Crystal structure of catena-poly[(4-bromoisophthalato-κ^2*O:O′*)-[1,1'-(1,3-propanediyl)bis(benzimidazole-κ^2*N:N′*)cobalt(II)], $C_{25}H_{19}BrCoN_4O_4$

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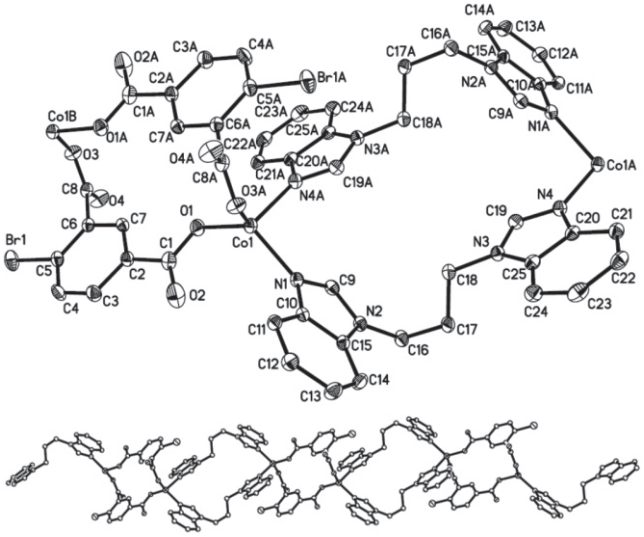

Abstract

$C_{25}H_{19}BrCoN_4O_4$, triclinic, $P\bar{1}$ (no. 2), a = 8.333(1) Å, b = 12.331(2) Å, c = 13.061(2) Å, α = 62.770(2)°, β = 85.658(2)°, γ = 79.584(2)°, V = 1173.6 Å^3, Z = 2, $R_{gt}(F)$ = 0.0406, $wR_{ref}(F^2)$ = 0.1063, T = 296 K.

Table 1. Data collection and handling.

Crystal:	red blocks, size 0.13×0.19×0.25 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	24.74 cm^{-1}
Diffractometer, scan mode:	CCD area detector, φ and ω
$2\theta_{max}$:	51°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	8763, 4328
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 3055
$N(param)_{refined}$:	316
Programs:	SHELX [12]

Source of material

The title compound was prepared under the hydrothermal conditions. A mixture of 4-bromoisophthalate (4-Br-H_2ip, 0.1 mmol), 1,1'-(1,3-propanediyl)bis(benzimidazole) (*pbbm*, 0.1 mmol) and $Co(OAc)_2{\cdot}4H_2O$ (0.1 mmol) in distilled water (15 mL) was stirred for 30 min, and the pH value of the solution was adjusted to about 4 with 1 M KOH. After stirring for another 30 min, the mixture was transferred to a 25 mL Teflon-lined stainless steel vessel and heated at 120 °C for 3 days. Then the reaction system was cooled to room temperature over 24 h, and red block crystals were obtained.

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Discussion

The design and synthesis of metal-organic frameworks (MOFs) have attracted considerable attention because of their potential applications as functional materials as well as their structural diversity and intriguing variety of topologies [1–7]. It is well known that carboxylate ligands play an important role in coordination chemistry, which may adopt diverse binding modes such as monodentate, chelating, and bridging in the syn-syn, syn-anti, and anti-anti configurations [8–9]. On the other hand, the flexible bis(*N*-containing heterocyclic ring) ligands containing 1- or 2-substituted tetrazole, 1-substituted imidazole, benzimidazole, benzotriazole or 1,2,3-triazole, and 1-or 4-substituted 1,2,4-triazole rings tethered by an alkyl spacer have been extensively used [10–11]. In this paper, we select 4-bromoisophthalate (4-Br-H_2ip) and 1,1'-(1,3-propanediyl)bis(benzimidazole) (*pbbm*) to react with Co(II) ions to obtain a new MOF. The asymmetric unit of the title structure consists of a Co(II) ion, a 4-Br-ip ligand, and a *pbbm* ligand (figure, top). The Co(II) ion adopts a distorted tetrahedral coordination geometry, coordinating to two carboxylic O atoms from two 4-Br-ip ligands (Co1–O1 = 1.929(3) Å and Co1–O3A = 1.950(3) Å) and two N atoms from two *pbbm* ligands (Co1–N1 = 2.014(3) Å and Co1–N4A = 2.034(3) Å). The title complex displays an interesting infinite 1D looped chains structure composed of two kinds of rings, the 16-membered ring and the 20-membered ring (figure, bottom). The 16-membered ring is formed by two 4-Br-ip ligands bridging two Co(II) ions and the Co(II)···Co(II) distance is 6.903 Å. The 20-membered ring is made up of two *pbbm* ligands bridging two Co(II) ions and the Co(II)···Co(II) distance is 10.206 Å. The two rings are connected alternately via Co(II) ions forming an infinite 1-D chain. Moreover, the adjacent looped chains are linked through hydrogen bonds by weak intermolecular C–H···O hydrogen bonds to generate a three-dimensional network. The bond lengths and angles of these weak hydrogen bonding parametres are in the range of 3.278(6) - 3.345(6) Å and 142-174°, respectively. The *pbbm* ligand adopts a bidentate-bridging conformation mode with the dihedral angle between the two benzimidazole rings of 62.94°.

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H(3)	2*i*	0.5768	0.1227	0.0512	0.065
H(4)	2*i*	0.5628	0.1368	–0.1304	0.067
H(7)	2*i*	0.6576	0.4722	–0.0896	0.045
H(9)	2*i*	1.0266	0.3069	0.3682	0.048
H(11)	2*i*	0.5377	0.1331	0.4776	0.047
H(12)	2*i*	0.5269	–0.0403	0.6514	0.058
H(13)	2*i*	0.7474	–0.1322	0.7745	0.064
H(14)	2*i*	0.9953	–0.0603	0.7246	0.058
H(16A)	2*i*	1.2619	0.1847	0.5016	0.059
H(16B)	2*i*	1.2455	0.0486	0.5905	0.059
H(17A)	2*i*	1.1446	0.1094	0.7285	0.058

Table 2. continued.

Atom	Site	*x*	*y*	*z*	U_{iso}
H(17B)	2*i*	1.3058	0.1642	0.6818	0.058
H(18A)	2*i*	1.1257	0.3511	0.5501	0.053
H(18B)	2*i*	0.9856	0.2944	0.6343	0.053
H(19)	2*i*	1.2428	0.4940	0.5917	0.050

Table 2. continued.

Atom	Site	*x*	*y*	*z*	U_{iso}
H(21)	2*i*	1.1713	0.4409	0.9765	0.053
H(22)	2*i*	1.0412	0.2834	1.1091	0.065
H(23)	2*i*	0.9649	0.1415	1.0629	0.071
H(24)	2*i*	1.0012	0.1558	0.8801	0.061

Table 3. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Co(1)	2*i*	0.66773(6)	0.37310(5)	0.27222(4)	0.0390(3)	0.0425(3)	0.0312(3)	–0.0105(2)	0.0021(2)	–0.0154(2)
Br(1)	2*i*	0.60458(6)	0.31543(5)	–0.36419(4)	0.0644(3)	0.1013(4)	0.0631(3)	–0.0236(3)	0.0106(2)	–0.0596(3)
O(1)	2*i*	0.6674(3)	0.3815(3)	0.1211(2)	0.057(2)	0.057(2)	0.040(2)	–0.011(1)	0.000(1)	–0.026(1)
O(2)	2*i*	0.6377(5)	0.1851(4)	0.2037(3)	0.147(4)	0.095(3)	0.039(2)	–0.077(3)	0.004(2)	–0.008(2)
O(3)	2*i*	0.5468(3)	0.6222(2)	–0.3424(2)	0.043(2)	0.047(2)	0.045(2)	–0.006(1)	0.007(1)	–0.010(1)
O(4)	2*i*	0.7983(4)	0.5378(3)	–0.3578(3)	0.045(2)	0.078(2)	0.065(2)	–0.012(2)	0.018(2)	–0.014(2)
N(1)	2*i*	0.8151(3)	0.2433(3)	0.4017(2)	0.033(2)	0.041(2)	0.036(2)	–0.011(1)	0.003(1)	–0.019(2)
N(2)	2*i*	1.0311(3)	0.1526(3)	0.5190(3)	0.027(2)	0.046(2)	0.047(2)	–0.006(1)	–0.001(1)	–0.026(2)
N(3)	2*i*	1.1422(4)	0.3488(3)	0.7033(2)	0.041(2)	0.042(2)	0.035(2)	–0.010(2)	0.003(1)	–0.018(2)
N(4)	2*i*	1.2263(4)	0.4816(3)	0.7494(2)	0.041(2)	0.045(2)	0.034(2)	–0.011(2)	0.005(1)	–0.018(2)
C(1)	2*i*	0.6401(5)	0.2845(4)	0.1179(3)	0.048(2)	0.064(3)	0.039(2)	–0.024(2)	0.007(2)	–0.020(2)
C(2)	2*i*	0.6223(4)	0.2961(4)	0.0000(3)	0.041(2)	0.044(2)	0.037(2)	–0.013(2)	0.001(2)	–0.017(2)
C(3)	2*i*	0.5922(5)	0.1954(4)	–0.0134(4)	0.069(3)	0.046(3)	0.047(3)	–0.024(2)	–0.002(2)	–0.014(2)
C(4)	2*i*	0.5852(5)	0.2034(4)	–0.1217(4)	0.070(3)	0.049(3)	0.063(3)	–0.022(2)	–0.001(2)	–0.033(2)
C(5)	2*i*	0.6112(5)	0.3099(4)	–0.2168(3)	0.040(2)	0.057(3)	0.044(2)	–0.010(2)	0.002(2)	–0.030(2)
C(6)	2*i*	0.6377(4)	0.4130(3)	–0.2072(3)	0.031(2)	0.044(2)	0.038(2)	–0.006(2)	0.002(2)	–0.021(2)
C(7)	2*i*	0.6416(4)	0.4038(3)	–0.0977(3)	0.036(2)	0.040(2)	0.042(2)	–0.010(2)	0.003(2)	–0.022(2)
C(8)	2*i*	0.6654(5)	0.5323(4)	–0.3115(3)	0.040(2)	0.051(2)	0.031(2)	–0.013(2)	0.003(2)	–0.017(2)
C(9)	2*i*	0.9684(4)	0.2463(4)	0.4193(3)	0.038(2)	0.043(2)	0.045(2)	–0.013(2)	0.006(2)	–0.024(2)
C(10)	2*i*	0.7762(4)	0.1396(3)	0.4979(3)	0.031(2)	0.037(2)	0.036(2)	–0.008(2)	0.002(2)	–0.020(2)
C(11)	2*i*	0.6281(4)	0.0951(3)	0.5264(3)	0.031(2)	0.043(2)	0.047(2)	–0.004(2)	–0.003(2)	–0.023(2)
C(12)	2*i*	0.6231(5)	–0.0074(4)	0.6299(3)	0.040(2)	0.049(3)	0.053(3)	–0.014(2)	0.001(2)	–0.018(2)
C(13)	2*i*	0.7573(5)	–0.0639(4)	0.7042(4)	0.054(3)	0.048(3)	0.045(2)	–0.012(2)	–0.004(2)	–0.007(2)
C(14)	2*i*	0.9046(5)	–0.0214(4)	0.6762(3)	0.046(2)	0.047(2)	0.043(2)	–0.002(2)	–0.012(2)	–0.013(2)
C(15)	2*i*	0.9091(4)	0.0822(3)	0.5722(3)	0.031(2)	0.043(2)	0.039(2)	–0.005(2)	–0.001(2)	–0.024(2)
C(16)	2*i*	1.1957(4)	0.1345(4)	0.5636(4)	0.029(2)	0.061(3)	0.071(3)	–0.001(2)	–0.008(2)	–0.042(2)
C(17)	2*i*	1.1944(5)	0.1686(4)	0.6615(4)	0.037(2)	0.053(3)	0.063(3)	–0.003(2)	–0.015(2)	–0.033(2)
C(18)	2*i*	1.1017(5)	0.2970(4)	0.6294(3)	0.048(2)	0.048(2)	0.041(2)	–0.008(2)	–0.004(2)	–0.023(2)
C(19)	2*i*	1.2101(5)	0.4500(3)	0.6672(3)	0.045(2)	0.041(2)	0.036(2)	–0.011(2)	0.006(2)	–0.016(2)
C(20)	2*i*	1.1596(4)	0.3939(3)	0.8475(3)	0.031(2)	0.043(2)	0.035(2)	–0.002(2)	0.001(2)	–0.014(2)
C(21)	2*i*	1.1367(5)	0.3851(4)	0.9570(3)	0.046(2)	0.048(2)	0.037(2)	–0.006(2)	–0.001(2)	–0.018(2)
C(22)	2*i*	1.0609(5)	0.2907(4)	1.0353(3)	0.053(3)	0.061(3)	0.033(2)	–0.002(2)	0.001(2)	–0.012(2)
C(23)	2*i*	1.0130(5)	0.2057(4)	1.0068(4)	0.053(3)	0.057(3)	0.045(3)	–0.015(2)	0.009(2)	–0.003(2)
C(24)	2*i*	1.0341(5)	0.2129(4)	0.8986(3)	0.051(3)	0.045(2)	0.050(3)	–0.016(2)	0.002(2)	–0.014(2)
C(25)	2*i*	1.1073(4)	0.3102(3)	0.8185(3)	0.032(2)	0.043(2)	0.040(2)	–0.004(2)	0.000(2)	–0.016(2)

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