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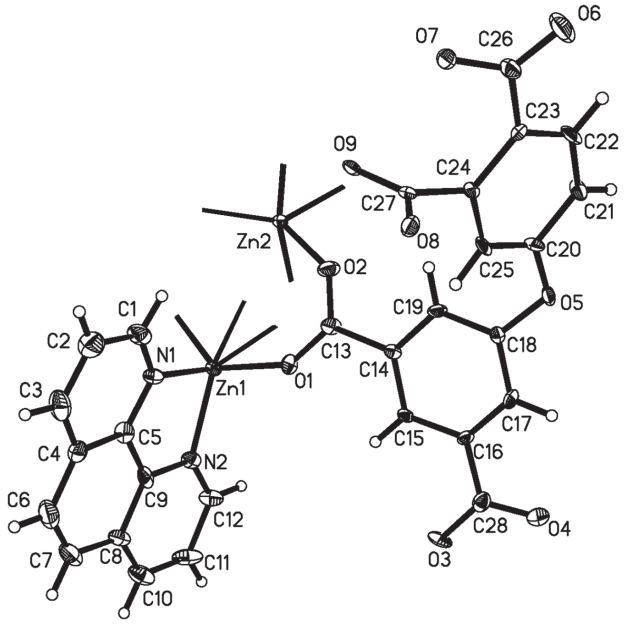
Crystal structure of poly[(μ_7-4-(3,5-dicarboxylatophenoxy)phthalato)-(1,10-phenanthroline-κ^2N,N')dizinc(II)], $C_{28}H_{14}N_2O_9Zn_2$



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Abstract

$C_{28}H_{14}N_2O_9Zn_2$, triclinic, $P\bar{1}$ (no. 2), $a = 9.6870(5)$ Å, $b = 10.1849(9)$ Å, $c = 12.7338(9)$ Å, $\alpha = 95.202(6)°$, $\beta = 107.027(5)°$, $\gamma = 91.896(5)°$, $V = 1193.97(14)$ Å^3, $Z = 2$, $R_{gt}(F) = 0.0516$, $wR_{ref}(F^2) = 0.1267$, $T = 293(2)$ 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.

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Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	0.43 × 0.32 × 0.29 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	2.07 mm^{-1}
Diffractometer, scan mode:	SuperNova, ω-scans
θ_{max}, completeness:	25.5°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	25935, 4433, 0.088
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 3738
$N(param)_{refined}$:	370
Programs:	CrysAlis^{PRO} [1], SHELX [2, 3]

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

Atom	x	y	z	U_{iso}*/U_{eq}
Zn1	0.80005(5)	0.87012(5)	0.39316(4)	0.02366(17)
Zn2	1.09938(5)	0.77784(5)	0.61098(4)	0.02333(17)
N1	0.7728(4)	0.7336(4)	0.2530(3)	0.0259(8)
N2	0.6048(4)	0.9252(4)	0.2878(3)	0.0272(9)
O1	0.7421(3)	0.7299(3)	0.4781(3)	0.0322(8)
O2	0.9303(3)	0.6692(3)	0.6101(3)	0.0400(9)
O3	0.2688(3)	0.7182(4)	0.5571(3)	0.0434(9)
O4	0.2619(3)	0.6486(4)	0.7112(3)	0.0439(9)
O5	0.6993(3)	0.3809(3)	0.8225(2)	0.0305(8)
O6	1.1044(5)	−0.0972(4)	0.8557(3)	0.0592(12)
O7	1.0988(3)	−0.0458(3)	0.6881(2)	0.0285(7)
O8	0.7932(3)	0.0029(3)	0.5239(2)	0.0262(7)
O9	0.9799(3)	0.1467(3)	0.5430(2)	0.0214(6)
C1	0.8503(5)	0.6316(5)	0.2414(4)	0.0351(12)
H1	0.9256	0.6129	0.3016	0.042*
C2	0.8231(6)	0.5513(5)	0.1420(4)	0.0427(13)
H2	0.8791	0.4801	0.1363	0.051*
C3	0.7145(6)	0.5781(6)	0.0542(5)	0.0478(14)
H3	0.6968	0.5260	−0.0127	0.057*
C4	0.6271(5)	0.6846(5)	0.0627(4)	0.0364(12)
C5	0.6614(5)	0.7582(5)	0.1663(4)	0.0276(10)
C6	0.5069(6)	0.7177(6)	−0.0238(4)	0.0463(14)
H6	0.4852	0.6704	−0.0932	0.056*
C7	0.4241(6)	0.8160(6)	−0.0073(4)	0.0432(14)
H7	0.3465	0.8353	−0.0656	0.052*
C8	0.4526(5)	0.8915(5)	0.0975(4)	0.0338(12)
C9	0.5707(5)	0.8628(4)	0.1847(4)	0.0266(10)
C10	0.3677(5)	0.9920(5)	0.1222(5)	0.0429(14)
H10	0.2891	1.0165	0.0672	0.052*
C11	0.4002(5)	1.0526(5)	0.2252(5)	0.0438(13)

Table 2 (continued)

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
H11	0.3431	1.1185	0.2414	0.053*
C12	0.5185(5)	1.0178(5)	0.3084(4)	0.0369(12)
H12	0.5380	1.0599	0.3795	0.044*
C13	0.7976(4)	0.6758(4)	0.5625(4)	0.0240(10)
C14	0.6968(4)	0.6116(4)	0.6162(3)	0.0212(9)
C15	0.5552(4)	0.6478(4)	0.5930(3)	0.0226(9)
H15	0.5197	0.7038	0.5389	0.027*
C16	0.4666(4)	0.6002(4)	0.6507(4)	0.0225(9)
C17	0.5149(4)	0.5069(4)	0.7240(4)	0.0238(10)
H17	0.4533	0.4709	0.7593	0.029*
C18	0.6546(4)	0.4678(4)	0.7442(3)	0.0207(9)
C19	0.7474(4)	0.5239(4)	0.6927(4)	0.0251(10)
H19	0.8434	0.5020	0.7099	0.030*
C20	0.7935(4)	0.2849(4)	0.8079(4)	0.0233(9)
C21	0.8803(5)	0.2402(5)	0.9018(4)	0.0282(10)
H21	0.8796	0.2777	0.9710	0.034*
C22	0.9689(5)	0.1388(4)	0.8926(4)	0.0260(10)
H22	1.0264	0.1067	0.9560	0.031*
C23	0.9732(4)	0.0837(4)	0.7886(3)	0.0222(9)
C24	0.8864(4)	0.1332(4)	0.6954(3)	0.0208(9)
C25	0.7932(4)	0.2320(4)	0.7047(4)	0.0226(9)
H25	0.7316	0.2618	0.6419	0.027*
C26	1.0673(5)	−0.0290(5)	0.7809(4)	0.0270(10)
C27	0.8866(4)	0.0867(4)	0.5799(3)	0.0194(9)
C28	0.3225(4)	0.6560(4)	0.6383(4)	0.0254(10)

Source of material

A mixture of $Zn(NO_3)_2{\cdot}6H_2O$ (0.1 mmol, 0.0297 g), 1,10-phenanthroline (0.1 mmol, 0.0180 g), 4-(3,5-dicarboxyphenoxy)phthalic acid (0.1 mmol, 35 mg), was dissolved in 10 mL H_2O. The solution was heated in a 25 mL Teflon-lined autoclave under autogenous pressure at 423 K for 5 days. After cooling to room temperature colourless block crystals were obtained.

Experimental details

All H atoms were positioned geometrically (N—H = 0.86 Å and C—H = 0.93 Å) and refined using a riding model, with $U_{iso}(H) = 1.2U_{eq}(C, N)$.

Discussion

Research on metal-organic coordination polymers (CPs) have made considerable progress in the fields of supramolecular chemistry and crystal engineering, owing to their intriguing architectures and applications [4–8]. Among the various ligands, the organic carboxylate ligands have been proven to be good candidates for the construction of CPs [7, 8]. Moreover, *N*-donor ligands have been proved to be efficient and typical building blocks in the assembly of CPs [9]. In addition, various aromatic *N*-donors also play an important role and frequently serve as ancillary ligands to adjust the supramolecular structure of the resulting network.

The asymmetric unit of the title structure contains two Zn(II) metal center, one 4-(3,5-dicarboxylatophenoxy) phthalato and one 1,10-phenanthroline ligand to construct a coordination polymer. The zinc atom 1 is six-coordinated [ZnN_2O_4], whereas the zinc atom 2 is penta-coordinated [ZnO_5] (*cf*. the figure). The Zn—O bond lengths range from 1.928(7)–2.473(7) Å. The Zn—N bond lengths range from 2.103(9) Å, 2.108(10) Å, respectively. The bond angles of O—Zn—O are in the range of 60.5(3)° to 172.1(3)°. In addition, there is a complex network of intermolecular hydrogen bonds. These interactions result in a three dimensional architecture.

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