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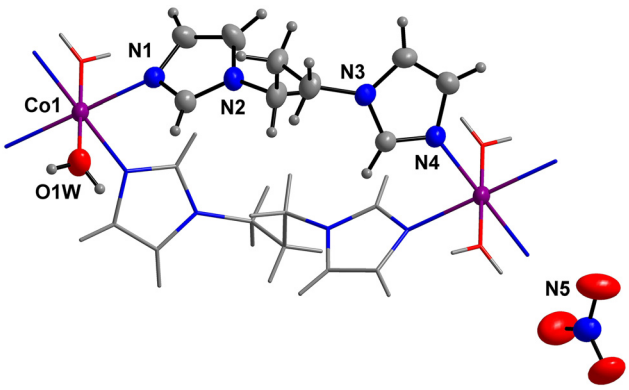
Crystal structure of *catena*-poly[diaqua-bis(μ_2-1,3-di(1*H*-imidazol-1-yl)propane-κ^2*N*:*N*′)cobalt(II)] dinitrate, $C_{18}H_{28}N_{10}O_8Co$



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Abstract

$C_{18}H_{28}N_{10}O_8Co$, monoclinic, $P2_1/c$ (no. 14), a = 9.2248(5) Å, b = 13.3140(8) Å, c = 10.6132(6) Å, β = 109.348(7)°, V = 1229.89(13) Å^3, Z = 2, $R_{gt}(F)$ = 0.0336, w$R_{ref}(F^2)$ = 0.1078, T = 293(2) K.

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A part of the polymer title crystal structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

The mixture of cobalt nitrate hexahydrate 43.7 mg (0.15 mmol), 1,3-di(1*H*-imidazol-1-yl)propane 20.1 mg (0.10 mmol), NaOH 12 mg (0.15 mmol) and *N*,*N*-dimethylformamide (10 mL) were placed in the autoclave lined with PTFE and heated at 120 °C for 36 h, then cooled to room temperature over 24 h. The pink crystals after cooling to room temperature were collected.

Table 1: Data collection and handling.

Crystal:	Pink block Size 0.22 × 0.17 × 0.11 mm
Wavelength:	MoKα radiation (0.71073 Å)
μ:	0.76 mm^{-1}
Diffractometer, scan mode:	φ and ω
θ_{max}, completeness:	25.0°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	4673, 2162, 0.021
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 1832
$N(param)_{refined}$:	177
Programs:	Bruker [1], SHELX [2, 3]

Experimental details

The structure was solved by direct methods and refined with the SHELX crystallographic software package [2]. The hydrogen atoms were placed at calculated positions and refined as riding atoms [3].

Comment

Construction of new metal coordination polymers (MCPs) has attracted attention due to their diverse structural topologies and potential applications as functional materials such as gas storage, magnetism, catalysis and luminescence [4–6]. Nitrogen-containing ligands have received considerable attention because of their versatile coordination models for the design of multifunctional coordination polymers. Meanwhile, the bis(imidazole)propane bearing alkyl spacers are a good choice [7], in which the flexible nature of spacers allows the ligands to bend and rotate when they coordinate to metal centers, and 1,3-di(1*H*-imidazol-1-yl)propane (diim) is known to serve as bridging ligand [8–12].

The asymmetric unit of the title structure contains one half of a Co(II) cation, one nitrate, one 1,3-di(1*H*-imidazol-1-

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Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	x	y	z	U_{iso}*/U_{eq}
C1	0.3940 (2)	0.05416 (17)	1.2024 (2)	0.0321 (5)
H1	0.471468	0.102216	1.221850	0.038*
C2	0.2384 (2)	−0.05767 (19)	1.2222 (2)	0.0374 (6)
H2	0.187534	−0.102797	1.259827	0.045*
C3	0.2063 (3)	−0.0431 (2)	1.0900 (2)	0.0421 (6)
H3	0.130918	−0.075143	1.020945	0.051*
C4	0.3159 (3)	0.07509 (19)	0.9561 (2)	0.0381 (6)
H4A	0.299236	0.024250	0.887292	0.046*
H4B	0.417952	0.102708	0.973264	0.046*
C5	0.1985 (3)	0.15753 (18)	0.9067 (2)	0.0385 (6)
H5A	0.195681	0.197653	0.982137	0.046*
H5B	0.097870	0.127613	0.866423	0.046*
C6	0.2328 (3)	0.22518 (18)	0.8057 (2)	0.0368 (5)
H6A	0.154034	0.276489	0.777182	0.044*
H6B	0.330558	0.258475	0.847418	0.044*
C7	0.3679 (2)	0.13740 (17)	0.6690 (2)	0.0311 (5)
H7	0.466620	0.152221	0.725340	0.037*
C8	0.1187 (2)	0.13311 (18)	0.5860 (2)	0.0351 (5)
H8	0.014847	0.142691	0.572897	0.042*
C9	0.1789 (2)	0.08086 (17)	0.5069 (2)	0.0346 (5)
H9	0.122564	0.048416	0.428302	0.042*
Co1	0.500000	0.000000	1.500000	0.02714 (18)
H1WA	0.634 (3)	0.1848 (11)	1.5237 (17)	0.063 (9)*
H1WB	0.6735 (18)	0.1383 (17)	1.4267 (17)	0.063 (10)*
N1	0.3566 (2)	0.00339 (13)	1.29321 (19)	0.0307 (5)
N2	0.3071 (2)	0.02839 (15)	1.07849 (17)	0.0333 (4)
N3	0.2389 (2)	0.16927 (14)	0.68880 (17)	0.0299 (4)
N4	0.3373 (2)	0.08272 (14)	0.56019 (16)	0.0314 (4)
N5	0.7730 (2)	0.18378 (16)	0.2096 (2)	0.0439 (5)
O1	0.8008 (3)	0.1280 (2)	0.3067 (2)	0.0852 (8)
O2	0.8722 (2)	0.21268 (19)	0.1652 (2)	0.0754 (7)
O3	0.6376 (2)	0.21036 (17)	0.1522 (2)	0.0728 (7)
O1W	0.6107 (2)	0.13547 (13)	1.46986 (16)	0.0439 (4)

yl)propane and one water ligand (see the Figure). Each Co(II) is six-coordinated by two water molecules, and four nitrogen atoms from four 1,3-di(1*H*-imidazol-1-yl)propane ligands, which exhibit distorted octahedral geometry. The average Co–N and Co–O bond lengths are in the normal range of 2.1231(17)–2.1551(19) and 2.1483(17) Å, respectively. The adjacent Co(II) ions are bridged by two bidentate diim ligands to afford a 1D loop-like chain.

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Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

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