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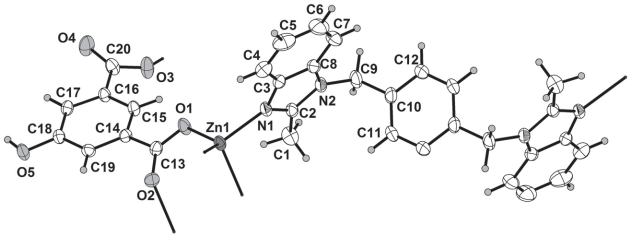
Crystal structure of *poly*-[bis(μ_3-5-hydroxyisophtalato-$\kappa^3O:O':O''$)(μ_2-1,4-bis(2-ethylbenzimidazol-1-ylmethyl)benzene-$\kappa^2N:N'$)dizinc(II)], $C_{40}H_{30}N_4O_5Zn_2$



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Abstract

$C_{40}H_{30}N_4O_5Zn_2$, triclinic, $P\bar{1}$ (No. 2), $a = 8.5232(17)$ Å, $b = 9.947(2)$ Å, $c = 11.555(2)$ Å, $\alpha = 72.76(3)°$, $\beta = 77.78(3)°$, $\gamma = 70.13(3)°$, $V = 873.2(3)$ Å^3, $Z = 1$, $R_{gt}(F) = 0.0363$, $wR_{ref}(F^2) = 0.0852$, $T = 293(2)$ K.

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Tables 1 and 2 contain details of the measurement method and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

A mixture of 1,4-bis(2-methylbenzimidazol-1-ylmethyl)benzene (73.2 mg, 0.2 mmol), $Zn(Ac)_2 \cdot 2H_2O$ (21.9 mg, 0.1 mmol), 5-hydroxyisophthalic acid (36.4 mg, 0.2 mmol), and H_2O (10 mL) were placed in a Teflon-lined stainless steel vessel, heated to 170 °C for 4 days, and then cooled to room temperature for 24 h. Colorless block crystals of the title complex were obtained.

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Table 1: Data collection and handling.

Crystal:	Colorless prism size 0.30 × 0.27 × 0.21 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	14.43 cm^{-1}
Diffractometer, scan mode:	Rigaku Saturn 724, φ and ω
$2\theta_{max}$, completeness:	58.24°, >99 %,
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	5750, 3014, 0.0243
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 2724
$N(param)_{refined}$:	255
Programs:	CrystalClear [10], SHELX [11]

Experimental details

Absorption corrections were applied by using multi-scan program. The structures were solved by direct methods and refined with full-matrix least-squares on F_2 [11]. The hydrogen atoms were placed at calculated positions and refined as riding atoms with fixed isotropic displacement parameters.

Discussion

Considerable attention has been paid to the design and synthesis of crystalline porous materials known as metal–organic frameworks (MOFs) [1–3], due to their large surface area and tunable pore environments, making them promising for a wide range of applications. Numerous MOFs with interesting structures have been synthesized, and their novel architectures have been developing continuously [4–6]. The semi-rigid ligand 1,4-bis(2-methylbenzimidazol-1-ylmethyl)benzene (bmb) contains a rigid spacer of phenyl ring and two freely rotating methylbenzimidazol *arms*. Moreover, the flexible $-CH_2-$ groups allow the two methylbenzimidazol groups to deviate significantly from coplanarity with a tendency to generate various conformations when bmb coordinates with metal centers [7]. The 2-position methyl group enhance the donated-electrons ability of benzimidazole ring, and the bmb ligand exhibits strong collaborative coordination ability with organic carboxylate. Moreover, the change of substitutional group and its position in carboxylate coligands

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.56897(4)	0.54820(4)	0.33109(3)	0.02717(13)
O1	0.3224(2)	0.6234(2)	0.35783(19)	0.0350(5)
O2	0.3544(3)	0.6363(2)	0.53883(19)	0.0343(5)
C13	0.2631(3)	0.6570(3)	0.4584(3)	0.0263(6)
C14	0.0783(3)	0.7306(3)	0.4800(2)	0.0228(6)
C19	0.0188(3)	0.8170(3)	0.5641(3)	0.0256(6)
H19	0.0921	0.8215	0.6112	0.031*
C18	−0.1501(3)	0.8966(3)	0.5778(3)	0.0241(6)
C17	−0.2577(3)	0.8873(3)	0.5074(3)	0.0261(6)
H17	−0.3698	0.9441	0.5131	0.031*
C16	−0.2002(3)	0.7944(3)	0.4289(3)	0.0239(6)
C15	−0.0312(3)	0.7163(3)	0.4142(3)	0.0265(6)
H15	0.0084	0.6549	0.3607	0.032*
O5	−0.2044(3)	0.9798(2)	0.66102(19)	0.0330(5)
H5	−0.3024	1.0295	0.6545	0.050*
C1	0.5154(4)	0.2575(4)	0.2764(3)	0.0396(8)
H1A	0.5992	0.1739	0.3163	0.059*
H1B	0.4439	0.2241	0.2445	0.059*
H1C	0.4492	0.3135	0.3342	0.059*
C2	0.5986(3)	0.3512(3)	0.1751(3)	0.0265(6)
N1	0.6263(3)	0.4716(3)	0.1819(2)	0.0254(5)
C3	0.7102(3)	0.5242(3)	0.0683(3)	0.0270(6)
C8	0.7295(4)	0.4313(3)	−0.0060(3)	0.0285(7)
N2	0.6564(3)	0.3235(3)	0.0637(2)	0.0287(6)
C4	0.7715(4)	0.6450(4)	0.0260(3)	0.0385(8)
H4	0.7583	0.7085	0.0748	0.046*
C5	0.8526(5)	0.6667(4)	−0.0911(4)	0.0524(10)
H5A	0.8956	0.7464	−0.1220	0.063*
C6	0.8721(5)	0.5722(4)	−0.1650(3)	0.0511(10)
H6	0.9284	0.5902	−0.2436	0.061*
C7	0.8105(4)	0.4535(4)	−0.1246(3)	0.0417(8)
H7	0.8224	0.3912	−0.1741	0.050*
C9	0.6599(4)	0.1960(4)	0.0227(3)	0.0373(8)
H9A	0.6175	0.2300	−0.0558	0.045*
H9B	0.5871	0.1437	0.0806	0.045*
C10	0.8361(4)	0.0926(3)	0.0113(3)	0.0332(7)
C11	0.9269(4)	0.0321(4)	0.1103(3)	0.0401(8)
H11	0.8776	0.0538	0.1851	0.048*
C12	0.9114(4)	0.0595(4)	−0.0995(3)	0.0421(9)
H12	0.8522	0.0995	−0.1669	0.051*
C20	−0.3263(4)	0.7767(4)	0.3642(3)	0.0312(7)
O4	−0.4578(3)	0.8757(3)	0.3452(2)	0.0474(6)
O3	−0.2823(3)	0.6533(3)	0.3350(2)	0.0417(6)

may adjust the structural features and build complicated and fascinating MOFs [8].

Single crystal structure analysis reveals that there is one half 1,4-bis(2-methylbenzimidazol-1-ylmethyl)benzene (bmb), one 5-hydroxyisophthalate (hip) and one Zn(II) ion in the asymmetric unit. As shown in the figure, the Zn(II) is four-coordinated in a tetrahedral geometry, ligated by three oxygen atoms (O1, O2, and O3) from three symmetry-related 5-hydroxyisophthalate, one nitrogen atoms (N1) from bmb. The bond lengths are Zn(1)—O(1) = 1.966(2) Å, Zn(1)—O(2) = 2.005(2) Å, Zn(1)—O(3) = 1.912(2) Å, and Zn(1)—N(1) = 1.990(2) Å, respectively. They are in the normal ranges [9]. The two methylbenzimidazol arms of bmb bend in opposite directions to bridge adjacent Zn(hip) chains to form a 2D layer structure.

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