

Poly[[diaquacobalt(II)]- μ -2,5-dicarboxybenzene-1,4-dicarboxylato- μ -di-4-pyridylethene]

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Key indicators

Single-crystal X-ray study

 $T = 298\text{ K}$ Mean $\sigma(\text{C}-\text{C}) = 0.004\text{ \AA}$ R factor = 0.032 wR factor = 0.079

Data-to-parameter ratio = 10.6

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

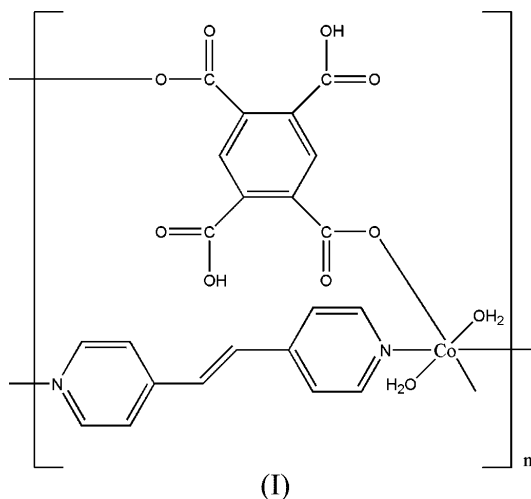
In the polymeric title complex, $[\text{Co}(\text{TBC})(\text{BPE})(\text{H}_2\text{O})_2]_n$ [TBC is the 2,5-dicarboxybenzene-1,4-dicarboxylate dianion ($\text{C}_{10}\text{H}_4\text{O}_8$) and BPE is 1,2-bis(4-pyridyl)ethene ($\text{C}_{12}\text{H}_{10}\text{N}_2$)], the Co^{II} ion, located on an inversion centre, assumes a distorted octahedral coordination geometry. The TBC and BPE ligands are located across individual inversion centres and bridge neighbouring Co^{II} ions to form two-dimensional polymeric sheets.

Received 8 May 2006

Accepted 27 May 2006

Comment

The rational design and synthesis of multinuclear coordination architectures is a rapidly developing field in current coordination chemistry for the development of novel functional materials (Fujita, 1999). As part of our ongoing investigation on polymeric complexes, the title two-dimensional Co^{II} polymeric complex, (I), has been prepared in our laboratory.



The coordination environment around the Co^{II} ion is shown in Fig. 1. The Co^{II} ion is located on an inversion centre and coordinated by two carboxylate O atoms from 2,5-dicarboxybenzene-1,4-dicarboxylate dianions (TBC), two N atoms from 1,2-bis(4-pyridyl)ethene (BPE) ligands and two water molecules, resulting in a distorted octahedral coordination geometry (Table 1). The TBC and BPE ligands are located across individual inversion centres and bridge neighbouring Co^{II} ions to form a two-dimensional polymeric structure (Fig. 2).

Neighbouring polymeric sheets are linked to each other *via* $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonding (Table 2) to form a three-dimensional supramolecular structure.

Experimental

An aqueous solution (16 ml) of H₂TBC (0.51 g, 2 mmol), BPE (0.41 g, 2 mmol) and CoSO₄·7H₂O (0.62 g, 2 mmol) in a 30 ml Teflon-lined stainless steel reactor was heated at 423 K for 4 d and then slowly cooled to room temperature to give pink prismatic single crystals.

Crystal data

[Co(C ₁₀ H ₄ O ₈)(C ₁₂ H ₁₀ N ₂)(H ₂ O) ₂]	$V = 494.64 (8) \text{ \AA}^3$
$M_r = 529.31$	$Z = 1$
Triclinic, $P\bar{1}$	$D_x = 1.777 \text{ Mg m}^{-3}$
$a = 6.8680 (7) \text{ \AA}$	Mo $K\alpha$ radiation
$b = 8.5558 (8) \text{ \AA}$	$\mu = 0.94 \text{ mm}^{-1}$
$c = 8.9769 (9) \text{ \AA}$	$T = 298 (2) \text{ K}$
$\alpha = 102.552 (2)^\circ$	Prism, pink
$\beta = 93.594 (2)^\circ$	$0.24 \times 0.16 \times 0.07 \text{ mm}$
$\gamma = 104.500 (2)^\circ$	

Data collection

Bruker APEX area-detector diffractometer	2614 measured reflections
φ and ω scans	1731 independent reflections
Absorption correction: multi-scan (SADABS; Bruker, 2002)	1657 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.84, T_{\max} = 0.94$	$R_{\text{int}} = 0.012$
	$\theta_{\max} = 25.1^\circ$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0386P)^2 + 0.4596P]$
$R[F^2 > 2\sigma(F^2)] = 0.032$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.079$	$(\Delta/\sigma)_{\max} < 0.001$
$S = 1.04$	$\Delta\rho_{\max} = 0.35 \text{ e \AA}^{-3}$
1731 reflections	$\Delta\rho_{\min} = -0.34 \text{ e \AA}^{-3}$
163 parameters	Extinction correction: SHELXL97
H-atom parameters constrained	Extinction coefficient: 0.048 (4)

Table 1

Selected bond lengths (Å).

Co1—O1	2.1426 (15)	Co1—N1	2.1455 (18)
Co1—O5	2.1019 (16)		

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O3—H3 \cdots O2 ⁱ	0.82	1.79	2.605 (2)	170
O5—H5A \cdots O4 ⁱⁱ	0.82	2.03	2.835 (2)	166
O5—H5B \cdots O2 ⁱⁱⁱ	0.82	2.04	2.766 (2)	147

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

Water H atoms and the carboxyl H atom were located in a difference Fourier map and refined as riding, with $O-H = 0.82 \text{ \AA}$ and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$. Other H atoms were positioned geometrically, with $C-H = 0.93 \text{ \AA}$, and refined in riding mode [$U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$].

Data collection: SMART (Bruker, 2002); cell refinement: SAINT (Bruker, 2002); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEPII (Johnson, 1976); software used to prepare material for publication: SHELXTL (Bruker, 2002).

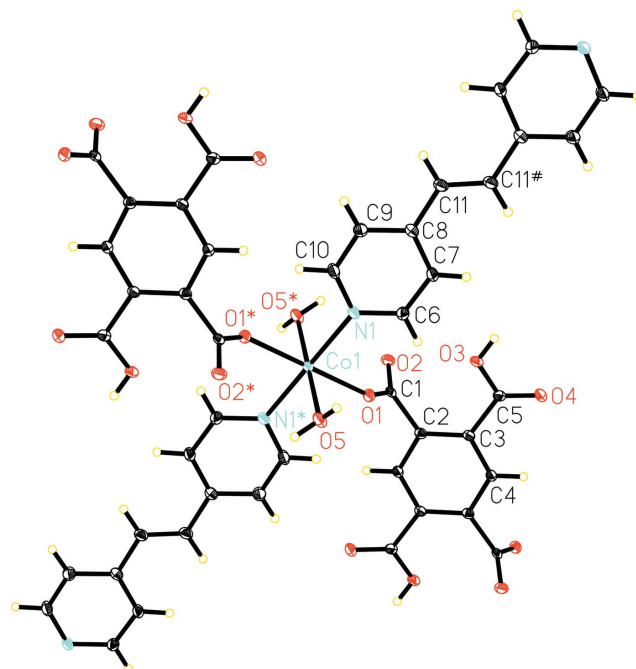


Figure 1

The coordination environment around the Co^{II} ion, with 50% probability displacement ellipsoids (arbitrary spheres for H atoms) [symmetry codes: (*) $1 - x, 1 - y, -z$; (#) $1 - x, 2 - y, -1 - z$].

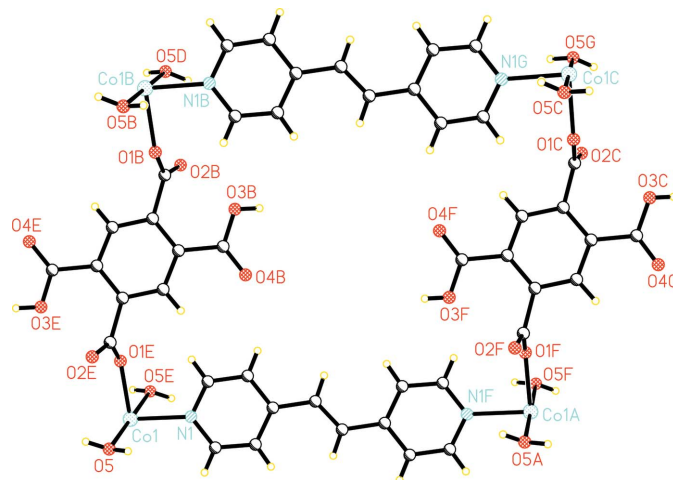


Figure 2

A segment of the two-dimensional complex sheet. [Symmetry codes: (A) $x, y + 1, z - 1$; (B) $x - 1, y - 1, z - 1$; (C) $x - 1, y, z - 2$; (D) $-x, -y, -z - 1$; (E) $1 - x, 1 - y, -z$; (F) $1 - x, 2 - y, -z - 1$; (G) $-x, 1 - y, -2 - z$].

We acknowledge financial support by Zhejiang Provincial Natural Science Foundation of China (grant No. Y404294) and the '551' Distinguished Person Foundation of Wenzhou.

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