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catena-Poly[piperazinium(2+) [tetraaquazinc(II)-μ-benzene-1,3,5-tricarboxylato-diaquacobalt(II)-μ-benzene-1,3,5-tricarboxylato] dihydrate]

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The asymmetric unit of the title polymer, $\{(C_4H_{12}N_2)[ZnCo(C_9H_3O_6)_2(H_2O)_6]\cdot 2H_2O\}_n$, contains one independent Zn^{II} atom and one independent Co^{II} atom, each of which is located on an inversion center. The benzene-1,3,5-tricarboxylate molecule bridges the Zn^{II} and Co^{II} atoms in two coordination modes, forming a one-dimensional polymeric zigzag chain structure; the chains are further linked by O—H···O and N—H···O hydrogen bonds, forming a three-dimensional network. In the micropore formed by the packing of the zigzag chains, there is one piperazinium(2+) cation and two water molecules.

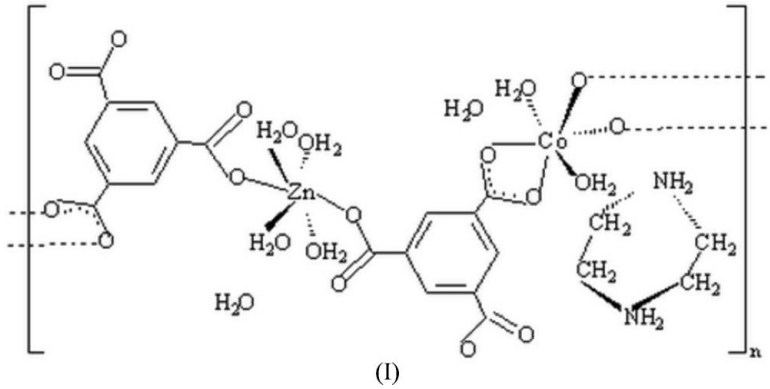
Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.005 Å
R factor = 0.041
wR factor = 0.119
Data-to-parameter ratio = 12.0

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

Comment

Benzene-1,3,5-tricarboxylate usually plays the role of a bridging ligand in metal complexes (Wang *et al.*, 2005; Wei *et al.*, 2006). We present here the structure of the title Zn^{II} and Co^{II} complex, (I), in which benzene-1,3,5-tricarboxylate (BTC) ligands link the Zn^{II} and Co^{II} atoms in two kinds of coordination modes, forming a polymeric complex.



(I)

The title polymer contains two independent atoms, Zn^{II} and Co^{II}, located at the centers of centrosymmetric ZnO_6 and CoO_6 octahedra (Fig. 1). Each BTC ligand bridges one Zn^{II} and one Co^{II} atom, forming a polymeric zigzag chain running along [011]. Two carboxylate group of the BTC coordinate to the Zn^{II} and Co^{II} atoms, one in a monodentate fashion and the other in a bidentate chelating fashion; the third carboxylate group of the BTC is not coordinated to the Zn^{II} and Co^{II} atoms. The packing of the chains forms quadrilateral pores, which are occupied by one piperazinium(2+) cation and two water molecules (Fig. 2).

Experimental

An aqueous solution (15 ml) of benzene-1,3,5-tricarboxylic acid (0.210 g) and piperazine hexahydrate (0.132 g) was mixed with an

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aqueous solution (5 ml) of zinc(II) nitrate hexahydrate (0.149 g) and cobalt(II) nitrate hexahydrate (0.146 g) with continuous stirring. The mixture was sealed in a 40 ml Teflon-lined stainless steel vessel and heated at 453 K for 96 h under autogenous conditions. After cooling to room temperature, the resulting product was filtered off to obtain pink crystals of (I) (about 76.2% yield based on the Zn source). IR (KBr, ν cm^{-1}): 3120, 2446, 2345, 1610, 1533, 1429, 1426, 1398, 1363, 1202, 1087, 754, 712, 542, 521, 459; elemental analysis calculated for $C_{22}H_{34}CoN_2O_{20}Zn$: C 34.25, H 4.45, N 3.63%; found: C 34.29, H 4.52, N 3.58%.

Crystal data

$(C_4H_{12}N_2)[ZnCo(C_9H_3O_6)_2(H_2O)_6]\cdot 2H_2O$	$\gamma = 102.538\ (6)^\circ$
$M_r = 770.81$	$V = 731.8\ (5)$ Å^3
Triclinic, $P\overline{1}$	$Z = 1$
$a = 7.189\ (3)$ Å	$D_x = 1.749$ Mg m^{-3}
$b = 10.588\ (4)$ Å	Mo $K\alpha$ radiation
$c = 10.593\ (4)$ Å	$\mu = 1.48$ mm^{-1}
$\alpha = 110.675\ (5)^\circ$	$T = 294\ (2)$ K
$\beta = 91.429\ (6)^\circ$	Block, pink
	0.20 × 0.18 × 0.14 mm

Data collection

Bruker SMART CCD area-detector diffractometer	3672 measured reflections
	2549 independent reflections
φ and ω scans	2137 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$R_{int} = 0.023$
	$\theta_{max} = 25.0^\circ$
$T_{min} = 0.485$, $T_{max} = 0.813$	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0648P)^2 + 1.1797P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.041$	
$wR(F^2) = 0.119$	
$S = 1.04$	$(\Delta/\sigma)_{max} < 0.001$
2549 reflections	$\Delta\rho_{max} = 0.72$ e Å^{-3}
212 parameters	$\Delta\rho_{min} = -0.77$ e Å^{-3}
H-atom parameters constrained	

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O7^{i}	0.90	2.05	2.901 (4)	156
O8—H8A···O5^{i}	0.84	1.84	2.672 (4)	170
O10—H10C···O6^{i}	0.85	1.90	2.751 (5)	180
N1—H1A···O8^{ii}	0.90	2.44	3.033 (4)	124
N1—H1B···O6^{iii}	0.90	1.87	2.758 (4)	169
O7—H7B···O5^{iv}	0.85	1.89	2.721 (4)	168
O8—H8B···O4^{iv}	0.85	1.92	2.755 (3)	167
O9—H9B···O2^{v}	0.85	1.80	2.641 (4)	168
O10—H10D···O9^{vi}	0.85	2.09	2.920 (5)	167
O9—H9A···O10	0.84	1.96	2.756 (5)	156
O7—H7A···O2	0.85	1.85	2.653 (4)	158

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

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H = 0.93–0.97 Å, N—H = 0.90 Å and O—H = 0.84–0.86 Å, and with U_{iso}(H) values set at $1.2U_{eq}$(C,N) or $1.5U_{eq}$(O).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

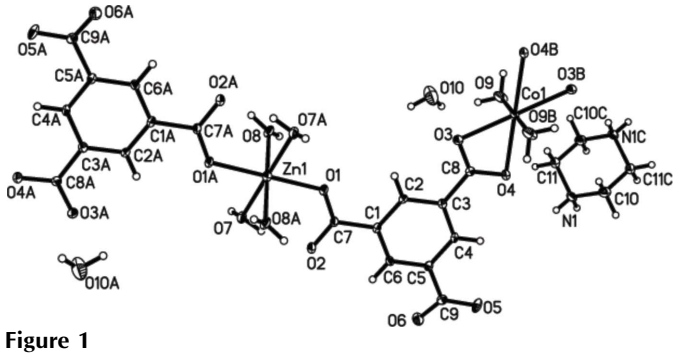

Figure 1
View of a segment of the title polymer (I) with 30% probability displacement ellipsoids (arbitratry spheres for H atoms) [Symmetry codes: (A) $-x, -y, -z+1$; (B) $-x, -y+1, -z$; (C) $-x+2, -y+2, -z$].

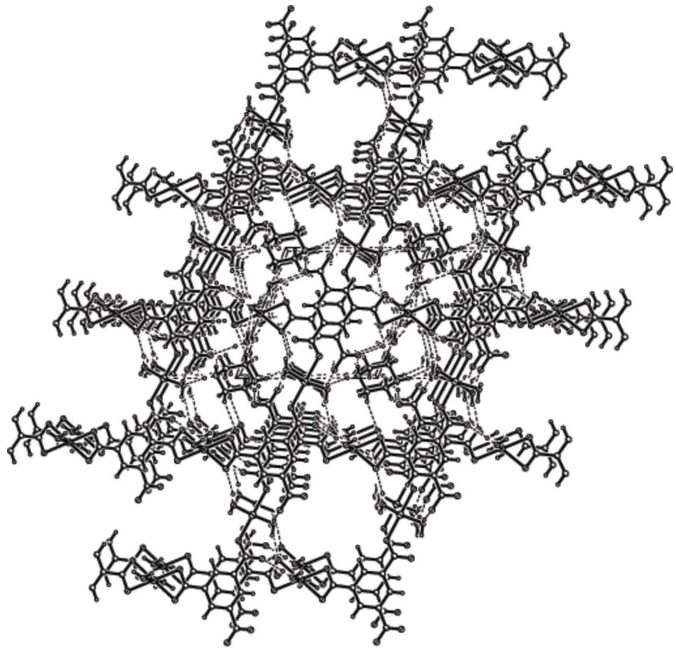

Figure 2
Packing of (I), viewed along the *a* axis. Dashed lines indicate hydrogen bonds.

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