Crystal structure of (1,2-bi(4-pyridyl)ethane)(5-bromoisophthalato)-cobalt(II), $\text{Co}(\text{C}_{12}\text{H}_{12}\text{N}_2)(\text{C}_8\text{H}_3\text{O}_4\text{Br})$

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Abstract

$\text{C}_{20}\text{H}_{15}\text{BrCoN}_2\text{O}_4$, triclinic, $P\bar{1}$ (no. 2), $a = 9.761(8)$ Å, $b = 10.086(8)$ Å, $c = 11.202(9)$ Å, $\alpha = 76.457(9)^\circ$, $\beta = 93.570(1)^\circ$, $\gamma = 68.399(9)^\circ$, $V = 983.3$ Å³, $Z = 2$, $R_g(F) = 0.038$, $wR_{\text{ref}}(F^2) = 0.098$, $T = 293$ K.

Source of material

A mixture of 5-bromoisophthalic acid ($\text{H}_2\text{5-Br-ip}$, 0.1 mmol, 24.5 mg), 1,2-bi(4-pyridyl)ethane (bpa, 0.1 mmol, 18.9 mg), $\text{Co}(\text{OAc})_2 \cdot 4\text{H}_2\text{O}$ (0.05 mmol, 12.0 mg), NaOH (0.1 mmol, 4.0 mg) and H_2O (15 mL) was placed in a Teflon-lined stainless steel vessel, heated to 120 °C for 3 days, and then cooled to room temperature over 24 h. Pink block-shaped crystals of the title compound were obtained.

Discussion

The rational design and construction of coordination polymers with unique structural motifs and chemical or physical properties have attracted extensive interest in supramolecular and materials chemistry [1–8]. In the past decade, plenty of metal-organic hybrids exhibiting fascinating structures and various properties such as luminescence, magnetism, sorption, ion exchange, nonlinear optics and electricity have been synthesized by chemists. Among the various ligands, organic aromatic poly-carboxylates have been extensively employed in the preparation of such metal-organic compounds. In comparison to the 1,3-benzenedicarboxylic acid, 1,3,5-benzenetricarboxylic acid, and 1,2,4,5-benzenetetracarboxylic acid ligands, 5-bromoisophthalic acid remains largely unexplored.

The asymmetric unit of the title structure contains one Co(II) cation, one bpa ligand and one 5-Br-ip anion. Each Co atom is octahedrally coordinated by two *trans* N atoms of two bpa ligands and four oxygen atoms from three 5-Br-ip ligands. The Co—N bond lengths are both 2.163(3) Å and the Co—O bond lengths are in the range of 2.011(3)–2.253(3) Å, respectively. X-ray structural analysis reveals that the title structure consists of a 2D layer constructed from the linkage of 1D $[\text{Co}(\text{bpa})]_n$ chains via flexible bpa. Along the [110] direction, the Co atoms are bridged by the 5-Br-ip anions to generate 1D ribbon-like chains containing alternative arrangement of 8- and 16-membered rings. Two carboxylate groups bridge two Co(II) ions to form an 8-membered ring and two 5-Br-ip ligands bridge two Co(II) ions to form a 16-membered ring. Within the 8-membered ring and 16-membered ring, the Co···Co separations are 4.5 and 7.0 Å, respectively. The adjacent ribbon chains are interlinked by the flexible bpa ligands to form a 2D layer.

Table 1. Data collection and handling.

Crystal:	pink block, size 0.06 × 0.25 × 0.35 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ :	11.55 cm ^{−1}
Diffractometer, scan mode:	Bruker SMART CCD, φ/ω
$2\theta_{\text{max}}$:	51°
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$:	6844, 3558
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2\sigma(I_{\text{obs}})$, 2605
$N(\text{param})_{\text{refined}}$:	253
Programs:	SHELXS-97 [9], SHELXL-97 [10], SHELXTL [11]

Table 2. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U_{iso}
H(2)	2i	0.9186	−0.0752	0.4102	0.034
H(4)	2i	0.8205	−0.2279	0.1488	0.037
H(6)	2i	0.8184	0.1808	0.0826	0.042
H(9)	2i	0.8023	0.1531	0.5405	0.052
H(10)	2i	0.6164	0.1401	0.6918	0.054
H(12)	2i	0.5166	0.5580	0.6916	0.074
H(13)	2i	0.7026	0.5617	0.5397	0.070
H(14A)	2i	0.4271	0.2413	0.8419	0.050
H(14B)	2i	0.3358	0.4048	0.7953	0.050
H(15A)	2i	0.4673	0.4759	0.9101	0.063
H(15B)	2i	0.5596	0.3127	0.9561	0.063
H(16)	2i	0.0096	0.5335	1.1306	0.052
H(17)	2i	0.1816	0.5414	0.9657	0.057
H(19)	2i	0.4709	0.2006	1.1544	0.057
H(20)	2i	0.2903	0.2035	1.3145	0.053

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Table 3. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
Co(1)	2i	0.95442(6)	0.36598(5)	0.38443(4)	0.0401(3)	0.0226(3)	0.0241(3)	-0.0199(2)	0.0027(2)	-0.0051(2)
Br(1)	2i	0.76664(6)	0.00259(5)	-0.06353(4)	0.0923(4)	0.0605(3)	0.0370(3)	-0.0345(3)	-0.0267(3)	-0.0017(2)
O(1)	2i	0.8411(3)	0.3168(3)	0.2498(2)	0.057(2)	0.021(1)	0.042(2)	-0.019(1)	-0.006(1)	-0.003(1)
O(2)	2i	0.9956(3)	0.1482(3)	0.3724(2)	0.051(2)	0.028(1)	0.028(1)	-0.025(1)	-0.002(1)	-0.005(1)
O(3)	2i	0.9061(3)	-0.3277(3)	0.4888(2)	0.053(2)	0.030(1)	0.027(2)	-0.023(1)	-0.009(1)	0.000(1)
O(4)	2i	0.8754(3)	-0.4147(3)	0.3349(2)	0.049(2)	0.025(1)	0.032(1)	-0.023(1)	0.002(1)	-0.007(1)
N(1)	2i	0.7721(4)	0.3591(3)	0.5234(3)	0.043(2)	0.033(2)	0.032(2)	-0.024(2)	0.007(2)	-0.008(1)
N(2)	2i	0.1317(4)	0.3681(3)	1.2391(3)	0.044(2)	0.032(2)	0.025(2)	-0.023(2)	0.005(1)	-0.005(1)
C(1)	2i	0.8753(4)	0.0684(4)	0.2523(3)	0.040(2)	0.025(2)	0.031(2)	-0.020(2)	-0.000(2)	-0.005(2)
C(2)	2i	0.8919(4)	-0.0617(4)	0.3313(3)	0.038(2)	0.028(2)	0.026(2)	-0.021(2)	0.001(2)	-0.007(2)
C(3)	2i	0.8689(4)	-0.1736(4)	0.2941(3)	0.036(2)	0.022(2)	0.026(2)	-0.017(2)	0.001(2)	-0.005(2)
C(4)	2i	0.8328(4)	-0.1529(4)	0.1758(3)	0.041(2)	0.028(2)	0.035(2)	-0.021(2)	-0.006(2)	-0.008(2)
C(5)	2i	0.8151(4)	-0.0217(4)	0.0978(3)	0.047(3)	0.035(2)	0.028(2)	-0.021(2)	-0.009(2)	-0.003(2)
C(6)	2i	0.8336(4)	0.0913(4)	0.1351(3)	0.053(3)	0.026(2)	0.031(2)	-0.021(2)	-0.008(2)	0.000(2)
C(7)	2i	0.9058(4)	0.1864(4)	0.2928(3)	0.040(2)	0.027(2)	0.026(2)	-0.021(2)	0.006(2)	-0.008(2)
C(8)	2i	0.8868(4)	-0.3161(4)	0.3800(3)	0.030(2)	0.023(2)	0.031(2)	-0.015(2)	0.000(2)	-0.005(2)
C(9)	2i	0.7441(5)	0.2365(4)	0.5712(4)	0.056(3)	0.037(2)	0.036(2)	-0.023(2)	0.017(2)	-0.008(2)
C(10)	2i	0.6333(5)	0.2276(5)	0.6635(4)	0.061(3)	0.043(2)	0.038(2)	-0.033(2)	0.013(2)	-0.009(2)
C(11)	2i	0.5481(4)	0.3453(4)	0.7139(3)	0.037(2)	0.048(2)	0.027(2)	-0.025(2)	0.003(2)	-0.006(2)
C(12)	2i	0.5746(6)	0.4730(5)	0.6632(4)	0.080(4)	0.048(3)	0.061(3)	-0.036(3)	0.037(3)	-0.029(2)
C(13)	2i	0.6860(6)	0.4744(5)	0.5710(4)	0.082(4)	0.044(3)	0.058(3)	-0.042(3)	0.032(3)	-0.022(2)
C(14)	2i	0.4316(5)	0.3387(5)	0.8203(4)	0.041(3)	0.057(3)	0.034(2)	-0.029(2)	0.007(2)	-0.012(2)
C(15)	2i	0.4633(5)	0.3783(6)	0.9320(4)	0.049(3)	0.086(4)	0.040(3)	-0.044(3)	0.016(2)	-0.023(2)
C(16)	2i	0.1043(5)	0.4650(5)	1.1359(4)	0.045(3)	0.044(2)	0.033(2)	-0.014(2)	0.008(2)	-0.004(2)
C(17)	2i	0.2073(5)	0.4706(5)	1.0360(4)	0.059(3)	0.049(3)	0.030(2)	-0.022(2)	0.007(2)	-0.001(2)
C(18)	2i	0.3484(5)	0.3713(5)	1.0404(4)	0.046(3)	0.055(3)	0.031(2)	-0.036(2)	0.008(2)	-0.014(2)
C(19)	2i	0.3772(5)	0.2706(5)	1.1469(4)	0.039(3)	0.059(3)	0.041(3)	-0.015(2)	0.005(2)	-0.013(2)
C(20)	2i	0.2675(5)	0.2728(5)	1.2431(4)	0.046(3)	0.049(3)	0.035(2)	-0.019(2)	0.001(2)	-0.005(2)

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