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Chunying Xu, Siye Tang* and Wenjuan Chu

Crystal structure of *poly*-[μ-1,4-bis(2-ethylbenzimidazol-1-ylmethyl)benzene-κ^2*N*:*N*′)-bis(μ$_4$-4,4′-sulfonyldibenzoato-κ^4*O*:*O*′:*O*″:*O*‴) dicadmium(II)] monohydrate, $C_{52}H_{42}N_4O_{14}Cd_2$

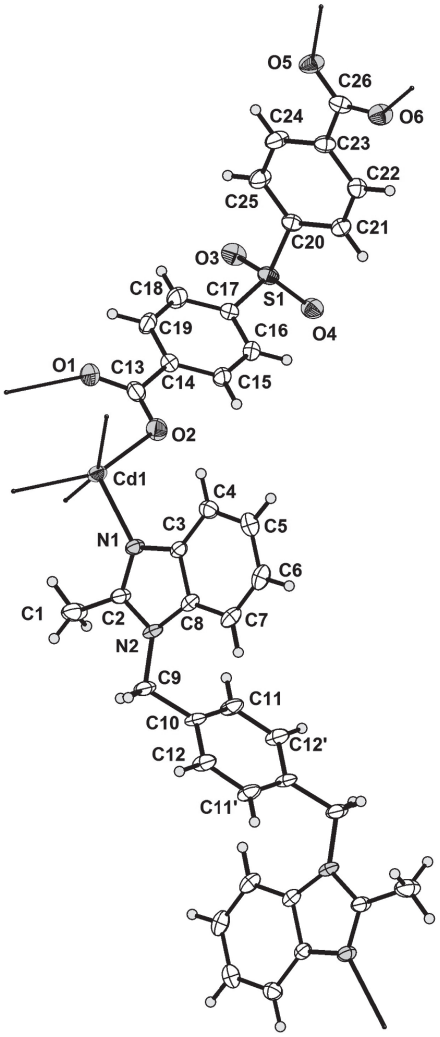

Figure 1: Coordination environment of Cd(II) ion in the title complex.

***Corresponding author: Siye Tang,** College of Chemistry and Chemical Engineering, Luoyang Normal University, Luoyang, Henan 471022, P. R. China, e-mail: tangsiyencs@163.com
Chunying Xu: College of Chemistry and Chemical Engineering, Luoyang Normal University, Luoyang, Henan 471022, P. R. China
Wenjuan Chu: Henan Tobacoo Industry Limited Liaility Company of Anyang Cigarette Factory, Anyang, Henan 455000, P. R. China

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Abstract

$C_{52}H_{42}N_4O_{14}Cd_2$, triclinic, $P\bar{1}$ (no. 2), $a = 9.0684(18)$ Å, $b = 12.585(3)$ Å, $c = 12.697(3)$ Å, $\alpha = 101.14(3)°$, $\beta = 106.98(3)°$, $y = 102.06(3)°$, $V = 1304.3(5)$ Å^3, $Z = 1$, $R_{gt}(F) = 0.0276$, $wR_{ref}(F^2) = 0.0853$, $T = 293(2)$ 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.

Table 1: Data collection and handling.

Crystal:	Colorless prism size 0.34×0.30×0.24 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	9.6 cm^{-1}
Diffractometer, scan mode:	Rigaku Saturn 724, ω
$2\theta_{max}$, completeness:	55.8°, 98.5%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	9207, 4512, 0.020
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 4183
$N(param)_{refined}$:	326
Programs:	SHELX [6], SQUEEZE [7]

Source of material

The title compound was prepared under the hydrothermal conditions. A mixture of 1,4-bis(2-methylbenzimidazol-1-ylmethyl)benzene, *bmb* (73.2 mg, 0.2 mmol), $Cd(Ac)_2{\cdot}H_2O$ (53.2 mg, 0.2 mmol), 4,4′-sulfonyldibenzoic acid, H_2ssb (61.2 mg, 0.2 mmol), and H_2O (10 mL) were placed in a Teflon-lined stainless steel vessel, heated to 140°C for 5 day, and then cooled to room temperature within 24 h. Colorless prismatic crystals of the title complex were obtained.

Experimental details

Absorption corrections were applied by using multi-scan program. The structure was solved by direct methods and

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

Atom	x	y	z	U_{iso}*/U_{eq}
C1	0.3827(5)	−0.1586(3)	0.6686(3)	0.0550(10)
H1A	0.2790	−0.1661	0.6150	0.083*
H1B	0.3745	−0.2175	0.7065	0.083*
H1C	0.4570	−0.1645	0.6287	0.083*
C2	0.4412(4)	−0.0465(3)	0.7550(3)	0.0319(7)
C3	0.4637(3)	0.1246(2)	0.8463(2)	0.0274(6)
C4	0.4455(4)	0.2312(3)	0.8823(3)	0.0333(7)
H4	0.3648	0.2552	0.8376	0.040*
C5	0.5520(4)	0.2999(3)	0.9871(3)	0.0405(8)
H5	0.5439	0.3722	1.0126	0.049*
C6	0.6713(4)	0.2639(3)	1.0554(3)	0.0461(9)
H6	0.7407	0.3123	1.1256	0.055*
C7	0.6886(4)	0.1577(3)	1.0211(3)	0.0410(8)
H7	0.7677	0.1334	1.0671	0.049*
C8	0.5836(3)	0.0887(3)	0.9155(2)	0.0306(6)
C9	0.6551(4)	−0.0982(3)	0.8948(3)	0.0403(8)
H9A	0.6337	−0.1625	0.8308	0.048*
H9B	0.6152	−0.1259	0.9504	0.048*
C10	0.8341(4)	−0.0452(3)	0.9488(3)	0.0326(7)
C11	0.9186(4)	0.0210(3)	0.9000(3)	0.0404(8)
H11	0.8643	0.0359	0.8325	0.048*
C12	0.9161(4)	−0.0662(3)	1.0504(3)	0.0396(8)
H12	0.8601	−0.1104	1.0848	0.048*
C13	0.1500(4)	0.1768(3)	0.4363(3)	0.0388(8)
C14	0.1973(4)	0.2536(3)	0.3666(3)	0.0343(7)
C15	0.3502(4)	0.3284(3)	0.4053(3)	0.0379(7)
H15	0.4241	0.3315	0.4750	0.045*
C16	0.3934(4)	0.3978(3)	0.3416(3)	0.0376(7)
H16	0.4956	0.4483	0.3683	0.045*
C17	0.2838(4)	0.3919(2)	0.2379(3)	0.0315(7)
C18	0.1314(4)	0.3159(3)	0.1970(3)	0.0456(9)
H18	0.0585	0.3108	0.1261	0.055*
C19	0.0903(4)	0.2486(3)	0.2625(3)	0.0453(8)
H19	−0.0122	0.1985	0.2361	0.054*
C20	0.2680(4)	0.6005(2)	0.2084(2)	0.0308(6)
C21	0.3762(4)	0.6913(3)	0.2978(3)	0.0326(7)
H21	0.4844	0.6945	0.3260	0.039*
C22	0.3209(4)	0.7760(3)	0.3436(3)	0.0341(7)
H22	0.3923	0.8371	0.4033	0.041*
C23	0.1584(4)	0.7714(3)	0.3017(3)	0.0332(7)
C24	0.0543(4)	0.6813(3)	0.2100(3)	0.0419(8)
H24	−0.0532	0.6792	0.1796	0.050*
C25	0.1073(4)	0.5959(3)	0.1637(3)	0.0421(8)
H25	0.0364	0.5356	0.1030	0.051*
C26	0.0963(4)	0.8584(3)	0.3601(3)	0.0360(7)
Cd1	0.17053(2)	0.041568(16)	0.602056(16)	0.02629(9)
N1	0.3768(3)	0.0376(2)	0.7462(2)	0.0302(6)
N2	0.5674(3)	−0.0199(2)	0.8543(2)	0.0311(6)
O1	0.0079(3)	0.1158(2)	0.3979(2)	0.0525(7)
O2	0.2547(3)	0.1794(2)	0.5267(2)	0.0485(6)
O3	0.2380(3)	0.4331(2)	0.03880(19)	0.0459(6)
O4	0.5065(3)	0.5213(2)	0.1916(2)	0.0441(6)
O5	−0.0483(3)	0.8542(2)	0.3133(2)	0.0468(6)
O6	0.1928(3)	0.9277(2)	0.45129(19)	0.0465(6)
S1	0.33440(10)	0.48522(7)	0.15741(6)	0.03336(18)

refined with the SHELX [6] software package. The hydrogen atoms were placed at calculated positions and refined as riding atoms with isotropic displacement parameters. The dataset was analyzed using the program SQUEEZE [7] giving 8.4 electrons. According to this value one water molecule is present in the crystal.

Discussion

Recently, much attention has been paid to the design and synthesis of coordination polymers not only owing to their underlying applications as functional solid materials in the fields of luminescence, molecular separation, ion exchange and heterogeneous catalysis, but also to their intriguing variety of molecular architectures [1, 2]. It is well established that the design and choice of ligands are crucial for the construction of network topology [3, 4].

As shown in Figure 1, the center Cd(II) is five-coordinated in a trigonal bipyramid geometry, ligated by four oxygen atoms (O1A, O2A, O5 and O6A) from four symmetry-related dianionic *ssb* ligand and one nitrogen atoms (N1) from *bmb*. The bond lengths are Cd(1)–O(1A) = 1.9979(17) Å, Cd(1)–O(2A) = 1.9804(16) Å, Cd(1)–O(5) = 2.0064(17) Å, Cd(1)–O(6A) = 2.0064(17) Å and Cd(1)–N(1) = 2.009(2) Å, respectively. They are in the normal range [5]. The dihedral angle between two benzene rings is 85°. Each pair of Cd(II) ions is bridged by four *sbb* anions to generate a well-known paddle-wheel binuclear clusters with a Cd···Cd separation of 3.209 Å. The binuclear clusters are further extended by *sbb* anions into a 1D chain. *bmb* adopts symmetric trans-conformation. The Cd(*sbb*) chains are pillared by *bmb* into a 2D framework.

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