{iv}	0.88 (2)	1.83 (2)	2.703 (2)	175 (3)
O7—H7A...O6 ^v	0.87 (3)	2.17 (3)	2.957 (2)	151 (2)
O7—H7B...O8 ^{vi}	0.87 (3)	1.94 (3)	2.794 (2)	166 (3)
O8—H8A...O3 ^{vii}	0.87 (2)	1.80 (2)	2.6226 (19)	158 (3)
O8—H8B...O2 ^{viii}	0.88 (2)	1.74 (2)	2.610 (2)	168 (2)

Symmetry codes: (iii) $-x + \frac{3}{2}, y, z + \frac{1}{2}$; (iv) $x - \frac{1}{2}, -y + 1, -z + \frac{3}{2}$; (v) $-x + 1, y - \frac{1}{2}, -z + \frac{3}{2}$; (vi) $-x + 1, y + \frac{1}{2}, -z + \frac{3}{2}$; (vii) $-x + \frac{3}{2}, -y + \frac{1}{2}, z$; (viii) $-x + 1, -y, -z + 1$.

The H atoms of the water molecules were located in difference Fourier maps and refined isotropically with the O—H distances restrained to 0.88 (1) Å. The hydroxyl H atom and the carbon-bonded H atoms were placed in idealized positions and constrained to ride on their parent atoms; O—H = 0.82 Å, C—H = 0.93 Å and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O,C})$.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINTE* (Bruker, 2000); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 1999); software used to prepare material for publication: *SHELXTL*.

The author sincerely thanks Yanán University for financial support.

References

Bruker (2000). *SMART* (Version 5.0) and *SAINTE* (Version 6.02). Bruker AXS Inc., Madison, Wisconsin, USA.

- Cao, X.-Y., Zhang, J.-A., Kang, Y., Cheng, J.-K., Li, Z.-J., Wang, X.-Q., Wen, Y.-H. & Yao, Y.-G. (2004a). *Acta Cryst.* **C60**, m350–m352.
- Cao, X.-Y., Zhang, J.-A., Kang, Y., Cheng, J.-K., Li, Z.-J., Wang, X.-Q., Wen, Y.-H. & Yao, Y.-G. (2004b). *Acta Cryst.* **E60**, m460–m461.
- Li, X.-H. & Chi, X.-X. (2004). *Acta Cryst.* **E60**, m1301–m1302.
- Li, X. J., Cao, R., Sun, D. F., Bi, W. H., Wang, Y. Q., Li, X. J. & Hong, M. C. (2004). *Cryst. Growth Des.* **4**, 775–780.
- North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* **A24**, 351–359.
- Plater, M. J., Foreman, M. R., Howie, R. A., Skakle, J. M., McWilliam, S. A., Coronado, E. G. & Gomez-Garcia, C. J. (2001). *Polyhedron*, **20**, 2293–2303.
- Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
- Sheldrick, G. M. (1999). *SHELXTL*. Version 6.10. Bruker AXS Inc., Madison, Wisconsin, USA.
- Xiao, H.-P., Shi, Q. & Ye, M.-D. (2004). *Acta Cryst.* **E60**, m1498–m1500.