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## Key indicators

Single-crystal X-ray study

T = 295 K

Mean  $\sigma(\text{C}-\text{C}) = 0.002 \text{ \AA}$ 

R factor = 0.027

wR factor = 0.067

Data-to-parameter ratio = 15.6

For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.**catena-Poly[[diaquabis(1*H*-benzimidazole- $\kappa\text{N}^3$ )-  
cobalt(II)]- $\mu$ -succinato- $\kappa\text{O}$ ]**

The crystal structure of the title compound  $[\text{Co}(\text{C}_4\text{H}_4\text{O}_4)(\text{C}_7\text{H}_6\text{N}_2)_2(\text{H}_2\text{O})_2]_n$ , consists of a polymeric  $\text{Co}^{\text{II}}$  complex bridged by a succinate dianion. Neighboring polymeric chains linked *via* hydrogen bonds. The overlapped arrangement and short separation of  $3.365(3) \text{ \AA}$  between parallel benzimidazole rings suggest the existence of  $\pi$ - $\pi$  stacking. The centrosymmetric complex has an octahedral coordination geometry.

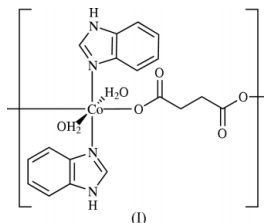
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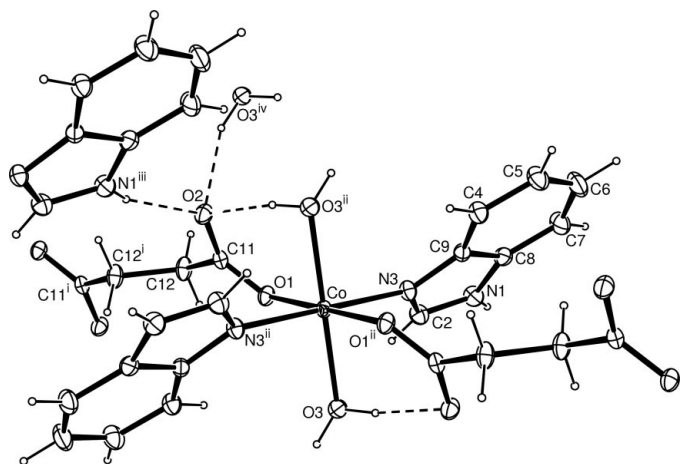
## Comment

$\pi$ - $\pi$  stacking between aromatic rings has been shown to be correlated with the electron-transfer process in some biological systems (Deisenhofer & Michel, 1989). As a part of an investigation of  $\pi$ - $\pi$  stacking in metal complexes (Chen *et al.*, 2003), the title polymeric  $\text{Co}^{\text{II}}$  complex, (I), has recently been prepared in our laboratory and its X-ray structure is presented here.

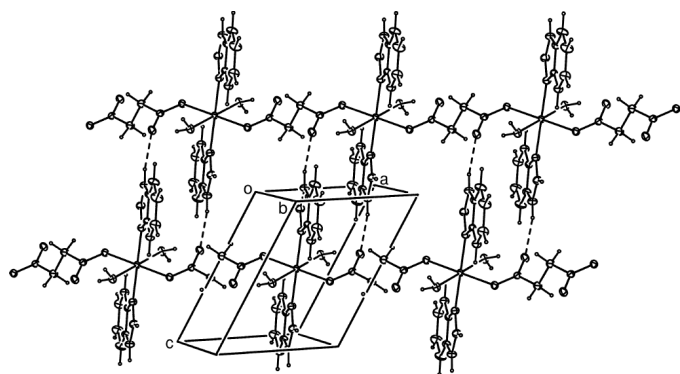


The title  $\text{Co}^{\text{II}}$  complex is isomorphous with the  $\text{Ni}^{\text{II}}$  complex reported recently (Liu *et al.*, 2003). The crystal structure consists of polymeric chains of the  $\text{Co}^{\text{II}}$  complex. The octahedral coordination environment around the  $\text{Co}^{\text{II}}$  atom, located on an inversion center, is illustrated in Fig. 1. The  $\text{Co}-\text{O}(\text{water})$  bond [ $2.1404(11) \text{ \AA}$ ] is longer than the  $\text{Co}-\text{O}(\text{carboxyl})$  bond [ $2.0898(11) \text{ \AA}$ ] (Table 1). The carboxyl group of the succinate is monodentate; the uncoordinated carboxyl atom O2 is hydrogen-bonded to the adjacent coordinated water and benzimidazole molecules, as shown in Fig. 1.

The succinate dianions bridge the  $\text{Co}^{\text{II}}$  atoms through both terminal carboxyl groups to form one-dimensional polymeric chains (Fig. 2). Adjacent chains are linked *via*  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds between benzimidazole and carboxyl groups and  $\text{O}-\text{H}\cdots\text{O}$  hydrogen bonds between coordinated water molecules and carboxyl groups (Table 2). Fig. 2 also shows the overlapped arrangement of parallel benzimidazole groups from adjacent polymeric chains. Neighboring benzimidazole rings related by  $(-x, 1-y, -z)$  are  $3.365(3) \text{ \AA}$  apart. These findings suggest the existence of  $\pi$ - $\pi$  stacking between adjacent polymeric chains.



**Figure 1**  
The coordination environment around the  $\text{Co}^{\text{II}}$  atom in (I), with 50% probability displacement ellipsoids. Dashed lines indicate hydrogen bonding. [Symmetry codes: (i)  $-x, -y, 1-z$ ; (ii)  $1-x, 1-y, 1-z$ ; (iii)  $x, y, 1+z$ ; (iv)  $x-1, y, z$ ].



**Figure 2**  
The molecular packing diagram, showing the  $\pi$ - $\pi$  stacking between benzimidazole rings from neighboring polymeric chains. Dashed lines indicate hydrogen bonds.

## Experimental

$\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$  (0.48 g, 2 mmol) was added to an aqueous solution (10 ml) containing succinic acid (0.24 g, 2 mmol) and NaOH (0.16 g, 4 mmol). After the mixture was refluxed for 1 h, an ethanol solution (10 ml) of benzimidazole (0.24 g, 2 mmol) was added with continuous stirring. The solution was refluxed for 2 h, then was cooled to room temperature and filtered. Pink single crystals were obtained from the filtrate after 3 d.

### Crystal data

$[\text{Co}(\text{C}_4\text{H}_4\text{O}_4)(\text{C}_7\text{H}_6\text{N}_2)_2\text{H}_2\text{O}_2]$   
 $M_r = 447.31$   
 Triclinic,  $P\bar{1}$   
 $a = 7.0717$  (9) Å  
 $b = 8.6326$  (11) Å  
 $c = 8.8223$  (12) Å  
 $\alpha = 100.699$  (7)°  
 $\beta = 112.489$  (9)°  
 $\gamma = 104.780$  (6)°  
 $V = 456.33$  (11) Å<sup>3</sup>

$Z = 1$   
 $D_x = 1.628$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 Cell parameters from 2067 reflections  
 $\theta = 2.5$ – $25.0$ °  
 $\mu = 0.99$  mm<sup>-1</sup>  
 $T = 295$  (2) K  
 Plate, pink  
 $0.28 \times 0.18 \times 0.06$  mm

### Data collection

Rigaku RAXIS-RAPID diffractometer

$\omega$  scans

Absorption correction: multi-scan

(*ABSCOR*; Higashi, 1995)

$T_{\text{min}} = 0.756$ ,  $T_{\text{max}} = 0.940$

4322 measured reflections

2074 independent reflections

1951 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.015$

$\theta_{\text{max}} = 27.5$ °

$h = -9 \rightarrow 9$

$k = -11 \rightarrow 11$

$l = -11 \rightarrow 11$

### Refinement

Refinement on  $F^2$

$R[F^2 > 2\sigma(F^2)] = 0.027$

$wR(F^2) = 0.067$

$S = 1.09$

2074 reflections

133 parameters

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.033P)^2 + 0.2062P]$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\text{max}} = 0.001$

$\Delta\rho_{\text{max}} = 0.28$  e Å<sup>-3</sup>

$\Delta\rho_{\text{min}} = -0.24$  e Å<sup>-3</sup>

**Table 1**

Selected geometric parameters (Å, °).

Co—O1	2.0894 (11)	O2—C11	1.2695 (19)
Co—N3	2.1309 (13)	C11—C12	1.517 (2)
Co—O3	2.1407 (11)	C12—C12 <sup>i</sup>	1.521 (3)
O1—C11	1.2568 (18)		
O1—Co—N3	91.30 (5)	N3—Co—O3	86.21 (5)
O1—Co—O3	90.50 (4)		

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

**Table 2**

Hydrogen-bonding geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O3—H32 <sup>..</sup> ·O2 <sup>ii</sup>	0.87	1.85	2.7020 (18)	167
N1—H1 <sup>..</sup> ·O2 <sup>v</sup>	0.86	2.07	2.8775 (19)	157
O3—H31 <sup>..</sup> ·O2 <sup>vi</sup>	0.89	2.00	2.860 (2)	160

Symmetry codes: (ii)  $1-x, 1-y, 1-z$ ; (v)  $x, y, z-1$ ; (vi)  $1+x, y, z$ .

H atoms of water molecules were located in a difference Fourier map and included in the structure-factor calculation, with fixed coordinates and isotropic displacement parameters of 0.05 Å<sup>2</sup>. Other H atoms were placed in calculated positions, with C—H = 0.93 Å (benzimidazole) or 0.97 Å (succinate) and N—H = 0.86 Å, and included in the final cycles of refinement in a riding model, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}$  of the carrier atoms.

Data collection: *PROCESS-AUTO* (Rigaku Corporation, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSO and Rigaku Corporation, 2002); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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## References

- Altomare, A., Cascarano, G., Giacovazzo, C. & Guagliardi, A. (1993). *J. Appl. Cryst.* **26**, 343–350.  
 Chen, Z., Xu, D.-J., Li, Z.-Y., Wu, J.-Y. & Chiang, M. Y. (2003). *J. Coord. Chem.* **56**, 253–259.  
 Deisenhofer, J. & Michel, H. (1989). *EMBO J.* **8**, 2149–2170.  
 Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.

- Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
- Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
- Liu, Y., Gu, J.-M. & Xu, D.-J. (2003). *Acta Cryst.* **E59**, m330–m332.
- Rigaku Corporation (1998). *PROCESS-AUTO*. Rigaku Corporation, Tokyo, Japan.
- Rigaku/MSK & Rigaku Corporation. (2002). *CrystalStructure*. Version 3.00. Rigaku/MSK, The Woodlands, TX, USA 77381-5209. Rigaku, Akishima, Tokyo, Japan.
- Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.