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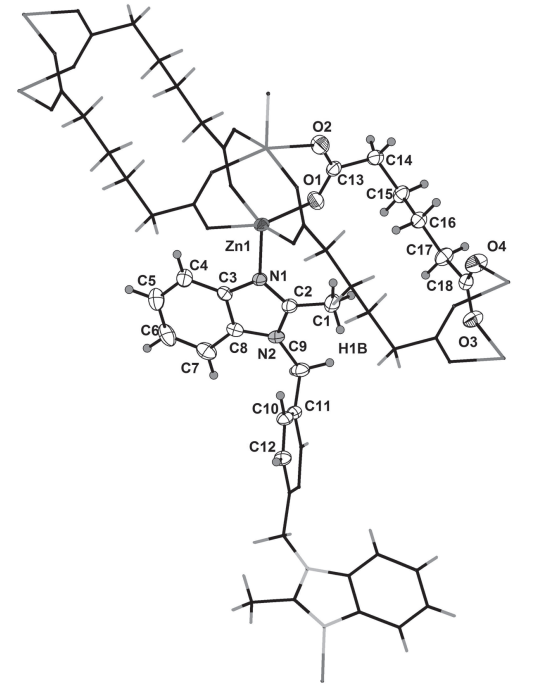
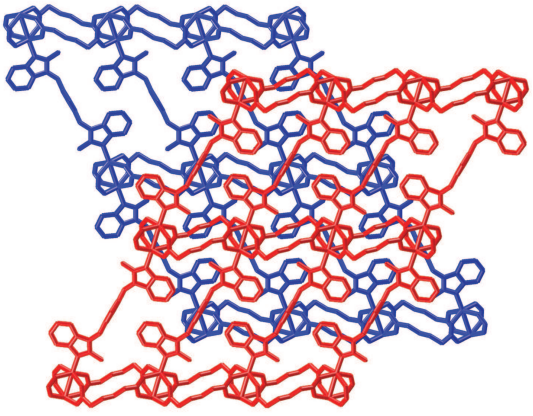
Crystal structure of poly[bis(adipate-κ⁴*O*,*O*′:*O*″,*O*‴)(1,4-bis(2-methyl-1*H*-benzo[*d*]imidazol-1-yl) benzene-κ²*N*:*N*′)dizinc(II), $C_{36}H_{38}N_4O_8Zn_2$





DOI 10.1515/ncrs-2016-0006
Received January 3, 2016; accepted March 26, 2016; available online April 21, 2016

Abstract

$C_{36}H_{38}N_4O_8Zn_2$, monoclinic, $P2_1/n$ (no. 14), $a = 13.144(3)$ Å, $b = 9.0091(18)$ Å, $c = 15.468(3)$ Å, $\beta = 112.56(3)°$, $V = 1691.6(6)$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0468$, $wR_{ref}(F^2) = 0.0980$, $T = 293(2)$ K.

CCDC no.: 1470648

Table 1: Data collection and handling.

Crystal:	Colorless Prisms Size 0.19 × 0.16 × 0.14 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	14.8 cm^{-1}
Diffractometer, scan mode:	Rigaku Saturn 724, ω
$2\theta_{max}$, completeness	58.2°, >99 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	22102, 4549, 0.037
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 4119
$N(param)_{refined}$:	227
Programs:	SHELX [13]

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 $Zn(Ac)_2 \cdot H_2O$ (43.9 mg, 0.2 mmol), adipic acid (29.2 mg, 0.2 mmol), NaOH (8.0 mg, 0.2 mmol) and 1,4-bis(2-methylbenzimidazol-1-ylmethyl) benzene (36.6 mg, 0.1 mmol) in 10 mL distilled H_2O was sealed in a 25 mL Teflon-lined stainless steel container and heated at 160°C for 4 days. After the mixture was cooled to room temperature at a rate of 5°C/h, colorless block crystals were obtained with a yield of 56% (based on Zn). Anal. Calc. for $C_{36}H_{38}N_4O_8Zn_2$ (%): C, 55.04; H, 4.88; N, 9.66. Found: C, 55.29; H, 5.03; N, 9.83. IR (KBr, cm-1): 2960(s), 2898(w), 1641(s), 1618(s), 1513(s), 1458(m), 1421(s), 1320(w), 1298(m), 1232(w), 1150(w),

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
O3	0.86930(16)	−0.3600(2)	0.03775(14)	0.0405(4)
O4	0.92071(18)	−0.2968(2)	−0.07855(15)	0.0466(5)
Zn1	0.96973(2)	0.45613(3)	0.079397(18)	0.02661(9)
C3	0.92730(18)	0.4812(3)	0.25859(15)	0.0250(5)
N2	0.88554(16)	0.2544(2)	0.28915(13)	0.0273(4)
N1	0.93696(16)	0.3861(2)	0.19127(13)	0.0250(4)
O1	0.85115(17)	0.3415(2)	−0.02559(13)	0.0430(5)
C10	0.92739(19)	0.0700(3)	0.41927(16)	0.0257(5)
C8	0.89479(19)	0.3992(3)	0.32010(16)	0.0281(5)
C2	0.91236(19)	0.2520(3)	0.21208(16)	0.0261(5)
C16	0.8151(2)	−0.0182(3)	−0.09923(18)	0.0311(5)
H16A	0.8281	−0.0517	−0.1537	0.037*
H16B	0.8829	0.0256	−0.0558	0.037*
C13	0.8432(2)	0.3328(3)	−0.10885(17)	0.0291(5)
C7	0.8773(2)	0.4640(3)	0.39470(19)	0.0398(6)
H7	0.8554	0.4084	0.4352	0.048*
C9	0.8444(2)	0.1336(3)	0.32932(17)	0.0340(6)
H9A	0.8189	0.0545	0.2835	0.041*
H9B	0.7813	0.1692	0.3412	0.041*
C4	0.9460(2)	0.6323(3)	0.27129(19)	0.0348(6)
H4	0.9694	0.6880	0.2318	0.042*
C12	0.8880(2)	0.0036(3)	0.48136(17)	0.0298(5)
H12	0.8130	0.0058	0.4692	0.036*
C14	0.7536(2)	0.2340(3)	−0.17440(18)	0.0357(6)
H14A	0.7762	0.2003	−0.2239	0.043*
H14B	0.6873	0.2930	−0.2033	0.043*
C11	1.0399(2)	0.0660(3)	0.43842(16)	0.0286(5)
H11	1.0669	0.1102	0.3972	0.034*
C15	0.7254(2)	0.0992(3)	−0.12909(19)	0.0333(5)
H15A	0.7118	0.1311	−0.0746	0.040*
H15B	0.6580	0.0553	−0.1729	0.040*
C1	0.9145(3)	0.1157(3)	0.1596(2)	0.0413(6)
H1A	0.8405	0.0826	0.1252	0.062*
H1B	0.9546	0.0396	0.2027	0.062*
H1C	0.9499	0.1362	0.1170	0.062*
C6	0.8940(3)	0.6139(4)	0.4055(2)	0.0485(7)
H6	0.8824	0.6618	0.4542	0.058*
C5	0.9281(3)	0.6965(3)	0.3452(2)	0.0456(7)
H5	0.9392	0.7981	0.3551	0.055*
O2	0.90226(16)	0.4011(2)	−0.14265(14)	0.0435(5)
C18	0.8652(2)	−0.2792(3)	−0.02928(17)	0.0295(5)
C17	0.7854(2)	−0.1504(3)	−0.0531(2)	0.0359(6)
H17A	0.7136	−0.1863	−0.0943	0.043*
H17B	0.7789	−0.1168	0.0041	0.043*

1139(m), 1013(m), 991(m), 877(m), 814(w), 778(w), 751(s), 709(w), 671(m), 606(m), 553(w), 482(m).

Experimental details

Absorption corrections were applied using the multi-scan method. The hydrogen atoms were placed at calculated positions and refined as riding atoms with isotropic displacement parameters [13].

Discussion

Metal–organic frameworks (MOFs) with various structures have received tremendous attention because of their potential applications in catalysis, luminescence, magnetism, gas storage and separation and so on [1–4]. Although a variety of MOFs have been successfully synthesized, rational control in constructing of coordination polymers with desired frameworks and properties remains a great challenge in crystal engineering. Therefore, tactical synthesis or selection of organic ligand and metal ions is key factor for achieving expected MOFs [5]. Recently, five-membered heterocycle ligands such as imidazole, pyrazole, triazole and tetrazole as well as their derivatives have been widely used to construct MOFs because of their various conformation in neutral or ionic forms [6–9]. In this paper, we selected 1,4-bis(2-methylbenzimidazol-1-ylmethyl)benzene (bmb) as N-donor ligands for several reasons: (1) the 2-position substituent methyl of bmb effectively enhances the donated electrons ability of benzimidazole ring; (2) bmb exhibit strong collaborative coordination ability with O-donor ligands [10–12].

The asymmetric unit of the title structure consists of one half of a 1,4-bis(2-methylbenzimidazol-1-ylmethyl) benzene (bmb), one adipiclate (adi^{2-}), and one Zn(II) in (upper part of the figure). The Zn(II) ion displays nearly ideal ZnO_4N square-pyramidal coordination environment, with the oxygen donors situated in the equatorial plane (Zn—O: 2.0368(19)–2.610(19) Å), and bmb nitrogen donors oriented in a *trans*-fashion in the axial positions (Zn—N 2.0372(18) Å). Each pair of Zn(II) ions is bridged by four *adi* carboxylate groups to generate a well-known paddle-wheel binuclear unit (upper part of the figure). The second carboxylate group of each *adi* anionic ligand coordinates to another paddle wheel unit, generating the extended one dimensional chain. Two bmb ligands occupy the axial positions of the dizinc paddle wheel and pillar these chains along c axis affording square grid-shaped layer. These layers offset along b axis affording hexagonal channels that run through the gross structure. Simplifying the binuclear Zn as a node, the structure shows a 4^4 topology. These 2-D structures are stacking in the offset fashion along the ac-plane with some displacement between two layers (lower part of the figure).

Acknowledgements: This work was financially supported by the Science and technology research key project of the Education Department of Henan Province (2014A150025) and the Provincial cultivation fund of Luoyang normal university (2013-PYJJ-005).

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