Crystal structure of *catena*-diaqua(5-methoxyisophthalate) [1,2-*bis*-(imidazol-1'-yl)ethane]-cadmium(II)-water(1:1), $C_{13}H_{17}CdN_2O_8$

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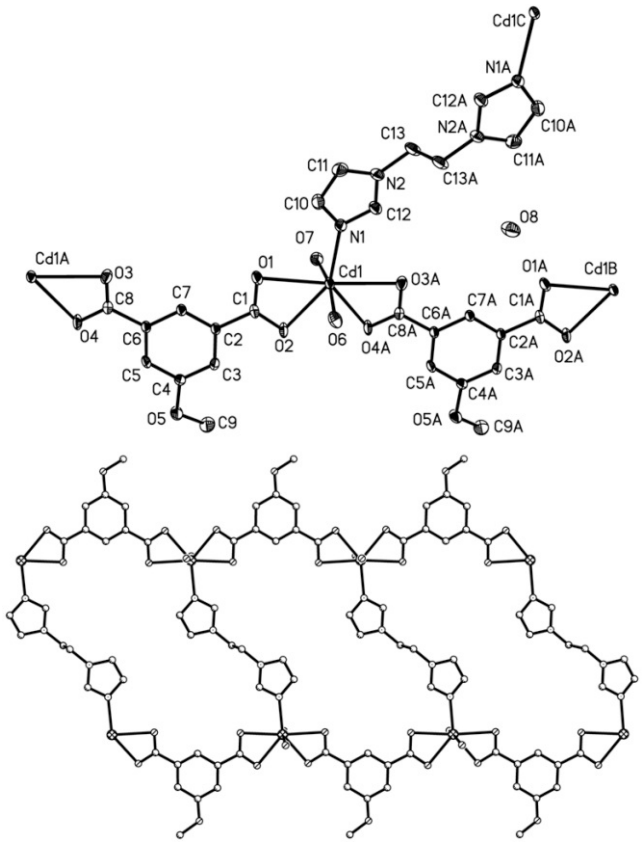

Abstract

$C_{13}H_{17}CdN_2O_8$, triclinic, $P\bar{1}$ (no. 2), a = 9.230(1) Å, b = 10.191(1) Å, c = 10.248(1) Å, α = 65.699(1)°, β = 65.896(1)°, γ = 79.459(1)°, V = 801.8 Å^3, Z = 2, $R_{gt}(F)$ = 0.0203, $wR_{ref}(F^2)$ = 0.0490, T = 296 K.

Table 1. Data collection and handling.

Crystal:	colourless blocks, size 0.08×0.12×0.22 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	14.07 cm^{-1}
Diffractometer, scan mode:	Bruker SMART CCD, φ and ω
$2\theta_{max}$:	51°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	6005, 2969
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2738
$N(param)_{refined}$:	218
Programs:	SHELXS-97, SHELXL-97 [11]

Source of material

The title compound was prepared under the hydrothermal conditions. A mixture of 5-methoxyisophthalate (0.1 mmol) and 1,2-*bis*-(imidazol-1'-yl)ethane (0.05 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 days, and then cooled to room temperature within 24 h. Colorless block 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 can be used as functional materials with potential applications in such fields as nonlinear optics, magnetism, molecular separation, catalysis, luminesence, and gas sorption [1-6]. It is well known that carboxylate ligands play an important role in coordination chemistry, which may adopt diverse binding modes such as monodentate, chelating, and bridging in the *syn-syn*, *syn-anti*, and *anti-anti* configurations [7-8]. So far, a great many metal-carboxylate complexes, in the presence of rigid or flexible N-donor bridging ligands, such as 4,4'-bipyridine and its derivatives or bis(imidazole) ligands have been designed and characterized widely [9-10]. In this paper, we select 5-methoxyisophthalate (CH_3O-ip) and 1,2-*bis*-(imidazol-1'-yl)-ethane (bime) to react with Cd(II) ions to obtain a new MOFs. The X-ray structure analysis shows that the title complex crystallizes in the triclinic system, space group $P\bar{1}$. The asymmetric unit of the title complex consists of a Cd^{2+} ion, a CH_3O-ip ligand, a half 1,2-*bis*-(imidazol-1'-yl)-ethane (bime) ligand, two coordinated water molecules and one free water molecule (figure, top). The Cd^{2+} ion is chelated by four oxygen atoms from two carboxylate groups of two CH_3O-ip ligands forming two chelating rings. One nitrogen atom from a bime ligand and two oxygen atoms from two coordinated water molecules complete the sevenfold coordination at the metal center. Thus, the coordination geometry around Cd^{2+} ion can be described as a distorted pentagonal bipyramid. Four chelating carboxylate oxygen-atoms and the nitrogen atom from the bime ligand comprise the equatorial plane around Cd^{2+} ion, while the two oxygens from watermolecules form the pyramidal apices with bond angles O6–Cd1–O7 of 168.773(3). The Cd–O bond lengths are in the range of 2.301(2) - 2.534(2) Å. The Cd–N bond length is 2.277(2) Å. The CH_3O-ip ligand takes the bidentate-chelating coordination mode to bridge the neighbouring Cd^{2+} ions to yield a 1D linear chain, with bridged Cd···Cd distance of 10.191(1) A. Every two of these 1D chains are linked into a 1D ladder-like chain by the bime ligand (figure, bottom). The Cd···Cd distance across the bime ligand is 11.817(1) Å. These 1D ladder-like chains are assembled by hydrogen bonds between coordinated or free water molecules and CH_3O-ip ligands yielding a three-dimensional supramolecular structure. The bond lengths and angles of these hydrogen bonding parametres are in the range of 2.721(2) - 2.925(3) Å and 153.0 - 179.4°, respectively.

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

Atom	Site	*x*	*y*	*z*	U_{iso}
H(1W)	2*i*	0.5908	0.6687	–0.0722	0.063
H(2W)	2*i*	0.659	0.7504	–0.0387	0.063
H(3W)	2*i*	0.309	0.4492	0.5581	0.057
H(4W)	2*i*	0.3169	0.5808	0.5449	0.057
H(5W)	2*i*	0.2864	0.0049	0.1719	0.099
H(6W)	2*i*	0.1417	0.0402	0.2198	0.099
H(3)	2*i*	0.7893	0.7977	0.343	0.037
H(5)	2*i*	0.7788	1.1818	0.3676	0.036
H(7)	2*i*	0.4502	1.0899	0.2564	0.031
H(9A)	2*i*	0.88	0.7563	0.5555	0.079
H(9B)	2*i*	1.0511	0.8001	0.5177	0.079
H(9C)	2*i*	1.0169	0.7628	0.3991	0.079
H(10)	2*i*	0.1812	0.8621	0.0778	0.047
H(11)	2*i*	–0.0187	0.8082	0.0092	0.052
H(12)	2*i*	0.1773	0.4439	0.2077	0.044
H(13A)	2*i*	–0.1461	0.5574	0.077	0.053
H(13B)	2*i*	–0.0659	0.4157	0.1596	0.053

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*	0.43038(2)	0.59596(2)	0.24804(2)	0.0327(1)	0.0223(1)	0.0371(1)	0.00163(7)	–0.02166(8)	–0.01406(7)
O(1)	2*i*	0.4159(2)	0.8483(2)	0.2441(2)	0.047(1)	0.035(1)	0.079(1)	0.0048(8)	–0.041(1)	–0.030(1)
O(2)	2*i*	0.6106(2)	0.6996(2)	0.2845(2)	0.053(1)	0.0190(8)	0.049(1)	0.0031(7)	–0.0307(9)	–0.0161(7)
O(3)	2*i*	0.4252(2)	1.3530(2)	0.2394(2)	0.051(1)	0.0284(9)	0.056(1)	0.0121(8)	–0.0360(9)	–0.0208(8)
O(4)	2*i*	0.5866(2)	1.3861(2)	0.3307(2)	0.053(1)	0.0230(8)	0.052(1)	0.0017(8)	–0.0290(9)	–0.0210(8)
O(5)	2*i*	0.9347(2)	0.9528(2)	0.4045(3)	0.049(1)	0.038(1)	0.102(2)	0.0120(9)	–0.055(1)	–0.032(1)
O(6)	2*i*	0.6139(2)	0.6702(2)	–0.0006(2)	0.054(1)	0.043(1)	0.036(1)	–0.0110(9)	–0.0193(9)	–0.0144(8)
O(7)	2*i*	0.2791(2)	0.5342(2)	0.5139(2)	0.043(1)	0.038(1)	0.041(1)	0.0028(8)	–0.0244(8)	–0.0154(8)
O(8)	2*i*	0.2267(3)	0.0763(2)	0.1448(3)	0.056(1)	0.039(1)	0.101(2)	–0.006(1)	–0.045(1)	–0.006(1)
N(1)	2*i*	0.2241(2)	0.6441(2)	0.1664(2)	0.036(1)	0.031(1)	0.041(1)	0.0042(9)	–0.023(1)	–0.0165(9)
N(2)	2*i*	0.0458(2)	0.5943(2)	0.1014(2)	0.031(1)	0.046(1)	0.043(1)	0.0008(9)	–0.021(1)	–0.021(1)
C(1)	2*i*	0.5402(3)	0.8194(2)	0.2726(3)	0.040(1)	0.022(1)	0.032(1)	–0.004(1)	–0.016(1)	–0.012(1)
C(2)	2*i*	0.6085(3)	0.9280(2)	0.2960(3)	0.030(1)	0.023(1)	0.030(1)	–0.0008(9)	–0.014(1)	–0.0130(9)
C(3)	2*i*	0.7418(3)	0.8879(2)	0.3357(3)	0.033(1)	0.023(1)	0.043(1)	0.0047(9)	–0.018(1)	–0.018(1)
C(4)	2*i*	0.8037(3)	0.9829(3)	0.3645(3)	0.028(1)	0.030(1)	0.045(1)	0.003(1)	–0.021(1)	–0.018(1)
C(5)	2*i*	0.7358(3)	1.1182(2)	0.3495(3)	0.034(1)	0.026(1)	0.042(1)	–0.004(1)	–0.019(1)	–0.017(1)
C(6)	2*i*	0.6042(3)	1.1603(2)	0.3079(3)	0.029(1)	0.022(1)	0.030(1)	–0.0012(9)	–0.012(1)	–0.0122(9)
C(7)	2*i*	0.5396(3)	1.0635(2)	0.2825(3)	0.029(1)	0.023(1)	0.033(1)	0.0009(9)	–0.017(1)	–0.013(1)
C(8)	2*i*	0.5343(3)	1.3085(2)	0.2919(3)	0.034(1)	0.021(1)	0.028(1)	–0.0008(9)	–0.012(1)	–0.0101(9)
C(9)	2*i*	0.9738(4)	0.8061(3)	0.4749(4)	0.058(2)	0.046(2)	0.071(2)	0.015(1)	–0.047(2)	–0.020(2)
C(10)	2*i*	0.1555(3)	0.7705(3)	0.0959(3)	0.048(2)	0.032(1)	0.045(2)	0.001(1)	–0.024(1)	–0.016(1)
C(11)	2*i*	0.0453(3)	0.7416(3)	0.0569(3)	0.044(2)	0.046(2)	0.048(2)	0.011(1)	–0.029(1)	–0.017(1)
C(12)	2*i*	0.1540(3)	0.5415(3)	0.1667(3)	0.041(1)	0.034(1)	0.048(2)	–0.001(1)	–0.028(1)	–0.015(1)
C(13)	2*i*	–0.0449(3)	0.5095(3)	0.0763(3)	0.034(1)	0.062(2)	0.051(2)	–0.009(1)	–0.020(1)	–0.026(1)

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