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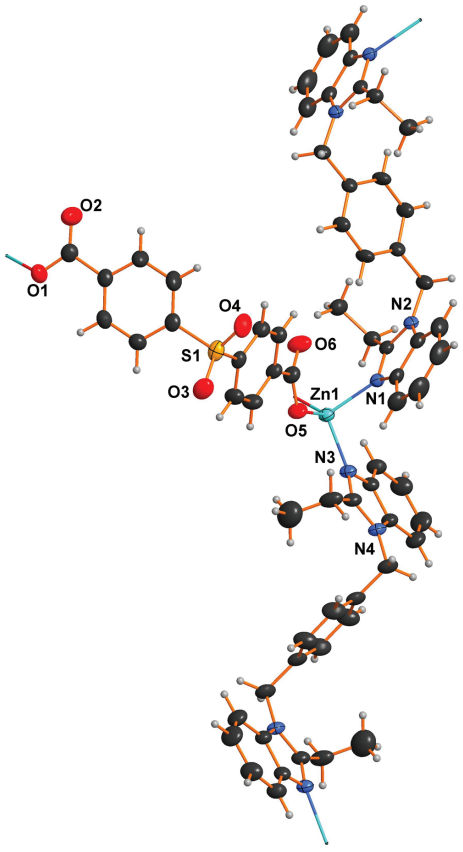
Crystal structure of poly[(μ_2-1,4-bis((2-ethyl-1*H*-benzo[*d*]imidazol-1-yl)methyl)benzene-$\kappa^2N:N'$)-(μ_2-4,4′-sulfonyldibenzoato-$\kappa^2O:O'$)zinc(II)], $C_{40}H_{34}N_4O_6SZn$



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Abstract

$C_{40}H_{34}N_4O_6SZn$, triclinic $P\bar{1}$ (no. 2), $a = 11.157(2)$ Å, $b = 11.867(2)$ Å, $c = 14.141(3)$ Å, $\alpha = 75.30(3)°$, $\beta = 86.09(3)°$, $\gamma = 84.91(3)°$, $V = 1801.8(6)$ Å^3, $Z = 2$, $R_{gt}(F) = 0.0419$, $\omega R_{ref}(F^2) = 0.1063$, $T = 293(2)$ K.

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The 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:	Prism, colourless
Size:	0.33 × 0.22 × 0.19 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	0.79 mm^{-1}
Diffractometer, scan mode:	Bruker SMART, φ and ω-scans
$2\theta_{max}$, completeness:	25.5°, >97%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	12744, 6572, 0.022
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 5779
$N(param)_{refined}$:	471
Programs:	Rigaku/MSC [1], SHELX [2]

Source of material

The title compound was prepared under the hydrothermal conditions. A mixture of 1,4-bis(2-ethylbenzimidazol-1-ylmethyl) benzene (73.2 mg, 0.2 mmol), $Zn(Ac)_2{\cdot}2H_2O$ (21.9 mg, 0.1 mmol), 4,4′-sulfonyldibenzoic acid (H_2sb; 32.8 mg, 0.2 mmol), and H_2O (10 mL) were placed in a teflon-lined stainless steel vessel, heated to 160 °C for 4 days, and then cooled to room temperature for 24 h. Colorless block crystals of the title complex were obtained.

Experimental details

The hydrogen atoms were placed at calculated positions and refined as riding atoms with isotropic displacement parameters.

Discussion

Metal–organic frameworks (MOFs) with entangled architectures, such as the most common interpenetrating nets, polyrotaxane structures, self-penetrating nets etc., are of great attention [3–6]. It is not only because of their intrinsic aesthetic appeal and complicated molecular architectures as well

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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}
Zn1	0.94384(3)	0.33679(3)	0.26407(2)	0.03138(11)
N1	0.92930(18)	0.18348(18)	0.36809(15)	0.0323(5)
N2	0.82997(19)	0.05301(19)	0.47911(16)	0.0355(5)
N3	1.12299(19)	0.35217(19)	0.24505(15)	0.0344(5)
N4	1.31701(19)	0.32032(19)	0.20597(16)	0.0356(5)
O1	0.14988(18)	0.53665(16)	−0.30268(14)	0.0456(5)
O2	0.0489(2)	0.3892(2)	−0.2128(2)	0.0710(7)
O3	0.69220(19)	0.1731(2)	−0.28050(14)	0.0546(6)
O4	0.58652(19)	0.01337(16)	−0.16585(15)	0.0514(5)
O5	0.89055(17)	0.31080(17)	0.14352(13)	0.0430(5)
O6	0.71992(18)	0.2523(2)	0.22503(15)	0.0553(6)
S1	0.61265(7)	0.13451(6)	−0.19700(5)	0.03993(18)
C1	1.1481(4)	0.4153(4)	0.0119(3)	0.0914(13)
H1A	1.0896	0.4643	0.0389	0.137*
H1B	1.1180	0.4012	−0.0458	0.137*
H1C	1.2218	0.4535	−0.0050	0.137*
C2	1.1707(3)	0.3042(3)	0.0840(2)	0.0521(8)
H2A	1.0993	0.2608	0.0943	0.063*
H2B	1.2359	0.2581	0.0595	0.063*
C3	1.2029(2)	0.3240(2)	0.1785(2)	0.0359(6)
C4	1.1899(2)	0.3701(2)	0.31838(19)	0.0328(6)
C5	1.1536(3)	0.4035(2)	0.4039(2)	0.0414(7)
H5	1.0725	0.4190	0.4196	0.050*
C6	1.2411(3)	0.4127(3)	0.4644(2)	0.0520(8)
H6	1.2189	0.4358	0.5217	0.062*
C7	1.3626(3)	0.3883(3)	0.4420(2)	0.0576(9)
H7	1.4193	0.3939	0.4854	0.069*
C8	1.4009(3)	0.3561(3)	0.3577(2)	0.0492(8)
H8	1.4821	0.3399	0.3429	0.059*
C9	1.3118(2)	0.3489(2)	0.29545(19)	0.0345(6)
C10	1.4282(2)	0.2968(3)	0.1501(2)	0.0431(7)
H10A	1.4171	0.2339	0.1198	0.052*
H10B	1.4930	0.2708	0.1948	0.052*
C11	1.4644(2)	0.4019(2)	0.0717(2)	0.0380(6)
C12	1.5015(3)	0.4979(3)	0.0966(2)	0.0502(8)
H12	1.5030	0.4975	0.1623	0.060*
C13	1.4639(3)	0.4059(3)	−0.0266(2)	0.0498(8)
H13	1.4397	0.3424	−0.0459	0.060*
C14	0.6823(2)	0.2996(3)	0.4812(2)	0.0462(7)
H14A	0.6711	0.3211	0.4120	0.069*
H14B	0.6619	0.3663	0.5074	0.069*
H14C	0.6314	0.2385	0.5124	0.069*
C15	0.8137(2)	0.2568(2)	0.49975(19)	0.0367(6)
H15A	0.8633	0.3226	0.4782	0.044*
H15B	0.8222	0.2258	0.5696	0.044*
C16	0.8581(2)	0.1658(2)	0.44899(19)	0.0313(6)
C17	0.9476(2)	0.0760(2)	0.3441(2)	0.0356(6)
C18	1.0130(3)	0.0438(3)	0.2673(2)	0.0507(8)
H18	1.0558	0.0975	0.2208	0.061*
C19	1.0129(3)	−0.0707(3)	0.2619(3)	0.0617(9)
H19	1.0561	−0.0943	0.2108	0.074*
C20	0.9491(3)	−0.1515(3)	0.3315(3)	0.0628(10)
H20	0.9508	−0.2280	0.3258	0.075*
C21	0.8836(3)	−0.1211(3)	0.4083(3)	0.0520(8)
H21	0.8404	−0.1748	0.4545	0.062*
C22	0.8855(2)	−0.0061(2)	0.4135(2)	0.0367(6)
C23	0.7453(2)	0.0031(3)	0.5588(2)	0.0421(7)
H23A	0.7422	0.0476	0.6078	0.050*
H23B	0.7748	−0.0764	0.5892	0.050*
C24	0.6186(2)	0.0021(2)	0.52568(19)	0.0336(6)
C25	0.5288(2)	−0.0333(2)	0.5964(2)	0.0401(7)
H25	0.5474	−0.0558	0.6619	0.048*
C26	0.5884(3)	0.0358(3)	0.4285(2)	0.0433(7)
H26	0.6475	0.0604	0.3797	0.052*
C27	0.7878(2)	0.2675(2)	0.1519(2)	0.0390(6)
C28	0.7516(2)	0.2324(2)	0.06298(19)	0.0338(6)
C29	0.6646(2)	0.1530(2)	0.0754(2)	0.0367(6)
H29	0.6334	0.1196	0.1380	0.044*
C30	0.6237(2)	0.1230(2)	−0.0039(2)	0.0382(6)
H30	0.5653	0.0695	0.0051	0.046*
C31	0.6699(2)	0.1726(2)	−0.09701(19)	0.0336(6)
C32	0.7588(3)	0.2508(3)	−0.1112(2)	0.0439(7)
H32	0.7904	0.2835	−0.1737	0.053*
C33	0.7997(3)	0.2792(3)	−0.0302(2)	0.0449(7)
H33	0.8602	0.3304	−0.0386	0.054*
C34	0.4741(2)	0.2188(2)	−0.21835(19)	0.0363(6)
C35	0.3680(3)	0.1727(3)	−0.1765(2)	0.0512(8)
H35	0.3689	0.0958	−0.1393	0.061*
C36	0.2612(3)	0.2405(3)	−0.1900(2)	0.0485(8)
H36	0.1898	0.2091	−0.1620	0.058*
C37	0.2589(2)	0.3554(2)	−0.24478(19)	0.0363(6)
C38	0.3652(3)	0.3998(2)	−0.2874(2)	0.0408(7)
H38	0.3641	0.4764	−0.3253	0.049*
C39	0.4733(3)	0.3327(2)	−0.2747(2)	0.0423(7)
H39	0.5445	0.3637	−0.3037	0.051*
C40	0.1411(3)	0.4308(3)	−0.2530(2)	0.0404(7)

as topological features [7–12], but also for their potential application, such as gas adsorption, molecular electronic devices, and so on [13–15]. Compared to the interpenetrating nets (the polymeric equivalents of catenanes and rotaxanes) and other intertwining nets, the self-penetrating frameworks, have attracted much higher interest [16, 17].

The title structure consists of a 1,4-bis(2-ethyl benzimidazol-1-ylmethyl) benzene (beb), one 4,4′-sulfonyldibenzoate (sb^{2-}), and one Zn(II) ion in the asymmetric unit. The Zn(II) ion presents a distorted tetrahedral coordination geometry, ligated by two oxygen atoms (O1A and O5) from two symmetry-related carboxylate groups of 4,4′-sulfonyldibenzoate and two nitrogen atoms N1 and N3) from different beb ligands. The bond lengths are Zn(1)—O(1A) = 1.9249(19) Å, Zn(1)—O(5) = 1.9471(18) Å, Zn(1)—N(1) = 2.039(2) Å, and Zn(1)—N(3) = Zn1 2.017(2) Å, respectively. They are in the normal range [18].

In the title complex, two beb ligands adopt symmetric trans-conformation with the $N_{donor}\cdots N—C_{sp^3}\cdots C$ torsion of 30.496° and 28.589° [19], respectively. Each Zn(II) ion links

two beb and two sb^{2-} resulting in a 2D sheet structure, similarily to related structures. The two sheets give parallel (2D → 2D) catenation.

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