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catena-Poly[bis[aqua(1,10-phenanthroline)-cobalt(II)]-μ_4-1,2,4,5-benzenetetracarboxylato]

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.013 Å
R factor = 0.074
wR factor = 0.195
Data-to-parameter ratio = 11.4

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

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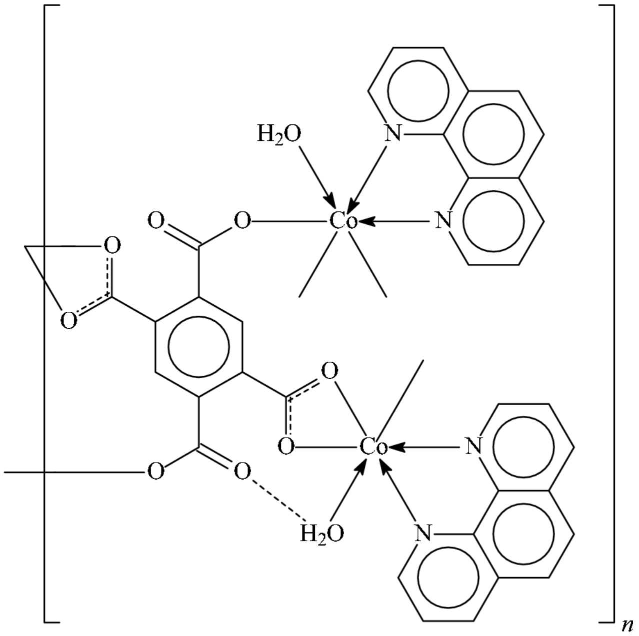
The title compound, $[Co_2(C_{10}H_2O_8)(C_{12}H_8N_2)_2(H_2O)_2]_n$, adopts a linear chain structure in which the tetra-anionic ligand, which lies on a special position of $\bar{1}$ site symmetry, uses two O atoms of one carboxylate group to bind to one Co atom and the O atom of the carboxyl group at the *ortho* position to bind to another Co atom. Each Co atom is also chelated by the *N*-heterocycle, and its sixth coordination site is occupied by a water molecule.

Comment

This study continues a recent study on cobalt(II) pyromellitate complexes (Fu *et al.*, 2004) and follows the report on $[(C_{10}H_2O_8)(C_{12}H_8N_2)_2Cu_2{\cdot}2H_2O]_n$ (Zhang *et al.*, 2003). Unlike the copper complex, which has the metal atom in a tetrahedral geometry, the title cobalt compound, (I), although having the same chemical formula with Co replacing Cu (Fig. 1), has a different architecture. The unique metal atom is chelated by the *N*-heterocycle and by one carboxyl $-CO_2$ arm of the 1,2,4,5-benzenetetracarboxylate (pyromellitate) tetra-anion, and is coordinated by the water molecule. It is also bonded to one O atom of a non-equivalent carboxyl unit of an adjacent tetra-anion, this unit displaying unambiguous carbon–oxygen single and double bonds. The double-bond O atom engages in hydrogen bonding with the water molecule (Fig. 2).



(I)

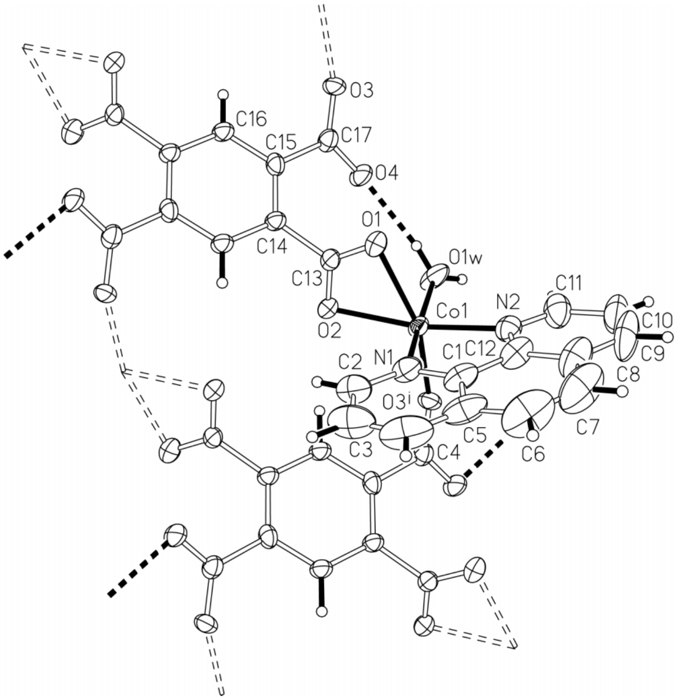


Figure 1
*ORTEP*II (Johnson, 1976) plot of a portion of $[Co_2(C_{10}H_2O_8)(C_{12}H_8N_2)_2(H_2O)_2]_n$. Displacement ellipsoids are drawn at the 50% probability level, and H atoms are drawn as spheres of arbitrary radii. [Symmetry code: (i) = 1 + *x*, *y*, *z*.]

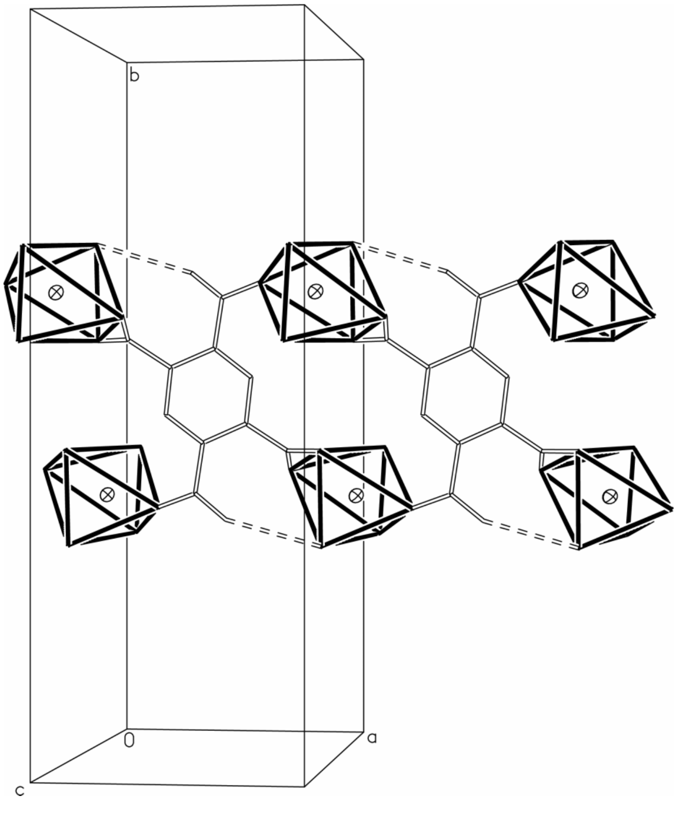


Figure 2
Schematic representation of the chain structure; the coordination geometry around the Co atom is depicted as an octahedron.

Only a few *N*-heterocycle adducts of cobalt(II) pyromellitate have been reported; among these are an imidazole adduct that was synthesized in aqueous solution (Wang *et al.*, 2000), an *N*-methylimidazole adduct that was synthesized hydrothermally (Cheng *et al.*, 2002) and a DMF adduct that was synthesized solvothermally (Fu *et al.*, 2004).

Experimental

Cobalt(II) nitrate hexahydrate (0.28 g, 1.0 mmol), pyromellitic acid (0.13 g, 0.5 mmol) and 1,10-phenanthroline (0.11 g, 1.0 mmol) were dissolved in *N*,*N*-dimethylformamide (10 ml). The mixture was sealed in a Teflon-lined stainless steel bomb, which was heated at 393 K for 4 d. Orange crystals were obtained when the bomb was cooled slowly to room temperature. Analysis found: C 53.44, H 2.78, N 7.34%; calculated for $C_{34}H_{22}Co_2N_4O_{10}$: C 53.42, H 2.90, N 7.33%.

Crystal data

$[Co_2(C_{10}H_2O_8)(C_{12}H_8N_2)_2(H_2O)_2]$
$M_r = 764.42$
Monoclinic, $P2_1/a$
$a = 7.542$ (2) Å
$b = 21.220$ (5) Å
$c = 9.478$ (2) Å
$\beta = 95.836$ (4)°
$V = 1509.1$ (6) Å^3
$Z = 2$
$D_x = 1.682$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 759 reflections
$\theta = 2.4–19.9°$
$\mu = 1.17$ mm^{-1}
$T = 295$ (2) K
Bar, orange
0.31 × 0.09 × 0.06 mm

Data collection

Bruker APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{min} = 0.157$, $T_{max} = 0.933$
7206 measured reflections
2647 independent reflections
1827 reflections with $I > 2\sigma(I)$
$R_{int} = 0.074$
$\theta_{max} = 25.0°$
$h = -8 \rightarrow 5$
$k = -22 \rightarrow 25$
$l = -8 \rightarrow 11$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.074$
$wR(F^2) = 0.195$
$S = 1.08$
2647 reflections
232 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0914P)^2 + 1.3411P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.32$ e Å^{-3}
$\Delta\rho_{min} = -0.44$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—O1	2.231 (5)	Co1—O1*w*	2.055 (5)
Co1—O2	2.128 (4)	Co1—N1	2.139 (6)
Co1—O3^i	2.024 (4)	Co1—N2	2.122 (6)
O1—Co1—O2	60.3 (2)	O2—Co1—N2	166.1 (2)
O1—Co1—O3^i	161.5 (2)	O2—Co1—O1*w*	85.5 (2)
O1—Co1—O1*w*	86.2 (2)	O3^i—Co1—O1*w*	91.7 (2)
O1—Co1—N1	87.4 (2)	O3^i—Co1—N1	96.6 (2)
O1—Co1—N2	106.1 (2)	O3^i—Co1—N2	92.4 (2)
O2—Co1—O3^i	101.3 (2)	O1*w*—Co1—N1	170.4 (2)
O2—Co1—N1	97.6 (2)	O1*w*—Co1—N2	97.0 (2)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O1w—H1w1···O4	0.85 (1)	2.08 (2)	2.916 (7)	167 (6)
O1w—H1w2···O4^{ii}	0.85 (1)	1.92 (2)	2.763 (6)	172 (6)

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

The quality of the diffraction measurements was not optimal. The water H atoms were located and refined with distance restraints of O—H = 0.85 (1) Å and H···H = 1.39 (1) Å, and with U_{iso}(H) = 1.2U_{eq}(O). Other H atoms were placed at calculated positions (C—H = 0.93 Å) and refined in the riding-model approximation, with U_{iso}(H) = 1.2U_{eq}(C). The final difference Fourier map had a large peak about 1 Å from atom O1 and 2 Å from atom Co1.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; 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.

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