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Key indicators

Single-crystal X-ray study

T = 295 K

Mean $\sigma(\text{C}-\text{C}) = 0.006 \text{ \AA}$

R factor = 0.048

wR factor = 0.131

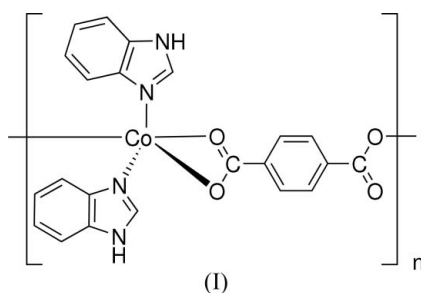
Data-to-parameter ratio = 12.6

For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.**catena-Poly[[bis(1*H*-benzimidazole- κN^3)cobalt(II)]- μ -terephthalato- $\kappa^3\text{O}^1, \text{O}^1': \text{O}^4$]**

In the title compound, $[\text{Co}(\text{C}_8\text{H}_4\text{O}_4)(\text{C}_7\text{H}_6\text{N}_2)_2]_n$, the terephthalate dianions bridge Co^{II} ions through terminal carboxyl groups to form polymeric complex chains; one carboxyl group coordinates in a monodentate manner and the other chelates to the Co atom. Two benzimidazole ligands also coordinate to the Co atom to complete a distorted trigonal-bipyramidal coordination geometry. The crystal packing is stabilized by $\text{N}-\text{H} \cdots \text{O}$ hydrogen bonds and $\pi-\pi$ stacking involving the benzimidazole ligands, with a face-to-face separation of 3.454 (11) \AA .

Comment

$\pi-\pi$ Stacking interactions between aromatic rings have attracted much attention because they are correlated with the electron transfer process in some biological systems (Deisenhofer & Michel, 1989). As part of our ongoing investigations of the nature of $\pi-\pi$ stacking (Pan & Xu, 2004, 2005), the title polymeric Co^{II} complex, (I), incorporating terephthalate (tp) dianions and benzimidazole (bzim) ligands, has been prepared and its crystal structure is presented here.



A segment of the polymeric structure of (I) is illustrated in Fig. 1. The Co^{II} ion is coordinated by two tp dianions and two bzim molecules. Each terephthalate bridges two neighboring Co^{II} atoms to form a polymeric chain (Fig. 2).

The $\text{Co}-\text{O}2$ distance of 2.515 (3) \AA is much longer than the $\text{Co}-\text{O}1$ and $\text{Co}-\text{O}3$ distances (Table 1), but is probably reasonable for a strained bidentate system. The $\text{Co}-\text{O}1-\text{C}1$ angle of 102.2 (2) $^\circ$ appears to be compressed to allow Co and O2 to approach each other. The other tp carboxylate group has a more typical $\text{Co}-\text{O}3^i-\text{C}8^i$ angle of 110.4 (2) $^\circ$ and a much longer $\text{Co}-\text{O}4^i$ bond distance of 2.789 (3) \AA , indicating that there is no bonding between Co and $\text{O}4^i$ [symmetry code: (i) $\frac{1}{2} + x, \frac{1}{2} - y, \frac{1}{2} + z$]. This is consistent with the situation found in related Mn^{II} (Liu *et al.*, 2005) and Cu^{II} complexes (Li *et al.*, 2005).

Thus in (I) the two tp carboxyl groups coordinate to the Co atom differently, one in a monodentate mode and the other in

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a chelating mode. The coordination geometry around the Co atom can be described as distorted trigonal-bipyramidal, with atoms O2 and O3 in the axial sites. The uncoordinated carboxyl O4 atom accepts an N—H···O hydrogen bond from a bzim ligand of a neighboring chain (Table 2).

A partially overlapped arrangement of bzim rings from neighboring polymeric chains is observed in (I) (Fig. 2). The face-to-face separation between neighboring parallel bzim rings, related by an inversion center at $(\frac{1}{2}, 1, \frac{1}{2})$, is 3.454 (11) Å, strongly suggesting the existence of π - π stacking.

Experimental

An aqueous solution (5 ml) containing $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$ (0.24 g, 1 mmol), NaOH (0.08 g, 2 mmol) and terephthalic acid (0.17 g, 1 mmol) was mixed with an ethanol solution (15 ml) of bzim (0.24 g, 2 mmol). The mixture was refluxed for 5 h. After cooling to room temperature, the solution was filtered. Red single crystals of (I) were obtained from the filtrate after two weeks.

Crystal data

$[\text{Co}(\text{C}_8\text{H}_4\text{O}_4)(\text{C}_7\text{H}_6\text{N}_2)_2]$
 $M_r = 459.32$
 Monoclinic, $P2_1/n$
 $a = 17.319$ (2) Å
 $b = 7.2711$ (7) Å
 $c = 17.8495$ (18) Å
 $\beta = 115.002$ (3)°
 $V = 2037.1$ (4) Å³
 $Z = 4$

$D_x = 1.498$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 7787 reflections
 $\theta = 2.6$ – 24.0 °
 $\mu = 0.88$ mm⁻¹
 $T = 295$ (2) K
 Plate, red
 $0.30 \times 0.21 \times 0.08$ mm

Data collection

Rigaku R-Axis RAPID diffractometer
 ω scans
 Absorption correction: multi-scan (ABSCOR; Higashi, 1995)
 $T_{\min} = 0.762$, $T_{\max} = 0.925$
 10571 measured reflections

3527 independent reflections
 2730 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.057$
 $\theta_{\text{max}} = 25.0$ °
 $h = -20 \rightarrow 20$
 $k = -8 \rightarrow 8$
 $l = -21 \rightarrow 21$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.048$
 $wR(F^2) = 0.131$
 $S = 1.01$
 3527 reflections
 280 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0744P)^2 + 0.8857P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.45$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.48$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Co—O1	2.022 (2)	C1—O1	1.262 (4)
Co—O2	2.515 (3)	C1—O2	1.235 (4)
Co—O3 ⁱ	2.000 (2)	C8—O3	1.268 (4)
Co—N13	2.034 (3)	C8—O4	1.246 (4)
Co—N23	2.039 (3)		
O1—Co—O2	56.01 (9)	O3 ⁱ —Co—N13	101.13 (10)
O1—Co—O3 ⁱ	107.21 (10)	O3 ⁱ —Co—N23	106.82 (11)
O1—Co—N13	110.78 (11)	N13—Co—N23	109.21 (12)
O1—Co—N23	119.93 (11)	Co—O1—C1	102.2 (2)
O2—Co—O3 ⁱ	163.22 (9)	Co—O2—C1	79.9 (2)
O2—Co—N13	86.92 (10)	Co ⁱⁱ —O3—C8	110.4 (2)
O2—Co—N23	83.92 (10)		

Symmetry codes: (i) $x + \frac{1}{2}, -y + \frac{1}{2}, z + \frac{1}{2}$; (ii) $x - \frac{1}{2}, -y + \frac{1}{2}, z - \frac{1}{2}$.

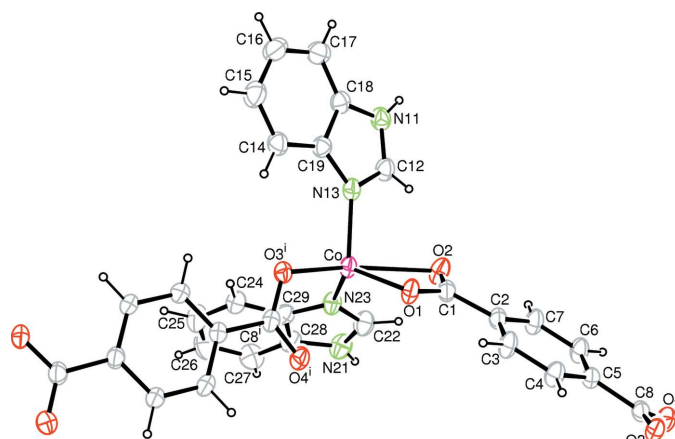


Figure 1
 Part of the polymeric structure of (I), shown with 30% probability displacement ellipsoids for the non-H atoms [symmetry code: (i) $\frac{1}{2} + x, \frac{1}{2} - y, \frac{1}{2} + z$].

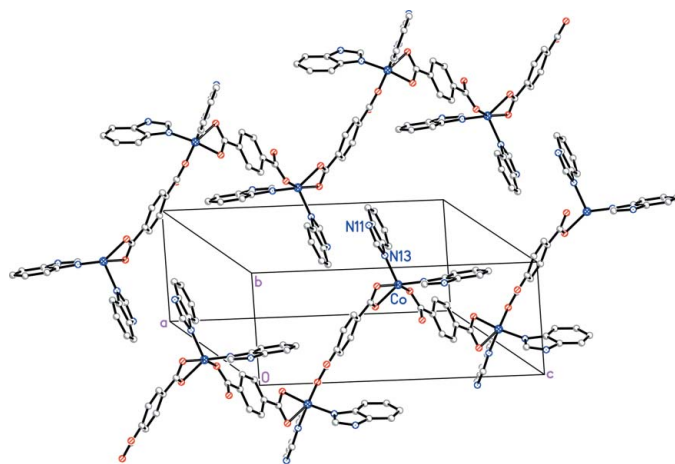


Figure 2
 Packing diagram for (I), showing the π - π stacking.

Table 2

Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N11—H11···O1 ⁱⁱⁱ	0.86	2.05	2.792 (4)	145
N21—H21···O4 ^{iv}	0.86	1.95	2.735 (4)	151

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

H atoms were placed in calculated positions, with C—H = 0.93 Å and N—H = 0.86 Å, and were included in the final cycles of refinement as riding, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{carrier})$.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku, 2002); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP3 for Windows* (Farrugia, 1997) and *XP* (Siemens, 1994); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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