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The crystal structure of *poly*[(*m*₄-4-bromoisophthalato- κ^4 O: O':O'':O''')zinc(II)], $C_8H_3BrO_4Zn$

Table 1: Data collection and handling.

Crystal:	Colourless plate
Size:	0.28 × 0.28 × 0.01 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	7.46 mm ⁻¹
Diffractometer, scan mode:	SuperNova, ω
$\theta_{\max}$, completeness:	26.4°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	3504, 1754, 0.032
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1491
$N(\text{param})_{\text{refined}}$:	127
Programs:	CrysAlis ^{PRO} [1], SHELX [2, 3]

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

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Br1	0.27909(18)	0.69278(5)	0.36560(6)	0.0493(3)
Zn1	1.20838(12)	0.60376(4)	1.02274(5)	0.0169(2)
O1	1.0300(8)	0.5767(3)	0.8725(3)	0.0241(9)
O2	0.6684(8)	0.4823(3)	0.8646(3)	0.0270(9)
O3	1.0145(7)	0.7997(3)	0.5849(3)	0.0249(9)
O4	0.5867(7)	0.8474(3)	0.5092(3)	0.0265(9)
C1	0.6498(11)	0.5860(4)	0.7202(4)	0.0187(11)
C2	0.7533(11)	0.6645(4)	0.6849(4)	0.0195(11)
C3	0.6330(10)	0.7027(3)	0.5844(4)	0.0163(11)
C4	0.4181(11)	0.6580(4)	0.5160(4)	0.0216(11)
C5	0.3111(13)	0.5808(4)	0.5505(5)	0.0287(13)
C6	0.4221(12)	0.5451(4)	0.6537(4)	0.0260(12)
C7	0.7910(11)	0.5451(4)	0.8276(4)	0.0199(11)
C8	0.7455(11)	0.7897(3)	0.5562(4)	0.0183(11)
H5	0.1633(13)	0.5527(4)	0.5040(5)	0.0345(16)*
H6	0.3451(12)	0.4944(4)	0.6781(4)	0.0312(15)*
H2	0.9063(11)	0.6916(4)	0.7298(4)	0.0234(13)*

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Abstract

$C_8H_3BrO_4Zn$, monoclinic, $P2_1/c$ (no. 14), $a = 4.7134(4)$ Å, $b = 15.4354(13)$ Å, $c = 12.0064(9)$ Å, $\beta = 98.942(8)^\circ$, $V = 862.89(12)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0445$, $wR_{\text{ref}}(F^2) = 0.1193$, $T = 292.67(10)$ K.

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A part of the molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

4-Bromo-1,3-benzenedicarboxylic acid (0.03 g, 0.1 mmol) and zinc nitrate hexahydrate (0.03 g, 0.1 mmol) were added to water (7 mL) in a Teflon-lined stainless steel reactor. The mixture was heated at 393 K for 3 days, and then slowly cooled to room temperature. Colourless crystals of the title compound were obtained.

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Experimental details

The hydrogen atoms were placed at calculated positions with the SHELX program (AFIX option: 43).

Comment

Over the past few decades, the design and assembly of metal organic coordination polymers molecular crystalline materials has gained considerable interest due to their potential applications in several fields [4–10]. Self-assembly of organic ligands and metal anions is widely used to construct complexes with different structures and properties, which facilitated the understanding of structure–property relationships and the fabrication of new molecule-based crystalline complexes. So we may change the conditions of a chemical reaction [11–15] to control the structure of coordination polymers. But adjustment and control of structure is still in an early stage, and successfully prepared samples are still limited. In order to further study the formation conditions of coordination polymers, we used 4-bromo-1,3-benzenedicarboxylic acid (H₂Brbdc) and zinc nitrate to prepare a coordination polymer [ZnBrbdc]_n.

The asymmetric unit possesses one crystallographically independent Zn(II) ion, and one completely deprotonated Brbdc ligand. Each Zn(II)1 is four-coordinated with a slightly distorted tetrahedral environment by four carboxylato O atoms from four different Brbdc ligands. The bond angles around Zn(II)1 range from 98.31(17)° to 123.61(17)°; the Zn(II)1–O bond lengths range from 1.914(3) to 1.966(3) Å. Two carboxylate groups (1-and 3-COO[−]) have a dihedral angle of 13.49° and 37.99° toward the plane of the corresponding phenyl ring, respectively. The neighbouring Zn(II) ions are connected by carboxyl of Brbdc ligands in bidentate coordination modes to furnish a one-dimensional second building unit (SBU). The adjacent SBUs are further linked by Brbdc ligands to extend into a three-dimensional network structure.

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