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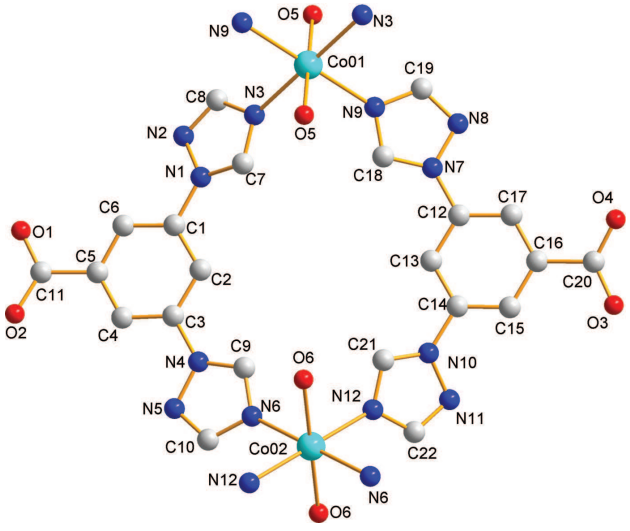
Crystal structure of catena-poly[diaqua-bis(μ$_2$-3,5-di(1*H*-1,2,4-triazol-1-yl)benzoate-κ^2*N*:*N*′) cobalt(II))] 2.5 hydrate, $C_{22}H_{23}CoN_{12}O_{8.50}$



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Abstract

$C_{22}H_{23}CoN_{12}O_{8.50}$, triclinic, $P\bar{1}$ (no. 2), $a = 9.6549(3)$ Å, $b = 10.6027(4)$ Å, $c = 13.4938(4)$ Å, $\alpha = 100.824(3)°$, $\beta = 99.707(3)°$, $\gamma = 96.642(3)°$, $V = 1321.76(8)$ Å^3, $Z = 2$, $R_{gt}(F) = 0.0366$, $wR_{ref}(F^2) = 0.0914$, $T = 288.03(10)$ K.

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The crystal structure is shown in the figure. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

The title compound was prepared by hydrothermal method. A mixture of $Co(OAc)_2 \cdot 4\ H_2O$ (0.049 g, 0.2 mmol), 3,5-di(1,2,4-triazole-4)benzenecarboxylic acid (0.0256 g, 0.1 mmol), and H_2O (10 mL) was sealed in a 25 mL Teflon-lined stainless steel vessel and heated at 160 °C for 4 days. The reaction mixture was slowly cooled to room temperature at a rate of 5 °C/h, and the red block crystals were collected, washed with water, and dried in air.

Table 1: Data collection and handling.

Crystal:	Clear light pink block
Size:	0.27 × 0.21 × 0.15 mm
Wavelength:	Mo *Kα* radiation (0.71073 Å)
μ:	0.73 mm^{-1}
Diffractometer, scan mode:	SuperNova, φ and ω
θ_{max}, completeness:	25.5°, 99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	14128, 4844, 0.028
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 4245
$N(param)_{refined}$:	412
Programs:	CrysAlis^{PRO} [1], SHELX [2, 3]

Experimental details

The hydrogen atoms were assigned with common isotropic displacement factors $U_{iso}(H) = 1.2$ times U_{eq} (C, aromatic ring), and $U_{iso}(H) = 1.5$ times U_{eq}(O, water). The final refinement by using geometrical restraints, with C—H = 0.93 Å (aromatic ring), and O—H = 0.85 Å (water).

Comment

Coordination polymer (CPs) or organic-inorganic hybrid materials, constructed by inorganic secondary building units and organic bridging ligands has taken wide attention owing to their intriguing structural as well as distinctive properties such as catalytic, luminescence, gas adsorption, and magnetism [4–6]. It is well known that the structures and properties of the CPs are strongly dependent on the organic ligands and the metal ions [7]. Bifunctional ligands containing carboxylate groups and nitrogen donors have attracted great interests in construction of CPs [8].

The asymmetric unit of the title compound consists of two-half Co(II) ions, two 3,5-di(1,2,4-triazole-4) benzenecarboxylic acid anions (L^-), two coordinated water molecules and two and a half lattice water molecules (Figure). The two Co1 centers are both six-coordinated with slightly distorted octahedral geometry. The coordinations are completed

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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}
Co01	0.5000	1.0000	1.0000	0.01936(12)
Co02	1.0000	0.5000	0.5000	0.01942(12)
O1	0.8678(2)	0.32659(17)	1.20232(13)	0.0390(5)
O2[a]	1.0096(6)	0.2309(5)	1.1044(4)	0.0367(9)
O2A[b]	0.9388(6)	0.1854(5)	1.0895(4)	0.0367(9)
O3	0.32773(19)	0.89171(18)	0.22653(13)	0.0358(4)
O4	0.2417(2)	1.03115(17)	0.33668(13)	0.0382(4)
O5	0.68976(17)	1.02834(16)	0.94737(12)	0.0301(4)
H5A	0.7482	1.0900	0.9896	0.045*
H5B	0.6749	1.0566	0.8915	0.045*
O6	1.03655(18)	0.67644(15)	0.60434(12)	0.0308(4)
H6A	1.0142	0.7357	0.5729	0.046*
H6B	1.1253	0.6977	0.6278	0.046*
O7	0.0488(3)	1.1038(2)	0.44923(19)	0.0608(6)
H7A	−0.0261	1.0482	0.4368	0.091*
H7B	0.1082	1.0741	0.4147	0.091*
O8	0.2284(2)	1.23730(19)	0.24516(16)	0.0502(5)
H8A	0.2373	1.1704	0.2704	0.075*
H8B	0.1486	1.2255	0.2043	0.075*
N1	0.6489(2)	0.63604(18)	1.00752(14)	0.0234(4)
N2	0.5733(2)	0.63768(19)	1.08453(15)	0.0300(5)
N3	0.5464(2)	0.80891(18)	1.01085(15)	0.0246(4)
N4	0.8938(2)	0.38858(17)	0.77082(14)	0.0219(4)
N5	0.9699(2)	0.29075(19)	0.74506(16)	0.0322(5)
N6	0.9464(2)	0.40871(18)	0.62279(14)	0.0246(4)
N7	0.3624(2)	0.88666(18)	0.67502(14)	0.0238(4)
N8	0.2540(2)	0.9546(2)	0.69348(16)	0.0337(5)
N9	0.3917(2)	0.94110(18)	0.84193(14)	0.0251(4)
N10	0.5937(2)	0.62392(18)	0.43906(14)	0.0248(4)
N11	0.5815(2)	0.5432(2)	0.34465(15)	0.0322(5)
N12	0.7849(2)	0.53384(18)	0.45077(15)	0.0252(4)
C1	0.7313(2)	0.5351(2)	0.98384(17)	0.0215(5)
C2	0.7654(2)	0.5079(2)	0.88717(17)	0.0224(5)
H2	0.7332	0.5528	0.8370	0.027*
C3	0.8490(2)	0.4117(2)	0.86740(17)	0.0211(5)
C4	0.8922(2)	0.3403(2)	0.93998(17)	0.0226(5)
H4	0.9466	0.2749	0.9250	0.027*
C5	0.8533(2)	0.3677(2)	1.03540(17)	0.0233(5)
C6	0.7742(2)	0.4670(2)	1.05818(17)	0.0235(5)
H6	0.7506	0.4874	1.1227	0.028*
C7	0.6313(3)	0.7386(2)	0.96515(18)	0.0258(5)
H7	0.6727	0.7578	0.9113	0.031*
C8	0.5141(3)	0.7425(2)	1.08300(18)	0.0276(5)
H8	0.4547	0.7694	1.1277	0.033*
C9	0.8823(3)	0.4569(2)	0.69663(17)	0.0256(5)
H9	0.8353	0.5288	0.6973	0.031*
C10	0.9978(3)	0.3065(2)	0.65592(19)	0.0297(6)
H10	1.0486	0.2523	0.6185	0.036*
C11	0.9023(3)	0.2952(2)	1.11814(18)	0.0299(6)
C12	0.3850(2)	0.8441(2)	0.57319(16)	0.0213(5)
C13	0.4696(2)	0.7488(2)	0.55503(17)	0.0239(5)
H13	0.5076	0.7096	0.6074	0.029*
C14	0.4963(2)	0.7136(2)	0.45687(17)	0.0221(5)
C15	0.4391(2)	0.7693(2)	0.37761(18)	0.0239(5)
H15	0.4573	0.7433	0.3119	0.029*
C16	0.3540(2)	0.8648(2)	0.39733(17)	0.0217(5)
C17	0.3276(2)	0.9030(2)	0.49574(17)	0.0228(5)
H17	0.2718	0.9675	0.5095	0.027*
C18	0.4417(2)	0.8808(2)	0.76462(17)	0.0256(5)
H18	0.5217	0.8396	0.7714	0.031*
C19	0.2761(3)	0.9841(3)	0.79417(19)	0.0323(6)
H19	0.2175	1.0306	0.8301	0.039*
C20	0.3017(2)	0.9342(2)	0.31297(18)	0.0243(5)
C21	0.7151(2)	0.6167(2)	0.49999(18)	0.0250(5)
H21	0.7460	0.6632	0.5674	0.030*
C22	0.6992(3)	0.4920(2)	0.35664(19)	0.0294(5)
H22	0.7220	0.4317	0.3047	0.035*
O9[c]	0.9241(4)	−0.0389(4)	1.0463(3)	0.0482(10)
H9A[c]	0.9693	−0.0714	1.0013	0.072*
H9B[c]	0.9477	0.0423	1.0491	0.072*

[a]Occupancy: 0.517(5), [b]Occupancy: 0.483(5), [c]Occupancy: 0.5.

by four nitrogen atoms from four different L^- anions, and two oxygen atoms from coordinated water molecules. The Co—N bond lengths are in the range of 2.1506(18)–2.1737(18) Å, and the Co—O bond lengths are 2.0840(16) and 2.0728(16) Å, respectively. In the title compound, each L^- ligand coordinated to two center Co(II) ions by two nitrogen atoms. Thus adjacent Co(II) ions are connected into 1D chain structure. The carboxyl group of L^- did not participate in the coordination.

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