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catena-Poly[[[diaquabis(*N*,*N*-dimethylformamide)-cobalt(II)]-μ-1,4-benzenedicarboxylato-κ^2O:O'] *N*,*N*-dimethylformamide solvate monohydrate]

Chun-Xiao Jia

Department of Chemistry, DeZhou University, DeZhou, ShanDong 253023, People's Republic of China

Correspondence e-mail:
jiachunxiao@yahoo.com.cn

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Key indicators

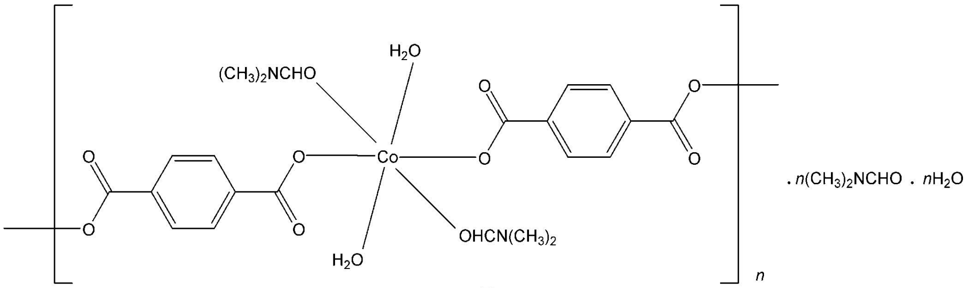
Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.004 Å
R factor = 0.044
wR factor = 0.125
Data-to-parameter ratio = 15.2

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

In the title compound, $\{[Co(C_8H_4O_4)(C_3H_7NO)_2(H_2O)_2]\cdot C_3H_7NO\cdot H_2O\}_n$, the Co^{II} atom, lying on an inversion center, is coordinated by six O atoms from two carboxylate groups, two water molecules and two N,N'-dimethylformamide molecules. The polymeric chain runs along the c axis, and neighboring chains are interlinked by hydrogen bonds involving uncoordinated water molecules, forming a two-dimensional supramolecular network.

Comment

Transition metal complexes of romatic dicarboxylates, such as 1,4-benzenedicarboxylate (Li *et al.*, 1998, 1999) and 4,4′-biphenyldicarboxylate (Rosi *et al.*, 2002), have attracted considerable interest because of their peculiar structures and unique properties. In an investigation of these potentially interesting structures, the title compound, (I), was synthesized by the reaction of benzenedicarboxylic acid and cobalt(II) nitrate.



(I)

The Co^{II} atom, lying on an inversion center, is coordinated by six O atoms from two carboxylate groups, two water molecules and two N,N-dimethylformamide molecules, giving an approximately octahedral geometry (Fig. 1). The 1,4-benzenedicarboxylate ligand bridges the Co^{II} atoms to form a chain running along the c axis. Adjacent chains are linked by O—H⋯O hydrogen bonds through uncoordinated water molecules (Table 1), resulting in a two-dimensional supramolecular framework (Fig. 2).

Experimental

A mixture of $Co(NO_3)_2$ (0.1 mmol) in H_2O (10 ml) and 1,4-benzenedicarboxylic acid (0.1 mmol) in H_2O (10 ml) was refluxed for 30 min. The resulting precipitate was filtered off and pale-red crystals of (I) were obtained from the filtrate after 10 d. Analysis calculated for $C_{20}H_{40}CoN_4O_{12}$: C 40.89, H 6.86, N 9.54%; found: C 40.66, H 6.82, N 9.21%.

Crystal data

$[Co(C_8H_4O_4)(C_3H_7NO)_2(H_2O)_2]\cdot C_3H_7NO\cdot H_2O$
$M_r = 587.49$
Triclinic, $P\overline{1}$
$a = 8.6025\ (10)$ Å
$b = 8.9590\ (11)$ Å
$c = 11.4191\ (13)$ Å
$\alpha = 83.598\ (1)^\circ$
$\beta = 74.289\ (1)^\circ$
$\gamma = 61.744\ (1)^\circ$
$V = 746.09\ (15)$ Å^3
$Z = 1$
$D_x = 1.308$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.63$ mm^{-1}
$T = 294\ (2)$ K
Block, red
$0.24 \times 0.21 \times 0.15$ mm

Data collection

Bruker APEX-II CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.859$, $T_{max} = 0.909$
4033 measured reflections
2590 independent reflections
2421 reflections with $I > 2\sigma(I)$
$R_{int} = 0.011$
$\theta_{max} = 25.0^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.125$
$S = 1.02$
2590 reflections
173 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0757P)^2 + 0.5318P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.63$ e Å^{-3}
$\Delta\rho_{min} = -0.39$ e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O4—H4A···O1	0.85	1.90	2.657 (3)	147
O4—H4B···O6^{i}	0.85	1.88	2.711 (4)	164
O6—H6D···O5^{ii}	0.85	1.90	2.738 (7)	167
O6—H6E···O1	0.85	1.99	2.725 (5)	144

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

H atoms were located in a difference Fourier map, but were then placed in calculated positions (C—H = 0.93–0.96 Å and O—H = 0.85 Å) and treated as riding, with $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}$(methyl C, O).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg & Berndt, 1999); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

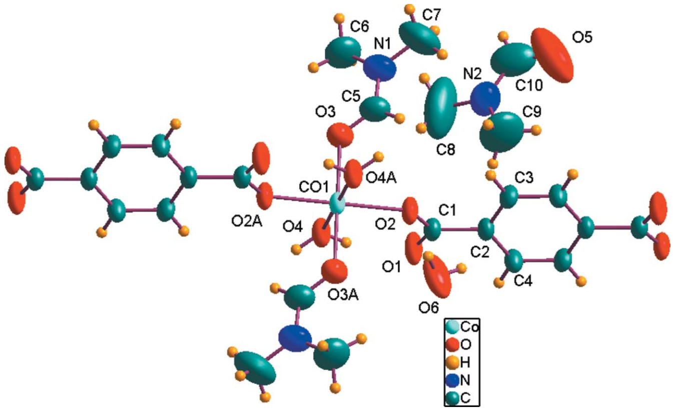


Figure 1
Part of the polymeric structure of (I). Displacement ellipsoids are drawn at the 30% probability level (symmetry code: A $-x + 1, -y, -z$).

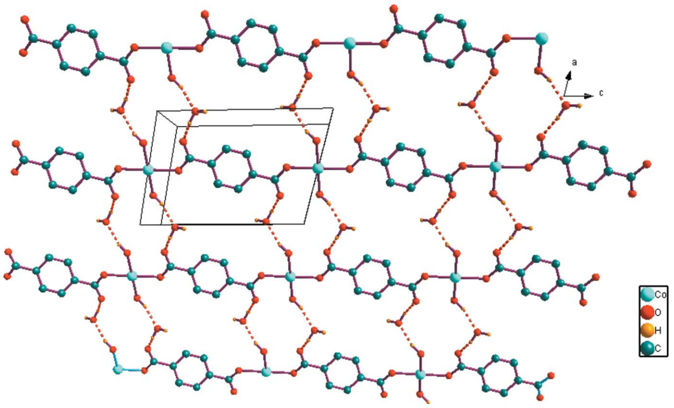


Figure 2
The two-dimensional supramolecular structure of (I), viewed down the b axis. Red dashed lines denote O—H···O hydrogen bonds. Dimethylformamide molecules and H atoms not involved in the hydrogen bonds have been omitted.

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