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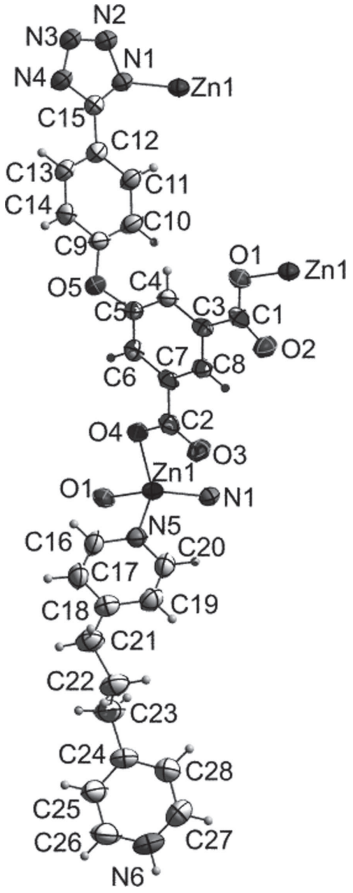
Crystal structure of catena-poly[(μ_3-5-(4-(tetrazol-1-id-5-yl)phenoxy)benzene-1,3-dicarboxyato-κ^3 *O*:*O'*:*N*)(4-(3-(pyridin-4-yl)propyl)pyridinium-κ*N*) zinc(II)], $C_{28}H_{22}ZnN_6O_5$



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Abstract

$C_{28}H_{22}ZnN_6O_5$, triclinic, $P\bar{1}$ (no. 2), $a = 9.9400(9)$ Å, $b = 10.1638(8)$ Å, $c = 13.0867(11)$ Å, $\alpha = 97.678(7)°$, $\beta = 94.730(7)°$, $\gamma = 98.694(7)°$, $V = 1288.09(19)$ Å^3, $Z = 2$, $R_{gt}(F) = 0.0692$, $wR_{ref}(F^2) = 0.1587$, $T = 293(2)$ K.

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Table 1: Data collection and handling.

Crystal:	Colorless, block, size 0.18×0.20×0.23 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	10.05 cm^{-1}
Diffractometer, scan mode:	multiwire proportional, φ and ω scans
$2\theta_{max}$:	51°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	9063, 4754
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 3298
$N(param)_{refined}$:	361
Programs:	SADABS [5], SHELX [6]

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

Atom	Site	*x*	*y*	*z*	U_{iso}
H(6A)	2*i*	1.4428	0.7233	1.1084	0.083
H(4)	2*i*	0.2883	0.2318	0.4597	0.045
H(6)	2*i*	0.2994	0.6246	0.4545	0.045
H(8)	2*i*	0.4370	0.4995	0.7135	0.045
H(10)	2*i*	0.0235	0.3209	0.4162	0.061
H(11)	2*i*	−0.1633	0.1685	0.3344	0.058
H(13)	2*i*	0.0242	0.1259	0.0772	0.060
H(14)	2*i*	0.2168	0.2661	0.1618	0.062
H(16)	2*i*	0.6298	0.0737	0.5647	0.065
H(17)	2*i*	0.8530	0.1604	0.5650	0.066
H(19)	2*i*	0.9086	0.1166	0.8627	0.067
H(20)	2*i*	0.6848	0.0234	0.8525	0.063
H(21A)	2*i*	1.0709	0.2547	0.6583	0.073
H(21B)	2*i*	1.1063	0.1238	0.6969	0.073
H(22A)	2*i*	1.1215	0.2347	0.8712	0.076
H(22B)	2*i*	1.2340	0.2992	0.8073	0.076
H(23A)	2*i*	1.0841	0.4616	0.7764	0.093
H(23B)	2*i*	1.0012	0.4075	0.8635	0.093
H(25)	2*i*	1.2617	0.6387	0.8292	0.087
H(26)	2*i*	1.4236	0.7711	0.9468	0.099
H(27)	2*i*	1.3197	0.5512	1.1595	0.112
H(28)	2*i*	1.1515	0.4188	1.0430	0.121

Table 3: Fractional coordinates and atomic displacement parameters (Å^2).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Zn(1)	2*i*	0.42707(7)	−0.01402(6)	0.69636(5)	0.0464(4)	0.0315(3)	0.0368(4)	0.0025(3)	0.0028(3)	0.0009(3)
O(1)	2*i*	0.3644(4)	0.1173(3)	0.6109(3)	0.056(3)	0.027(2)	0.048(2)	0.005(2)	0.004(2)	0.005(2)
O(2)	2*i*	0.4714(4)	0.2700(4)	0.7402(3)	0.073(3)	0.037(2)	0.044(2)	0.008(2)	−0.009(2)	0.003(2)
O(3)	2*i*	0.4612(5)	0.7509(4)	0.7369(3)	0.097(4)	0.037(2)	0.042(2)	0.007(2)	−0.008(2)	0.001(2)
O(4)	2*i*	0.3779(4)	0.8181(3)	0.5965(3)	0.055(2)	0.028(2)	0.038(2)	0.007(2)	0.003(2)	0.003(2)
O(5)	2*i*	0.2486(4)	0.4049(4)	0.3361(3)	0.055(3)	0.048(2)	0.036(2)	−0.008(2)	−0.004(2)	0.005(2)
N(1)	2*i*	−0.3282(5)	−0.0026(4)	0.1753(3)	0.049(3)	0.037(2)	0.035(2)	−0.003(2)	0.006(2)	−0.003(2)
N(2)	2*i*	−0.4029(5)	−0.0871(5)	0.0962(4)	0.052(3)	0.051(3)	0.038(3)	−0.007(2)	0.001(2)	0.000(2)
N(3)	2*i*	−0.3326(6)	−0.0942(5)	0.0178(4)	0.062(4)	0.066(3)	0.035(3)	−0.014(3)	0.002(3)	−0.003(2)
N(4)	2*i*	−0.2092(6)	−0.0136(5)	0.0422(4)	0.063(4)	0.070(3)	0.036(3)	−0.015(3)	0.005(3)	−0.006(3)
N(5)	2*i*	0.6344(5)	0.0410(4)	0.7078(3)	0.041(3)	0.035(2)	0.040(3)	0.004(2)	0.000(2)	0.003(2)
N(6)	2*i*	1.3825(6)	0.6719(6)	1.0637(5)	0.067(4)	0.064(4)	0.063(4)	−0.002(3)	−0.013(3)	−0.013(3)
C(1)	2*i*	0.4048(6)	0.2380(5)	0.6553(4)	0.039(3)	0.032(3)	0.048(3)	0.006(2)	0.010(3)	0.007(3)
C(2)	2*i*	0.4085(6)	0.7267(5)	0.6476(4)	0.040(3)	0.035(3)	0.045(3)	0.005(3)	0.013(3)	0.004(3)
C(3)	2*i*	0.3680(5)	0.3467(5)	0.5967(4)	0.031(3)	0.031(3)	0.041(3)	0.003(2)	0.007(2)	0.006(2)
C(4)	2*i*	0.3110(5)	0.3200(5)	0.4934(4)	0.035(3)	0.033(3)	0.040(3)	−0.002(2)	0.001(3)	0.000(2)
C(5)	2*i*	0.2890(6)	0.4250(5)	0.4423(4)	0.044(3)	0.032(3)	0.033(3)	−0.001(2)	−0.001(2)	0.005(2)
C(6)	2*i*	0.3175(5)	0.5553(5)	0.4906(4)	0.037(3)	0.037(3)	0.041(3)	0.009(2)	0.001(3)	0.009(2)
C(7)	2*i*	0.3731(6)	0.5845(5)	0.5931(4)	0.044(3)	0.026(3)	0.045(3)	0.004(2)	0.012(3)	0.004(2)
C(8)	2*i*	0.3986(5)	0.4805(5)	0.6449(4)	0.037(3)	0.034(3)	0.038(3)	0.003(2)	0.006(3)	0.000(2)
C(9)	2*i*	0.1359(6)	0.3101(5)	0.2957(4)	0.045(3)	0.034(3)	0.040(3)	−0.001(3)	−0.006(3)	0.002(2)
C(10)	2*i*	0.0240(6)	0.2809(6)	0.3481(4)	0.044(4)	0.063(4)	0.036(3)	0.000(3)	−0.001(3)	−0.010(3)
C(11)	2*i*	−0.0884(6)	0.1909(6)	0.2983(4)	0.038(3)	0.067(4)	0.034(3)	0.001(3)	0.001(3)	−0.003(3)
C(12)	2*i*	−0.0913(6)	0.1338(5)	0.1958(4)	0.053(4)	0.043(3)	0.034(3)	0.003(3)	0.003(3)	0.002(3)
C(13)	2*i*	0.0238(6)	0.1640(6)	0.1458(4)	0.059(4)	0.054(4)	0.031(3)	−0.005(3)	0.007(3)	−0.005(3)
C(14)	2*i*	0.1386(6)	0.2496(6)	0.1956(4)	0.055(4)	0.056(4)	0.037(3)	−0.008(3)	0.014(3)	−0.002(3)
C(15)	2*i*	−0.2100(6)	0.0402(5)	0.1398(4)	0.044(3)	0.042(3)	0.032(3)	−0.002(3)	0.002(3)	0.005(2)
C(16)	2*i*	0.6874(7)	0.0817(6)	0.6257(4)	0.055(4)	0.075(4)	0.032(3)	0.005(3)	0.006(3)	0.010(3)
C(17)	2*i*	0.8212(6)	0.1344(6)	0.6253(5)	0.053(4)	0.073(4)	0.039(3)	0.003(3)	0.011(3)	0.014(3)
C(18)	2*i*	0.9104(6)	0.1494(6)	0.7146(5)	0.042(3)	0.046(3)	0.048(3)	0.007(3)	0.000(3)	0.000(3)
C(19)	2*i*	0.8539(6)	0.1075(6)	0.8002(5)	0.049(4)	0.072(4)	0.043(4)	0.004(3)	−0.006(3)	0.008(3)
C(20)	2*i*	0.7191(7)	0.0532(6)	0.7941(5)	0.059(4)	0.061(4)	0.038(3)	0.009(3)	0.004(3)	0.014(3)
C(21)	2*i*	1.0608(6)	0.2007(7)	0.7139(5)	0.041(4)	0.069(4)	0.064(4)	0.000(3)	0.001(3)	−0.003(3)
C(22)	2*i*	1.1365(7)	0.2848(7)	0.8139(5)	0.046(4)	0.069(4)	0.066(4)	0.002(3)	−0.006(3)	−0.005(4)
C(23)	2*i*	1.0909(8)	0.4200(7)	0.8387(6)	0.079(5)	0.062(4)	0.079(5)	−0.008(4)	−0.019(4)	0.001(4)
C(24)	2*i*	1.1917(7)	0.5111(6)	0.9205(5)	0.054(4)	0.056(4)	0.059(4)	−0.008(3)	−0.007(3)	−0.002(3)
C(25)	2*i*	1.2722(8)	0.6185(7)	0.8963(6)	0.085(5)	0.057(4)	0.065(5)	−0.010(4)	−0.022(4)	0.013(4)
C(26)	2*i*	1.3681(8)	0.6984(7)	0.9662(7)	0.090(6)	0.055(4)	0.089(6)	−0.015(4)	−0.021(5)	0.008(4)
C(27)	2*i*	1.3069(9)	0.5697(9)	1.0920(6)	0.107(7)	0.107(7)	0.050(4)	−0.021(6)	−0.015(5)	0.012(5)
C(28)	2*i*	1.208(1)	0.4892(9)	1.0217(6)	0.117(7)	0.095(6)	0.068(5)	−0.045(5)	−0.020(5)	0.026(5)

The figure shows a part of the title structure (asymmetric unit and symmetry related Zn). Tables 1–3 contain details of the methods used and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

The title complex was synthesized under hydrothermal conditions. A mixture of $Zn(NO_3)_2 \cdot 6H_2O$ (0.1485 g, 0.5 mmol), 1,3-bis(4-pyridyl)propane (0.0991 g, 0.5 mmol; bpp), 5-(4′-(tetrazol-5″-yl)phenoxy)isophthalic acid (0.0653 g, 0.2 mmol; TPI) and 10 mL deionized water was sealed in a Teflon-lined stainless vessel (25 mL) and heated at 423 K for 48 h under autogenous pressure, then cooled slowly to room temperature. Colorless block crystals were obtained by filtration.

Experimental details

The hydrogen atoms were idealized and refined using a riding model with the help of the SHELX-97 programm (AFIX 43, 23 option) [6].

Discussion

The coordination chemistry of pyridinecarboxylic, pyrazolecarboxylic, imidazolecarboxylic and tetrazolecarboxylic acids based heterocyclic acids has been extensively studied and is mostly related to their good coordination ability and diverse coordination modes [1–4]. In this study, we report the structure of a new zinc(II) complex with the mixture of 1,3-bis(4-pyridyl)propane (bpp) and 5-(4′-(tetrazol-5″-yl)phenoxy) isophthalic acid (TPI). The asymmetric unit of

title complex contains one crystallographically independent Zn(II) atom, one protonated bpp ligand, and one deprotonated TPI ligand. Each Zn(II) center is four-coordinated by two nitrogen atoms from one bpp and one TPI ligand, two oxygen atoms from TPI ligands to furnish a distorted tetrahedral coordination geometry. The Zn-N/O bond lengths are in the range of 2.015(4)–2.040(4) Å and 1.976(3)–1.989(4) Å, respectively. Both carboxylate groups of the anionic TPI ligand exhibit a monodentate coordination mode. Each TPI ligand bridges three Zn(II) centers to construct a 1D polymeric ladder structure with the half-coordinated bpp ligands grafting on two sides. Each ladder is further interlinked to form a 2D supramolecular layer motif through N—H···O hydrogen-bonding (H···O = 2.080 Å) interactions between pyridine rings and carboxylate oxygen atoms.

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