Crystal structure of poly[[μ_2-1,2-benzenedicarboxylato-κ^4*O,O′:O″,O‴*]-[μ_2-2-((1*H*-imidazol-1-yl)-6-methyl)-1*H*-benzoimidazole-κ^2*N:N′*]-cadmium(II)], $C_{20}H_{15}CdN_4O_4$

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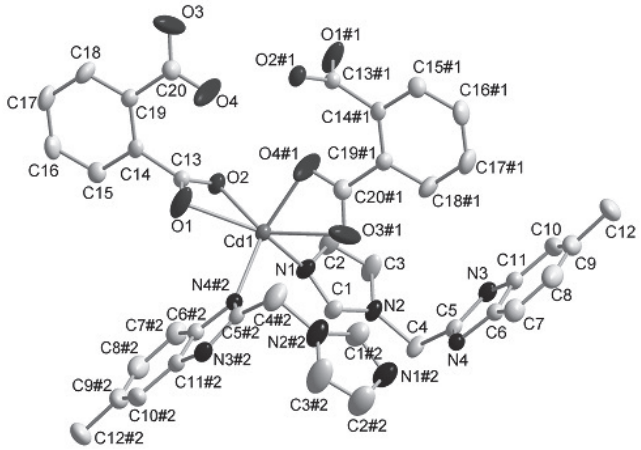

Abstract

$C_{20}H_{15}CdN_4O_4$, triclinic, $P\bar{1}$ (no. 2), a = 9.927(2) Å, b = 9.970(2) Å, c = 11.046(2) Å, α = 80.94(3)°, β = 75.54(3)°, γ = 68.27(3)°, V = 980.8(3) Å^3, Z = 2, $R_{gt}(F)$ = 0.0281, $wR_{ref}(F^2)$ = 0.0703, T = 293 K.

Table 1. Data collection and handling.

Crystal:	light yellow blocks, size 0.20 mm×0.18 mm×0.15 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	11.48 cm^{-1}
Diffractometer, scan mode:	Rigaku Saturn724, ω
$2\theta_{max}$:	52°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	9156, 3831
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 3639
$N(param)_{refined}$:	272
Programs:	SHELX [6], DIAMOND [7]

Source of material

Single crystals of $C_{20}H_{15}CdN_4O_4$ were prepared by a solvothermal reaction. 2-((1*H*-imidazol-1-yl)-6-methyl)-1*H*-benzoimidazole (*immb*, 0.05 mmol), $CdSO_4 \cdot 8/3H_2O$ (0.05 mmol), sodium phthalate (0.05 mmol), methanol (2 mL) and water (4 mL) was sealed in a Teflon-lined autoclave and heated at 393K for 72 h. Then the mixture was cooled to room temperature. The light yellow block-like crystals suitable for X-ray analysis were obtained.

Experimental details

The hydrogen atoms were positioned geometrically and refined using a riding model, with d(N–H) = 0.86 Å and U_{iso}(H) = 1.2 U_{eq}(N), d(C–H) = 0.93-0.97 Å and U_{iso}(H) = 1.2-1.5 U_{eq}(C).

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Discussion

In recent decades, the rational design and synthesis of metal-organic frameworks (MOFs) have attracted significant interest due to their intriguing structures and potential application in many fields, such as nonlinear optics, magnetism, catalytisis, adsorption, ion exchange, luminescence [1–3]. In the formation of complexes, the structure of the target product is influenced by several factors. And it's well known that the selection of appropriate organic ligands is foremost to consider [4]. Among all the potential organic ligands, multicarboxylates and N-heterocyclic compounds have turned to be nice building blocks due to their excellent traits. N-heterocyclic compound, such as N-donor with imidazole and benzimidazole groups, can coordinate with metal ions in versatile ways. Moreover, multicarboxylates as O-donor are able to coordinate to metal ions via monodentate, bidentate, or chelating mode. Based on the features mentioned above, we have successfully synthesized the title complex $[Cd(pa)(immb)]_n$ (pa^{2-} = phthalate, *immb* = 2-((1*H*-imidazol-1-yl)-6-methyl)-1*H*-benzoimidazole) bearing N and O-donors. The asymmetric unit contains one Cd(II) cation, one *immb* molecule and one phthalate anion. The Cd(II) ion is in a six coordination environment, and is connected with two nitrogen atoms (N1 and $N4^{\#2}$) from two *immb* ligands, four oxygen atoms (O1, O2, $O3^{\#1}$, $O4^{\#1}$) from two carboxylates with chelating mode (symmetry codes: #1: $-x$+1, $-y$+2, $-z$+1; #2: $-x$+2, $-y$+1, $-z$+1). Most of the bond angles around the central Cd(II) ion deviate dramatically from the ideal angles of 90° or 180° expected for an octahedral geometry. The Cd–N and Cd–O distances are similar to those in reported Cd(II) complexes [5]. The Cd(II) ions are linked by phthalates and *immb* ligands alternately leading to 1D chains. Adjacent chains are connected by N–H···O hydrogen bonds between benzimidazole ring and carboxylate forming the 2D layer structure.

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

Atom	Site	Occ.	x	y	z	U_{iso}
H(3A)	2*i*		0.7439	0.1497	0.5251	0.056
H(1A)	2*i*		0.9556	0.4650	0.6424	0.054
H(2A)	2*i*		0.5257	0.5931	0.7585	0.072
H(3B)	2*i*		0.6124	0.3333	0.7423	0.076
H(4A)	2*i*		0.8853	0.1293	0.6998	0.057
H(4B)	2*i*		1.0196	0.1856	0.6602	0.057
H(7A)	2*i*		1.1378	0.2305	0.1604	0.070
H(10A)	2*i*		0.6942	0.1341	0.2844	0.082
H(12A)	2*i*	0.550(7)	0.6960	0.1477	0.0539	0.111
H(12B)	2*i*	0.550(7)	0.8576	0.0945	–0.0270	0.111
H(12C)	2*i*	0.550(7)	0.7675	0.2607	–0.0204	0.111
H(12D)	2*i*	0.450(7)	1.1010	0.2254	–0.0621	0.123
H(12E)	2*i*	0.450(7)	0.9313	0.2810	–0.0626	0.123
H(12F)	2*i*	0.450(7)	1.0219	0.1145	–0.059	0.123

Table 2. continued.

Atom	Site	Occ.	x	y	z	U_{iso}
H(15A)	2*i*		0.5437	1.0988	0.9476	0.054
H(16A)	2*i*		0.4025	1.3042	1.0528	0.066

Table 2. continued.

Atom	Site	Occ.	x	y	z	U_{iso}
H(17A)	2*i*		0.2278	1.4879	0.9649	0.078
H(18A)	2*i*		0.1793	1.462	0.7768	0.073

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

Atom	Site	Occ.	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cd(1)	2*i*		0.7331	0.7963	0.5973	0.0377(1)	0.0318(1)	0.0461(1)	–0.00883(8)	–0.00873(8)	–0.00790(8)
N(1)	2*i*		0.7417(3)	0.5808(2)	0.6979(2)	0.042(1)	0.032(1)	0.065(2)	–0.010(1)	–0.003(1)	–0.006(1)
N(2)	2*i*		0.8216(3)	0.3467(2)	0.6854(2)	0.052(1)	0.030(1)	0.040(1)	–0.013(1)	0.004(1)	–0.0053(9)
N(3)	2*i*		0.8197(3)	0.1661(2)	0.4767(2)	0.039(1)	0.040(1)	0.060(2)	–0.017(1)	0.001(1)	–0.009(1)
N(4)	2*i*		1.0294(2)	0.2117(2)	0.4184(2)	0.038(1)	0.035(1)	0.042(1)	–0.0117(9)	–0.0067(9)	–0.0055(9)
O(1)	2*i*		0.6650(3)	1.0287(3)	0.6593(3)	0.062(2)	0.052(1)	0.115(2)	–0.032(1)	0.045(1)	–0.037(1)
O(2)	2*i*		0.5200(2)	0.9110(2)	0.7533(2)	0.050(1)	0.034(1)	0.055(1)	–0.0174(9)	–0.0014(9)	–0.0075(8)
O(3)	2*i*		0.1945(3)	1.3339(5)	0.5927(3)	0.064(2)	0.199(4)	0.100(2)	0.028(2)	–0.046(2)	–0.077(3)
O(4)	2*i*		0.3860(5)	1.1553(3)	0.5611(3)	0.212(4)	0.085(2)	0.079(2)	0.068(2)	–0.093(2)	–0.048(2)
C(1)	2*i*		0.8592(3)	0.4649(3)	0.6697(3)	0.041(1)	0.033(1)	0.059(2)	–0.012(1)	–0.006(1)	–0.004(1)
C(2)	2*i*		0.6238(4)	0.5343(3)	0.7329(3)	0.044(2)	0.048(2)	0.078(2)	–0.017(1)	0.012(2)	–0.017(2)
C(3)	2*i*		0.6708(4)	0.3912(4)	0.7247(4)	0.057(2)	0.048(2)	0.079(2)	–0.030(2)	0.023(2)	–0.019(2)
C(4)	2*i*		0.9211(4)	0.2023(3)	0.6480(3)	0.065(2)	0.027(1)	0.041(1)	–0.010(1)	–0.004(1)	–0.000(1)
C(5)	2*i*		0.9277(3)	0.1902(3)	0.5135(2)	0.040(1)	0.027(1)	0.042(1)	–0.008(1)	–0.002(1)	–0.005(1)
C(6)	2*i*		0.9835(3)	0.2004(3)	0.3121(2)	0.044(1)	0.034(1)	0.042(1)	–0.010(1)	–0.011(1)	–0.004(1)
C(7)	2*i*		1.0488(4)	0.2129(4)	0.1856(3)	0.068(2)	0.058(2)	0.045(2)	–0.021(2)	–0.005(1)	–0.005(1)
C(8)	2*i*		0.9777(5)	0.1984(4)	0.0991(3)	0.093(3)	0.066(2)	0.052(2)	–0.009(2)	–0.026(2)	–0.012(2)
C(9)	2*i*		0.8464(5)	0.1695(4)	0.1360(4)	0.086(3)	0.064(2)	0.080(3)	0.001(2)	–0.047(2)	–0.026(2)
C(10)	2*i*		0.7815(4)	0.1548(4)	0.2600(4)	0.055(2)	0.054(2)	0.103(3)	–0.009(2)	–0.036(2)	–0.024(2)
C(11)	2*i*		0.8522(3)	0.1722(3)	0.3486(3)	0.043(2)	0.037(1)	0.060(2)	–0.009(1)	–0.014(1)	–0.011(1)
C(12)	2*i*	0.550(7)	0.7866(8)	0.1680(8)	0.0259(7)	0.075(5)	0.086(5)	0.076(5)	–0.027(4)	–0.037(4)	–0.018(4)
C(12')	2*i*	0.450(7)	1.011(1)	0.205(1)	–0.0313(8)	0.102(7)	0.088(7)	0.056(5)	–0.033(6)	–0.018(5)	–0.005(4)
C(13)	2*i*		0.5476(3)	1.0232(3)	0.7313(2)	0.035(1)	0.034(1)	0.039(1)	–0.012(1)	–0.006(1)	–0.004(1)
C(14)	2*i*		0.4477(3)	1.1564(3)	0.7974(2)	0.038(1)	0.033(1)	0.036(1)	–0.018(1)	–0.000(1)	–0.005(1)
C(15)	2*i*		0.4709(3)	1.1720(3)	0.9125(3)	0.055(2)	0.044(2)	0.039(1)	–0.024(1)	–0.008(1)	0.001(1)
C(16)	2*i*		0.3870(4)	1.2952(3)	0.9752(3)	0.076(2)	0.061(2)	0.034(1)	–0.031(2)	–0.004(1)	–0.015(1)
C(17)	2*i*		0.2816(4)	1.4036(4)	0.9237(3)	0.078(2)	0.050(2)	0.057(2)	–0.011(2)	–0.001(2)	–0.027(2)
C(18)	2*i*		0.2539(4)	1.3891(3)	0.8101(3)	0.066(2)	0.042(2)	0.058(2)	0.004(2)	–0.008(2)	–0.018(1)
C(19)	2*i*		0.3376(3)	1.2659(3)	0.7466(2)	0.040(1)	0.041(1)	0.042(1)	–0.009(1)	–0.006(1)	–0.011(1)
C(20)	2*i*		0.3047(4)	1.2512(3)	0.6251(3)	0.058(2)	0.050(2)	0.045(2)	–0.016(2)	–0.013(1)	–0.008(1)

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