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Crystal structure of poly[(μ_4 -5-tert-butylisophthalato- $\kappa^4 O:O':O'':O'''$)-(1,3-dimethyl-2-imidazolidinone- κO)zinc(II)] $C_{17}H_{22}N_2O_5Zn$

Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	0.32 × 0.15 × 0.11 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	1.30 mm ⁻¹
Diffractometer, scan mode:	Bruker SMART, φ and ω -scans
$\theta_{\max}$, completeness:	25.5°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	3592, 3592, 0.0466
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 2894
$N(\text{param})_{\text{refined}}$:	245
Programs:	Bruker programs [1], SHELX [2, 3]

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Abstract

$C_{17}H_{22}N_2O_5Zn$, monoclinic, $P2_1/c$ (no. 14), $a = 12.577(3)$ Å, $b = 10.932(2)$ Å, $c = 14.726(3)$ Å, $\beta = 107.145(2)^\circ$, $V = 1934.7(7)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0329$, $wR_{\text{ref}}(F^2) = 0.0808$, $T = 296(2)$ K.

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The crystal structure is shown in the figure. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

In a typical experiment 5-tert-butylisophthalic acid (0.02 g, 0.1 mmol), and zinc acetate (0.02 g, 0.1 mmol) were added to 1,3-dimethyl-2-imidazolidinone (10 mL) in a teflon-lined stainless steel reactor. The mixture was heated at 373 K for 3 days, and then slowly cooled down to room temperature. Colorless block crystals of the title compound were obtained.

Experimental details

The hydrogen atoms were placed at calculated positions with the SHELX program (AFIX options: 43 and 147).

Discussion

In the past few decades, the preparation and study of coordination polymers has attracted people's continuous attention and effort, because of their potential applications in many areas, for example, magnetism, adsorption, catalysis, and luminescence, as well as their charming architectures and topologies [4–12]. Generally, the construction of intriguing structural topologies depends upon many factors, mainly including the medium, the template, pH value, temperature, the inbeing of the metal ions, the nature of organic ligands, and other factors [13, 14]. Traditional synthetic methods of coordination polymers are hydrothermal and solvothermal methods. In addition, the urothermal synthesis has been successfully introduced to the preparation of coordination polymers [15–19]. In this synthetic method, urea and its derivatives act as the solvents, potential templates, or end group ligands in the formation of coordination polymers [20]. To continue the study about the influence of urea and its derivatives on synthesizing Zn(II) CPs based on bridging carboxylate ligands, we select DMI as solvent and 5-tert-butylisophthalate as ligand.

The asymmetric unit possesses one crystallographically unique Zn(II) ions, one 5-tert-butylisophthalate and one 1,3-dimethyl-2-imidazolidinone ligand. Each Zn1(II) ion is five-coordinated by four oxygen atoms from four different tbip²⁻

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Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
Zn1	0.08568(2)	0.40200(3)	0.02282(3)	0.02324(11)
O1	0.1665(3)	0.5040(3)	0.1369(2)	0.0460(9)
O2	0.0312(2)	0.6453(3)	0.1019(2)	0.0440(7)
O3	0.0278(2)	0.8554(3)	0.4080(2)	0.0452(8)
O4	0.1619(3)	0.9957(3)	0.4460(2)	0.0454(8)
O5	0.17793(15)	0.2530(2)	0.0435(5)	0.0424(5)
N1	0.1615(4)	0.0688(4)	0.1119(3)	0.0656(13)
N2	0.1648(4)	0.0722(4)	−0.0347(3)	0.0666(13)
C1	0.1852(3)	0.6793(3)	0.2346(2)	0.0283(8)
C2	0.1271(2)	0.7510(3)	0.2797(5)	0.0279(6)
H2	0.0497	0.7497	0.2600	0.033 [*]
C3	0.1836(3)	0.8260(3)	0.3552(3)	0.0281(8)
C4	0.2985(3)	0.8323(4)	0.3809(3)	0.0370(10)
H4	0.3356	0.8868	0.4282	0.044 [*]
C5	0.3594(2)	0.7592(3)	0.3375(7)	0.0422(8)
C6	0.3007(3)	0.6817(4)	0.2645(3)	0.0375(10)
H6	0.3399	0.6305	0.2353	0.045 [*]
C7	0.1226(3)	0.6031(4)	0.1511(3)	0.0314(9)
C8	0.1190(3)	0.8988(4)	0.4074(3)	0.0307(8)
C9	0.4874(3)	0.7642(4)	0.3677(6)	0.0705(13)
C10 ^a	0.5306(8)	0.6354(7)	0.4032(9)	0.099(3)
H10A ^a	0.5041	0.5774	0.3526	0.149 [*]
H10B ^a	0.5040	0.6131	0.4557	0.149 [*]
H10C ^a	0.6105	0.6356	0.4233	0.149 [*]
C10 ^b	0.5402(11)	0.6754(11)	0.3176(10)	0.099(3)
H10D ^b	0.6186	0.6916	0.3335	0.149 [*]
H10E ^b	0.5074	0.6835	0.2502	0.149 [*]
H10F ^b	0.5287	0.5937	0.3367	0.149 [*]
C11 ^a	0.5263(12)	0.7905(12)	0.2799(8)	0.107(3)
H11A ^a	0.6058	0.7984	0.2990	0.160 [*]
H11B ^a	0.4930	0.8651	0.2505	0.160 [*]
H11C ^a	0.5043	0.7243	0.2355	0.160 [*]
C11 ^b	0.5187(11)	0.8964(8)	0.3496(11)	0.107(3)
H11D ^b	0.5957	0.9106	0.3830	0.160 [*]
H11E ^b	0.4733	0.9526	0.3719	0.160 [*]
H11F ^b	0.5067	0.9083	0.2828	0.160 [*]
C12 ^a	0.5397(9)	0.8569(9)	0.4434(8)	0.102(3)
H12A ^a	0.6190	0.8553	0.4560	0.153 [*]
H12B ^a	0.5211	0.8374	0.5004	0.153 [*]
H12C ^a	0.5122	0.9370	0.4219	0.153 [*]
C12 ^b	0.5297(15)	0.7451(12)	0.4758(8)	0.102(3)
H12D ^b	0.5118	0.6637	0.4909	0.153 [*]
H12E ^b	0.4948	0.8033	0.5067	0.153 [*]
H12F ^b	0.6089	0.7564	0.4973	0.153 [*]
C13	0.1674(2)	0.1398(3)	0.0400(4)	0.0355(7)
C14	0.1595(7)	−0.0583(5)	0.0877(6)	0.091(2)
H14A	0.0929	−0.0978	0.0939	0.109 [*]
H14B	0.2243	−0.1005	0.1277	0.109 [*]
C15	0.1604(7)	−0.0563(5)	−0.0144(6)	0.093(2)
H15A	0.2249	−0.0989	−0.0219	0.111 [*]
H15B	0.0936	−0.0936	−0.0557	0.111 [*]
C16	0.1677(6)	0.1145(6)	0.2052(4)	0.091(2)
H16A	0.1707	0.2022	0.2050	0.136 [*]

Table 2 (continued)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
H16B	0.2333	0.0830	0.2506	0.136 [*]
H16C	0.1031	0.0886	0.2222	0.136 [*]
C17	0.1715(6)	0.1177(6)	−0.1239(4)	0.099(2)
H17A	0.1715	0.2055	−0.1228	0.148 [*]
H17B	0.1086	0.0891	−0.1739	0.148 [*]
H17C	0.2388	0.0890	−0.1347	0.148 [*]

Occupancies: ^a = 0.544(8), ^b = 0.456(8).

ligands and one oxygen atom from one DMI molecule to form a irregular polyhedra geometry. The bond angles around Zn1 vary from 72.47(8) to 159.13(13)°, and the Zn1–O bond distances range from 2.022(3) to 2.052(3) Å. Each thbp^{2−} connects four Zn(II) lions and neighbouring Zn(II) ions are bridged by thbp^{2−} to form a 2D layer structure.

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