Crystal structure of *catena*-triaqua(5-methoxyisophthalate)-cadmium(II) — water (1:2), $[Cd(C_9H_6O_5)(H_2O)_3] \cdot 2H_2O$

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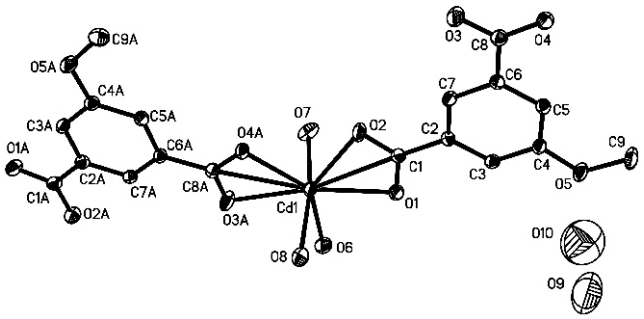

Abstract

$C_9H_{16}CdO_{10}$, monoclinic, *C*12/*c*1 (no. 15), a = 16.133(2) Å, b = 17.828(2) Å, c = 10.249(1) Å, β = 116.650(2)°, V = 2634.6 Å^3, Z = 8, $R_{gt}(F)$ = 0.033, $wR_{ref}(F^2)$ = 0.096, T = 296 K.

Source of material

The title compound was prepared under hydrothermal conditions. A mixture of 5-methoxyisophthalate (0.1 mmol), $Cd(ClO_4)_2$ (0.1 mmol), NaOH (0.1mmol) and H_2O (15 mL) was placed in a Teflon-lined stainless-steel vessel, heated to 170 °C for 4 days, and then cooled to room temperature for 24 h. Colorless block-shaped crystals of the title complex were obtained.

Discussion

The design and preparation of metal-organic frameworks (MOFs) has become an attractive research field. The motivation comes not only from their application as functional materials but is also due to the intriguing structural architectures [1-4]. In principle, the most effective approach for the construction of MOFs is to rationally modify the building blocks and to control the assembled motifs for required products via selecting different organic ligands [5,6]. 5-methoxyisophthalate (CH_3O-H_2ip) may serve as a suitable building block to construct novel coordination polymers due to the existence of a noncoordinating CH_3O group on the aromatic backbone, which will have a profound impact on the electron density of such a ligand and therefore different physical and chemical properties [7-9].

The asymmetric unit of the title crystal structure consists of a Cd^{2+} ion, a CH_3O-ip ligand, three coordinated water molecules and two free water molecules. The Cd^{2+} ion is chelated by four oxygen atoms from carboxylate of CH_3O-ip ligand forming two chelating rings, and the oxygen atoms from three coordinated water molecules complete the seven-fold coordination at the metal center. Thus, the coordination geometry about Cd^{2+} ion can be described as a distorted pentagonal bipyramid. Four chelating carboxylate oxygens and an oxygen from water complete the equatorial plane, while the other two oxygens from water form the pyramidal apices with bond angles ∠O7–Cd1–O8 = 170.7(1)°. The Cd—O bond lengths are in the range of 2.275(3) - 2.397(3) Å. The CH_3O-ip ligand takes the bidentate-chelating coordination mode to bridge the neighbouring Cd^{2+} ions and yield a chain. These chains are assembled by hydrogen bonds between coordinated water molecules and free water molecules to afford a three-dimensional supramolecular structure. The bond lengths and angles of these hydrogen bonding parameters are in the range of 1.95(2) - 3.03(1) Å and 120.3 - 179.3°, respectively. It is obvious that the water and ethanol molecules make a crucial contribution to the stability of the host.

Table 1. Data collection and handling.

Crystal:	colorless block, size 0.13 × 0.19 × 0.27 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	17.06 cm^{-1}
Diffractometer, scan mode:	Bruker SMART CCD, φ/ω
$2\theta_{max}$:	51°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	9778, 2454
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 1944
$N(param)_{refined}$:	182
Programs:	SHELXS-97, SHELXL-97, SHELXTL [10]

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

Atom	Site	x	y	z	U_{iso}
H(1W)	8*f*	0.1409	1.1080	1.0651	0.088
H(2W)	8*f*	0.1077	1.1536	0.9547	0.088
H(3W)	8*f*	0.0114	1.0632	0.6044	0.104
H(4W)	8*f*	0.0786	1.0417	0.5673	0.104
H(5W)	8*f*	0.3247	1.0880	1.1087	0.093
H(6W)	8*f*	0.3039	1.0107	1.1404	0.093
H(7W)	8*f*	0.3105	0.2438	0.1391	0.376
H(8W)	8*f*	0.3235	0.1710	0.1715	0.376
H(9W)	8*f*	0.3857	0.2500	0.1153	0.555
H(10W)	8*f*	0.4859	0.2805	0.2245	0.555
H(3)	8*f*	0.0667	0.8088	0.9778	0.047
H(5)	8*f*	0.1145	0.6007	0.8783	0.045
H(7)	8*f*	0.2055	0.7793	0.7406	0.045
H(9A)	8*f*	–0.0048	0.5758	0.9368	0.095
H(9B)	8*f*	–0.0017	0.5876	1.0904	0.095
H(9C)	8*f*	0.0905	0.5749	1.0777	0.095

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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)	8*f*	0.19119(3)	1.03929(2)	0.86135(4)	0.0549(3)	0.0316(2)	0.0448(2)	–0.0030(2)	0.0321(2)	–0.0006(2)
O(1)	8*f*	0.1277(3)	0.9337(2)	0.9264(4)	0.088(3)	0.033(2)	0.057(2)	–0.006(2)	0.047(2)	–0.006(2)
O(2)	8*f*	0.1907(3)	0.9143(2)	0.7795(4)	0.081(3)	0.036(2)	0.071(3)	–0.005(2)	0.053(2)	0.006(2)
O(3)	8*f*	0.2558(3)	0.6604(2)	0.6709(5)	0.093(3)	0.046(2)	0.088(3)	–0.001(2)	0.074(3)	–0.005(2)
O(4)	8*f*	0.2046(3)	0.5621(2)	0.7391(4)	0.071(2)	0.032(2)	0.054(2)	0.009(2)	0.040(2)	0.003(2)
O(5)	8*f*	0.0384(3)	0.6758(2)	1.0191(4)	0.073(3)	0.047(2)	0.066(2)	–0.003(2)	0.053(2)	0.006(2)
O(6)	8*f*	0.1144(3)	1.1068(2)	0.9723(4)	0.077(3)	0.055(2)	0.062(2)	–0.002(2)	0.046(2)	–0.009(2)
O(7)	8*f*	0.0698(3)	1.0585(3)	0.6377(4)	0.060(3)	0.106(3)	0.049(2)	0.011(2)	0.031(2)	0.013(2)
O(8)	8*f*	0.3176(3)	1.0414(2)	1.0896(4)	0.074(3)	0.057(2)	0.053(2)	–0.007(2)	0.027(2)	0.011(2)
O(9)	8*f*	0.3371(9)	0.2052(8)	0.127(1)	0.269(9)	0.246(9)	0.236(9)	0.047(7)	0.111(7)	–0.068(7)
O(10)	8*f*	0.443(1)	0.260(1)	0.149(2)	0.39(1)	0.36(1)	0.37(1)	0.033(9)	0.18(1)	0.023(9)
C(1)	8*f*	0.1519(4)	0.8900(3)	0.8541(5)	0.057(3)	0.034(3)	0.036(3)	–0.003(2)	0.021(2)	–0.001(2)
C(2)	8*f*	0.1375(3)	0.8071(3)	0.8587(5)	0.040(3)	0.031(2)	0.035(2)	–0.002(2)	0.017(2)	–0.000(2)
C(3)	8*f*	0.0919(3)	0.7771(3)	0.9329(5)	0.050(3)	0.035(2)	0.039(3)	0.002(2)	0.027(2)	–0.002(2)
C(4)	8*f*	0.0833(3)	0.7001(3)	0.9409(5)	0.042(3)	0.038(3)	0.040(3)	–0.002(2)	0.024(2)	0.003(2)
C(5)	8*f*	0.1205(3)	0.6524(3)	0.8736(5)	0.045(3)	0.031(2)	0.041(3)	0.001(2)	0.022(2)	0.001(2)
C(6)	8*f*	0.1670(3)	0.6824(2)	0.7988(5)	0.040(3)	0.032(2)	0.037(2)	0.001(2)	0.020(2)	–0.002(2)
C(7)	8*f*	0.1750(3)	0.7593(3)	0.7911(5)	0.042(3)	0.038(3)	0.037(2)	0.001(2)	0.023(2)	0.005(2)
C(8)	8*f*	0.2113(3)	0.6324(3)	0.7322(5)	0.046(3)	0.039(3)	0.042(3)	0.003(2)	0.024(2)	0.000(2)
C(9)	8*f*	0.0299(5)	0.5972(3)	1.0321(7)	0.081(4)	0.046(3)	0.080(4)	–0.006(3)	0.052(4)	0.017(3)

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