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Crystal structure of poly[bis(μ_2 -4-bromoisophthalate- $\kappa^2 O:O'$)-tris(μ_2 -1-(3-((1H-1,2,4-triazol-1-yl)methyl)benzyl)-1H-1,2,4-triazole- $\kappa^2 N:N'$)dicobalt(II)] monohydrate, $C_{26}H_{23}CoN_9O_5Br$

Table 1: Data collection and handling.

Crystal:	Block, clear dark violet
Size:	0.25 × 0.20 × 0.16 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	2.09 mm ⁻¹
Diffractometer, scan mode:	Bruker SMART, φ and ω -scans
$\theta_{\max}$, completeness:	25.5°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	12897, 5223, 0.028
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 3940
$N(\text{param})_{\text{refined}}$:	382
Programs:	Bruker programs [1], SHELX [2], OLEX2 [3]

Source of material

A mixture of 4-bromoisophthalic acid (H_2Brip , 24.5 mg, 0.1 mmol), $Co(NO_3)_2 \cdot 6H_2O$ (29.1 mg, 0.1 mmol), and 1-(3-((1H-1,2,4-triazol-1-yl)methyl)benzyl)-1H-1,2,4-triazole (bmbt, 24.0 mg, 0.1 mmol), was added to water (9 mL) in a 25 mL Teflon-lined autoclave. The mixture was heated at 423 K for 3 days and then slowly cooled down to room temperature. Red block crystals of the title compound were obtained.

Experimental details

The hydrogen atoms were placed in calculated positions riding on attached atoms with isotropic thermal parameters 1.2 times those of their carrier atoms. The U_{iso} values of the hydrogen atoms of methyl groups and oxygen were set to 1.5 $U_{\text{eq}}(C, O)$.

Discussion

MOFs and CPs with fascinating networks and potential applications have attracted great attention [4–6]. Among the construction strategies, the mixed-ligand synthetic method, especially the combination of multicarboxylate ligands and nitrogen-donor ligands, play a greatly significant role for the preparation of MOFs and CPs [7–9]. The flexible linkers with nitrogen donors have been widely utilized in the construction of MOFs and CPs due to the variable coordination modes. Bis(imidazole)/bis(triazol) ligands are the broadest organic building blocks to construct MOFs [10–12]. In this work, through the combinatorial fashion of 4-bromoisophthalic

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Abstract

$C_{26}H_{23}CoN_9O_5Br$, triclinic, $P\bar{1}$ (no. 2), $a = 8.3522(10)$ Å, $b = 13.6076(16)$ Å, $c = 14.1028(17)$ Å, $\alpha = 64.664(1)^\circ$, $\beta = 76.130(1)^\circ$, $\gamma = 79.045(1)^\circ$, $V = 1405.4(3)$ Å³, $Z = 2$, $R_{\text{gt}}(F) = 0.0445$, $wR_{\text{ref}}(F^2) = 0.1156$, $T = 296(2)$ K.

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A part of 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.

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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}
Co1	0.5	0.5	0.0	0.02896(18)
Co2	−0.5	0.0	0.5	0.02858(18)
Br1	−0.43887(6)	0.37395(4)	0.45668(5)	0.0699(2)
O1	−0.3513(3)	0.1307(2)	0.4192(2)	0.0410(7)
O2	−0.1830(5)	0.0994(3)	0.5298(3)	0.0858(14)
O3	0.3071(3)	0.4260(2)	0.1228(2)	0.0408(7)
O4	0.3191(3)	0.2434(2)	0.1971(2)	0.0447(7)
O5	−0.6146(3)	0.0521(2)	0.3643(2)	0.0429(7)
H5a	−0.6637(3)	0.1152(2)	0.3560(2)	0.0644(10)*
H5b	−0.6849(3)	0.0055(2)	0.3886(2)	0.0644(10)*
N1	−0.3235(4)	−0.0985(2)	0.4337(2)	0.0346(7)
N2	−0.2318(4)	−0.2035(3)	0.3415(3)	0.0446(9)
N3	−0.1103(4)	−0.1983(3)	0.3881(3)	0.0377(8)
N4	0.5394(4)	0.5815(3)	0.0891(3)	0.0371(8)
N5	0.6100(4)	0.7030(3)	0.1277(3)	0.0414(8)
N6	0.4709(6)	0.6674(4)	0.1990(3)	0.0676(13)
N7	0.6963(4)	0.3703(2)	0.0594(3)	0.0363(8)
N8	0.8372(4)	0.2109(3)	0.1142(3)	0.0413(8)
N9	0.9536(4)	0.2823(3)	0.0588(3)	0.0451(9)
C1	−0.2388(5)	0.1535(3)	0.4472(3)	0.0356(9)
C2	−0.1593(4)	0.2586(3)	0.3737(3)	0.0307(8)
C3	−0.2329(5)	0.3604(3)	0.3697(3)	0.0392(9)
C4	−0.1541(5)	0.4535(3)	0.3080(3)	0.0428(10)
H4	−0.2053(5)	0.5210(3)	0.3064(3)	0.0513(12)*
C5	0.0008(5)	0.4460(3)	0.2487(3)	0.0377(9)
H5	0.0539(5)	0.5089(3)	0.2069(3)	0.0452(11)*
C6	0.0785(4)	0.3462(3)	0.2505(3)	0.0289(8)
C7	−0.0027(4)	0.2526(3)	0.3141(3)	0.0295(8)
H7	0.0493(4)	0.1850(3)	0.3166(3)	0.0354(10)*
C8	0.2503(4)	0.3364(3)	0.1862(3)	0.0329(9)
C9	−0.3554(5)	−0.1427(3)	0.3719(3)	0.0406(10)
H9	−0.4583(5)	−0.1306(3)	0.3523(3)	0.0487(12)*
C10	−0.1670(5)	−0.1359(3)	0.4426(3)	0.0374(9)
H10	−0.1059(5)	−0.1208(3)	0.4810(3)	0.0449(11)*
C11	0.0451(5)	−0.2685(3)	0.3869(4)	0.0455(11)
H11a	0.0966(5)	−0.2549(3)	0.3139(4)	0.0547(13)*
H11b	0.1199(5)	−0.2503(3)	0.4185(4)	0.0547(13)*
C12	0.0194(5)	−0.3885(3)	0.4467(3)	0.0365(9)
C13	0.1426(5)	−0.4655(3)	0.4293(3)	0.0415(10)
H13	0.2400(5)	−0.4428(3)	0.3817(3)	0.0498(12)*
C14	0.1235(5)	−0.5755(3)	0.4813(3)	0.0430(10)
H14	0.2075(5)	−0.6260(3)	0.4679(3)	0.0516(12)*
C15	0.4355(6)	0.5939(4)	0.1727(4)	0.0601(14)
H15	0.3454(6)	0.5533(4)	0.2090(4)	0.0721(16)*
C16	0.6471(5)	0.6515(3)	0.0635(3)	0.0373(9)
H16	0.7370(5)	0.6631(3)	0.0079(3)	0.0448(11)*
C17	0.6834(6)	0.7965(4)	0.1184(4)	0.0520(12)
H17a	0.6827(6)	0.7923(4)	0.1887(4)	0.0624(14)*
H17b	0.7977(6)	0.7954(4)	0.0821(4)	0.0624(14)*
C18	0.5051(6)	0.9724(4)	0.1047(4)	0.0550(12)
H18	0.5080(6)	0.9541(4)	0.1755(4)	0.0660(15)*
C19	0.5868(6)	0.9017(3)	0.0573(4)	0.0470(11)
C20	0.5801(6)	0.9308(4)	−0.0484(4)	0.0548(12)
H20	0.6337(6)	0.8844(4)	−0.0815(4)	0.0657(15)*
C21	0.8617(5)	0.3758(3)	0.0281(3)	0.0413(10)

Table 2 (continued)

Atom	x	y	z	<i>U</i> _{iso} */ <i>U</i> _{eq}
H21	0.9073(5)	0.4418(3)	−0.0125(3)	0.0495(12)*
C22	0.6870(5)	0.2647(3)	0.1137(3)	0.0436(10)
H22	0.5887(5)	0.2322(3)	0.1470(3)	0.0523(12)*
C23	0.8843(6)	0.0932(3)	0.1581(4)	0.0560(13)
H23a	0.9713(6)	0.0775(3)	0.1987(4)	0.0672(15)*
H23b	0.7895(6)	0.0567(3)	0.2065(4)	0.0672(15)*
C24	1.0568(6)	−0.0453(3)	0.0939(4)	0.0501(11)
H24	1.0970(6)	−0.0764(3)	0.1573(4)	0.0601(14)*
C25	0.9444(5)	0.0471(3)	0.0742(3)	0.0417(10)
C26	0.8898(6)	0.0920(3)	−0.0207(4)	0.0506(12)
H26	0.8158(6)	0.1548(3)	−0.0363(4)	0.0607(14)*

acid (H₂brip) and 1-(3-((1*H*-1,2,4-triazol-1-yl)methyl)benzyl)-1*H*-1,2,4-triazole (bmbt), a 3D framework was synthesized *via* hydrothermal process.

The asymmetric unit consists of one Co(II) ion, distributed on two special sites (see table2) one brip and one and half located on three inversion centers bmbt molecules. The assembly of Co(II) ions and the neutral bmbt molecules generate two kinds of chain structures. In one kind of chain, Co(II) is six-coordinated with a pseudo-square planar environment by two nitrogen atoms from two bmbt ligands, two oxygen atoms from two brip linkers and two oxygen atoms from two coordinated water molecules. Bmbt ligands adopt a m₂-coordination to form this chain. For the other chain, Co(II) is six-coordinated by four nitrogen atoms from four bmbt ligands, two oxygen atoms from two Brip. The Zn–N bond lengths are in the range of 2.100(2)–2.192(2) Å, and the Co–O bond length is 2.105(2)–2.138(3) Å. These one dimensional motifs were further bridged to form a 3D structure.

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