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Key indicators

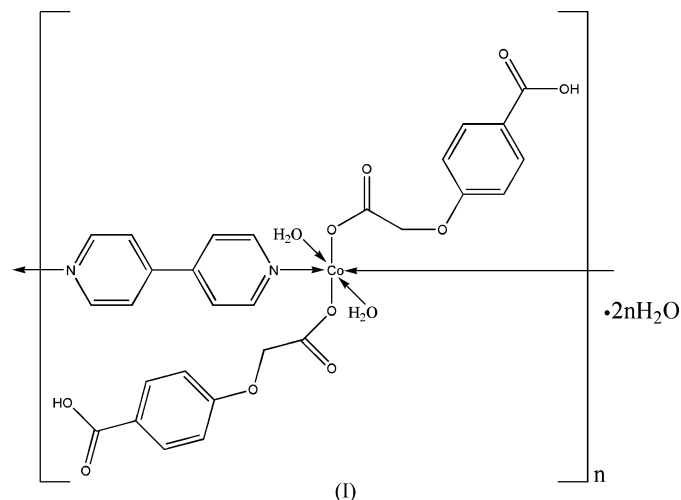
Single-crystal X-ray study
 $T = 295$ K
Mean $\sigma(\text{C}-\text{C}) = 0.005$ Å
 R factor = 0.052
 wR factor = 0.135
Data-to-parameter ratio = 15.2For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.**catena-Poly[[[diaquabis(4-carboxyphenoxy-acetato- κ O)cobalt(II)]- μ -4,4'-bipyridine- κ^2 N,N'] dihydrate]**

The title compound, $\{[\text{Co}(\text{C}_9\text{H}_7\text{O}_5)_2(\text{C}_{10}\text{H}_8\text{N}_2)(\text{H}_2\text{O})_2] \cdot 2\text{H}_2\text{O}\}_n$, has an infinite one-dimensional chain structure along the a axis. The Co atom and the mid-point of the bipyridine group are located on inversion centres. A three-dimensional supramolecular network is built up by $\text{O}-\text{H} \cdots \text{O}$ hydrogen-bonding interactions between water molecules, carboxyl hydroxy groups and carboxylate groups.

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Comment

In recent years, much interest has been focused on using aromatic carboxylic acid ligands to construct supramolecular architectures by self-assembly (Zhang *et al.*, 2004). 4-Carboxyphenoxyacetic acid is a multidentate flexible ligand with versatile binding abilities and the capability of participating in hydrogen bonds as both a donor and an acceptor, thus representing an excellent candidate for the construction of supramolecular complexes. Recently, four one-dimensional Co^{II} polymers based on the 4-carboxyphenoxyacetic acid ligand were reported, namely $\{[\text{Co}(4\text{-carboxyphenoxyacetate})(3\text{-hydroxypyridine})_2(\text{H}_2\text{O})_2](\text{H}_2\text{O})\}_n$ (Gao *et al.*, 2004), $[\text{Co}(4\text{-carboxyphenoxyacetate})(2,2'\text{-bipyridine})(\text{H}_2\text{O})]_n$ (Gao, Huo, Gu, Liu & Zhao, 2005), $[\text{Co}(4\text{-carboxyphenoxyacetate})(1,10\text{-phenanthroline})(\text{H}_2\text{O})]_n$ (Gao, Huo, Gu, Zhao & Zhao, 2005) and $[\text{Co}(4\text{-carboxyphenoxyacetate})_2(4,4'\text{-bipyridine})_2(\text{H}_2\text{O})_2] \cdot 4\text{H}_2\text{O}$ (Deng *et al.*, 2005). In this paper, we report the new title compound, (I), synthesized by the reaction of 4-carboxyphenoxyacetic acid, 4,4'-bipyridine and cobalt dinitrate hexahydrate in an aqueous solution, which forms an infinite one-dimensional chain structure.



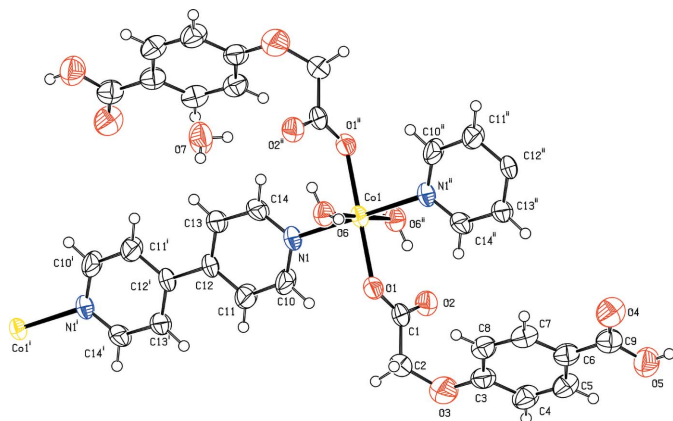


Figure 1
Part of the polymeric structure of the title complex, with the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are represented as spheres of arbitrary radii. [Symmetry codes: (i) $-x, 1 - y, 1 - z$; (ii) $1 - x, 1 - y, 1 - z$].

Complex (I) consists of an infinite one-dimensional chain and uncoordinated water molecules (Fig. 1). The Co atom is located on an inversion centre and is hexacoordinated by two N atoms of the 4,4'-bipyridine ligands, two O atoms of the 4-carboxyphenoxyacetate groups and two water molecules. There is another inversion centre at the mid-point of the central C—C bond of the 4,4'-bipyridine unit.

In the crystal structure, a three-dimensional supramolecular network is constructed *via* O—H...O hydrogen-bonding interactions between water molecules, carboxylic acid hydroxy groups and carboxylate O atoms (Table 1, Fig. 2).

Experimental

4-Carboxyphenoxyacetic acid was prepared by the reaction of chloroacetic acid with 4-hydroxybenzoic acid, and all other chemicals were of analytical grade and used without further purification. 4-Carboxyphenoxyacetic acid (0.98 g, 5 mmol) and 4,4'-bipyridine (0.78 g, 5 mmol) were dissolved in hot water (10 ml), and the pH was adjusted to about 6 using 0.2 M NaOH solution with stirring. Cobalt(II) nitrate hexahydrate (1.46 g, 5 mmol) was added to the mixed solution. The resulting solution was filtered, and the filtrate was allowed to stand in a desiccator at room temperature for several days. Pink block crystals of (I) were obtained.

Crystal data

$[\text{Co}(\text{C}_9\text{H}_7\text{O}_5)_2(\text{C}_{10}\text{H}_8\text{N}_2)(\text{H}_2\text{O})_2] \cdot 2\text{H}_2\text{O}$	$V = 1460.6 (6) \text{ \AA}^3$
$M_r = 677.47$	$Z = 2$
Monoclinic, $P2_1/c$	$D_x = 1.540 \text{ Mg m}^{-3}$
$a = 11.726 (2) \text{ \AA}$	Mo $K\alpha$ radiation
$b = 11.135 (2) \text{ \AA}$	$\mu = 0.66 \text{ mm}^{-1}$
$c = 12.485 (3) \text{ \AA}$	$T = 295 (2) \text{ K}$
$\beta = 116.37 (3)^\circ$	Block, pink
	$0.39 \times 0.36 \times 0.26 \text{ mm}$

Data collection

Rigaku R-AXIS RAPID diffractometer	13737 measured reflections
ω scans	3324 independent reflections
Absorption correction: multi-scan (Higashi, 1995)	2475 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.780, T_{\max} = 0.844$	$R_{\text{int}} = 0.054$
	$\theta_{\text{max}} = 27.5^\circ$

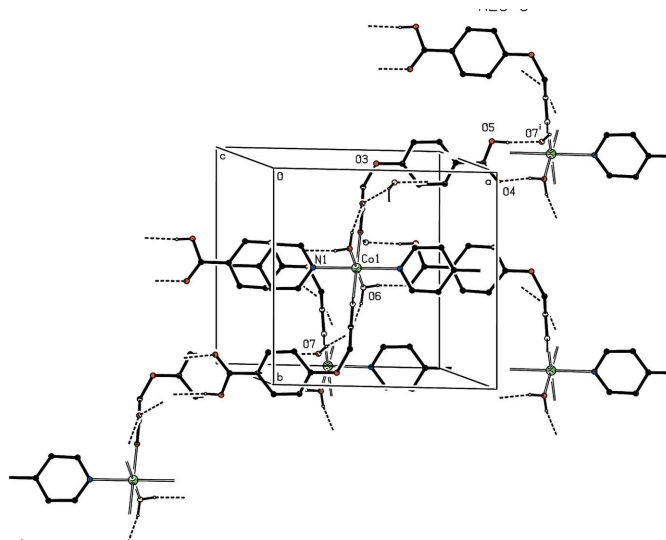


Figure 2
A partial packing view, showing the three-dimensional hydrogen-bonding network. Dashed lines indicate the hydrogen-bonding interactions. H atoms not involved in hydrogen bonds have been omitted for clarity. [Symmetry code: (i) $1 + x, y - 1, z$].

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.074P)^2 + 0.3963P]$
$R[F^2 > 2\sigma(F^2)] = 0.052$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.135$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.06$	$\Delta\rho_{\text{max}} = 0.45 \text{ e \AA}^{-3}$
3324 reflections	$\Delta\rho_{\text{min}} = -0.51 \text{ e \AA}^{-3}$
218 parameters	
H atoms treated by a mixture of independent and constrained refinement	

Table 1

Hydrogen-bond geometry ($\text{\AA}, ^\circ$).

$D\text{---}H \cdots A$	$D\text{---}H$	$H \cdots A$	$D \cdots A$	$D\text{---}H \cdots A$
O5—H5A...O7 ⁱ	0.82	1.77	2.586 (3)	175
O6—H61...O2 ⁱⁱ	0.835 (15)	1.860 (14)	2.648 (3)	157 (3)
O6—H62...O4 ⁱⁱⁱ	0.82 (4)	1.879 (11)	2.695 (3)	171 (3)
O7—H71...O2 ⁱⁱ	0.83 (4)	1.93 (4)	2.751 (3)	169 (5)
O7—H72...O1 ^{iv}	0.83 (4)	2.044 (17)	2.838 (3)	159 (4)

Symmetry codes: (i) $x + 1, y - 1, z$; (ii) $-x + 1, -y + 1, -z + 1$; (iii) $-x + 2, y + \frac{1}{2}, -z + \frac{3}{2}$; (iv) $-x + 1, y + \frac{1}{2}, -z + \frac{3}{2}$.

H atoms bound to C atoms and to the hydroxy group were placed in calculated positions and treated as riding on their parent atoms, with C—H = 0.93 (C_{aromatic}) or 0.97 \AA ($C_{\text{methylene}}$) and O—H = 0.82 \AA , and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C}, \text{O})$. Water H atoms were located in a difference Fourier map and refined using restrained distances O—H = 0.82 (1) \AA and H...H = 1.39 (2) \AA , with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$.

Data collection: *PROCESS-AUTO* (Rigaku, 2002); 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: *ORTEPIII* (Burnett & Johnson, 1996) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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