catena-Poly[[triaquacobalt(II)]-μ-2,3-pyridinedicarboxylato-κ²O²:O³]

Xian-Ming Zhang,ᵃ Rui-Qin Fang,ᵃ Hai-Shun Wuᵃ and Seik Weng Ngᵇ*

ᵃSchool of Chemistry and Material Science, Shanxi Normal University, Linfen 041004, People's Republic of China, and ᵇDepartment of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia

Correspondence e-mail: seikweng@um.edu.my

Key indicators

Single-crystal X-ray study
$T = 298$ K
Mean σ(C–C) = 0.006 Å
R factor = 0.035
wR factor = 0.068
Data-to-parameter ratio = 9.1

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

The structure of the title one-dimensional coordination polymer, $[Co(C_7H_3NO_4)(H_2O)_3]_n$, contains a Co^{II} ion, a pyridine-2,3-dicarboxylate dianion and three water molecules in the asymmetric unit. The coordination polymer forms a one-dimensional zigzag chain structure along the c axis. The chains are interconnected by O—H···O hydrogen bonds into a three-dimensional framework.

Comment

Recently, Zhang & You (2003) reported the structure of a one-dimensional zigzag coordination polymer of diaqua(pyridine-2,3-dicarboxylato)cobalt(II). In that structure, each cobalt(II) ion is bound to three pyridine-2,3-dicarboxylate ligands and two water molecules. In each ligand, one of the carboxylate groups is involved in N,O-chelation [Co—N = 2.107 (2) Å and Co—O = 2.061 (2) Å], while the other is used to bridge Co^{II} atoms [Co—O = 2.182 (2) and 2.192 (2) Å]. A variation of the synthesis yielded the title compound, triaqua(pyridine-2,3-dicarboxylato)cobalt(II), (I). We present its structure here.

(I)
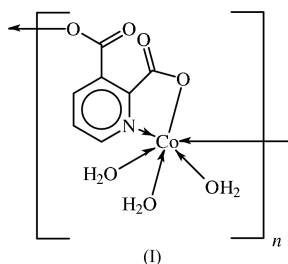
In the title compound, the Co^{II} atom is in a distorted octahedral coordination environment (see Fig. 1 and Table 1 for details), with the pyridyl atom N1, two carboxylate O atoms [O1 and O3^i; symmetry code: (i) $\frac{1}{2} - x$, y, $z - \frac{1}{2}$] and three water O atoms (O1w, O2w and O3w) occupying the vertices. The carboxylate group in the 2-position, which is involved in the N,O-chelation, is coplanar with the pyridine ring [dihedral angle = 2.9 (9)°]. The other carboxylate group in the 3-position is perpendicular to the pyridine ring [dihedral angle = 89.5 (1)°]. As can be seen in Fig. 2, the coordination polymer forms a one-dimensional zigzag chain structure along the c axis. The chains are interconnected by O—H···O hydrogen bonds (Table 2) into a three-dimensional network structure.

Experimental

Cobalt diacetate tetrahydrate (0.25 g, 1 mmol) and pyridine-2,3-dicarboxylic acid (0.17 g, 1 mmol) were dissolved in water (7 ml) to which sodium hydroxide (4 M) was added so that the pH = 7. The

metal-organic papers
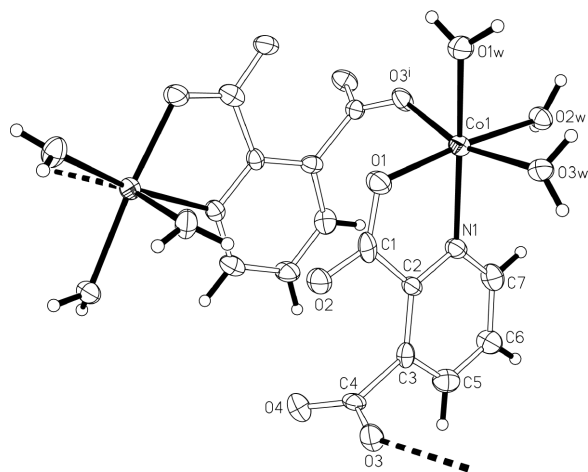
Figure 1
*ORTEP*II (Johnson, 1976) plot of a part of the polymeric [Co(C$_7$H$_3$-NO$_4$)(H$_2$O)$_3$]$_n$ chain, with displacement ellipsoids drawn at the 50% probability level. [Symmetry code: (i) $\frac{1}{2} - x$, y, $z - \frac{1}{2}$.]

Figure 2
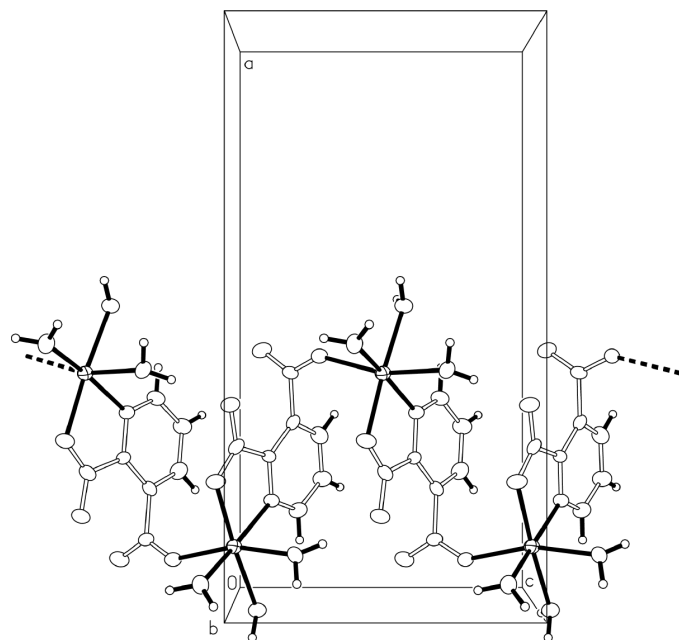*ORTEP*II (Johnson, 1976) plot, showing the zigzag chain formation along the *c* axis of the orthorhombic cell.

solution was transferred into a 15 ml Teflon-lined stainless-steel bomb and it was held at 443 K for 120 h. The bomb was cooled slowly to room temperature, to yield red plate-shaped crystals of the title compound in about 65% yield. CHN analysis, found: C 50.55, H 2.46, N 8.41%; calculated for C$_7$H$_9$CoNO$_4$: C 50.61, H 2.43, N 8.43%.

Crystal data

[Co(C$_7$H$_3$NO$_4$)(H$_2$O)$_3$]
$M_r = 278.08$
Orthorhombic, $Pca2_1$
$a = 16.082\ (3)$ Å
$b = 6.745\ (1)$ Å
$c = 8.467\ (2)$ Å
$V = 918.4\ (3)$ Å^3
$Z = 4$
$D_x = 2.011$ Mg m^{-3}

Mo $K\alpha$ radiation
Cell parameters from 25
   reflections
$\theta = 7.5–15.0°$
$\mu = 1.89$ mm^{-1}
$T = 298\ (2)$ K
Plate, red
$0.28 \times 0.20 \times 0.04$ mm

Data collection

Siemens *R3m* four-circle
   diffractometer
ω scans
Absorption correction: ψ scan
   (North *et al.*, 1968)
   $T_{\min} = 0.62$, $T_{\max} = 0.93$
3513 measured reflections
1480 independent reflections
1380 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.036$
$\theta_{\max} = 25.0°$
$h = -19 \rightarrow 14$
$k = -8 \rightarrow 8$
$l = -8 \rightarrow 10$
2 standard reflections
   every 120 reflections
   intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.068$
$S = 0.97$
1480 reflections
163 parameters
H atoms treated by a mixture of
   independent and constrained
   refinement

$w = 1/[\sigma^2(F_o^2) + (0.0348P)^2]$
   where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.30$ e Å^{-3}
$\Delta\rho_{\min} = -0.34$ e Å^{-3}
Absolute structure: Flack (1988);
   691 Friedel pairs
Flack parameter = 0.06 (2)

Table 1
Selected geometric parameters (Å, °).

Co1—O1	2.044 (3)	Co1—O2w	2.175 (3)
Co1—O3^i	2.087 (3)	Co1—O3w	2.057 (3)
Co1—O1w	2.084 (3)	Co1—N1	2.133 (3)
O1—Co1—O3^i	97.8 (1)	O3^i—Co1—N1	104.1 (1)
O1—Co1—O1w	92.3 (1)	O1w—Co1—O2w	92.9 (1)
O1—Co1—O2w	174.8 (1)	O1w—Co1—O3w	83.9 (1)
O1—Co1—O3w	95.8 (1)	O1w—Co1—N1	167.4 (1)
O1—Co1—N1	78.5 (1)	O2w—Co1—O3w	83.7 (1)
O3^i—Co1—O1w	85.5 (1)	O2w—Co1—N1	96.3 (1)
O3^i—Co1—O2w	83.7 (1)	O3w—Co1—N1	88.5 (1)
O3^i—Co1—O3w	163.1 (1)		

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

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O1w—H1w1$\cdots$O4^{ii}	0.85 (1)	1.87 (1)	2.720 (4)	172 (3)
O1w—H1w2$\cdots$O2w^{iii}	0.85 (1)	1.98 (1)	2.825 (5)	175 (4)
O2w—H2w2$\cdots$O2^{ii}	0.86 (1)	1.86 (1)	2.700 (4)	167 (4)
O2w—H2w1$\cdots$O4^{iv}	0.86 (1)	1.87 (2)	2.697 (4)	161 (4)
O3w—H3w2$\cdots$O3^{ii}	0.84 (1)	1.93 (2)	2.752 (4)	165 (4)
O3w—H3w1$\cdots$O2^v	0.85 (1)	1.85 (1)	2.698 (5)	176 (4)

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

Water H atoms were located in a difference map and their positional parameters were refined subject to an O—H restraint of 0.85 (1) Å and an H$\cdots$H restraint of 1.39 (1) Å (ten restraints in total). The aromatic H atoms were placed at calculated positions in the riding-model approximation (C—H = 0.93 Å). The isotropic displacement parameters of all H atoms were set to 1.2 times U_{eq} of the parent atoms.

Data collection: *R3m Software* (Siemens, 1990); cell refinement: *R3m Software*; data reduction: *R3m Software*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

References

Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Johnson, C. K. (1976). *ORTEP*II. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.
Siemens (1990). *R3m Software*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Zhang, H.-T. & You, X. Z. (2003). *Acta Cryst.* C**59**, m313–m314.