

**catena-Poly[[diaquabis(benzimidazole- $\kappa N$ )-cobalt(II)]- $\mu$ -fumarato- $\kappa^2 O^1:O^4$ ]**Yu Liu,<sup>a</sup> Duan-Jun Xu,<sup>a\*</sup>  
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The title polymeric complex,  $[\text{Co}(\mu\text{-C}_4\text{H}_2\text{O}_4)(\text{C}_7\text{H}_6\text{N}_2)_2(\text{H}_2\text{O})_2]_n$ , displays a one-dimensional chain structure bridged by fumarate dianions. In the crystal structure, the polymeric chains are linked to each other by hydrogen bonds. The overlapped arrangement and the short separation of 3.35 (2) Å suggest the existence of  $\pi$ - $\pi$  stacking between parallel benzimidazole rings. The  $\text{Co}^{\text{II}}$  atom exists in a centrosymmetric octahedral geometry.

**Key indicators**

Single-crystal X-ray study

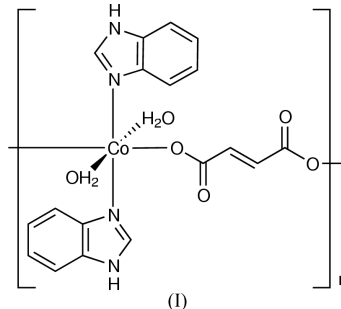
 $T = 150 \text{ K}$ Mean  $\sigma(\text{C}-\text{C}) = 0.008 \text{ \AA}$  $R$  factor = 0.045 $wR$  factor = 0.113

Data-to-parameter ratio = 12.2

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

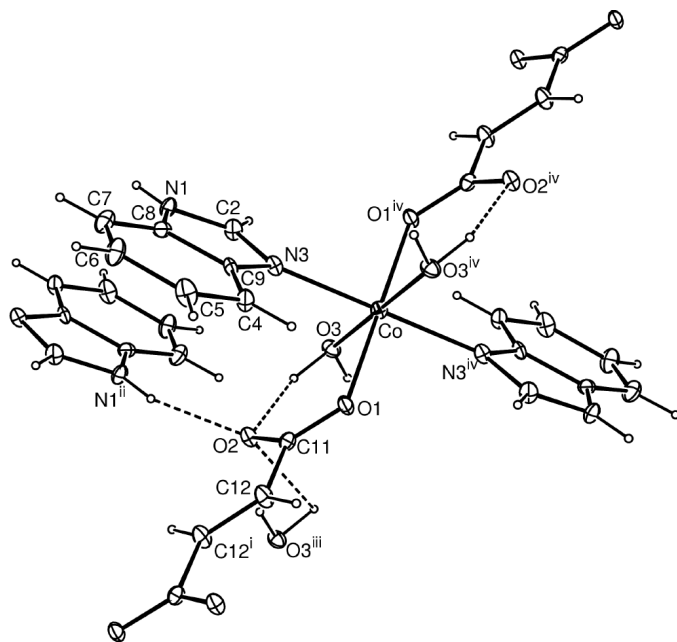
**Comment**

Aromatic  $\pi$ - $\pi$ -stacking interaction has shown to be correlated with electron transfer in some biological systems (Deisenhofer & Michel, 1989). As part of an investigation on the  $\pi$ - $\pi$ -stacking interaction in metal complexes (Chen *et al.*, 2003), the title polymeric  $\text{Co}^{\text{II}}$  complex, (I), with the benzimidazole ligand has recently been prepared in this laboratory.



The coordination environment around the  $\text{Co}^{\text{II}}$  atom in (I) is illustrated in Fig. 1. The  $\text{Co}^{\text{II}}$  atom is located at an inversion center and exhibits an octahedral coordination, formed by benzimidazole molecules, water molecules and fumarate dianions; bond lengths and angles are normal (Table 1). The carboxyl group of the fumarate dianion coordinates in a monodentate manner to the  $\text{Co}^{\text{II}}$  atom. The uncoordinated carboxyl O atom (O2) is hydrogen bonded to the neighboring benzimidazole and coordinated water molecules (Fig. 1).

Each fumarate dianion bridges two  $\text{Co}^{\text{II}}$  atoms through both terminal carboxyl groups, to form polymeric complex chains as shown in Fig. 2. Adjacent polymeric chains are linked to each other by hydrogen bonds (Table 2). An overlapped arrangement of benzimidazole rings is observed between adjacent complex molecules related by an inversion center (Fig. 3). The short separation of 3.35 (2) Å between neighboring parallel benzimidazole rings suggests the existence of  $\pi$ - $\pi$  stacking.



**Figure 1**  
The coordination environment around the Co<sup>II</sup> atom in (I), with 50% probability displacement ellipsoids. Dashed lines indicate hydrogen bonds [symmetry codes: (i)  $-x, -y, 1 - z$ ; (ii)  $1 - x, 1 - y, 2 - z$ ; (iii)  $-x, 1 - y, 1 - z$ ; (iv)  $1 - x, 1 - y, 1 - z$ ].

## Experimental

An ethanol solution (5 ml) of benzimidazole (0.24 g, 2 mmol) was mixed with an aqueous solution (5 ml) of CoCl<sub>2</sub>·6H<sub>2</sub>O (0.24 g, 1 mmol) at room temperature. After refluxing the solution for 30 min, an aqueous solution (5 ml) containing fumaric acid (0.12 g, 1 mmol) and NaOH (0.08 g, 2 mmol) was added. The mixture was refluxed for 1 h and filtered. Pink single crystals were obtained after 2 d.

### Crystal data

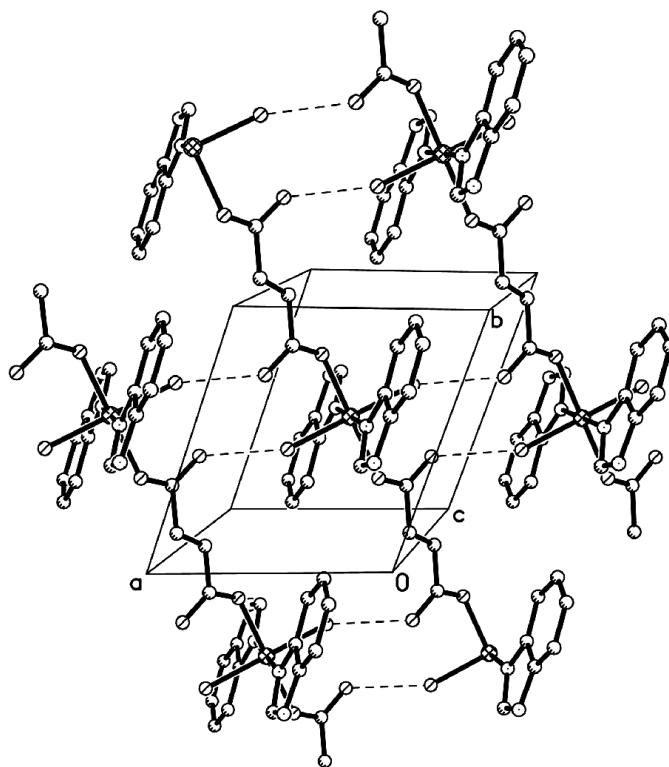
[Co(C <sub>4</sub> H <sub>2</sub> O <sub>4</sub> )(C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> ) <sub>2</sub> (H <sub>2</sub> O) <sub>2</sub> ]	$Z = 1$
$M_r = 445.29$	$D_x = 1.625 \text{ Mg m}^{-3}$
Triclinic, $P\bar{1}$	Mo $K\alpha$ radiation
$a = 7.0668 (10) \text{ \AA}$	Cell parameters from 1988 reflections
$b = 8.5150 (12) \text{ \AA}$	$\theta = 2.0\text{--}23.0^\circ$
$c = 8.7929 (13) \text{ \AA}$	$\mu = 0.99 \text{ mm}^{-1}$
$\alpha = 99.358 (11)^\circ$	$T = 150 (1) \text{ K}$
$\beta = 113.322 (13)^\circ$	Prism, pink
$\gamma = 102.787 (12)^\circ$	$0.32 \times 0.30 \times 0.22 \text{ mm}$
$V = 454.95 (13) \text{ \AA}^3$	

### Data collection

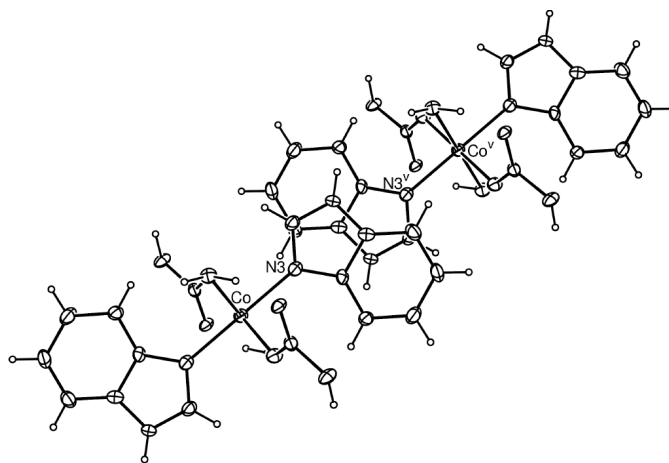
Bruker SMART CCD diffractometer	1623 independent reflections
$\omega$ and $\varphi$ scans	996 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Bruker, 1999)	$R_{\text{int}} = 0.053$
$T_{\text{min}} = 0.722, T_{\text{max}} = 0.802$	$\theta_{\text{max}} = 25.2^\circ$
2497 measured reflections	$h = -8 \rightarrow 4$
	$k = -9 \rightarrow 10$
	$l = -10 \rightarrow 10$

### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.0269P)^2 + 0.2058P]$
$R[F^2 > 2\sigma(F^2)] = 0.045$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.113$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 0.91$	$\Delta\rho_{\text{max}} = 0.51 \text{ e \AA}^{-3}$
1623 reflections	$\Delta\rho_{\text{min}} = -0.50 \text{ e \AA}^{-3}$
133 parameters	
H-atom parameters constrained	



**Figure 2**  
A crystal packing diagram. Dashed lines indicate the hydrogen bonding between adjacent polymeric chains.



**Figure 3**  
A diagram showing the  $\pi$ - $\pi$  stacking between neighboring benzimidazole rings [symmetry code: (v)  $2 - x, 1 - y, 2 - z$ ].

**Table 1**

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

Co—O1	2.075 (3)	O2—C11	1.278 (5)
Co—N3	2.110 (4)	C11—C12	1.502 (7)
Co—O3	2.125 (3)	C12—C12 <sup>i</sup>	1.315 (8)
O1—C11	1.253 (5)		
O1—Co—N3	87.60 (13)	N3—Co—O3	85.64 (14)
O1—Co—O3	89.97 (12)		

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—H31 $\cdots$ O2	0.99	1.77	2.712 (5)	159
O3—H32 $\cdots$ O2 <sup>iii</sup>	0.91	1.99	2.871 (5)	163
N1—H1 $\cdots$ O2 <sup>ii</sup>	0.86	2.01	2.827 (5)	158

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

H atoms of the water molecule were located in a difference Fourier map and were included in structure-factor calculations with fixed positional parameters and  $U_{\text{iso}} = 0.05 \text{ \AA}^2$ . Other H atoms were placed in calculated positions with C—H distances of 0.93 Å and N—H distances of 0.86 Å, and were included in the final cycles of refinement in the riding model, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}$  of the carrier atom.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; 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) and *XP* (Siemens, 1994);

software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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