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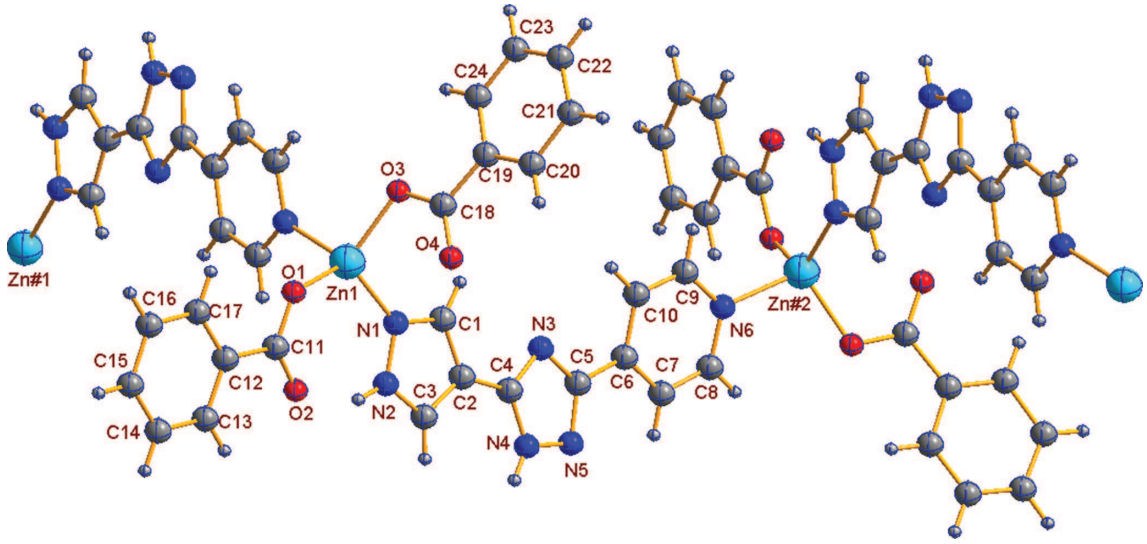
Crystal structure of *catena*-poly[(μ_2-3-(1*H*-pyrazol-4-yl)-5-(pyridin-4-yl)-1,2,4-triazole-κ *N*:*N*′)-bis(benzoato-κ*O*)zinc(II)], $C_{24}H_{18}N_6O_4Zn$



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Abstract

$C_{24}H_{18}N_6O_4Zn$, monoclinic, $P2_1/c$ (no. 14), $a = 13.7579(8)$ Å, $b = 8.5684(6)$ Å, $c = 19.7973(10)$ Å, $\beta = 96.500(6)°$, $V = 2318.8(2)$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0521$, $wR_{ref}(F^2) = 0.1297$, $T = 288$ K.

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A part of the title 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.

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.21 × 0.20 × 0.18 mm
Wavelength:	Mo *Kα* radiation (0.71073 Å)
μ:	11.0 cm^{-1}
Diffractometer, scan mode:	SuperNova, ω-scans
$2\theta_{max}$, completeness:	52°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	12462, 4407, 0.036
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 3181
$N(param)_{refined}$:	320
Programs:	SHELX [1], CrysAlis^{PRO} [2], OLEX2 [3]

Source of material

3-(1*H*-pyrazol-4-yl)-5-(pyridin-4-yl)-1,2,4-triazole (H_2L) (21.2 mg, 0.10 mmol), benzoic acid (hbc) (36.6 mg, 0.30 mmol), $Zn(NO_3)_2{\cdot}6H_2O$ (89.2 mg, 0.30 mmol) and KOH (5.6 mg, 0.10 mmol) were dissolved in H_2O, and then sealed in a 25 mL teflon-lined stainless steel autoclave at 165 °C for 54 h, finally cooled to room temperature at a rate of 5 °C/h^{-1}. Light yellow block-shaped crystals were obtained.

Experimental details

Hydrogen atoms were placed in calculated positions and were included in the refinement using the riding model approximation, with $U_{iso}(H) = 1.2U_{eq}(C/N)$.

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.29353(3)	0.81352(5)	0.54562(2)	0.04250(18)
O1	0.2647(2)	0.9212(3)	0.46001(11)	0.0570(8)
O2	0.4133(2)	0.9184(4)	0.42777(14)	0.0713(9)
O3	0.19285(19)	0.6837(3)	0.57744(14)	0.0561(7)
O4	0.2301(2)	0.5242(4)	0.49667(12)	0.0640(8)
N1	0.4245(2)	0.7065(4)	0.56499(14)	0.0401(7)
N2	0.4952(2)	0.7247(4)	0.52355(14)	0.0411(7)
H2	0.4898	0.7841	0.4883	0.049*
N3	0.6037(2)	0.3936(4)	0.70165(13)	0.0391(7)
N4	0.7125(2)	0.4162(4)	0.63046(14)	0.0383(7)
N5	0.7556(2)	0.3225(4)	0.68005(14)	0.0406(7)
N6	0.7072(2)	−0.0048(4)	0.88695(13)	0.0391(7)
C1	0.4632(3)	0.6051(5)	0.61251(17)	0.0457(9)
H1	0.4310	0.5694	0.6484	0.055*
C2	0.5577(2)	0.5600(4)	0.60135(16)	0.0360(8)
C3	0.5741(3)	0.6400(4)	0.54364(16)	0.0399(9)
H3	0.6309	0.6358	0.5223	0.048*
C4	0.6229(2)	0.4572(4)	0.64315(15)	0.0342(8)
C5	0.6870(2)	0.3127(4)	0.72188(15)	0.0345(8)
C6	0.6980(2)	0.2127(4)	0.78195(16)	0.0345(8)
C7	0.7833(3)	0.1312(5)	0.80180(17)	0.0432(9)
H7	0.8389	0.1489	0.7802	0.052*
C8	0.7853(3)	0.0239(5)	0.85348(17)	0.0448(9)
H8	0.8429	−0.0311	0.8659	0.054*
C9	0.6268(3)	0.0794(5)	0.86986(17)	0.0440(9)
H9	0.5733	0.0638	0.8939	0.053*
C10	0.6189(3)	0.1871(5)	0.81899(17)	0.0427(9)
H10	0.5612	0.2433	0.8090	0.051*
C11	0.3279(3)	0.9606(5)	0.42129(17)	0.0456(10)
C12	0.2926(3)	1.0681(5)	0.36351(17)	0.0467(10)
C13	0.3576(3)	1.1100(5)	0.31745(17)	0.0545(11)
H13	0.4203	1.0681	0.3218	0.065*
C14	0.3296(5)	1.2126(6)	0.2659(2)	0.0718(15)
H14	0.3736	1.2406	0.2357	0.086*
C15	0.2384(5)	1.2734(6)	0.2587(3)	0.0851(18)
H15	0.2197	1.3420	0.2232	0.102*
C16	0.1732(5)	1.2340(7)	0.3039(3)	0.0882(17)
H16	0.1106	1.2768	0.2991	0.106*
C17	0.2010(4)	1.1292(6)	0.3571(2)	0.0656(12)
H17	0.1572	1.1020	0.3876	0.079*
C18	0.1815(3)	0.5569(5)	0.54376(17)	0.0436(9)
C19	0.1068(3)	0.4465(5)	0.56424(17)	0.0437(9)
C20	0.0850(4)	0.3140(6)	0.5289(2)	0.0732(14)
H20	0.1188	0.2874	0.4924	0.088*
C21	0.0085(4)	0.2143(6)	0.5484(4)	0.0947(19)
H21	−0.0085	0.1234	0.5243	0.114*
C22	−0.0382(4)	0.2548(8)	0.6025(4)	0.0885(17)
H22	−0.0873	0.1905	0.6156	0.106*
C23	−0.0155(4)	0.3828(8)	0.6368(3)	0.0839(16)
H23	−0.0480	0.4077	0.6741	0.101*
C24	0.0553(3)	0.4797(6)	0.6184(2)	0.0607(12)
H24	0.0693	0.5710	0.6430	0.073*
H4	0.741(3)	0.439(4)	0.5961(18)	0.048(11)*

Discussion

Largely due to applications in gas storage and separation, luminescence, catalysis, magnetism and sensing, metal-organic framework/coordination polymer synthetic investigations have continued unabated over the past decade which drives the design and development of new metal-organic framework materials [4–8]. In that regard, the *N*-donor ligands and aromatic carboxylic acid are perhaps the most promising candidates, because they can interact with a metal surface by both π electrons and the lone-pair electrons at the nitrogen atom and oxygen atom. Hence, they provide access to diverse coordination polymer topologies [9–12]. In light of the interesting structural diversity in previously reported zinc(II) Metal–Organic frameworks based on triazole-carboxylate [13, 14], we set about attempts to prepare transition metal coordination polymers containing the easily prepared 3-(1*H*-pyrazol-4-yl)-5-(pyridin-4-yl)-1,2,4-triazole and the bezoate ligand (bc^-). A perspective view of the molecular structure of $[Zn(bc)_2(H_2L)]n$ is show in the figure.

The asymmetric unit consists of one Zn(II) ion, two bc^- ligands and one H_2L ligand. The Zn(II) ion is four-coordinated by one nitrogen atom N(1) of H_2L ligand and two oxygen atoms [O(1), O(3)] from two different bc^- ligands. The connection to the next unit is realized by the Zn-N coordination (Zn1-N6#1) of the next H_2L ligand (*cf*. the figure). The bond lengths of Zn—N are 2.021(3) and 2.052(3) Å, and Zn—O are 1.930(3) and 1.937(3) Å, which are in the normal range [15]. It should be noted that these connections lead to a one-dimensional chain.

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