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Polymeric aqua(benzimidazole-*κN*)(*μ*-malonato)cobalt(II)

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Key indicators

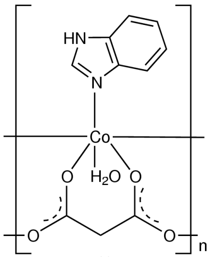
Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.006 Å
R factor = 0.039
wR factor = 0.101
Data-to-parameter ratio = 12.2

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

The crystal structure of the title compound, [Co($C_3H_2O_4$)($C_7H_6N_2$)(H_2O)]$_n$, consists of two-dimensional polymeric Co^{II} complex layers. The octahedral coordination around a Co^{II} atom is composed of a chelate malonate, two monodentate malonate anions from the adjacent asymmetric unit, a bezimidazole ligand and a coordinated water molecule. Each malonate dianion links three Co^{II} atoms related by an *n*-glide plane to form polymeric layers in the (010) plane. π–π stacking of the benzimidazole ligands occurs between adjacent polymeric layers, the separation between parallel benzimidazole rings being 3.42 (2) Å.

Comment

Aromatic π–π-stacking interaction has been observed in some metal complexes with aromatic heteropolycyclic ligands, such as phenanthroline, bithiazole and benzimidazole (Chen *et al.*, 2003). A new polymeric complex, (I), with the benzimidazole ligand has recently been prepared in this laboratory and its X-ray structure, showing the π–π stacking between the polymeric complex layers, is presented here.



(I)

The crystal structure of (I) consists of polymeric sheets of (I). The coordination geometry around a Co^{II} atom is illustrated in Fig. 1. The octahedral coordination is formed by a chelate malonate, two monodentate malonates from adjacent asymmetric units, a benzimidazole ligand and a coordinated water molecule. The malonate chelates to the Co^{II} atom through the terminal carboxyl groups in a boat configuration. The Co—O(water) distance of 2.169 (2) Å is significantly longer than the average Co—O(carboxyl) distance of 2.092 (2) Å, these distances ranging from 2.074 (2) to 2.121 (2) Å. The coordinated water molecule forms hydrogen bonds to neighboring carboxyl groups, as shown in Fig. 1 and Table 2.

The malonate dianion plays a bridging role in the structure. Each malonate dianion links three Co^{II} atoms, related by an *n*-glide plane, to form infinite two-dimensional polymer layers in the (010) plane (Fig. 2). The molecular packing, including the parallel disposition of benzimidazole rings in neighboring

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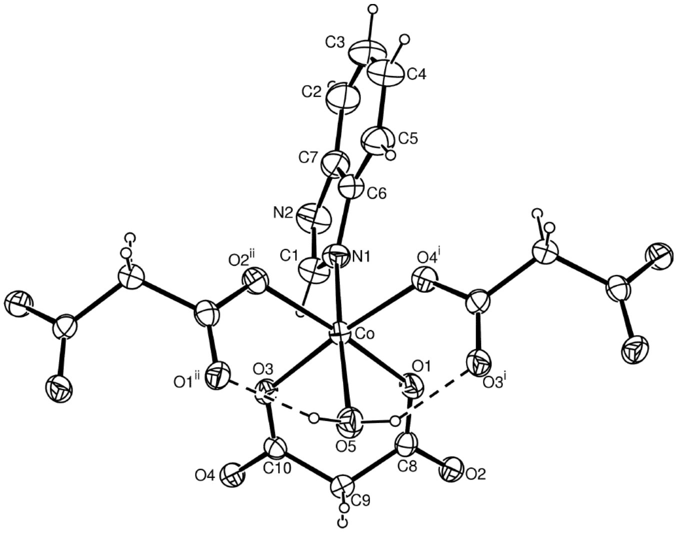

Figure 1
The coordination environment around the Co^{II} atom in (I), with 30% probability displacement ellipsoids. Dashed lines indicate hydrogen bonds [symmetry codes: (i) $x-\frac{1}{2}, \frac{1}{2}-y, \frac{1}{2}+z$; (ii) $x-\frac{1}{2}, \frac{1}{2}-y, z-\frac{1}{2}$].

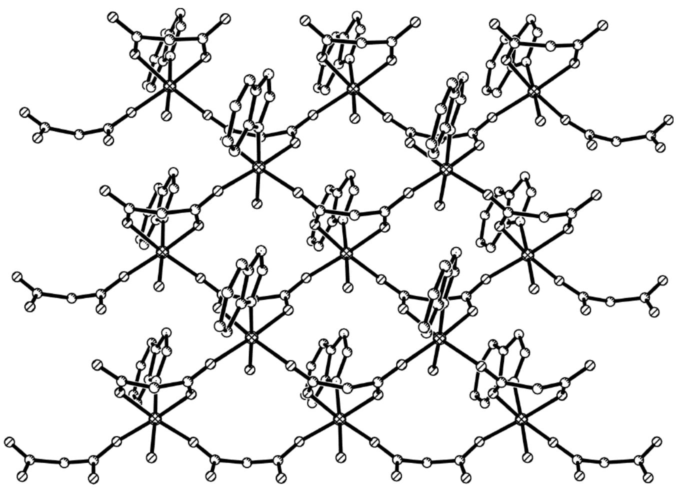

Figure 2
The polymeric layer structure formed by malonate linkages.

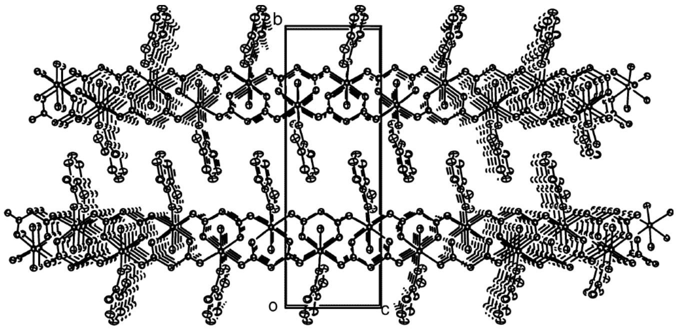

Figure 3
The molecular packing, showing the π–π stacking between benzimidazole rings.

polymer layers, is shown in Fig. 3. The shorter separation of 3.42 (2) Å between neighboring benzimidazole rings suggests the existence of π–π stacking between adjacent polymer layers.

Experimental

An ethanol solution (5 ml) of benzimidazole (0.236 g, 2 mmol) was mixed with an aqueous solution (10 ml) of $CoCl_2.6H_2O$ (0.237 g, 1 mmol) at room temperature. An aqueous solution (8 ml) containing malonic acid (0.104 g, 1 mmol) and Na_2CO_3 (0.106 g, 1 mmol) was added to the above solution with stirring at room temperature. The mixture was then refluxed for 2 h and filtered. Pink single crystals were obtained after 5 d.

Crystal data

$[Co(C_3H_2O_4)(C_7H_6N_2)(H_2O)]$
$M_r = 297.13$
Monoclinic, $P2_1/n$
$a = 6.7654$ (10) Å
$b = 21.9841$ (18) Å
$c = 7.4945$ (14) Å
$\beta = 91.944$ (2)°
$V = 1114.0$ (3) Å^3
$Z = 4$

$D_x = 1.772$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 6128 reflections
$\theta = 2.9$–25.0°
$\mu = 1.56$ mm^{-1}
$T = 295$ (2) K
Plate, pink
0.25 × 0.18 × 0.10 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.672$, $T_{max} = 0.851$
7470 measured reflections

1995 independent reflections
1828 reflections with $I > 2\sigma(I)$
$R_{int} = 0.019$
$\theta_{max} = 25.3°$
$h = -7 \rightarrow 8$
$k = -26 \rightarrow 26$
$l = -9 \rightarrow 8$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.101$
$S = 1.12$
1995 reflections
163 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0401P)^2 + 2.9317P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.44$ e Å^{-3}
$\Delta\rho_{min} = -0.79$ e Å^{-3}

Table 1
Selected geometric parameters (Å).

Co—O1	2.074 (2)	Co—N1	2.114 (3)
Co—O4^i	2.085 (2)	Co—O2^{ii}	2.121 (2)
Co—O3	2.087 (2)	Co—O5	2.169 (2)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O5—H52···O3^i	0.98	1.85	2.689 (3)	143
O5—H51···O1^{ii}	0.89	1.90	2.672 (3)	143
N2—H2···O2^{iii}	0.86	2.43	3.078 (4)	132

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

The H atoms of the water molecule were located in a difference Fourier map and were included in the structure-factor calculations with fixed positional parameters and $U_{iso} = 0.05$ Å^2. Other H atoms were placed in calculated positions with C—H = 0.93 Å (benzimidazole) or 0.97 Å (malonate) and N—H = 0.86 Å, and included in the final cycles of refinement in theriding model, with U_{iso}(H) = 1.2 times U_{eq} of the carrier atom.

Data collection: *PROCESS-AUTO* (Rigaku Corporation, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC and Rigaku, 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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