Crystal structure of catena-(5-*tert*-butylisophthalic)cadmium(II)-[1,4-*bis*-(2-methyl-imidazol-1-yl)butane], $[Cd(C_{12}H_{12}O_4)(C_{12}H_{18}N_4)]_n$, $C_{18}H_{21}CdN_2O_4$

Wei-Wei Lu[*, I] and Feng-Yang Ju[II]

[I] Chemical Engineering & Pharmaceutics College, Henan University of Science and Technology, Luoyang 471003, Henan Province, P. R. China
[II] LuoYang Normal University, College of Chemistry and Chemical Engineering, Luoyang 471022, Henan Province, P. R. China

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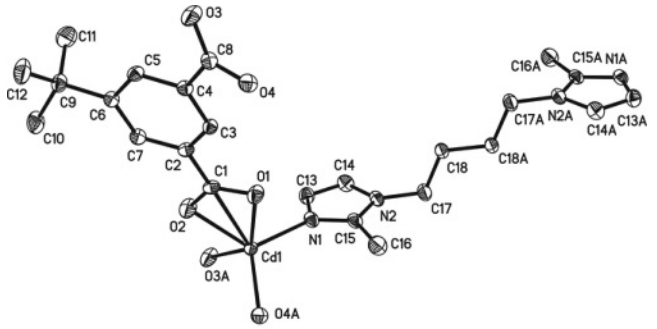

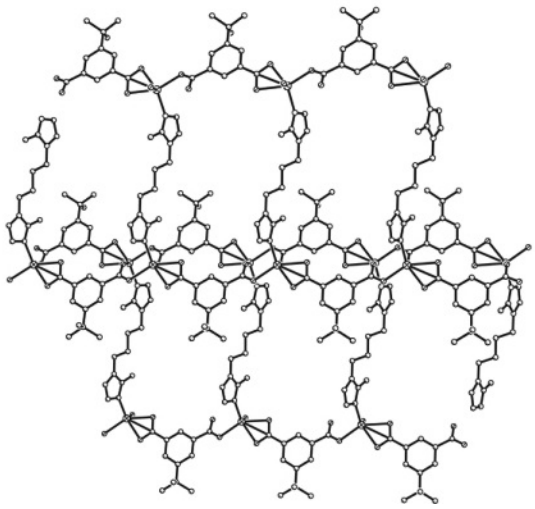

Abstract

$C_{18}H_{21}CdN_2O_4$, triclinic, $P\bar{1}$ (no. 2), a = 9.101(1) Å, b = 10.175(1) Å, c = 10.962(1) Å, α = 65.170(1)°, β = 75.095(1)°, γ = 88.586(1)°, V = 886.1 Å^3, Z = 2, $R_{gt}(F)$ = 0.0216, $wR_{ref}(F^2)$ = 0.0557, T = 296 K.

Table 1. Data collection and handling.

Crystal:	colourless blocks, size 0.13×0.17×0.25 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	12.57 cm^{-1}
Diffractometer, scan mode:	CCD area detector, φ and ω
$2\theta_{max}$:	51°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	6634, 3274
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 3039
$N(param)_{refined}$:	230
Programs:	SHELX [10]

* Correspondence author (e-mail: lyhnkjd@126.com)

Source of material

The title compound was prepared under hydrothermal conditions. A mixture of 5-*tert*-butylisophthalic (0.1 mmol) and1,4-*bis*(2-methyl-imidazol-1-yl)butane (0.1 mmol), $Cd(NO_3)_2$ (0.1 mmol), NaOH (0.1mmol) and H_2O (15 mL) were placed in a Teflon-lined stainless steel vessel, heated to 440 K for 4 day, and then cooled to room temperature within 24 h. Colourless block-shaped crystals of the title complex were obtained.

Discussion

In recent years, the design and synthesis of metal-organic frameworks (MOFs) with well-regulated architectures have caused increasing attention because they may act as functional materials with potential applications in such fields as nonlinear optics, magnetism, molecular separation, catalysis, luminescence, and gas sorption [1-5]. Among the various ligands, isophthalic acid (H_2isop) and its derivatives with special conformations, such as a 120° angle between two carboxylic groups, have been extensively used to prepare a variety of coordination polymers in virtue of the robust and versatile coordination capability of carboxylates [6-7]. On the other hand, the flexible *bis*(*N*-containing heterocyclic ring) ligands containing 1- or 2-substituted tetrazole, 1-substituted imidazole, benzimidazole, benzotriazole or 1,2,3-triazole,and 1-or 4-substituted 1,2,4-triazole rings tethered by an alkyl spacer have been extensively used [8-9]. In this paper, we select 5-*tert*-butylisophthalic (H_2tbip) and 1,4-*bis*(2-methyl-imidazol-1-yl)butane (bib) to react with Cd(II) ions to obtain a new MOF. The X-ray structure analysis shows that the title complex crystallizes in the triclinic system, space group $P\bar{1}$. The structure of the title complex consists of a 2D network containing noncentrosymmetric dinuclear Cd units as nodes. The asymmetric structure unit of the title complex consists of a Cd(II) ion, a tbip ligand, and a bib ligand (figure, top). The Cd(II) ion is chelated by four oxygen atoms from two carboxylate of two tbip ligands forming two chelating rings, one oxygen atom from another tbip ligand and one nitrogen atom from a bib ligand complete the six-coordination at the metal center. The Cd–O bond lengths are in the range of 2.2184(17)-2.7050(3) Å and the Cd–N bond length is 2.223(2) Å. In this structure, the Cd···Cd distance in the $[Cd_2(COO)_2]$ dimeric unit is 3.9523(4) Å. Each tbip ligand serves as a tridentate ligand to link the Cd(II) ions to generate a 1D polymeric motif. These 1D motifs are further connected by bib ligands to form a 2D layer (figure, bottom). The bib ligand adopts a bidentate-bridging conformation mode with the dihedral angle between the two imidazol rings of 0°, suggesting that these imidazole rings of each flexible bib ligand are parallel to each other. The Cd···Cd separation across the tbip and bib ligand are 10.1747(13) and 14.3251(14) Å, respectively.

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H(3)	2*i*	0.5835	–0.0681	0.3620	0.032
H(5)	2*i*	0.9752	–0.2335	0.2538	0.036
H(7)	2*i*	0.9875	0.1442	0.2834	0.036
H(10A)	2*i*	1.2334	0.1713	0.2024	0.082
H(10B)	2*i*	1.3686	0.0745	0.2301	0.082
H(10C)	2*i*	1.2219	0.0497	0.3525	0.082
H(11A)	2*i*	1.1960	–0.0559	0.0388	0.091
H(11B)	2*i*	1.3483	0.0206	0.0300	0.091
H(11C)	2*i*	1.2043	0.1074	0.0141	0.091
H(12A)	2*i*	1.2066	–0.2143	0.3934	0.090
H(12B)	2*i*	1.3530	–0.1742	0.2674	0.090
H(12C)	2*i*	1.2055	–0.2518	0.2688	0.090
H(13)	2*i*	0.5988	0.6628	0.0440	0.049
H(14)	2*i*	0.4030	0.7360	–0.0789	0.051
H(16A)	2*i*	0.2160	0.3091	0.3956	0.077
H(16B)	2*i*	0.0846	0.3770	0.3271	0.077
H(16C)	2*i*	0.1415	0.4418	0.4157	0.077
H(17A)	2*i*	0.1031	0.6971	0.0043	0.050
H(17B)	2*i*	0.0262	0.5811	0.1568	0.050
H(18A)	2*i*	0.0798	0.3938	0.0840	0.042
H(18B)	2*i*	0.1571	0.5098	–0.0686	0.042

Table 3. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cd(1)	2*i*	0.57173(2)	0.41693(2)	0.36368(2)	0.0258(1)	0.0226(1)	0.0353(1)	0.00271(6)	–0.00843(7)	–0.01606(7)
O(1)	2*i*	0.5555(2)	0.1876(2)	0.3532(2)	0.035(1)	0.0348(9)	0.066(1)	0.0099(8)	–0.0139(9)	–0.0303(9)
O(2)	2*i*	0.7749(2)	0.2844(2)	0.3393(2)	0.039(1)	0.0297(9)	0.078(1)	0.0051(8)	–0.0149(9)	–0.033(1)
O(3)	2*i*	0.7475(2)	–0.3874(2)	0.2810(2)	0.035(1)	0.035(1)	0.085(1)	0.0006(8)	–0.0055(9)	–0.041(1)
O(4)	2*i*	0.5436(2)	–0.3419(2)	0.4107(2)	0.0340(9)	0.0337(9)	0.0350(9)	–0.0087(7)	–0.0034(7)	–0.0143(7)
N(1)	2*i*	0.4327(2)	0.5196(2)	0.2141(2)	0.038(1)	0.031(1)	0.043(1)	0.0056(9)	–0.0179(9)	–0.0183(9)
N(2)	2*i*	0.2548(2)	0.5871(2)	0.1040(2)	0.037(1)	0.038(1)	0.042(1)	0.0049(9)	–0.019(1)	–0.020(1)
C(1)	2*i*	0.6958(3)	0.1841(2)	0.3408(2)	0.037(1)	0.023(1)	0.028(1)	0.004(1)	–0.006(1)	–0.0112(9)
C(2)	2*i*	0.7739(3)	0.0589(2)	0.3222(2)	0.032(1)	0.021(1)	0.027(1)	0.0025(9)	–0.0058(9)	–0.0104(9)
C(3)	2*i*	0.6896(3)	–0.0618(2)	0.3370(2)	0.025(1)	0.024(1)	0.030(1)	0.0026(9)	–0.0066(9)	–0.0118(9)
C(4)	2*i*	0.7660(3)	–0.1727(2)	0.3139(2)	0.030(1)	0.021(1)	0.030(1)	–0.0007(9)	–0.0072(9)	–0.0117(9)
C(5)	2*i*	0.9255(3)	–0.1611(2)	0.2738(2)	0.032(1)	0.023(1)	0.035(1)	0.0040(9)	–0.006(1)	–0.015(1)
C(6)	2*i*	1.0123(3)	–0.0432(2)	0.2631(2)	0.029(1)	0.025(1)	0.031(1)	0.0005(9)	–0.0071(9)	–0.0111(9)
C(7)	2*i*	0.9328(3)	0.0650(2)	0.2887(2)	0.033(1)	0.021(1)	0.037(1)	–0.0010(9)	–0.009(1)	–0.013(1)
C(8)	2*i*	0.6810(3)	–0.3095(2)	0.3362(2)	0.032(1)	0.020(1)	0.036(1)	0.0023(9)	–0.012(1)	–0.011(1)
C(9)	2*i*	1.1875(3)	–0.0338(3)	0.2193(3)	0.028(1)	0.035(1)	0.048(2)	0.003(1)	–0.010(1)	–0.019(1)
C(10)	2*i*	1.2596(3)	0.0756(3)	0.2544(4)	0.035(2)	0.054(2)	0.085(2)	–0.002(1)	–0.019(2)	–0.037(2)
C(11)	2*i*	1.2388(3)	0.0140(4)	0.0607(3)	0.038(2)	0.079(2)	0.057(2)	–0.005(2)	0.003(1)	–0.031(2)
C(12)	2*i*	1.2434(4)	–0.1824(3)	0.2942(4)	0.043(2)	0.053(2)	0.095(3)	0.018(1)	–0.031(2)	–0.036(2)
C(13)	2*i*	0.4967(3)	0.6258(3)	0.0807(3)	0.035(1)	0.041(2)	0.044(2)	–0.003(1)	–0.009(1)	–0.017(1)
C(14)	2*i*	0.3895(3)	0.6669(3)	0.0126(3)	0.047(2)	0.039(1)	0.038(1)	–0.000(1)	–0.014(1)	–0.012(1)
C(15)	2*i*	0.2866(3)	0.4990(3)	0.2246(3)	0.038(1)	0.033(1)	0.042(1)	0.002(1)	–0.015(1)	–0.022(1)
C(16)	2*i*	0.1721(3)	0.3978(3)	0.3520(3)	0.050(2)	0.054(2)	0.043(2)	–0.009(1)	–0.009(1)	–0.015(1)
C(17)	2*i*	0.1066(3)	0.5989(3)	0.0724(3)	0.037(1)	0.045(2)	0.054(2)	0.009(1)	–0.022(1)	–0.026(1)
C(18)	2*i*	0.0772(3)	0.4923(3)	0.0159(3)	0.032(1)	0.040(1)	0.041(1)	0.004(1)	–0.014(1)	–0.021(1)

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