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Poly[piperazinium(2+) [hexaaquabis(μ_3-benzene-1,3,5-tricarboxylato)dinickel(II)] dihydrate]

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.030
wR factor = 0.084
Data-to-parameter ratio = 11.8

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

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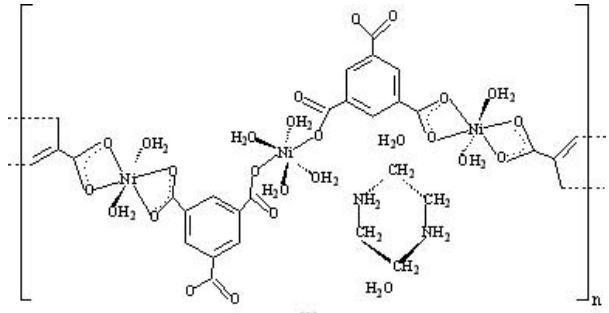
The title polymer, $\{(C_4H_{12}N_2)[Ni_2(C_9H_3O_6)_2(H_2O)_6]\cdot 2H_2O\}_n$, contains two independent Ni^{II} atoms, both of which are located on inversion centers. The benzene-1,3,5-tricarboxylate molecule bridges the Ni^{II} atoms in two coordination modes to form a one-dimensional polymeric structure. In the micropore formed by packing of the zigzag chains, there are one piperazinium(2+) cation and two water molecules.

Comment

Benzene-1,3,5-tricarboxylate usually plays the role of a bridging ligand in metal complexes (Wang *et al.*, 2005; Wei & Han, 2005). We present here the structure of the title Ni^{II} complex, $\{(C_4H_{12}N_2)[Ni_2(BTC)_2(H_2O)_6]\cdot 2H_2O\}_n$ (BTC is benzene-1,3,5-tricarboxylate), (I), in which BTC ligands link the Ni^{II} atoms in two coordination modes to form the polymeric complex.



(I)

The title polymer contains two independent Ni^{II} atoms, which are located at the centers of different centrosymmetric NiO_6 octahedra (Fig. 1). Each BTC bridges two Ni^{II} atoms to form a polymeric zigzag chain running along [01$\bar{1}$]. Two carboxylate groups of the BTC coordinate to Ni^{II} atoms, one in a monodentate fashion and the other in a bidentate chelating fashion, respectively, while the third is not coordinated to Ni^{II}. 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 aqueous solution (5 ml) of nickel(II) nitrate hexahydrate (0.146 g) and cobalt(II) nitrate hexahydrate (0.145 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

yield pale-green crystal of (I) (about 56.8% yield based on the Ni source). IR (KBr, ν cm^{-1}): 3120, 2445, 2345, 1610, 1533, 1454, 1426, 1398, 1363, 1202, 1087, 754, 712, 542, 521, 459; Elemental analysis calculated for $C_{22}H_{34}N_2Ni_2O_{20}$: C 34.56, H 4.49%; found: C 34.29, H 4.58%. The compound does not contain any Co substituted for Ni, as shown by both the ICP analysis (Inductively Coupled Plasma Atomic Emission Spectrometer) and the color of the product.

Crystal data

$(C_4H_{12}N_2)[Ni_2(C_9H_3O_6)_2(H_2O)_6]\cdot 2H_2O$	$Z = 1$
$M_r = 763.93$	$D_x = 1.768$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo $K\alpha$ radiation
$a = 7.136$ (3) Å	Cell parameters from 1723 reflections
$b = 10.515$ (4) Å	$\theta = 2.4$–$27.3°$
$c = 10.517$ (4) Å	$\mu = 1.41$ mm^{-1}
$\alpha = 110.553$ (4)°	$T = 293$ (2) K
$\beta = 91.344$ (5)°	Block, pale-green
$\gamma = 102.424$ (5)°	0.22 × 0.14 × 0.12 mm
$V = 717.4$ (5) Å^3	

Data collection

Bruker APEX-II CCD area-detector diffractometer	2491 independent reflections
φ and ω scans	2068 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$R_{int} = 0.015$
$T_{min} = 0.759$, $T_{max} = 0.845$	$\theta_{max} = 25.0°$
3896 measured reflections	$h = -8 \rightarrow 8$
	$k = -12 \rightarrow 12$
	$l = -8 \rightarrow 12$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0444P)^2 + 0.4741P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.030$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.084$	$\Delta\rho_{max} = 0.32$ e Å^{-3}
$S = 1.06$	$\Delta\rho_{min} = -0.42$ e Å^{-3}
2491 reflections	
211 parameters	
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Ni1—O2	2.0596 (18)	Ni2—O3	2.093 (2)
Ni1—O7	2.0970 (19)	Ni2—O4	2.189 (2)
Ni1—O8	2.0714 (19)	Ni2—O9	2.029 (2)
O2—Ni1—O7	93.59 (7)	O3—Ni2—O4	61.27 (8)
O2—Ni1—O8	87.27 (8)	O9—Ni2—O3	89.28 (9)
O8—Ni1—O7	95.16 (8)	O9—Ni2—O4	89.36 (8)

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 = 0.85 Å. U_{iso}(H) values were 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); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1996); software used to prepare material for publication: *SHELXTL*.

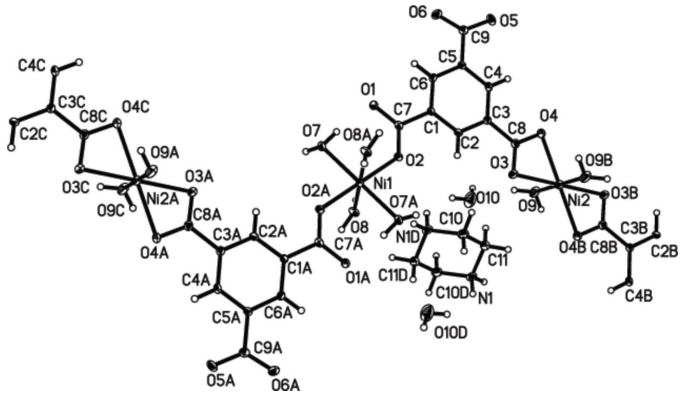


Figure 1
View of a segment of the title polymer (I) with 50% probability displacement ellipsoids [symmetry codes: (A) $-x+1, -y+1, -z$; (B) $-x+1, -y, -z+1$; (C) $x, y+1, z-1$; (D) $x, y, z-1$].

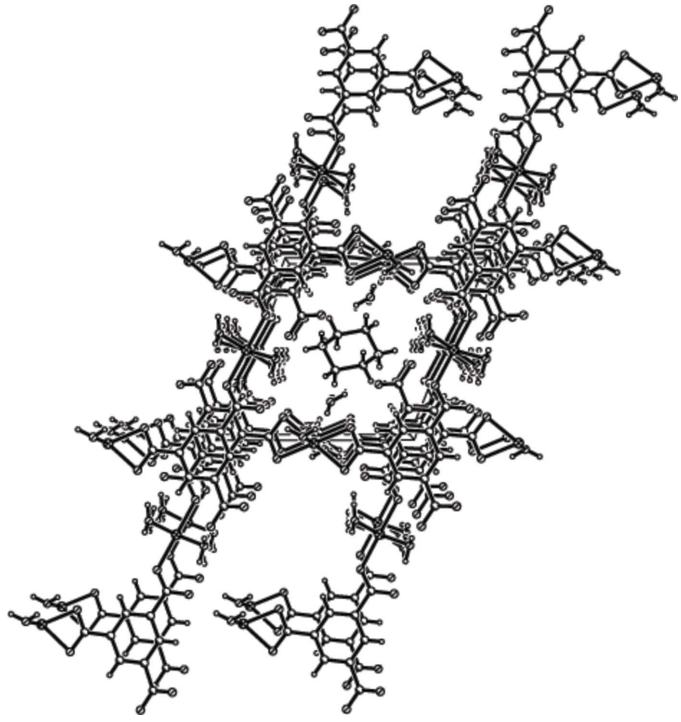


Figure 2
Packing of (I), viewed along the *a* axis.

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