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The crystal structure of diaqua-bis(2-(3-(1H-pyrazol-4-yl)-1H-1,2,4-triazol-5-yl)pyridine- $\kappa^2N:N'$)-bis(3,5-dicarboxybenzoato- κ^1O)cobalt(II), $C_{38}H_{30}CoN_{12}O_{14}$

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Abstract

$C_{38}H_{30}CoN_{12}O_{14}$, triclinic, $P\bar{1}$ (no. 2), $a = 6.9503(3)$ Å, $b = 7.0244(4)$ Å, $c = 20.1182(9)$ Å, $\alpha = 92.261(4)^\circ$, $\beta = 95.206(4)^\circ$, $\gamma = 104.600(4)^\circ$, $V = 944.59(8)$ Å³, $Z = 1$, $R_{gt}(F) = 0.0408$, $wR_{ref}(F^2) = 0.0910$, $T = 287$ K.

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Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

A mixture of H_2L (2-(3-(1H-pyrazol-4-yl)-1H-1,2,4-triazol-5-yl)pyridine, 43 mg, 0.2 mmol), 1,3,5- H_3 btc (trimesic acid,

Table 1: Data collection and handling.

Crystal:	Red block
Size:	$0.22 \times 0.20 \times 0.20$ mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	0.55 mm^{-1}
Diffractometer, scan mode:	SuperNova, ω
$\theta_{\max}$, completeness:	26.0° , >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	10271, 3596, 0.028
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 3171
$N(\text{param})_{\text{refined}}$:	301
Programs:	CrysAlis ^{PRO} [1], Olex2 [2], SHELXL [3]

42 mg, 0.2 mmol), $Co(OAc)_2 \cdot 4H_2O$ (50 mg, 0.2 mmol) and acetonitrile/ H_2O (10 mL, 1:4 v/v) was stirred for 30 min. The mixture was transferred to a 25 mL Teflon-lined stainless steel vessel and heated at 150°C for three days, and then cooled to room temperature over 48 h. Red crystals of the title compound were obtained.

Experimental details

Using Olex2, the structure was solved with the SIR2004 structure solution program using Direct Methods and refined with the ShelXL refinement package using least squares minimisation.

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Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($\text{\AA}^2$).

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}/U_{\text{eq}}$
Co1	1.0000	0.5000	0.5000	0.02531 (14)
O1	0.7888 (2)	0.3507 (3)	0.56972 (8)	0.0337 (4)
O2	0.4727 (2)	0.2397 (3)	0.52567 (8)	0.0467 (5)
O3	−0.0570 (2)	−0.0866 (3)	0.65400 (8)	0.0448 (5)
O4	0.0079 (2)	−0.1189 (3)	0.76239 (8)	0.0448 (5)
H4	−0.1119	−0.1736	0.7591	0.067
H5	0.785 (5)	0.186 (5)	0.9115 (19)	0.095 (12)
O5	0.6819 (2)	0.1568 (3)	0.87433 (8)	0.0416 (5)
O6	0.9289 (2)	0.3063 (3)	0.81664 (9)	0.0457 (5)
O7	0.9114 (2)	0.7563 (3)	0.51634 (8)	0.0361 (4)
H7A	0.9227	0.7886	0.5585	0.054
H7B	0.7883	0.7380	0.5007	0.054
N1	0.7965 (2)	0.4308 (3)	0.40978 (9)	0.0257 (4)
N2	0.6028 (3)	0.3405 (3)	0.41353 (9)	0.0329 (5)
H2	0.5542	0.3026	0.4500	0.039
N3	0.3761 (2)	0.3211 (3)	0.20651 (8)	0.0230 (4)
N4	0.6855 (3)	0.4617 (3)	0.19194 (9)	0.0305 (5)
H4A	0.8117	0.5136	0.2010	0.037
N5	0.5864 (3)	0.4395 (3)	0.12980 (9)	0.0352 (5)
N6	−0.0539 (3)	0.2287 (3)	−0.02322 (10)	0.0360 (5)
C1	0.4959 (3)	0.3168 (4)	0.35455 (11)	0.0324 (6)
H1	0.3594	0.2590	0.3462	0.039
C2	0.6213 (3)	0.3922 (3)	0.30801 (10)	0.0218 (5)
C3	0.8077 (3)	0.4614 (4)	0.34540 (11)	0.0280 (5)
H3	0.9249	0.5214	0.3274	0.034
C4	0.5611 (3)	0.3922 (3)	0.23727 (10)	0.0219 (5)
C5	0.4012 (3)	0.3537 (3)	0.14062 (11)	0.0263 (5)
C6	0.2415 (3)	0.3059 (3)	0.08491 (11)	0.0267 (5)
C7	0.2891 (3)	0.2944 (4)	0.01942 (11)	0.0359 (6)
H7	0.4215	0.3121	0.0108	0.043
C8	0.1389 (4)	0.2567 (4)	−0.03250 (12)	0.0383 (6)
H8	0.1731	0.2504	−0.0760	0.046
C9	−0.0995 (4)	0.2391 (4)	0.03947 (12)	0.0378 (6)
H9	−0.2333	0.2197	0.0466	0.045
C10	0.0415 (3)	0.2773 (4)	0.09430 (11)	0.0342 (6)
H10	0.0028	0.2838	0.1372	0.041
C11	0.6088 (3)	0.2695 (3)	0.57336 (11)	0.0263 (5)
C12	0.5408 (3)	0.2016 (3)	0.63992 (10)	0.0229 (5)
C13	0.6716 (3)	0.2332 (3)	0.69762 (11)	0.0255 (5)
H13	0.8062	0.2932	0.6954	0.031
C14	0.6057 (3)	0.1771 (3)	0.75882 (10)	0.0237 (5)
C15	0.4056 (3)	0.0831 (3)	0.76228 (11)	0.0244 (5)
H15	0.3605	0.0440	0.8030	0.029
C16	0.2737 (3)	0.0482 (3)	0.70434 (10)	0.0223 (5)
C17	0.3408 (3)	0.1068 (3)	0.64369 (10)	0.0239 (5)
H17	0.2513	0.0825	0.6052	0.029
C18	0.0590 (3)	−0.0585 (3)	0.70380 (11)	0.0261 (5)
C19	0.7542 (3)	0.2188 (4)	0.81949 (11)	0.0301 (5)

Comment

The design and synthesis of coordination compound materials have been extensively studied owing to the widespread

applications in the areas of absorption, sensors, magnetism, catalysis and molecular recognition etc. [4–6]. Generally, the structure of functional compounds depends on the selection of metal centers and rational design of ligands. Especially, the physical and chemical characteristics of ligands play a crucial role in regulating the properties of functional compounds [7–9]. Triazole pyridine derivatives are very interesting polydentate ligands with multiple N atoms, and they are promising building motifs [10–12]. The oligo-carboxylate ligands have versatile coordination conformations and a strong coordination ability [13]. So mixed ligands incorporating the triazole ligands and aromatic carboxylates prove to construct intriguing compounds [14, 15]. Moreover, cobalt ion exhibits a good ability when coordinating with the ligands containing nitrogen and oxygen atoms. In addition, it is more environmental friendly compared with the toxic heavy metal ions as lead and mercury [16].

In the title compound, the asymmetric unit contains one half of Co(II) ion, one H_2L ligand, one H_2btc^- ligand and one coordinated H_2O molecule (figure). The Co(II) ion is located on an inversion centre, therefore, H_2L , H_2btc^- ligands and H_2O molecules are in trans positions. The Co(II) ion is six-coordinated in a distorted octahedral N_2O_4 environment. The equatorial plane is formed by two nitrogen atoms of two different H_2L ligands and two oxygen atoms from two H_2btc^- ligands. The Co1–N1 and Co1–N1A bond distances are 2.1562(16). The Co–O bond distances are 2.2214(15) Å for Co1–O1 and Co1–O1A. The angles of N–Co–O are in the range of 82.52(6)–97.48(6)°. The axial sites are occupied by two oxygen atoms from two H_2O molecules, and the Co–O bond distances are 2.0679(17) for Co1–O7 and Co1–O7A. Symmetry code: $A\ 2 - x, 1 - y, 1 - z$. Pyrazole, triazole, and trimesic acid rings are almost in the same equatorial plane, and the angles between the equatorial plane and the corresponding rings are 5.3°, 6.4° and 5.0°, respectively. The angles are both 25.94° between the equatorial plane and the pyridine rings.

In addition, there are abundant intermolecular hydrogen bonds in the crystal structure. The adjacent groups are connected via intermolecular hydrogen bonds ($N2-H2\cdots O2$ 1.71 Å, $N4-H4A\cdots O6^3$ 1.99 Å, $O4-H4\cdots N3^1$ 2.06 Å, $O5-H5\cdots N6^4$ 1.61 Å) between triazole nitrogen atoms and carboxyl oxygen atoms to yield a layered structure. The adjacent layers are stacked by intermolecular hydrogen ($O7-H7B\cdots O2^2$ 1.89 Å, $O7-H7A\cdots O3$ 2.06 Å) between carboxyl oxygen atoms and the coordinating water molecule to form a 3D supramolecular network. Symmetry code: $^1-x, -y, 1-z$; $^21-x, 1-y, 1-z$; $^32-x, 1-y, 1-z$; $^41+x, +y, 1+z$.

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