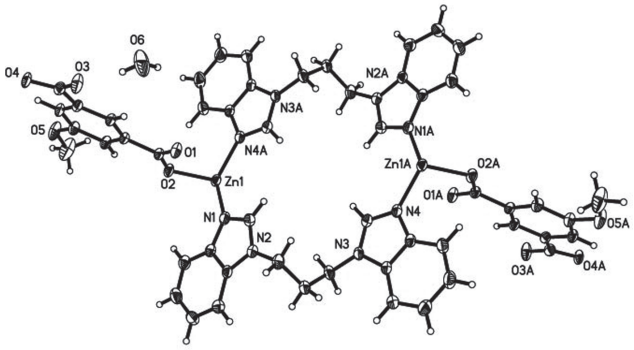
Zhan Zhou*, Zhe Zhou and Peng-Jing Jing

Crystal structure of *catena*-poly[(μ_2-1,3-bis(benzimidazol-1-yl)propane $\kappa^2N:N'$)-(μ_2-5-methoxyisophthalato-$\kappa^2O:O'$)zinc(II)] hydrate, $C_{26}H_{24}ZnN_4O_6$



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Abstract

$C_{26}H_{24}ZnN_4O_6$, triclinic, $P\bar{1}$ (no. 2), $a = 9.724(3)$ Å, $b = 10.173(3)$ Å, $c = 14.642(4)$ Å, $\alpha = 70.380(3)°$, $\beta = 85.642(4)°$, $\gamma = 63.925(3)°$, $V = 1221.2(6)$ Å^3, $Z = 2$, $R_{gt}(F) = 0.0411$, $wR_{ref}(F^2) = 0.0981$, $T = 296$ K.

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A part of the polymeric title crystal structure is shown in the figure. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Table 1: Data collection and handling.

Crystal:	Pink block
Size:	0.27 × 0.19 × 0.07 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	1.06 mm^{-1}
Diffractometer, scan mode:	Bruker SMART, φ and ω-scans
$2\theta_{max}$, completeness:	25.5°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	9118, 4513, 0.033
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 3296
$N(param)_{refined}$:	335
Programs:	Bruker programs [1], SHELX [2]

Source of material

A mixture of 5-methoxyisophthalic acid (39.2 mg, 0.2 mmol), $Zn(OAc)_2{\cdot}2H_2O$ (24 mg, 0.1 mmol), 1,3-bis(benzimidazol-1-yl)propane) (bbip; 27.6 mg, 0.1 mmol), and KOH (22.0 mg, 0.1 mmol) were added to water (10 mL) in a 25 mL Teflon-lined autoclave. The mixture was heated at 413 K for 3 days and then slowly cooled down to room temperature. Pink block crystals of the title compound were obtained.

Experimental details

The hydrogen atoms were placed in calculated positions and refined riding on the attached atoms with isotropic thermal parameters 1.2 times those of their carrier atoms. The methyl groups were idealized and refined using rigid groups allowed to rotate about the C—C bond (AFIX 137 option of the SHELXL-2014 program [2]). The U_{iso} values of the hydrogen atoms of methyl groups and oxygen were set to $1.5U_{eq}$ (C, O).

Discussion

In the last decades, the design and construction of metal-organic frameworks is of interest in the field of molecular magnetism and materials chemistry due to their fascinating structural diversities and potential application as functional materials [3–7]. Many carboxylates have been used to construct coordination polymers [8, 9]. The structural transformation mediated by 4-*R*-phthalic acid ($R = -C(CH_3)_3$ or $-CH_3$) and *N*-donor ligands has been studied [10]. The 1,3-bis(benzimidazol-1-yl)propane (bbip), a flexible ligand, serves as bridging ligand, which are employed to constrcut CPs [11–13]. It can be used as bidentate ligand to link two metal ions [14].

As shown in the Figure, one Zn(II) ion, one bbip ligand, one miph ligand, and one free water molecule form the asymmetric unit of the title crystal structure. This complex displays a distorted tetrahedral geometry due to Zn1 coordinate with

***Corresponding author: Zhan Zhou,** College of Chemistry and Chemical Engineering, Henan Key Laboratory of Function-Oriented Porous Materials, Luoyang Normal University, Luoyang, Henan 471934, P. R. China, e-mail: zhouzhan0406@163.com
Zhe Zhou and Peng-Jing Jing: College of Chemistry and Chemical Engineering, Henan Key Laboratory of Function-Oriented Porous Materials, Luoyang Normal University, Luoyang, Henan 471934, P. R. China

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.67374(4)	0.85971(4)	0.25058(3)	0.03569(13)
O1	0.6651(3)	0.5787(3)	0.30059(16)	0.0465(6)
O2	0.7169(2)	0.7303(2)	0.16859(15)	0.0417(5)
O3	0.6311(3)	0.1136(3)	0.29168(17)	0.0600(7)
O4	0.6824(3)	0.0506(2)	0.15918(15)	0.0443(6)
O5	0.7405(3)	0.4878(3)	−0.08975(16)	0.0633(8)
O6	0.4664(4)	0.2241(3)	0.4244(2)	0.1006(12)
H1W	0.5212	0.2007	0.3790	0.151*
H2W	0.4364	0.3218	0.4057	0.151*
N1	0.8401(3)	0.7623(3)	0.35784(18)	0.0396(6)
N2	0.9512(3)	0.6979(3)	0.50377(18)	0.0378(6)
N3	0.7787(3)	0.9817(3)	0.66940(18)	0.0365(6)
N4	0.5498(3)	1.0666(3)	0.72666(18)	0.0360(6)
C1	0.6888(3)	0.6144(3)	0.2136(2)	0.0353(7)
C2	0.6864(3)	0.5183(3)	0.1556(2)	0.0340(7)
C3	0.7145(4)	0.5554(3)	0.0577(2)	0.0395(8)
H3	0.7336	0.6412	0.0269	0.047*
C4	0.7138(4)	0.4630(4)	0.0063(2)	0.0403(8)
C5	0.6889(4)	0.3331(4)	0.0527(2)	0.0384(8)
H5	0.6885	0.2716	0.0180	0.046*
C6	0.6646(3)	0.2949(3)	0.1503(2)	0.0343(7)
C7	0.6609(3)	0.3894(3)	0.2010(2)	0.0347(7)
H7	0.6410	0.3656	0.2661	0.042*
C8	0.6565(4)	0.1448(4)	0.2044(2)	0.0405(8)
C9	0.7731(7)	0.6149(5)	−0.1399(3)	0.0965(18)
H9A	0.6906	0.7090	−0.1358	0.145*
H9B	0.7841	0.6225	−0.2070	0.145*
H9C	0.8669	0.5993	−0.1111	0.145*
C10	0.9983(4)	0.7120(3)	0.3511(2)	0.0365(7)
C11	1.0828(4)	0.7002(4)	0.2709(2)	0.0472(9)
H11	1.0364	0.7254	0.2103	0.057*
C12	1.2384(4)	0.6494(4)	0.2858(3)	0.0563(10)
H12	1.2984	0.6409	0.2335	0.068*
C13	1.3089(4)	0.6101(4)	0.3769(3)	0.0536(9)
H13	1.4143	0.5780	0.3835	0.064*
C14	1.2262(4)	0.6177(4)	0.4575(3)	0.0460(8)
H14	1.2732	0.5888	0.5186	0.055*
C15	1.0687(4)	0.6710(3)	0.4420(2)	0.0366(7)
C16	0.8201(4)	0.7518(4)	0.4500(2)	0.0419(8)
H16	0.7245	0.7792	0.4750	0.050*
C17	0.9659(4)	0.6711(4)	0.6081(2)	0.0449(8)
H17A	1.0411	0.5649	0.6406	0.054*
H17B	0.8681	0.6834	0.6344	0.054*
C18	1.0144(4)	0.7811(4)	0.6295(2)	0.0455(8)
H18A	1.1057	0.7769	0.5963	0.055*
H18B	1.0426	0.7437	0.6988	0.055*
C19	0.8951(4)	0.9502(4)	0.6003(2)	0.0444(8)
H19A	0.9471	1.0149	0.5936	0.053*
H19B	0.8444	0.9794	0.5372	0.053*
C20	0.8049(4)	0.9720(3)	0.7639(2)	0.0363(7)
C21	0.9383(4)	0.9238(4)	0.8197(3)	0.0544(10)
H21	1.0343	0.8905	0.7953	0.065*
C22	0.9214(5)	0.9279(5)	0.9128(3)	0.0663(12)
H22	1.0083	0.8959	0.9526	0.080*
C23	0.7779(5)	0.9785(4)	0.9493(3)	0.0612(11)
H23	0.7713	0.9793	1.0129	0.073*
C24	0.6465(4)	1.0271(4)	0.8942(2)	0.0466(9)
H24	0.5508	1.0608	0.9189	0.056*
C25	0.6614(4)	1.0242(3)	0.7994(2)	0.0347(7)
C26	0.6263(4)	1.0396(3)	0.6522(2)	0.0385(8)
H26	0.5794	1.0587	0.5931	0.046*

four atoms, which is inculding the two O atoms from two miph ligands, two N atoms from two bbip ligands. The Zn—O bond lengths are 1.962(2) and 1.987(2) Å, and the Zn—N ones are 1.999(3) and 2.006(3) Å, respectively. Two zinc(II) centers and two bbip ligands form centrosymmetric dimers (*cf*. the figure). These dimeric units are linked by miph to form an infinite chain. And the free water molecules are located in voids of the crystal structure, fixed by hydrogen-bonding between free water, and carboxylic oxygen atoms O(6)—H(1W)···O(3) 167.6°). Therefore, hydrogen bonds contribute to the stability of the structure. Bond lenghths and angles are in the expected ranges [15].

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