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Diaquatetrakis(1*H*-imidazole-κN^3)cobalt(II) terephthalate

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Key indicators

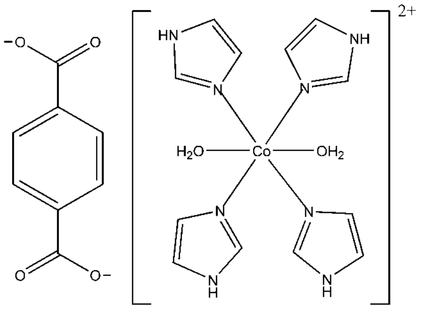
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
R factor = 0.044
wR factor = 0.133
Data-to-parameter ratio = 9.9

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

In the title complex, $[Co(C_3H_4N_2)_4(H_2O)_2](C_8H_4O_4)$, the octahedrally coordinated Co atom lies on a center of symmetry and is bonded by four imidazole and two water molecules. The terephthalate anion also lies on a center of symmetry but does not coordinate to the Co atom. Hydrogen bonding leads to a three-dimensional structure.

Comment

As a multidentate bridging ligand, terephthalate (tpt) has been used in the architecture of polymeric metal complexes because of its ability to form short bridges *via* one carboxylato group or long bridges *via* the benzene ring (Ma *et al.*, 2003; Zhang *et al.*, 2003; Yuan *et al.*, 2003). Recently, we tried to prepare a polymeric Co^{II} complex bridged by the tpt group, but X-ray diffraction analysis revealed an unexpected structure consisting of an uncoordinated tpt anion and a complex Co^{II} cation, *viz.* diaquatetrakis(imidazole)cobalt(II) terephthalate, (I).



(I)

As shown in Fig. 1, the crystal structure contains a complex Co^{II} cation and a terephthalate anion, which exhibits an isostructural structure to those of the reported complexes $[M(C_3H_4N_2)_4(H_2O)_2](C_8H_4O_4)$ (*M* = Ni, Cu, Mn) (Niu *et al.*, 1999; Zeng *et al.*, 1997; Liu *et al.*, 2001). The Co atom, located on an inversion centre, exhibits octahedral coordination geometry. Four imidazole and two water molecules coordinate to the Co atom with normal bond distances and angles. The terephthalate anion does not coordinate to the Co atom but links the complex cations through an extensive hydrogen-bonding network (Fig. 2).

Experimental

To a solution of imidazole (4.7 mmol), terephthalic acid (1.9 mmol) and water (20 ml) was added $CoCl_2.6H_2O$ (1.6 mmol). After stirring for 20 min, the mixture was allowed to stand at room temperature undisturbed for about 6 d, resulting in purple crystals.

Crystal data

$[Co(C_3H_4N_2)_4(H_2O)_2](C_8H_4O_4)$
$M_r = 531.40$
Monoclinic, $C2/c$
$a = 22.2830\ (7)$ Å
$b = 7.6818\ (3)$ Å
$c = 16.1127\ (3)$ Å
$\beta = 120.630\ (2)^\circ$
$V = 2373.25\ (12)$ Å^3
$Z = 4$

$D_x = 1.487$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 82 reflections
$\theta = 2.1$–25.1°
$\mu = 0.78$ mm^{-1}
$T = 293\ (2)$ K
Prism, purple
$0.32 \times 0.21 \times 0.06$ mm

Data collection

Bruker SMART CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.736$, $T_{max} = 0.950$
3377 measured reflections

2071 independent reflections
1731 reflections with $I > 2\sigma(I)$
$R_{int} = 0.024$
$\theta_{max} = 25.1^\circ$
$h = -12 \rightarrow 25$
$k = -8 \rightarrow 9$
$l = -19 \rightarrow 17$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.133$
$S = 1.08$
2071 reflections
209 parameters
All H-atom parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.0643P)^2 + 7.3403P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.40$ e Å^{-3}
$\Delta\rho_{min} = -0.34$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0019 (4)

Table 1
Selected geometric parameters (Å, °).

Co1—O3	2.144 (3)	Co1—N1	2.149 (3)
Co1—N3	2.146 (3)		
O3—Co1—N3	88.11 (11)	O3—Co1—N1	88.59 (11)

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O1	0.86 (5)	1.91 (5)	2.765 (4)	175 (5)
N4—H4A···O1^{ii}	0.79 (5)	1.97 (5)	2.743 (4)	165 (5)
O3—H3B···O2^{iii}	0.88 (5)	1.82 (5)	2.699 (3)	174 (4)
O3—H3A···O2^{iv}	0.80 (5)	2.05 (5)	2.813 (4)	159 (5)

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1994); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1994); software used to prepare material for publication: *SHELXS*97.

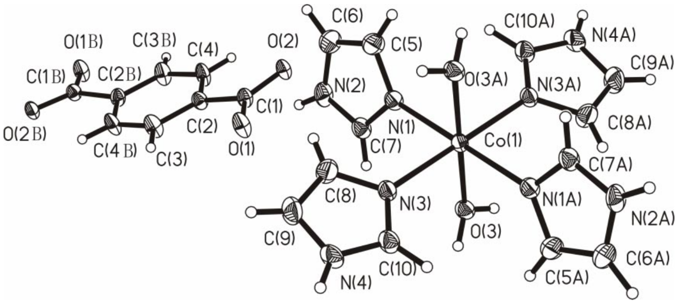


Figure 1
A perspective view of the complete centrosymmetric molecule of (I). Displacement ellipsoids are drawn at the 30% probability level [symmetry codes: (A) $\frac{1}{2} - x, \frac{1}{2} - y, -z$; ($B$) $1 - x, y, \frac{3}{2} - z$].

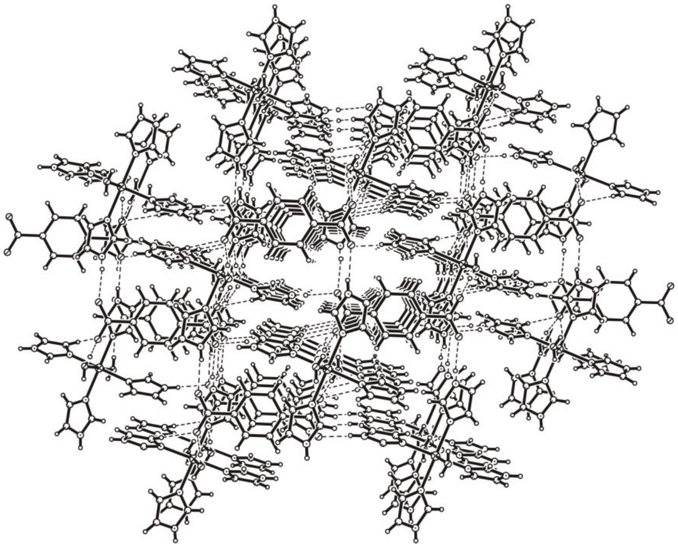


Figure 2
The three-dimensional structure of (I), viewed along the b axis. Hydrogen bonding is indicated by dashed lines.

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