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Bis[tetraaqua(1,10-phenanthroline-κ^2N,N')-cobalt(II)] 1,2,4,5-benzenetetracarboxylate

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The title compound, $[Co(C_{12}H_8N_2)(H_2O)_4]_2(C_{10}H_2O_8)$, consists of discrete tetraaqua(1,10-phenanthroline)cobalt(II) cations and 1,2,4,5-benzenetetracarboxylate anions. The Co^{II} atom is octahedrally coordinated by two N atoms of the 1,10-phenanthroline ligand and four O atoms of water molecules. The anion lies on an inversion centre. A two-dimensional hydrogen-bonding network is formed by O atoms of benzenetetracarboxylate and the coordinated water molecules.

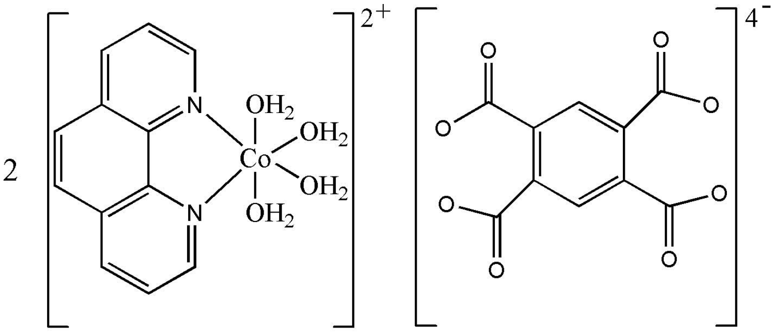
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.035
wR factor = 0.087
Data-to-parameter ratio = 13.9

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

Comment

Polycarboxylate ligands are of considerable theoretical and practical interest. 1,2,4,5-Benzenetetracarboxylate has four carboxylate groups and can act as a versatile bridging or chelating ligand, leading to extended metal-organic networks. It can coordinate to metal cations in numerous ways, in one-atom bridging, three-atom bridging and chelating modes. It can also form hydrogen bonds with uncoordinated or coordinated water molecules (Zou *et al.*, 1998). Many coordination compounds with new interesting structures have been reported, such as $[C_{10}H_2Ag_4O_8]_n$ and $[C_{10}H_6Ag_4O_{10}]_n$ (Sun *et al.*, 2004), $[C_{12}H_6Co_3O_{14}]_n$ (Li *et al.*, 2003), $[C_{22}H_{18}Co_2N_8O_8]_n$ (Zhang *et al.*, 2003), $[C_{20}H_{20}Co_4O_{24}]_n.4nH_2O$ (Kumagai *et al.*, 2002), and $[C_{20}H_{10}Nd_2O_{18}]_n$ (Sun *et al.*, 2002). In this paper, we report the crystal structure of the title compound, 2[Co(phen)$(H_2O)_4$](btc), (I), where phen is 1,10-phenanthroline and btc is 1,2,4,5-benzenetetracarboxylate.



(I)

The structure of (I) consists of Co^{II} complex cations and btc counter-anions (Fig. 1). In the cation, the Co^{II} atom is coordinated by two N atoms (N1 and N2) from the phen ligand and four O atoms (O1, O2, O3 and O4) from the water molecules. The average Cu—N and Cu—O bond lengths are 2.130 (2) and 2.090 (2) Å, respectively, which are comparable to the values found in the compounds $[Co(H_2O)_6](H_2btc)$ (Kumagai *et al.*, 2002) and $[Co_2(phen)_2(H_2btc)_2(H_2O)_2]_n$ (Hu

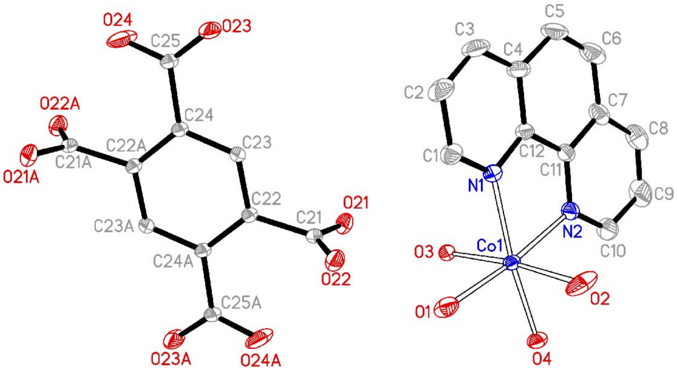


Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme. H atoms have been omitted for clarity. Atoms with the suffix *A* are generated by the symmetry code ($-x$, $1 - y$, $-z$).

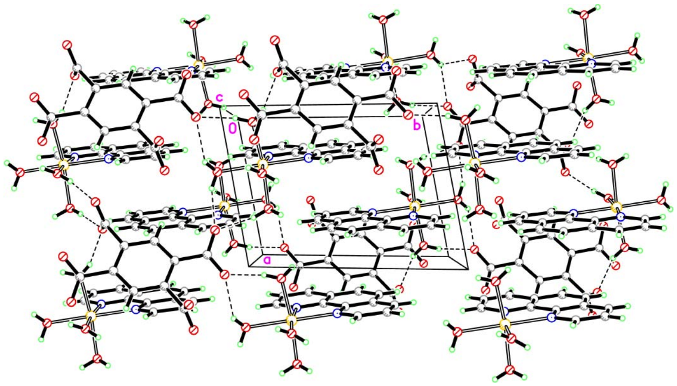


Figure 2
The packing diagram of (I), showing the hydrogen-bonding scheme as dashed lines.

et al., 2004). Although the O atoms of the carboxylate ligands do not coordinate to the Co^{II} atom, they form a two-dimensional hydrogen-bonding network with the O atoms of the coordinated water molecules (Fig. 2).

Experimental

An ethanol solution (10 ml) of cobalt(II) acetate tetrahydrate (25 mg, 0.1 mmol) was carefully layered with a mixed solvent solution (10 ml, ethanol/water, 25:75) of sodium 1,2,4,5-benzenetetracarboxylate (34 mg, 0.1 mmol) and phenanthroline (18 mg, 0.1 mmol). Red needle-shaped crystals suitable for X-ray diffraction determination were formed after several days. Analysis found: C 45.78, H 3.69, N 6.18%; calculated for $C_{17}H_{17}CoN_2O_8$: C 46.80, H 3.93, N 6.42%.

Crystal data

$[Co(C_{12}H_8N_2)(H_2O)_4]_2(C_{10}H_2O_8)$
$M_r = 872.52$
Triclinic, $P\overline{1}$
$a = 7.3184$ (4) Å
$b = 9.8767$ (6) Å
$c = 12.5639$ (7) Å
$\alpha = 76.600$ (3)°
$\beta = 88.384$ (3)°
$\gamma = 79.414$ (3)°
$V = 868.28$ (9) Å^3

$Z = 1$
$D_x = 1.669$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 6047 reflections
$\theta = 2.2$–27.4°
$\mu = 1.04$ mm^{-1}
$T = 293$ (2) K
Needle, red
0.38 × 0.12 × 0.12 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Oscillation scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.693$, $T_{max} = 0.885$
6047 measured reflections

3866 independent reflections
3295 reflections with $I > 2\sigma(I)$
$R_{int} = 0.031$
$\theta_{max} = 27.4°$
$h = -9 \rightarrow 9$
$k = -12 \rightarrow 12$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.087$
$S = 1.03$
3866 reflections
278 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0453P)^2 + 0.4128P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.38$ e Å^{-3}
$\Delta\rho_{min} = -0.39$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0101 (15)

Table 1
Selected geometric parameters (Å, °).

Co1—O1	2.0750 (17)	Co1—O4	2.1524 (15)
Co1—O2	2.0350 (18)	Co1—N1	2.1397 (16)
Co1—O3	2.1016 (15)	Co1—N2	2.1204 (18)
O1—Co1—O2	91.32 (9)	O2—Co1—N2	90.37 (9)
O1—Co1—O3	86.90 (7)	O3—Co1—O4	86.99 (6)
O1—Co1—O4	93.85 (7)	O3—Co1—N1	90.44 (6)
O1—Co1—N1	95.59 (7)	O3—Co1—N2	92.07 (6)
O1—Co1—N2	173.67 (7)	O4—Co1—N1	170.07 (6)
O2—Co1—O3	173.48 (6)	O4—Co1—N2	92.33 (6)
O2—Co1—O4	86.87 (7)	N1—Co1—N2	78.17 (7)
O2—Co1—N1	95.98 (7)		

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
O1—H1A⋯O22	0.82 (3)	1.83 (3)	2.646 (3)	173 (4)
O1—H1C⋯O1^{i}	0.80 (3)	2.39 (3)	2.874 (3)	120 (3)
O1—H1C⋯O23^{ii}	0.80 (3)	2.44 (3)	2.979 (3)	126 (3)
O2—H2A⋯O24^{iii}	0.82 (3)	1.81 (2)	2.623 (3)	168 (3)
O2—H2C⋯O21^{iv}	0.82 (3)	1.90 (3)	2.670 (3)	157 (3)
O3—H3A⋯O23^{v}	0.82 (3)	1.90 (3)	2.705 (2)	168 (3)
O3—H3C⋯O21	0.82 (3)	1.86 (3)	2.682 (2)	177 (4)
O4—H4A⋯O23^{v}	0.82 (2)	1.96 (2)	2.740 (3)	157 (4)
O4—H4B⋯O22^{i}	0.82 (3)	2.27 (3)	2.919 (2)	137 (3)
O4—H4B⋯O24^{iii}	0.82 (3)	2.17 (3)	2.845 (3)	140 (3)

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

Water H atoms were located in a difference Fourier map and refined with restrained O—H bond lengths [0.82 (2) Å] and fixed isotropic displacement parameters (0.08 Å^2). Other H atoms were placed at calculated positions and refined using a riding model, with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *RAPID-AUTO* (Rigaku, 2001); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* (Siemens, 1994); software used to prepare material for publication: *SHELXTL* (Siemens, 1995).

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