Crystal structure of catena-poly[aqua-μ-1,4-benzenedicarboxylato-κ^2*O*:*O*'-3,5-dimethyl-4-phenyl-1,2,4-triazole-κ*N*-zinc(II)] monohydrate, $Zn(H_2O)(C_8H_4O_4)(C_{10}H_{11}N_3)\cdot H_2O$, $C_{18}H_{17}N_3O_6Zn$

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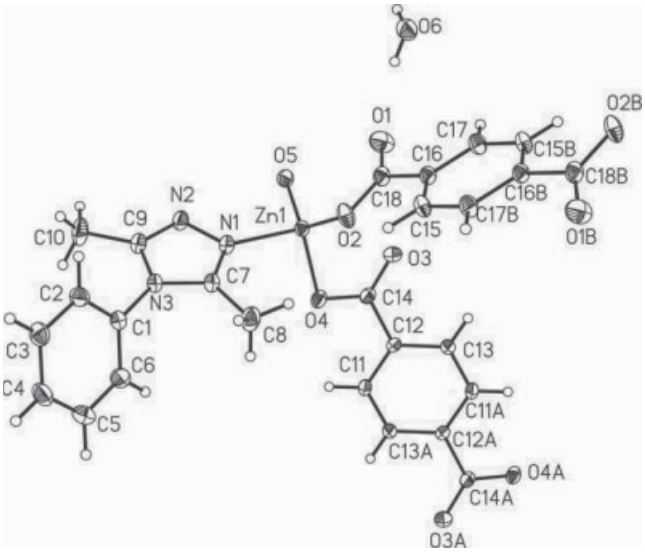

Abstract

$C_{18}H_{17}N_3O_6Zn$, triclinic, $P\bar{1}$ (no. 2), a = 10.0780(5) Å, b = 10.1678(5) Å, c = 10.3591(5) Å, α = 83.119(1)°, β = 81.178(2)°, γ = 64.753(1)°, V = 947.0 Å^3, Z = 2, $R_{gt}(F)$ = 0.0285, $wR_{ref}(F^2)$ = 0.1213, T = 296 K.

Table 1. Data collection and handling.

Crystal:	colourless blocks, size 0.18×0.21×0.25 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	13.37 cm^{-1}
Diffractometer, scan mode:	Bruker SMART APEXII CCD, φ and ω
$2\theta_{max}$:	55.3°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	11433, 4319
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 4041
$N(param)_{refined}$:	255
Programs:	SHELX [10]

Source of material

All reagents and solvents were used as obtained commercially without further purification. A mixture containing zinc acetate dihydrate (0.044 g, 0.2 mmol), 3,5-dimethyl-4-phenyl-1,2,4-triazole (*L*, 17.3 mg, 0.1 mmol), terephthalic acid (H_2pbda, 16.6 mg, 0.1 mmol), DMF (*N*:*N*'-dimethylformamide, 1 mL), 10 ml H_2O was sealed in a 16 ml Teflon-lined stainless steel container and heated at 453 K for 72 h. After cooling to room temperature within 12 h, colourless crystals of the title compound suitable for X-ray diffraction analysis were obtained in 48% yield. **Elemental analysis** calcd (%): C, 49.27; H, 4.36; N, 9.58%; found: C, 49.48; H, 4.29; N, 9.39%.

Experimental details

H atoms bonded to C atoms were placed geometrically and treated as riding, with C–H distances 0.93 Å and U_{iso}(H) = 1.2 U_{eq}(C) for the CH while U_{iso}(H) = 1.5 U_{eq}(C) for the CH_3 groups of *L* molecule. The H atoms of the water molecules were located from difference maps and refined with the O–H distances restrained to 0.82 Å and U_{iso}(H) = 1.2 U_{eq}(O).

Discussion

The rational design and construction of novel metal-organic frameworks (MOFs) are of current interest in the field of crystal engineering not only because of their promising applications in gas storage, separation, luminescence, heterogeneous catalysis and ion exchange, but also owing to their intriguing molecular architectures and topologies [1-4]. Generally, the multidentate organic ligands containing coordination sites of N donors such as triazole have favourable coordinate abilities and are widely utilized as building blocks in the construction of MOFs. The derivatives of 1,2,4-triazole can adopt the monodentate terminal or didentate *N*,*N*'-bridging coordination mode, which makes them easily link two adjacent metal ions to yield dinuclear, linear, trinuclear, or linear polymeric metal compounds with double or triple triazole bridges [5, 6]. On the other hand, carboxylate ligands such benzenedicarboxylate, benzenetricarboxylate, biphenyldicarboxylate are most extensively studied organic ligands in the construction of MOFs due to their variable coordination modes, structural diversity, and thermodynamic stability. Particularly, the mixed ligands of polycarboxylate and N-containing are good candidates to yield novel MOFs with more tunable factors proved in our previous studies [7, 8]. In this paper, we focus our attention on the reaction of mixed organic ligands containing 3,5-dimethyl-4-phenyl-1,2,4-triazole (*L*) and terephthalic acid ligands (H_2pbda) and zinc ions to synthesize a new complex. In the structure of the title compound, each Zn^{II} ion is 4-coordinated with a slightly distorted tetrahedral geometry, by three oxygen atoms (O2, O4, and O5) from two different $pbda^{2-}$ ligands and one water molecule, and one nitrogen atom (N1) from the *L* ligand. The Zn–O distances range from 1.9337(15) to 2.0011(14) Å, while the Zn–N distance is 2.0291(17) Å. The Zn–N and Zn–O distances are comparable to those found in other crystallographically characterized Zn^{II} complexes [9]. The $pbda^{2-}$ ligands link Zn^{II} ion ions using its carboxylate groups to form a 1D double chain, while the *L* ligands are terminal coordinated. It is worthwhile to note that hydrogen bonding interactions are usually important in the synthesis of supramolecular architec-

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ture. There exist medium strong O–H···O hydrogen bonding interactions between the coordination polymer and the solvent water molecule.

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

Atom	Site	*x*	*y*	*z*	U_{iso}
H(2)	2*i*	1.1473	0.5964	0.7810	0.043
H(3)	2*i*	1.2666	0.6856	0.6061	0.051
H(4)	2*i*	1.1345	0.8375	0.4433	0.055
H(5)	2*i*	0.8878	0.8923	0.4488	0.061
H(6)	2*i*	0.7707	0.7914	0.6135	0.051
H(8A)	2*i*	0.6249	0.9000	0.8433	0.077
H(8B)	2*i*	0.7590	0.8961	0.9055	0.077
H(8C)	2*i*	0.6258	0.8806	0.9956	0.077
H(10A)	2*i*	1.1248	0.3579	0.7828	0.082
H(10B)	2*i*	1.0155	0.3755	0.6827	0.082
H(10C)	2*i*	1.0292	0.2677	0.8067	0.082
H(11)	2*i*	0.1934	0.8572	0.8551	0.039
H(13)	2*i*	0.0247	0.9774	1.2209	0.038
H(15)	2*i*	0.6141	0.9823	1.2870	0.041
H(17)	2*i*	0.4248	0.8212	1.5959	0.041
H(6A)	2*i*	0.6683	0.4501	1.6692	0.058
H(6B)	2*i*	0.6351	0.5610	1.5731	0.058

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}
Zn(1)	2*i*	0.55426(2)	0.63819(2)	1.12417(2)	0.0240(2)	0.0265(2)	0.0236(2)	–0.0092(1)	–0.00257(9)	–0.00629(9)
C(1)	2*i*	0.9481(2)	0.6856(2)	0.7129(2)	0.0292(9)	0.0312(9)	0.0272(9)	–0.0135(8)	0.0014(7)	–0.0049(7)
C(2)	2*i*	1.0958(2)	0.6539(3)	0.7128(2)	0.031(1)	0.044(1)	0.034(1)	–0.0170(9)	–0.0037(8)	0.0025(9)
C(3)	2*i*	1.1663(3)	0.7092(3)	0.6092(2)	0.036(1)	0.051(1)	0.042(1)	–0.023(1)	0.0031(9)	–0.003(1)
C(4)	2*i*	1.0879(3)	0.7986(3)	0.5114(2)	0.054(1)	0.048(1)	0.034(1)	–0.025(1)	0.008(1)	–0.0008(9)
C(5)	2*i*	0.9405(3)	0.8305(3)	0.5146(2)	0.054(2)	0.057(2)	0.034(1)	–0.017(1)	–0.007(1)	0.010(1)
C(6)	2*i*	0.8695(3)	0.7724(3)	0.6137(2)	0.032(1)	0.053(1)	0.037(1)	–0.012(1)	–0.0058(9)	0.002(1)
C(7)	2*i*	0.7604(2)	0.6969(2)	0.9047(2)	0.0253(9)	0.0316(9)	0.0316(9)	–0.0107(7)	0.0022(7)	–0.0063(7)
C(8)	2*i*	0.6860(3)	0.8576(3)	0.9130(3)	0.055(2)	0.029(1)	0.059(2)	–0.013(1)	0.015(1)	–0.006(1)
C(9)	2*i*	0.9120(2)	0.4783(2)	0.8482(2)	0.0287(9)	0.0299(9)	0.038(1)	–0.0115(8)	0.0029(8)	–0.0088(8)
C(10)	2*i*	1.0309(3)	0.3594(3)	0.7735(3)	0.051(1)	0.034(1)	0.069(2)	–0.014(1)	0.024(1)	–0.020(1)
C(11)	2*i*	0.1158(2)	0.9143(2)	0.9134(2)	0.0272(9)	0.032(1)	0.0270(9)	–0.0021(7)	0.0001(7)	–0.0072(7)
C(12)	2*i*	0.1311(2)	0.8999(2)	1.0459(2)	0.0235(8)	0.0218(8)	0.0269(8)	–0.0056(7)	–0.0037(7)	–0.0013(6)
C(13)	2*i*	0.0147(2)	0.9864(2)	1.1321(2)	0.031(1)	0.033(1)	0.0223(8)	–0.0038(8)	–0.0040(7)	–0.0033(7)
C(14)	2*i*	0.2715(2)	0.7929(2)	1.0982(2)	0.0266(9)	0.0249(8)	0.0326(9)	–0.0066(7)	–0.0060(7)	–0.0048(7)
C(15)	2*i*	0.5680(3)	0.9893(2)	1.3725(2)	0.039(1)	0.041(1)	0.0266(9)	–0.0194(9)	0.0025(8)	–0.0115(8)
C(16)	2*i*	0.5228(2)	0.8828(2)	1.4287(2)	0.0305(9)	0.0305(9)	0.0276(9)	–0.0101(7)	–0.0053(7)	–0.0095(7)
C(17)	2*i*	0.4548(3)	0.8929(2)	1.5573(2)	0.041(1)	0.036(1)	0.030(1)	–0.0207(9)	0.0003(8)	–0.0082(8)
C(18)	2*i*	0.5453(2)	0.7557(2)	1.3529(2)	0.033(1)	0.034(1)	0.034(1)	–0.0108(8)	–0.0070(8)	–0.0141(8)
N(1)	2*i*	0.7277(2)	0.6008(2)	0.9831(2)	0.0272(8)	0.0290(8)	0.0317(8)	–0.0106(6)	0.0029(6)	–0.0077(6)
N(2)	2*i*	0.8236(2)	0.4615(2)	0.9472(2)	0.0314(8)	0.0268(8)	0.0387(9)	–0.0095(7)	0.0039(7)	–0.0061(7)
N(3)	2*i*	0.8773(2)	0.6236(2)	0.8176(2)	0.0255(7)	0.0301(8)	0.0293(8)	–0.0113(6)	0.0028(6)	–0.0063(6)
O(1)	2*i*	0.5351(3)	0.6468(2)	1.4103(2)	0.089(2)	0.0361(9)	0.046(1)	–0.0287(9)	–0.019(1)	–0.0055(7)
O(2)	2*i*	0.5725(2)	0.7733(2)	1.2292(2)	0.0489(9)	0.0518(9)	0.0324(8)	–0.0296(8)	0.0054(7)	–0.0202(7)
O(3)	2*i*	0.2745(2)	0.7600(2)	1.2163(2)	0.0394(8)	0.0450(9)	0.0318(8)	–0.0033(7)	–0.0109(6)	0.0019(6)
O(4)	2*i*	0.3875(2)	0.7417(2)	1.0148(1)	0.0234(6)	0.0331(7)	0.0357(7)	–0.0052(5)	–0.0055(5)	–0.0092(6)
O(5)	2*i*	0.5704(2)	0.4389(2)	1.1772(1)	0.0385(8)	0.0271(7)	0.0329(7)	–0.0114(6)	–0.0023(6)	–0.0057(5)
O(6)	2*i*	0.6570(2)	0.5342(2)	1.6478(2)	0.053(1)	0.048(1)	0.0401(9)	–0.0201(8)	0.0006(8)	–0.0010(7)

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