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Tetraaqua-1,2,4,5-benzenetetracarboxylato-(pyrazine)dicobalt(II) dihydrate

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The Co(II) atom in polymeric $\{[Co_2(C_{10}H_2O_8)(C_4H_4N_2)(H_2O)_4]\cdot 2H_2O\}_n$ exists in an octahedral coordination environment defined by the two O atoms of a chelating carboxyl group, the O atom of a monodentate carboxyl group of another benzenetetracarboxylato unit, two water molecules and the N atom of the pyrazine. The tetraanionic ligand and the *N*-heterocycle are located on inversion centers. The layer structure is linked by hydrogen bonds into a network structure.

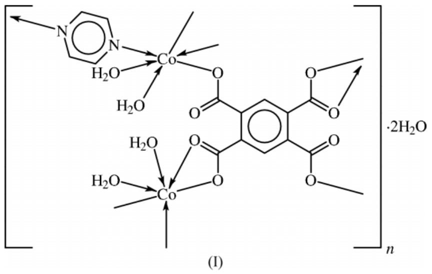
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.035
wR factor = 0.082
Data-to-parameter ratio = 12.3

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

Comment

A recent study documented the structure of polymeric tetraaqua(1,2,4,5-benzenetetracarboxylato)(pyrazine)dinickel(II) dihydrate (Yang *et al.*, 2003). The cobalt(II) analog was synthesized under similar reaction conditions in this study. The structure of the Ni compound has been presented in detail; a similar description applies to the present isomorphous compound (Fig. 1).



(I)

Experimental

Sodium hydroxide (0.16 g, 4 mmol) and pyromellitic anhydride (0.22 g, 1 mmol) were dissolved in water (15 ml). Cobalt(II) nitrate hexahydrate (0.58 g, 2 mmol) and pyrazine (0.16 g, 2 mmol) were dissolved in water (3 ml) and the two solutions were mixed. The mixture was placed in a 20 ml Teflon-lined stainless-steel bomb. The bomb was heated at 423 K for 20 h. Crystals separated from the solution when the bomb was cooled to room temperature at 5 K h^{-1}.

Crystal data

$[Co_2(C_{10}H_2O_8)(C_4H_4N_2)(H_2O)_4]\cdot 2H_2O$
M_r = 556.16
Triclinic, $P\bar{1}$
a = 7.2342 (4) Å
b = 8.0693 (5) Å
c = 9.3975 (6) Å
α = 96.114 (1)°
β = 102.350 (1)°
γ = 116.053 (1)°
V = 468.71 (5) Å^3
Z = 1
D_x = 1.970 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3407 reflections
θ = 2.3–28.3°
μ = 1.85 mm^{-1}
T = 298 (2) K
Prism, red
0.48 × 0.27 × 0.16 mm

Data collection

Bruker SMART APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.406$, $T_{\max} = 0.744$
4046 measured reflections
2084 independent reflections
1780 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.030$
$\theta_{\max} = 27.5°$
$h = -9 \rightarrow 9$
$k = -10 \rightarrow 10$
$l = -12 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.082$
$S = 0.95$
2084 reflections
169 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0368P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.58$ e Å^{-3}
$\Delta\rho_{\min} = -0.56$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—O1	2.179 (2)	Co1—O1*w*	2.077 (2)
Co1—O2	2.147 (2)	Co1—O2*w*	2.030 (2)
Co1—O3$^{\rm i}$	2.047 (2)	Co1—N1	2.123 (2)
O1—Co1—O2	60.5 (1)	O2—Co1—N1	85.3 (1)
O1—Co1—O3$^{\rm i}$	84.6 (1)	O3$^{\rm i}$—Co1—O1*w*	93.4 (1)
O1—Co1—O1*w*	100.7 (1)	O3$^{\rm i}$—Co1—O2*w*	90.1 (1)
O1—Co1—O2*w*	163.7 (1)	O3$^{\rm i}$—Co1—N1	173.3 (1)
O1—Co1—N1	91.4 (1)	O1*w*—Co1—O2*w*	95.0 (1)
O2—Co1—O3$^{\rm i}$	88.1 (1)	O1*w*—Co1—N1	92.7 (1)
O2—Co1—O1*w*	160.9 (1)	O2*w*—Co1—N1	92.3 (1)
O2—Co1—O2*w*	104.1 (1)		

Symmetry code: (i) $1 - x, 1 - y, 2 - z$.

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O1*w*—H1*w*2$\cdots$O1$^{\rm ii}$	0.84 (1)	1.90 (2)	2.645 (3)	147 (3)
O1*w*—H1*w*1$\cdots$O4$^{\rm i}$	0.85 (1)	1.87 (2)	2.645 (3)	152 (3)
O2*w*—H2*w*2$\cdots$O1*w*$^{\rm iii}$	0.84 (1)	1.98 (1)	2.816 (3)	171 (4)
O2*w*—H2*w*1$\cdots$O3*w*$^{\rm iv}$	0.85 (1)	1.89 (1)	2.723 (3)	167 (4)
O3*w*—H3*w*1$\cdots$O2	0.85 (1)	2.25 (2)	3.069 (3)	165 (4)
O3*w*—H3*w*2$\cdots$O3$^{\rm v}$	0.84 (1)	1.99 (1)	2.833 (3)	175 (4)

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

A value of 0.50 was used in the θ-dependent absorption correction in *SADABS* (Sheldrick, 1996). The atomic coordinates of the published Ni compound (Yang *et al.*, 2003) were used as the starting point for refinement.

The aromatic H atoms were positioned geometrically (C—H 0.93 Å) and were allowed to ride on the C atoms, with U(H) = $1.2U_{\rm eq}$(C). The water H-atoms were located and refined with an O—H 0.85 (1) Å distance restraint.

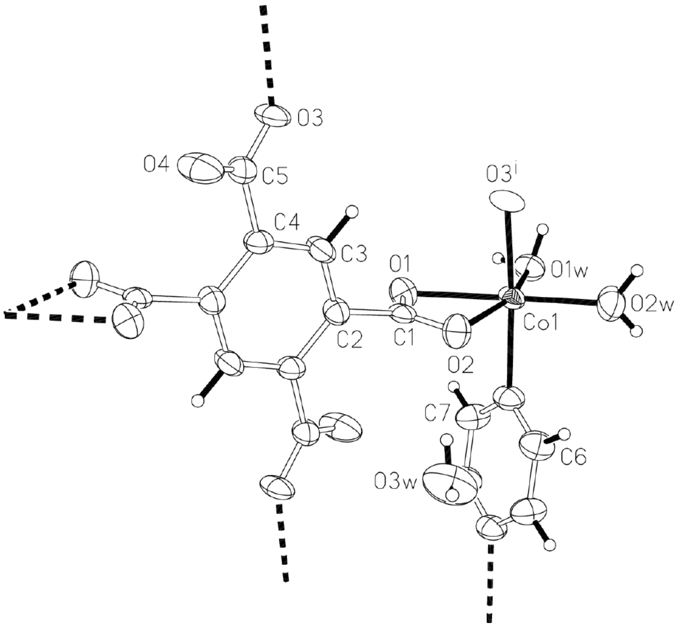


Figure 1
ORTEP (Johnson, 1976) plot of a segment of the title structure, with displacement ellipsoids drawn at the 75% probability level. [Symmetry code: (i) $1 - x, 1 - y, 2 - z$.]

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; method used to solve structure: atomic coordinates taken from isomorphous Ni compound (Yang *et al.*, 2003); 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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