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catena-Poly[bis[aqua(1,10-phenanthroline-κ^2N,N')-cobalt(II)]-di-μ-4,4′-oxydibenzoato-1:2$\kappa^4O:O'$]

Hong-Ping Xiao,[a]* Xin-Hua Li[a] and Seik Weng Ng[b]

[a]School of Chemistry and Materials Science, Wenzhou Normal College, Wenzhou 325027, People's Republic of China, and [b]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia

Correspondence e-mail: hp_xiao@wznc.zj.cn

Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.003 Å
R factor = 0.034
wR factor = 0.092
Data-to-parameter ratio = 15.2

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

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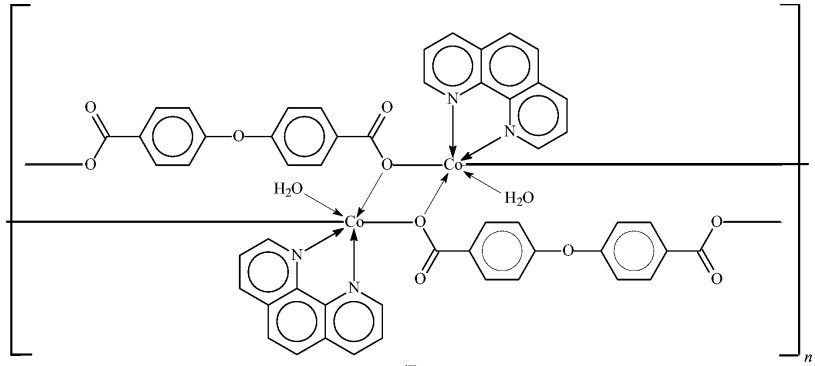
In the crystal structure of the title compound, $[Co_2(C_{14}H_8O_5)_2(C_{12}H_8N_2)_2(H_2O)_2]_n$, the dianion functions as a bridging ligand, bonding through both carboxyl $-CO_2$ end groups to link symmetry-related $[Co(C_{12}H_8N_2)(H_2O)]$ entities into a ribbon structure.

Comment

In the compound $[Co(C_{14}H_8O_5)(C_{10}H_8N_2)]_n$, the bidentate bonding mode of the carboxylate dianion leads to a linear chain motif (Skakle *et al.*, 2001). The reaction of cobalt(II) acetate, 4,4′-oxybisbenzoic acid and 1,10-phenanthroline affords the related polymeric title compound, $[Co_2(C_{12}H_8N_2)_2(C_{14}H_8O_5)_2(H_2O)_2]_n$, (I), in which 1,10-phenanthroline replaces 2,2′-bipyridine. The hydrothermal synthesis yields a compound having two water molecules in the formula unit.



(I)

Although the dicarboxylate moiety of (I) links the $[Co(C_{12}H_8N_2)(H_2O)]$ entities into a linear chain, as in the 2,2′-bipyridine compound, in (I) the two carboxyl $-CO_2$ fragments are only monodentate in the chain. The O atom of one repeat unit bonds to a Co atom of a symmetry-related unit, completing the distorted octahedral Co environment (Fig. 1). This gives rise to the formation of a ribbon structure (Fig. 2).

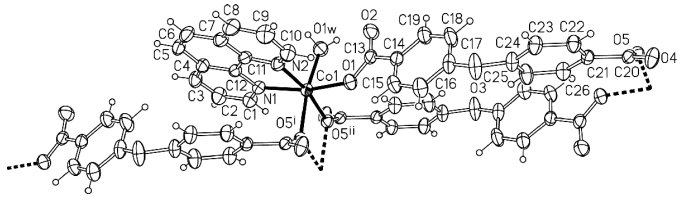


Figure 1
A plot illustrating the octahedral geometry of the Co atom in a fragment of the ribbon structure of (I). Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii. [Symmetry codes: (i) $1-x, 2-y, 1-z$; (ii) $x, y, z-1$].

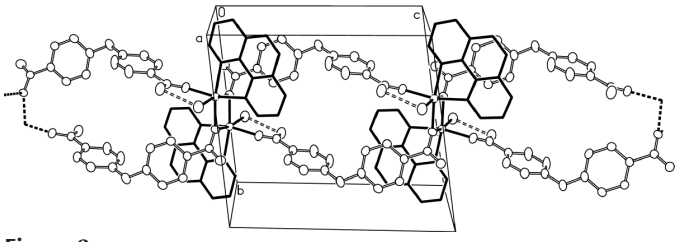


Figure 2
An illustration of the ribbon structure of (I). Dashed lines indicate hydrogen bonds.

The ribbons are linked into layers by O—H···O hydrogen bonds (Table 2).

Experimental

Cobalt(II) acetate tetrahydrate (0.125 g, 0.5 mmol), 4,4′-oxybisbenzoic acid (0.129 g, 0.5 mmol) and 1,10-phenanthroline (0.180 g, 1.0 mmol) were placed in a 30 ml Teflon-lined stainless-steel Parr bomb, together with water (20 ml). The bomb was heated at 423 K for 6 d and then cooled slowly to room temperature to furnish red crystals of (I).

Crystal data

$[Co_2(C_{14}H_8O_5)_2(C_{12}H_8N_2)_2(H_2O)_2]$
M_r = 1026.71
Triclinic, $P\overline{1}$
a = 7.7129 (4) Å
b = 11.5063 (6) Å
c = 13.3854 (7) Å
α = 82.614 (1)°
β = 83.165 (1)°
γ = 72.724 (1)°
V = 1120.8 (1) Å^3
Z = 1
D_x = 1.521 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 5331 reflections
θ = 2.5–28.3°
μ = 0.81 mm^{-1}
T = 295 (2) K
Prism, red
0.34 × 0.27 × 0.23 mm

Data collection

Bruker APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
T_{min} = 0.770, T_{max} = 0.835
9587 measured reflections
4919 independent reflections
4510 reflections with $I > 2\sigma(I)$
R_{int} = 0.014
θ_{max} = 27.5°
$h = -10 \rightarrow 10$
$k = -14 \rightarrow 14$
$l = -17 \rightarrow 17$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.092
S = 1.03
4919 reflections
324 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0553P)^2 + 0.3018P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—O1	2.053 (1)	Co1—O1*W*	2.094 (1)
Co1—O5^{iii}	2.108 (1)	Co1—N1	2.121 (1)
Co1—O5^{iv}	2.122 (1)	Co1—N2	2.161 (1)
O1—Co1—O5^{iii}	91.30 (5)	O5^{iii}—Co1—N2	94.16 (5)
O1—Co1—O5^{iv}	98.51 (5)	O5^{iv}—Co1—O1*W*	88.92 (5)
O1—Co1—O1*W*	88.10 (5)	O5^{iv}—Co1—N1	96.53 (5)
O1—Co1—N1	164.66 (5)	O5^{iv}—Co1—N2	169.23 (5)
O1—Co1—N2	88.34 (5)	O1*W*—Co1—N1	89.18 (6)
O5^{iii}—Co1—O5^{iv}	77.47 (5)	O1*W*—Co1—N2	99.66 (6)
O5^{iii}—Co1—O1*W*	166.14 (5)	N1—Co1—N2	77.24 (6)
O5^{iii}—Co1—N1	94.90 (5)		

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

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*1···O2	0.85 (1)	1.86 (2)	2.675 (2)	161 (3)
O1*W*—H1*W*2···O4^{v}	0.84 (1)	1.93 (1)	2.764 (2)	175 (2)

Symmetry codes: (v) $x+1, y, z+1$.

H atoms bonded to C atoms were included in the refinement in calculated positions in the riding-model approximation, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C). The water H atoms were located and refined with a distance restraint of 0.85 (1) Å and with U_{iso}(H) = 1.2U_{eq}(O).

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: *SHELXL97*.

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