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Crystal structure of *catena*-poly[*diaqua*-bis(3,4,5,6-tetrabromo-carboxybenzoato- $\kappa^1 O$)-(μ₂-4,4'-bipyridine- $\kappa^2 N:N'$)cobalt(II)], C₂₆H₁₄Br₈CoN₂O₁₀

Table 1: Data collection and handling.

Crystal:	Pink block
Size:	0.20 × 0.19 × 0.17 mm
Wavelength:	Cu Kα radiation (1.54184 Å)
μ:	16.1 mm ⁻¹
Diffractometer, scan mode:	XtaLAB Pro, ω
θ _{max} , completeness:	66.6°, >99%
<i>N</i> (<i>hkl</i>) _{measured} , <i>N</i> (<i>hkl</i>) _{unique} , <i>R</i> _{int} :	9804, 2887, 0.033
Criterion for <i>I</i> _{obs} , <i>N</i> (<i>hkl</i>) _{gt} :	<i>I</i> _{obs} > 2 σ(<i>I</i> _{obs}), 2688
<i>N</i> (<i>param</i>) _{refined} :	217
Programs:	SHELX [1, 2], CrysAlis ^{PRO} [3]

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Abstract

C₂₆H₁₄Br₈CoN₂O₁₀, orthorhombic, *Pbcn* (no. 60), *a* = 24.3935(3) Å, *b* = 11.4505(1) Å, *c* = 11.7004(1) Å, *V* = 3268.13(6) Å³, *Z* = 4, *R*_{gt}(*F*) = 0.0313, *wR*_{ref}(*F*²) = 0.0819, *T* = 293 K.

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A part of the title crystal structure is shown in the figure (' = 1 − *x*, *y*, 1.5 − *z*; '' = *x*, 1 + *y*, *z*). 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 3,4,5,6-tetrabromo-phthalic acid (H₂Br₄ph, 19 mg, 0.04 mmol), 4,4''-bipyridyl (31 mg, 0.02 mmol), and Co(ClO₄)₂ · 6H₂O (29 mg, 0.08 mmol) were added to water

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

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} ^{*/} / <i>U</i> _{eq}
Br1	0.67663(2)	0.81863(4)	0.77556(4)	0.04235(15)
Br2	0.80868(2)	0.79724(4)	0.74510(4)	0.03983(15)
Br3	0.86073(2)	0.58826(5)	0.58367(5)	0.04598(15)
Br4	0.77724(2)	0.41005(4)	0.44627(4)	0.03593(14)
C1	0.60882(15)	0.6428(3)	0.6292(3)	0.0235(7)
C2	0.65170(14)	0.4730(3)	0.4791(3)	0.0237(7)
C3	0.67066(14)	0.6293(3)	0.6207(3)	0.0214(7)
C4	0.69230(14)	0.5462(3)	0.5456(3)	0.0211(7)
C5	0.74888(15)	0.5325(3)	0.5362(3)	0.0230(7)
C6	0.78415(15)	0.6054(3)	0.5965(3)	0.0265(8)
C7	0.76308(15)	0.6927(3)	0.6669(3)	0.0253(8)
C8	0.70604(15)	0.7026(3)	0.6804(3)	0.0247(7)
C9	0.46030(16)	0.3651(3)	0.7000(4)	0.0333(9)
H9	0.4321	0.4057	0.6645	0.040*
C10	0.45862(16)	0.2441(3)	0.6980(4)	0.0338(9)
H10	0.4298	0.2056	0.6618	0.041*
C11	0.5000	0.1809(4)	0.7500	0.0237(11)
C12	0.5000	0.0510(4)	0.7500	0.0239(11)
C13	0.46980(19)	−0.0134(3)	0.6720(4)	0.0404(10)
H13	0.4489	0.0247	0.6170	0.048*
C14	0.47057(18)	−0.1336(3)	0.6753(4)	0.0381(10)
H14	0.4494	−0.1741	0.6225	0.046*
Co1	0.5000	0.61512(6)	0.7500	0.01751(19)
N1	0.5000	0.4266(4)	0.7500	0.0220(9)
N2	0.5000	−0.1951(3)	0.7500	0.0243(9)
O1	0.58695(10)	0.6146(2)	0.7241(2)	0.0218(5)
O2	0.58553(11)	0.6785(3)	0.5430(2)	0.0436(8)
O3	0.61640(12)	0.4166(3)	0.5263(2)	0.0418(7)

Table 2 (continued)

Atom	x	y	z	U_{iso}^*/U_{eq}
O4	0.65766(10)	0.4816(2)	0.3684(2)	0.0279(6)
H4	0.6351	0.4397	0.3364	0.042*
O5	0.51672(11)	0.6149(2)	0.9226(2)	0.0316(6)
H5A	0.5053	0.6796	0.9532	0.047*
H5B	0.5519	0.6169	0.9352	0.047*

(6 mL) in a 25 mL Teflon-lined autoclave. The mixture was heated at 393 K for 3 days and then slowly cooled down to room temperature. Light pink block crystals of the title compound were obtained.

Experimental details

The carbon bound hydrogen atoms were placed in calculated positions and refined using a riding model on attached atoms.

Comment

In the last two decades, a large number of cobalt(II)-based metal-organic frameworks (MOFs) and coordination polymers have been reported in the literature [3–8]. Organic aromatic multicarboxylates, such as phthalic acid (1,2-benzenedicarboxylic acid) and its derivatives, as the mediators between the metal centers, can yield predetermined networks and have been widely utilized to construct coordination polymers [9–12]. On the other hand, 4,4'-bipyridine (4,4'-bipy), as a nitrogen donor ligand, serves as a bridging ligand, which can act as bidentate ligand to coordinate to two metal ions [13–16].

In the title complex, there are one half of a Co(II) ion, one coordinated water molecule, one HBr₄ph ligands, and one half of 4,4'-bipy ligand in the asymmetric unit (figure). Co1 is six-coordinated with a distorted octahedral geometry by two O atoms from two HBr₄ph and a pair of N atoms of two 4,4'-bipy ligands, located at the basal equatorial plane, and two coordinated water molecules from the axial positions with a O5-Co1-O5' angle of 179.83(16)°. The Co–N bond lengths are 2.159(4) and 2.173(4) Å and the Co–O ones are in the range of 2.060(3) and 2.143(2) Å. Co(II) ions are linked by 4,4'-bipy ligands to form a 1-D polymer. In the title complex, there are three kinds of hydrogen bonds: (a) hydrogen bonding between water and carboxylate O atoms with d(O···O) = 2.62 Å; (b) hydrogen bonding between water and carboxylate O atoms with d(O···O) = 2.74 Å; (c) hydrogen bonding between carboxy O atoms and carboxylate O atoms with d(O···O) = 2.65 Å. An extended three-dimensional network of hydrogen bonds contributes to the stability of the structure.

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