

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

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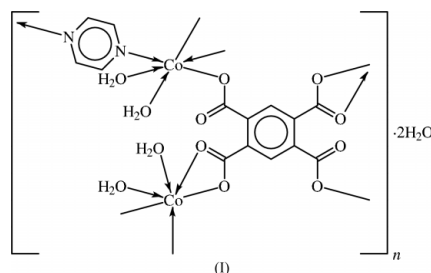
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The Co(II) atom in polymeric  $\{[\text{Co}_2(\text{C}_{10}\text{H}_2\text{O}_8)(\text{C}_4\text{H}_4\text{N}_2)(\text{H}_2\text{O})_4] \cdot 2\text{H}_2\text{O}\}_n$  exists in an octahedral coordination environment defined by the two O atoms of a 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.

## Comment

A recent study documented the structure of polymeric tetraqua(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).



## Key indicators

Single-crystal X-ray study

T = 298 K

Mean  $\sigma(\text{C}-\text{C}) = 0.004 \text{ \AA}$ 

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>.

## 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  $5 \text{ K h}^{-1}$ .

## Crystal data

 $[\text{Co}_2(\text{C}_{10}\text{H}_2\text{O}_8)(\text{C}_4\text{H}_4\text{N}_2)(\text{H}_2\text{O})_4] \cdot 2\text{H}_2\text{O}$ 
 $M_r = 556.16$ Triclinic,  $P\bar{1}$  $a = 7.2342 (4) \text{ \AA}$  $b = 8.0693 (5) \text{ \AA}$  $c = 9.3975 (6) \text{ \AA}$  $\alpha = 96.114 (1)^\circ$  $\beta = 102.350 (1)^\circ$  $\gamma = 116.053 (1)^\circ$  $V = 468.71 (5) \text{ \AA}^3$ 

Z = 1

 $D_x = 1.970 \text{ Mg m}^{-3}$ Mo  $K\alpha$  radiation

Cell parameters from 3407

reflections

 $\theta = 2.3\text{--}28.3^\circ$  $\mu = 1.85 \text{ mm}^{-1}$ 

T = 298 (2) K

Prism, red

 $0.48 \times 0.27 \times 0.16 \text{ mm}$

Data collection

Bruker SMART APEX area-detector diffractometer  
 $\varphi$  and  $\omega$  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  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.030$   
 $\theta_{\text{max}} = 27.5^\circ$   
 $h = -9 \rightarrow 9$   
 $k = -10 \rightarrow 10$   
 $l = -12 \rightarrow 12$

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  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.001$   
 $\Delta\rho_{\text{max}} = 0.58 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.56 \text{ e } \text{\AA}^{-3}$

Table 1

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

Co1—O1	2.179 (2)	Co1—O1w	2.077 (2)
Co1—O2	2.147 (2)	Co1—O2w	2.030 (2)
Co1—O3 <sup>i</sup>	2.047 (2)	Co1—N1	2.123 (2)
O1—Co1—O2	60.5 (1)	O2—Co1—N1	85.3 (1)
O1—Co1—O3 <sup>i</sup>	84.6 (1)	O3 <sup>i</sup> —Co1—O1w	93.4 (1)
O1—Co1—O1w	100.7 (1)	O3 <sup>i</sup> —Co1—O2w	90.1 (1)
O1—Co1—O2w	163.7 (1)	O3 <sup>i</sup> —Co1—N1	173.3 (1)
O1—Co1—N1	91.4 (1)	O1w—Co1—O2w	95.0 (1)
O2—Co1—O3 <sup>i</sup>	88.1 (1)	O1w—Co1—N1	92.7 (1)
O2—Co1—O1w	160.9 (1)	O2w—Co1—N1	92.3 (1)
O2—Co1—O2w	104.1 (1)		

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

Table 2

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

D—H...A	D—H	H...A	D...A	D—H...A
O1w—H1w2...O1 <sup>ii</sup>	0.84 (1)	1.90 (2)	2.645 (3)	147 (3)
O1w—H1w1...O4 <sup>i</sup>	0.85 (1)	1.87 (2)	2.645 (3)	152 (3)
O2w—H2w2...O1w <sup>iii</sup>	0.84 (1)	1.98 (1)	2.816 (3)	171 (4)
O2w—H2w1...O3w <sup>iv</sup>	0.85 (1)	1.89 (1)	2.723 (3)	167 (4)
O3w—H3w1...O2	0.85 (1)	2.25 (2)	3.069 (3)	165 (4)
O3w—H3w2...O3 <sup>v</sup>	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  $\theta$ -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  $\text{\AA}$ ) and were allowed to ride on the C atoms, with  $U(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ . The water H-atoms were located and refined with an O—H 0.85 (1)  $\text{\AA}$  distance restraint.

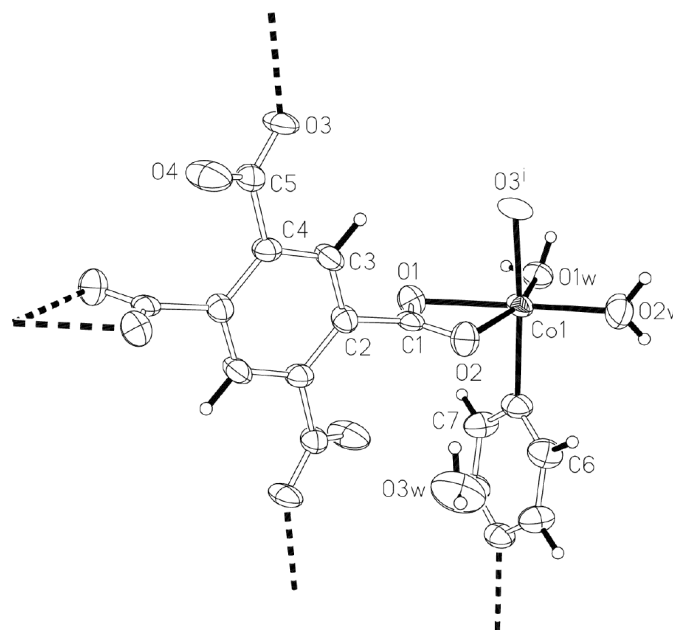


Figure 1

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: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEPII (Johnson, 1976); software used to prepare material for publication: SHELXL97.

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