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Crystal structure of *catena*-poly[triaqua-(μ_2 -1,3-di(1*H*-imidazol-1-yl)propane- $\kappa^2 N:N'$)-(4,4'-(1*H*-1,2,4-triazole-3,5-diyl)dibenzoato- $\kappa^1 O$)cobalt(II)] – *N,N'*-dimethylformamide (1/1), $C_{28}H_{34}N_8O_8Co$

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Abstract

$C_{28}H_{34}N_8O_8Co$, monoclinic, $P2_1/c$ (no. 14), $a = 14.8071(17)$ Å, $b = 19.676(2)$ Å, $c = 10.8580(13)$ Å, $V = 3066.7(6)$ Å³, $Z = 4$, $R_{gt}(F) = 0.0377$, $wR_{ref}(F^2) = 0.1228$, $T = 293(2)$ 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.

Table 1: Data collection and handling.

Crystal:	Purple block
Size:	0.30 × 0.26 × 0.22 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.62 mm ^{−1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
θ_{max} , completeness:	25.0°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int} :	15,494, 5398, 0.030
Criterion for I_{obs} , $N(hkl)_{gt}$:	$I_{obs} > 2\sigma(I_{obs})$, 4402
$N(param)_{refined}$:	432
Programs:	BRUKER [1], SHELX [2, 3]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	x	y	z	<i>U</i> _{iso} */ <i>U</i> _{eq}
C1	0.50779 (17)	0.31614 (13)	0.1611 (3)	0.0313 (6)
C2	0.42304 (15)	0.31747 (12)	0.2150 (2)	0.0259 (5)
C3	0.33596 (16)	0.30079 (12)	0.1381 (2)	0.0288 (5)
H3	0.330326	0.288938	0.053661	0.035*
C4	0.25775 (16)	0.30169 (12)	0.1864 (2)	0.0270 (5)
H4	0.199916	0.290641	0.134063	0.032*
C5	0.26497 (15)	0.31900 (11)	0.3126 (2)	0.0231 (5)
C6	0.35258 (17)	0.33298 (13)	0.3909 (2)	0.0307 (6)
H6	0.358706	0.342520	0.476403	0.037*
C7	0.43054 (17)	0.33275 (13)	0.3420 (2)	0.0310 (6)
H7	0.488559	0.342919	0.394806	0.037*
C8	0.18236 (15)	0.32421 (11)	0.3645 (2)	0.0224 (5)
C9	0.09161 (15)	0.33264 (11)	0.4867 (2)	0.0231 (5)
C10	0.05894 (16)	0.33660 (11)	0.6043 (2)	0.0247 (5)
C11	−0.03455 (16)	0.32827 (12)	0.6024 (2)	0.0278 (5)
H11	−0.078334	0.322493	0.525532	0.033*
C12	−0.06245 (16)	0.32858 (12)	0.7148 (2)	0.0274 (5)
H12	−0.125056	0.322385	0.712849	0.033*
C13	0.00123 (16)	0.33797 (11)	0.8305 (2)	0.0247 (5)
C14	0.09423 (17)	0.34823 (14)	0.8314 (2)	0.0352 (6)
H14	0.137608	0.356118	0.907875	0.042*
C15	0.12275 (17)	0.34679 (14)	0.7194 (2)	0.0344 (6)
H15	0.185400	0.352737	0.721408	0.041*
C16	−0.02672 (17)	0.33697 (12)	0.9552 (2)	0.0270 (5)
C17	0.73279 (17)	0.40166 (13)	0.4738 (2)	0.0352 (6)
H17	0.691002	0.371281	0.495271	0.042*
C18	0.8238 (2)	0.45083 (15)	0.3768 (3)	0.0502 (8)
H18	0.856887	0.460894	0.316583	0.060*
C19	0.8279 (2)	0.48688 (16)	0.4832 (3)	0.0588 (9)
H19	0.863594	0.525479	0.509688	0.071*
C20	0.7430 (2)	0.48164 (17)	0.6602 (3)	0.0583 (9)
H20A	0.712197	0.525229	0.640574	0.070*
H20B	0.698963	0.450544	0.683186	0.070*
C21	0.8240 (3)	0.48986 (17)	0.7700 (3)	0.0588 (9)
H21A	0.872320	0.515071	0.743561	0.071*
H21B	0.848859	0.445397	0.798637	0.071*
C22	0.7985 (3)	0.52726 (15)	0.8809 (3)	0.0616 (10)
H22A	0.855616	0.539592	0.942208	0.074*
H22B	0.766506	0.569040	0.848813	0.074*
C23	0.7685 (2)	0.43792 (15)	1.0268 (3)	0.0460 (7)
H23	0.829240	0.421472	1.047154	0.055*
C24	0.6485 (3)	0.49750 (16)	0.9409 (3)	0.0625 (9)
H24	0.608943	0.529354	0.892010	0.075*
C25	0.6252 (2)	0.45108 (16)	1.0204 (3)	0.0518 (8)
H25	0.566317	0.445973	1.035191	0.062*
C26	0.5347 (2)	0.35516 (16)	0.7545 (3)	0.0514 (8)
H26	0.529842	0.317976	0.805412	0.062*
C27	0.4654 (3)	0.4567 (2)	0.6490 (4)	0.0825 (12)
H27A	0.464972	0.496727	0.699306	0.124*
H27B	0.411987	0.456934	0.577949	0.124*
H27C	0.521141	0.455933	0.618767	0.124*
C28	0.3793 (2)	0.3826 (2)	0.7693 (4)	0.0852 (13)
H28A	0.388342	0.341690	0.819033	0.128*
H28B	0.327342	0.376873	0.697246	0.128*
H28C	0.367207	0.419723	0.820305	0.128*

Table 2: (continued)

Atom	x	y	z	<i>U</i> _{iso} */ <i>U</i> _{eq}
Co1	0.71736 (2)	0.33227 (2)	0.21032 (3)	0.02478 (13)
H1WA	0.8745 (13)	0.3160 (19)	0.1281 (11)	0.097 (14)*
H2WA	0.6914 (12)	0.2609 (16)	−0.0095 (10)	0.066 (10)*
H3WA	0.7852 (7)	0.2215 (9)	0.355 (2)	0.046 (9)*
H1WB	0.9040 (8)	0.3263 (14)	0.2545 (13)	0.051 (10)*
H2WB	0.61340 (17)	0.2618 (17)	0.0339 (17)	0.066 (11)*
H3WB	0.6972 (12)	0.2118 (9)	0.286 (3)	0.091 (14)*
N1	0.76356 (14)	0.39688 (10)	0.36983 (19)	0.0317 (5)
N2	0.76886 (17)	0.45543 (12)	0.5449 (2)	0.0438 (6)
N3	0.73996 (19)	0.48875 (11)	0.9462 (2)	0.0435 (6)
N4	0.70160 (15)	0.41308 (11)	1.07520 (19)	0.0346 (5)
N5	0.18354 (13)	0.32736 (10)	0.48790 (18)	0.0259 (5)
N6	0.03503 (13)	0.33368 (10)	0.37130 (19)	0.0291 (5)
N7	0.09464 (13)	0.32816 (10)	0.29422 (19)	0.0283 (5)
H7A	0.078325	0.327327	0.212562	0.034*
N8	0.46264 (16)	0.39692 (14)	0.7259 (2)	0.0515 (7)
O1	0.58372 (12)	0.33499 (9)	0.23504 (17)	0.0362 (5)
O2	0.49831 (12)	0.29606 (13)	0.05016 (18)	0.0588 (6)
O3	0.03239 (13)	0.35640 (12)	1.05105 (17)	0.0508 (6)
O4	−0.10732 (11)	0.31730 (10)	0.95673 (16)	0.0368 (4)
O5	0.60708 (15)	0.36085 (11)	0.7205 (2)	0.0636 (6)
O1W	0.85508 (11)	0.32205 (10)	0.19474 (17)	0.0336 (4)
O2W	0.67246 (12)	0.25997 (10)	0.05834 (15)	0.0339 (4)
O3W	0.73298 (12)	0.24134 (9)	0.32979 (17)	0.0324 (4)

Source of material

The mixture of 3,5-bis(4'-carboxy-phenyl)-1,2,4-triazole 30.9 mg (0.1 mmol), 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 (6 mL) were placed in the autoclave lined with PTFE and heated at 150 °C for 24 h, then cooled up to room temperature over 24 h. The pink crystals were collected after cooling to room temperature.

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 with isotropic displacement parameters [3].

Comment

Mixed ligands-CPs can be constructed from metal ions and carboxylic acid and nitrogen-containing ligands. In most situations, N containing ligands are electrically neutral,

while carboxylate ligands are negatively charged. Multicarboxylates like the 3,5-bis(4'-carboxy-phenyl)-1,2,4-triazole have been widely utilized to construct such networks [4–7]. On the other hand, 1,3-di(1*H*-imidazol-1-yl)propane (diim) is known to serve as bridging ligand [8–10].

The asymmetric unit of the title structure contains one Co(II) cation, one free *N,N*-dimethylformamide, one 1,3-di(1*H*-imidazol-1-yl)propane, one dianionic 4,4'-(1*H*-1,2,4-triazole-3,5-diyl)dibenzoate (bct) and three coordination water molecules. Each Co(II) is six-coordinated by three oxygen atom from three coordination water molecules, one oxygen atom from one bct ligand and two nitrogen atom from two 1,3-di(1*H*-imidazol-1-yl)propane ligands. The water ligands show almost identical Co–O distances. Co(1)–O(1W) 0.20977(18) nm Co(1)–O(2W) 0.21561(19) nm Co(1)–O(3W) 0.21894(19) nm], which exhibit a twisted octahedral geometry. The bridging diim ligands also link Co cations to form a 1D chain [11]. Then by intermolecular hydrogen bonding a 3D supramolecular structure formed.

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