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Key indicators

Single-crystal X-ray study
 $T = 295\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.005\text{ \AA}$
 R factor = 0.051
 wR factor = 0.136
Data-to-parameter ratio = 15.4For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.**catena-Poly[[aqua(1,10-phenanthroline- $\kappa^2\text{N},\text{N}'$)-
cobalt(II)]- μ -4-carboxyphenoxyacetato- $\kappa^3\text{O},\text{O}':\text{O}''$]**

The Co^{II} atom in the title coordination polymer, $[\text{Co}(\text{C}_9\text{H}_6\text{O}_5)(\text{C}_{12}\text{H}_8\text{N}_2)(\text{H}_2\text{O})]_n$, displays a distorted octahedral geometry defined by three carboxyl O atoms from two independent 4-carboxyphenoxyacetate groups, two N atoms from one 1,10-phenanthroline molecule and one water molecule. The Co^{II} atoms are bridged by carboxylate groups in monodentate and bidentate modes, forming a chain structure. Adjacent polymeric chains are connected *via* hydrogen-bond interactions into a double-chain structure. Furthermore, these chains are stacked through π - π interactions to construct a two-dimensional supramolecular network.

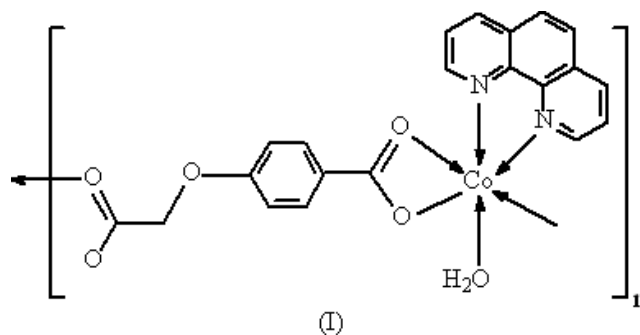
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Comment

4-Carboxyphenoxyacetic acid (4-CPOAH₂) is a multidentate carboxylate with both rigid and flexible parts, and hence it can be an excellent candidate for the construction of supramolecular architectures. Recently, we have reported the structures of some one-dimensional polymers in which the 4-CPOA²⁻ ligand shows various coordination modes, including bi-, tri- and tetradentate (Gu, Gao, Huo *et al.*, 2004; Gu, Gao, Zhao *et al.*, 2004; Gao *et al.*, 2004b). In the reported polymer, namely $[\text{Co}(4\text{-CPOA})(3\text{-hydroxypyridine})_2(\text{H}_2\text{O})_2]\cdot\text{H}_2\text{O}_n$, the octahedral Co^{II} atoms are bridged by bis-monodentate 4-CPOA²⁻ ligands, forming a chain structure (Gao *et al.*, 2004a). For the present study, we used 1,10-phenanthroline (phen) instead of 3-hydroxypyridine in the reaction and have synthesized $[\text{Co}(4\text{-CPOA})(1,10\text{-phen})(\text{H}_2\text{O})]_n$, (I).



As illustrated in Fig. 1, the Co^{II} centre is in a distorted octahedral environment with three carboxyl O atoms from two different 4-CPOA²⁻ groups, two N atoms from one bidentate chelate 1,10-phen molecule and one water molecule.

It is noteworthy that the oxyacetate group functions in a monodentate mode through atom O4, while the carboxyl group chelates the Co^{II} center through carboxylate atoms O1 and O2. The oxyacetate group is twisted out of the plane of the aromatic ring, the C17–O3–C20–C21 torsion angle being

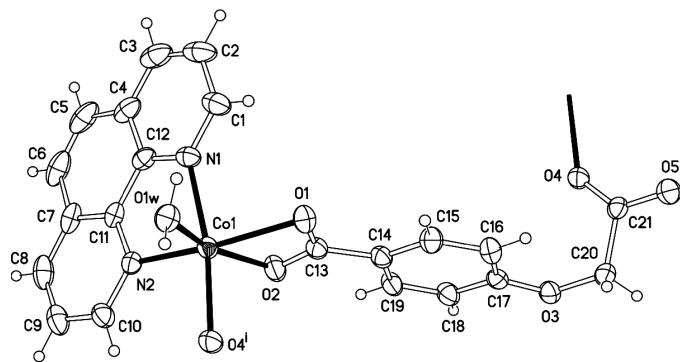


Figure 1
ORTEP plot (Johnson, 1976) of the title complex, with displacement ellipsoids drawn at the 30% probability level. See Table 1 for symmetry codes.

$-72.7(3)^\circ$, whereas the dihedral angle between the carboxylate group (O1/C13/O2) and the aromatic ring is $58.1(3)^\circ$.

Adjacent Co^{II} atoms are joined by 4-CPOA $^{2-}$ ligands, forming a one-dimensional chain structure. Two adjacent chains are further interlinked through hydrogen bonds between the coordinated water molecule and O atoms of carboxylate groups (Table 2), leading to a double-chain structure, as shown in Fig. 2. Furthermore, there are π - π stacking interactions in an offset manner between the phen rings at $3.662(3) \text{ \AA}$. The polymeric chains align in a manner that facilitates both hydrogen-bonding and π - π interactions in the two-dimensional supramolecular network.

Experimental

The title complex was prepared by the addition of 1,10-phenanthroline (0.40 g, 2 mmol) and cobalt diacetate trihydrate (0.48 g, 2 mmol) to an aqueous solution of 4-carboxyphenoxyacetic acid (0.39 g, 2 mmol), and the pH was adjusted to 6 with 0.1 M sodium hydroxide. The mixture was sealed in a 23 ml Teflon-lined stainless steel bomb and held at 423 K for 4 d. The bomb was cooled naturally to room temperature and pink prismatic crystals were obtained after several days. Analysis calculated for $\text{C}_{21}\text{H}_{16}\text{CoN}_2\text{O}_6$: C 55.89, H 3.57, N 6.21%; found: C 55.71, H 3.60, N 6.19%.

Crystal data

$[\text{Co}(\text{C}_9\text{H}_6\text{O}_5)(\text{C}_{12}\text{H}_8\text{N}_2)(\text{H}_2\text{O})]$
 $M_r = 451.29$
 Triclinic, $P\bar{1}$
 $a = 9.5043(19) \text{ \AA}$
 $b = 9.812(2) \text{ \AA}$
 $c = 11.584(2) \text{ \AA}$
 $\alpha = 70.73(3)^\circ$
 $\beta = 67.49(3)^\circ$
 $\gamma = 83.26(3)^\circ$
 $V = 942.0(4) \text{ \AA}^3$

$Z = 2$
 $D_x = 1.591 \text{ Mg m}^{-3}$
 Mo $K\alpha$ radiation
 Cell parameters from 7059 reflections
 $\theta = 3.9\text{--}27.4^\circ$
 $\mu = 0.95 \text{ mm}^{-1}$
 $T = 295(2) \text{ K}$
 Prism, pink
 $0.37 \times 0.25 \times 0.18 \text{ mm}$

Data collection

Rigaku R-Axis RAPID diffractometer
 ω scans
 Absorption correction: multi-scan (ABSCOR; Higashi, 1995)
 $T_{\text{min}} = 0.719$, $T_{\text{max}} = 0.847$
 8864 measured reflections

4264 independent reflections
 3639 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.037$
 $\theta_{\text{max}} = 27.5^\circ$
 $h = -11 \rightarrow 12$
 $k = -12 \rightarrow 12$
 $l = -14 \rightarrow 14$

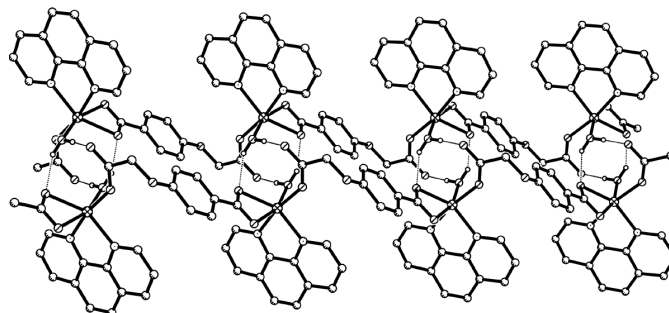


Figure 2
A double-chain structure constructed by hydrogen bonds (dashed lines). C-bound H atoms on C atoms have been omitted.

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.051$
 $wR(F^2) = 0.136$
 $S = 1.04$
 4264 reflections
 277 parameters
 H atoms treated by a mixture of independent and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.082P)^2 + 0.3727P]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

$$(\Delta/\sigma)_{\text{max}} < 0.001$$

$$\Delta\rho_{\text{max}} = 0.82 \text{ e \AA}^{-3}$$

$$\Delta\rho_{\text{min}} = -0.54 \text{ e \AA}^{-3}$$

Table 1

Selected geometric parameters (\AA , $^\circ$).

Co1—O1	2.163 (2)	Co1—N2	2.113 (2)
Co1—O2	2.205 (2)	O1—C13	1.270 (3)
Co1—O4 ⁱ	2.066 (2)	O2—C13	1.258 (3)
Co1—O1W	2.040 (2)	O4—C21	1.248 (3)
Co1—N1	2.168 (2)	O5—C21	1.253 (3)
O1—Co1—O2	60.35 (8)	O1W—Co1—O4 ⁱ	91.15 (9)
O1—Co1—N1	88.70 (9)	O1W—Co1—N1	88.36 (9)
O4 ⁱ —Co1—O1	101.03 (8)	O1W—Co1—N2	104.71 (9)
O4 ⁱ —Co1—O2	89.74 (9)	N1—Co1—O2	94.01 (9)
O4 ⁱ —Co1—N1	170.19 (9)	N2—Co1—O1	150.79 (8)
O4 ⁱ —Co1—N2	93.52 (8)	N2—Co1—O2	94.88 (9)
O1W—Co1—O1	100.21 (8)	N2—Co1—N1	77.15 (9)
O1W—Co1—O2	160.29 (8)		

Symmetry code: (i) $1 + x, y, z$.

Table 2

Hydrogen-bonding geometry (\AA , $^\circ$).

$D\text{---}H\cdots A$	$D\text{---}H$	$H\cdots A$	$D\cdots A$	$D\text{---}H\cdots A$
O1W—H1W1 \cdots O5 ⁱⁱ	0.85 (3)	1.78 (3)	2.619 (3)	172 (4)
O1W—H1W2 \cdots O1 ⁱⁱⁱ	0.84 (3)	2.06 (2)	2.760 (3)	141 (3)

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

C-bound H atoms were placed in calculated positions, with $C\text{---}H = 0.93$ or 0.97 \AA and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$, and were refined in the riding-model approximation. The H atoms of water molecules were located in difference Fourier maps and refined with $O\text{---}H$ and $H\cdots H$ distance restraints of $0.85(1)$ and $1.39(1) \text{ \AA}$, respectively, and with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MS, 2002); 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: *SHELXL97*.

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