Crystal structure of bis[triaqua-(5-*tert*-butylisophthalato-*O,O'*)-cadmium(II)] monohydrate, $[\text{Cd}(\text{H}_2\text{O})_3(\text{C}_{12}\text{H}_{12}\text{O}_4)]_2 \cdot \text{H}_2\text{O}$

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Abstract

$\text{C}_{24}\text{H}_{38}\text{Cd}_2\text{O}_{15}$, orthorhombic, *Pccn* (no. 56), $a = 16.429(2)$ Å, $b = 17.565(2)$ Å, $c = 10.503(1)$ Å, $V = 3030.8$ Å³, $Z = 4$, $R_g(F) = 0.024$, $wR_{\text{ref}}(F^2) = 0.065$, $T = 291$ K.

Source of material

A mixture of 5-*tert*-butylisophthalic acid (H_2tbp , 0.1 mmol, 24.6 mg), 1,2-bis(4-pyridyl)ethane (bpa, 0.1 mmol, 18.4 mg), $\text{Cd}(\text{OAc})_2 \cdot 2\text{H}_2\text{O}$ (26.5 mg, 0.1 mmol), KOH (0.1 mmol, 5.6 mg) and H_2O (15 ml) was placed in a Teflon-lined stainless steel vessel, heated to 160 °C for 3 days, and then cooled to room temperature over 24 h. Colorless block crystals of the title compound were obtained.

Experimental details

O8 was disordered on a two-fold axis and its site occupancy was set to 0.5.

Discussion

Crystal engineering of coordination polymers is a very active research field, the potentiality of these compounds as functional materials as well as their flexibility in aspects such as composition and topology being very appealing [1–8]. It is well known that organic ligands play crucial roles in the design and construction of desirable frameworks. Multicarboxylate acid 1,3-benzenedicarboxylates with variously oriented carboxylate groups, whose coordination modes are very abundant, have widely been utilized to construct coordination polymers [9–11]. In this contribution, we have chosen the structurally similar 5-*tert*-butylisophthalic acid as a bridging ligand to construct new coordination polymers.

The molecular structure unit of the title compound consists of one Cd(II) ion, one tbip, three coordinating water molecules and one lattice water molecule. Each Cd(II) center is in a distorted pentagonal bipyramidal coordination. Two chelating carboxylate groups from different tbip ligands and one water molecule com-

prise the equatorial basal plane. The other two water molecules occupy the apical sites. The Cd—O bond distances are in the range of 2.307(3)–2.497(3) Å. The Cd(II) centers are connected through tbip anions via its chelating bis-bidentate mode to yield a 1D chain along the [100]. It is interesting to note that the 1D chains are then linked by intermolecular hydrogen-bonding to result in a 3D dimensional network structure. These hydrogen bonds involve coordinated oxygen atoms of tbip ligands, coordinated water molecules and free water molecule. The intermolecular hydrogen bonds play an important role in creating such a high-dimensional structure.

Table 1. Data collection and handling.

Crystal:	colorless block, size $0.25 \times 0.25 \times 0.37$ mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ :	14.71 cm ^{−1}
Diffraction, scan mode:	Bruker SMART CCD, φ/ω
$2\theta_{\text{max}}$:	51°
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$:	21534, 2822
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2\sigma(I_{\text{obs}})$, 2517
$N(\text{param})_{\text{refined}}$:	193
Programs:	SHELXS-97 [12], SHELXL-97 [13], SHELXTL [14]

Table 2. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	Occ.	x	y	z	U_{iso}
H(1W)	8e		1.2280	0.2777	0.2335	0.082
H(2W)	8e		1.1740	0.3181	0.1639	0.082
H(3W)	8e		0.9924	0.2599	0.5709	0.098
H(4W)	8e		0.9698	0.3367	0.5103	0.098
H(5W)	8e		1.1484	0.3372	0.5951	0.141
H(6W)	8e		1.1267	0.4063	0.5232	0.141
H(2)	8e		0.9632	0.5341	0.2227	0.035
H(4)	8e		0.8163	0.5547	−0.0812	0.036
H(6)	8e		0.9024	0.3498	0.0175	0.035
H(10A)	8e		0.9086	0.3725	−0.2544	0.121
H(10B)	8e		0.8303	0.3301	−0.3020	0.121
H(10C)	8e		0.8692	0.3084	−0.1707	0.121
H(11A)	8e		0.7016	0.3435	−0.1787	0.112
H(11B)	8e		0.6927	0.4077	−0.0758	0.112
H(11C)	8e		0.7436	0.3344	−0.0455	0.112
H(12A)	8e		0.8266	0.4948	−0.2910	0.110
H(12B)	8e		0.7420	0.5031	−0.2232	0.110
H(12C)	8e		0.7536	0.4426	−0.3315	0.110
H(7W)	8e	0.50	0.9711	0.4608	0.4417	0.258
H(8W)	8e	0.50	0.9465	0.5295	0.4874	0.258

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Table 3. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	Occ.	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
Cd(1)	8e		1.08588(1)	0.29593(1)	0.37286(2)	0.0414(1)	0.0263(1)	0.0339(1)	0.00446(8)	−0.00673(9)	0.00323(8)
O(1)	8e		1.0288(1)	0.4152(1)	0.3108(2)	0.057(1)	0.036(1)	0.039(1)	0.004(1)	−0.022(1)	−0.0007(9)
O(2)	8e		0.9978(2)	0.3151(1)	0.1980(2)	0.066(2)	0.032(1)	0.040(1)	0.016(1)	−0.016(1)	−0.0033(9)
O(3)	8e		0.9159(2)	0.6688(1)	0.1966(3)	0.085(2)	0.030(1)	0.086(2)	0.000(1)	−0.036(2)	−0.013(1)
O(4)	8e		0.8509(2)	0.6847(1)	0.0172(2)	0.104(2)	0.030(1)	0.047(1)	0.015(1)	0.000(1)	0.006(1)
O(5)	8e		1.1960(1)	0.3157(1)	0.2335(2)	0.045(1)	0.054(1)	0.065(2)	0.006(1)	−0.003(1)	0.017(1)
O(6)	8e		0.9783(2)	0.2890(1)	0.5135(3)	0.083(2)	0.055(2)	0.058(2)	0.016(1)	0.020(1)	0.020(1)
O(7)	8e		1.1526(2)	0.3647(2)	0.5323(3)	0.122(3)	0.061(2)	0.098(2)	−0.023(2)	−0.070(2)	0.008(2)
C(1)	8e		0.9404(2)	0.4344(2)	0.1331(2)	0.028(1)	0.029(1)	0.025(1)	0.001(1)	0.000(1)	0.001(1)
C(2)	8e		0.9353(2)	0.5122(2)	0.1549(3)	0.030(1)	0.029(1)	0.030(1)	−0.002(1)	−0.001(1)	−0.003(1)
C(3)	8e		0.8881(2)	0.5574(2)	0.0745(3)	0.031(1)	0.026(1)	0.033(1)	−0.001(1)	0.003(1)	0.002(1)
C(4)	8e		0.8473(2)	0.5241(2)	−0.0275(3)	0.030(1)	0.030(1)	0.031(1)	0.002(1)	−0.002(1)	0.006(1)
C(5)	8e		0.8515(2)	0.4459(2)	−0.0516(2)	0.026(1)	0.032(1)	0.027(1)	0.001(1)	0.000(1)	−0.000(1)
C(6)	8e		0.8987(2)	0.4020(2)	0.0309(2)	0.032(1)	0.024(1)	0.030(1)	0.002(1)	−0.000(1)	−0.002(1)
C(7)	8e		0.9918(2)	0.3855(2)	0.2188(2)	0.034(1)	0.029(1)	0.026(1)	0.004(1)	0.001(1)	0.002(1)
C(8)	8e		0.8843(2)	0.6417(2)	0.0971(3)	0.040(2)	0.026(1)	0.049(2)	0.001(1)	0.007(1)	0.001(1)
C(9)	8e		0.8051(2)	0.4089(2)	−0.1625(3)	0.038(2)	0.040(2)	0.033(1)	0.001(1)	−0.008(1)	−0.005(1)
C(10)	8e		0.8583(3)	0.3495(3)	−0.2285(4)	0.076(3)	0.103(3)	0.062(2)	0.026(2)	−0.024(2)	−0.049(2)
C(11)	8e		0.7286(3)	0.3700(3)	−0.1108(4)	0.069(3)	0.090(3)	0.064(2)	−0.037(2)	−0.005(2)	−0.014(2)
C(12)	8e		0.7794(3)	0.4678(2)	−0.2612(4)	0.096(3)	0.070(2)	0.054(2)	−0.011(2)	−0.043(2)	0.005(2)
O(8)	8e	0.50	0.9437(7)	0.4819(7)	0.501(1)	0.190(8)	0.191(8)	0.135(6)	−0.035(7)	0.037(6)	−0.092(6)

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