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catena-Poly[[bis(1*H*-benzimidazole-κN^3)-cobalt(II)]-μ-isophthalato-κ^2O:O']

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Key indicators

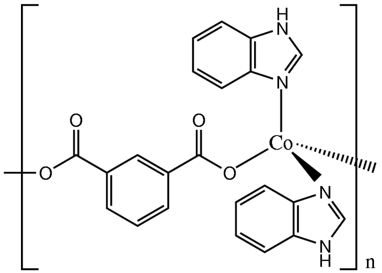
Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.006 Å
R factor = 0.046
wR factor = 0.091
Data-to-parameter ratio = 16.1

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

In the title polymeric complex, $[Co(C_8H_4O_4)(C_7H_6N_2)_2]_n$, the Co^{II} atom assumes distorted tetrahedral coordination geometry formed by two isophthalate dianions and two benzimidazole molecules. The isophthalate dianions bridge Co^{II} atoms through carboxy groups to form a one-dimensional polymeric association. C—H$\cdots\pi$ interactions occur between adjacent aromatic rings.

Comment

As part of our ongoing research on non-covalent interactions, the title Co^{II} complex, (I), bridged by isophthalate dianions, has been prepared, and its crystal structure is presented here to discuss the interaction between aromatic rings.



(I)

The asymmetric unit of (I) consists of a Co^{II} cation, a $(C_8H_4O_4)^{2-}$ isophthalate dianion and two $C_7H_6N_2$ BZIM (benzimidazole) molecules (Fig. 1). While two BZIM species coordinate to a Co^{II} atom, two isophthalate dianions, related by translation symmetry along the c axis, each coordinate in a monodentate manner to the Co^{II} atom to complete the

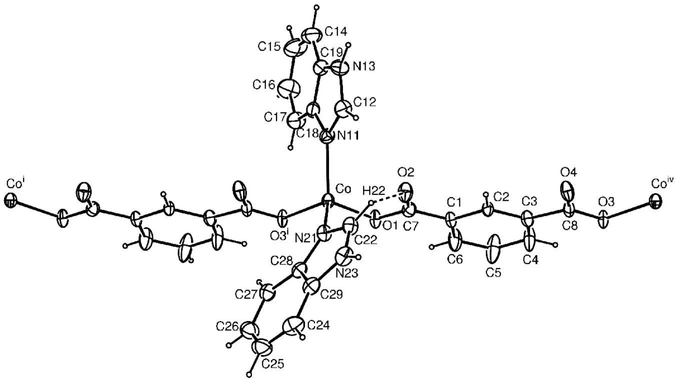


Figure 1
The molecular structure of (I) shown with 30% probability displacement ellipsoids and H atoms represented by small spheres. The dashed line shows the C—H$\cdots$O interaction [symmetry codes: (i) $x, y, z - 1$; (iv) $x, y, 1 + z$].

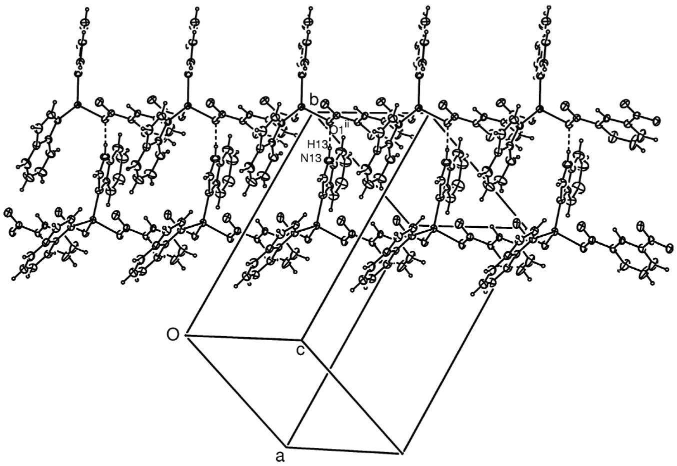


Figure 2
The molecular packing of (I); dashed lines indicate the hydrogen bonding between N13–BZIM and the carboxy group from the adjacent polymeric chain. [Symmetry code: (ii) $x - \frac{1}{2}, \frac{3}{2} - y, z$.]

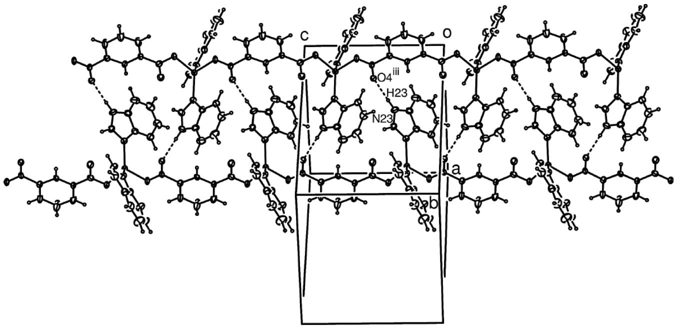


Figure 3
The molecular packing of (I); dashed lines indicate the hydrogen bonding between N23–BZIM and the carboxy group from the adjacent polymeric chain. [Symmetry code: (iii) $-x, 1 - y, z - \frac{1}{2}$.]

distorted tetrahedral coordination geometry. The N11—Co—N21 bond angle is some 24.00 (15)° larger than the O1—Co—O3 bond angle (Table 1). Uncoordinated carboxy atoms O1 and O4 accept hydrogen bonds from BZIM N—H moieties of an adjacent polymeric chain, as shown in Figs. 2 and 3.

The following H$\cdots$*Cg* distances and C—H$\cdots$*Cg* angles (*Cg* = the centroid of the ring) indicate the presence of C—H$\cdots\pi$ interactions between aromatic rings in (I): H14$\cdots$*Cg*(isophthalate^{v}) = 2.81 Å and C14—H14$\cdots$*Cg*(isophthalate^{v}) = 156° [symmetry code: (v) $\frac{1}{2} - x, \frac{1}{2} + y, z - \frac{1}{2}$]; H26$\cdots$*Cg*(N11–BZIM^{vi}) = 2.91 Å and C26—H26$\cdots$*Cg*(N11–BZIM^{vi}) = 175° [symmetry codes: (vi) $\frac{1}{2} - x, y - \frac{1}{2}, z - \frac{1}{2}$].

Aromatic π–π stacking has commonly been found between BZIM rings in metal complexes (Liu *et al.*, 2004), but does not occur in (I).

Experimental

An ethanol solution (5 ml) of BZIM (0.24 g, 2 mmol) was mixed with an aqueous solution (5 ml) of $CoCl_2 \cdot 6H_2O$ (0.48 g, 2 mmol), and the mixture was refluxed for 20 min. Then an aqueous solution (8 ml) containing isophthalic acid (0.33 g, 2 mmol) and NaOH (0.16 g, 4 mmol) was added into the above mixture, and the solution was refluxed for a further 2.5 h. After cooling to room temperature, the solution was filtered. Red single crystals of (I) were obtained from the filtrate after one week.

Crystal data

$[Co(C_8H_4O_4)(C_7H_6N_2)_2]$
M_r = 459.32
Orthorhombic, $Pna2_1$
a = 11.5641 (5) Å
b = 17.8801 (3) Å
c = 10.1058 (4) Å
V = 2089.55 (13) Å^3
Z = 4
D_x = 1.460 Mg m^{-3}

Mo *Kα* radiation
Cell parameters from 11734 reflections
θ = 2.5–26.0°
μ = 0.86 mm^{-1}
T = 295 (2) K
Plate, red
0.31 × 0.14 × 0.07 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.87, T_{max} = 0.94
19285 measured reflections

4412 independent reflections
3681 reflections with $I > 2\sigma(I)$
R_{int} = 0.059
θ_{max} = 27.5°
$h = -15 \rightarrow 15$
$k = -23 \rightarrow 23$
$l = -13 \rightarrow 11$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.091
S = 1.11
4412 reflections
274 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0332P)^2 + 1.1303P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}
Absolute structure: Flack (1983), 1880 Friedel Pairs
Flack parameter = −0.007 (18)

Table 1
Selected geometric parameters (Å, °).

Co—O1	2.018 (3)	Co—N11	2.022 (2)
Co—O3^{i}	1.984 (3)	Co—N21	2.033 (2)
O1—Co—O3^{i}	94.91 (11)	O3^{i}—Co—N11	105.74 (13)
O1—Co—N11	107.21 (12)	O3^{i}—Co—N21	111.23 (13)
O1—Co—N21	115.82 (13)	N11—Co—N21	118.91 (10)

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

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N13—H13$\cdots$O1^{ii}	0.86	1.92	2.781 (5)	176
N23—H23$\cdots$O4^{iii}	0.86	1.89	2.735 (4)	169
C22—H22$\cdots$O2	0.93	2.53	2.978 (5)	110

Symmetry codes: (ii) $x - \frac{1}{2}, \frac{3}{2} - y, z$; (iii) $-x, 1 - y, z - \frac{1}{2}$.

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 in riding mode, with U_{iso}(H) = 1.2U_{eq}(carrier atom).

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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