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Synthesis and crystal structure of *catena*-poly[bis(2-(2-(2,6-dichlorophenyl)amino)phenyl)acetato- $\kappa O;\kappa^2 O',O''$)-(μ_2 -1,4-di(pyridin-4-yl)benzene- $\kappa^2 N:N'$)zinc(II)], $C_{44}H_{32}N_4ZnCl_4O_4$

A part of the title crystal structure is shown in the figure. The asymmetric unit is shown as ellipsoids. 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:	0.43 × 0.38 × 0.28 mm
Wavelength:	Cu K α radiation (1.54178 Å)
μ :	3.66 mm ⁻¹
Diffractometer, scan mode:	Multiwire proportional, φ and ω -scans
θ_{max} , completeness:	73.7°, >97%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int} :	13919, 7939, 0.022
Criterion for I_{obs} , $N(hkl)_{gt}$:	$I_{obs} > 2 \sigma(I_{obs})$, 7446
$N(param)_{refined}$:	514
Programs:	SHELX [1], OLEX2 [2]

Source of material

A mixture of $Zn(OAc)_2 \cdot 2H_2O$ (22 mg, 0.1 mmol), 2-(2-(2,6-dichlorophenylamino)phenyl)acetic acid (0.1 mmol, 891 mg), 1,4-di(pyridin-4-yl)benzene (0.1 mmol, 232 mg) and distilled water (10 mL) was heated in a 25 mL stainless steel reactor with a Teflon liner 403 K for 40 h, followed by slow cooling to room temperature. Colourless crystals of the title compound formed.

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

The design and construction of metal-organic frameworks (MOFs) with well-regulated network structures has been provoked significant interest on these functional materials with predictable properties, such as electrochemistry, photophysics, catalysis, adsorption and separation [3–6]. The organic ligands, which have their differences in the size, the flexibility, the coordination ability, the number of the carboxylate groups, the positions of the carboxylate groups and

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Abstract

$C_{44}H_{32}N_4O_4Cl_4Zn$, triclinic, $P\bar{1}$ (no. 2), $a = 7.3158(2)$ Å, $b = 13.6944(5)$ Å, $c = 20.4081(6)$ Å, $\alpha = 82.930(3)^\circ$, $\beta = 89.667(2)^\circ$, $\gamma = 88.034(3)^\circ$, $V = 2027.85(11)$ Å³, $Z = 2$, $R_{gt}(F) = 0.0430$, $wR_{ref}(F^2) = 0.1141$, $T = 293(2)$ K.

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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	0.85335(4)	0.094975(19)	0.276362(12)	0.03856(9)
Cl1	1.02038(9)	−0.30368(5)	0.02582(4)	0.06427(17)
Cl2	0.70340(8)	0.05848(5)	0.02184(4)	0.06053(16)
Cl3	0.67319(15)	0.39976(9)	0.41599(7)	0.1189(4)
Cl4	1.27725(16)	0.61367(8)	0.37503(6)	0.1062(3)
N1	0.8585(3)	−0.13274(14)	0.08806(9)	0.0478(4)
H1	0.9363	−0.0993	0.1066	0.057*
N2	1.0483(3)	0.43836(15)	0.36368(10)	0.0540(5)
H2	1.0745	0.3815	0.3850	0.065*
N3	0.6405(2)	0.06947(14)	0.34169(8)	0.0435(4)
N4	0.7269(2)	0.20702(12)	0.20920(8)	0.0369(3)
O1	0.9812(3)	0.22950(14)	0.35832(11)	0.0687(5)
O2	1.0906(2)	0.15582(13)	0.27609(9)	0.0568(4)
O3	0.9753(3)	−0.06010(18)	0.29957(11)	0.0796(6)
O4	0.8284(3)	−0.01314(12)	0.20909(9)	0.0621(5)
C1	0.9138(3)	−0.07810(17)	0.24570(12)	0.0492(5)
C2	0.9432(3)	−0.17937(16)	0.22551(12)	0.0492(5)
H2A	1.0434	−0.1781	0.1941	0.059*
H2B	0.9792	−0.2244	0.2641	0.059*
C3	0.7785(3)	−0.21814(15)	0.19517(11)	0.0431(4)
C4	0.6583(4)	−0.2775(2)	0.23394(13)	0.0601(6)
H4	0.6789	−0.2910	0.2791	0.072*
C5	0.5097(5)	−0.3168(3)	0.20689(16)	0.0823(10)
H5	0.4323	−0.3571	0.2335	0.099*
C6	0.4762(5)	−0.2961(3)	0.14028(16)	0.0839(10)
H6	0.3761	−0.3227	0.1218	0.101*
C7	0.5910(4)	−0.2359(2)	0.10071(13)	0.0638(7)
H7	0.5673	−0.2217	0.0558	0.077*
C8	0.7412(3)	−0.19641(16)	0.12769(11)	0.0434(4)
C9	0.8483(3)	−0.12414(16)	0.01918(10)	0.0422(4)
C10	0.9142(3)	−0.19946(17)	−0.01636(11)	0.0459(5)
C11	0.9041(3)	−0.1923(2)	−0.08425(12)	0.0547(6)
H11	0.9465	−0.2443	−0.1062	0.066*
C12	0.8312(4)	−0.1079(2)	−0.11942(12)	0.0600(7)
H12	0.8222	−0.1033	−0.1651	0.072*
C13	0.7713(3)	−0.0299(2)	−0.08693(12)	0.0560(6)
H13	0.7261	0.0282	−0.1106	0.067*
C14	0.7796(3)	−0.03931(17)	−0.01865(11)	0.0455(5)
C15	1.0997(3)	0.21889(16)	0.31613(12)	0.0477(5)
C16	1.2563(3)	0.28910(17)	0.30694(13)	0.0490(5)
H16A	1.2991	0.3033	0.3496	0.059*
H16B	1.3573	0.2596	0.2845	0.059*
C17	1.1878(3)	0.38304(15)	0.26633(11)	0.0428(4)
C18	1.2157(3)	0.39833(19)	0.19850(13)	0.0533(6)
H18	1.2799	0.3504	0.1783	0.064*
C19	1.1508(4)	0.4829(2)	0.16003(13)	0.0616(6)
H19	1.1725	0.4918	0.1148	0.074*
C20	1.0540(4)	0.55316(19)	0.18967(13)	0.0601(6)
H20	1.0107	0.6104	0.1645	0.072*
C21	1.0211(4)	0.53902(17)	0.25655(13)	0.0547(6)
H21	0.9540	0.5868	0.2760	0.066*
C22	1.0859(3)	0.45487(16)	0.29569(11)	0.0441(5)
C23	0.9693(4)	0.5119(2)	0.39767(13)	0.0602(6)
C24	1.0609(5)	0.5969(2)	0.40656(17)	0.0772(9)
C25	0.9845(7)	0.6676(3)	0.4431(2)	0.1037(14)

Table 2 (continued)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} */ <i>U</i> _{eq}
H25	1.0483	0.7236	0.4487	0.124*
C26	0.8149(8)	0.6541(3)	0.4707(2)	0.1174(17)
H26	0.7637	0.7010	0.4953	0.141*
C27	0.7198(6)	0.5717(3)	0.4626(2)	0.1091(15)
H27	0.6049	0.5626	0.4816	0.131*
C28	0.7961(5)	0.5027(3)	0.42594(18)	0.0791(9)
C29	0.6081(3)	0.11793(17)	0.39369(12)	0.0497(5)
H29	0.6912	0.1640	0.4035	0.060*
C30	0.4559(3)	0.10233(18)	0.43357(12)	0.0510(5)
H30	0.4391	0.1378	0.4693	0.061*
C31	0.3284(3)	0.03487(16)	0.42106(10)	0.0420(4)
C32	0.3648(4)	−0.0151(2)	0.36717(13)	0.0639(7)
H32	0.2846	−0.0619	0.3564	0.077*
C33	0.5187(4)	0.0040(2)	0.32947(13)	0.0643(7)
H33	0.5388	−0.0307	0.2935	0.077*
C34	0.1604(3)	0.01693(16)	0.46185(10)	0.0420(4)
C35	0.1208(5)	0.0667(3)	0.51470(17)	0.0828(11)
H35	0.2017	0.1130	0.5258	0.099*
C36	0.0355(4)	−0.0501(3)	0.44794(16)	0.0781(10)
H36	0.0568	−0.0854	0.4124	0.094*
C37	0.6428(3)	0.18362(15)	0.15536(10)	0.0417(4)
H37	0.6221	0.1177	0.1523	0.050*
C38	0.5856(3)	0.25321(15)	0.10414(10)	0.0411(4)
H38	0.5280	0.2335	0.0677	0.049*
C39	0.6135(2)	0.35227(14)	0.10676(9)	0.0345(4)
C40	0.6955(3)	0.37628(15)	0.16376(11)	0.0421(4)
H40	0.7143	0.4418	0.1686	0.050*
C41	0.7489(3)	0.30297(15)	0.21297(10)	0.0416(4)
H41	0.8030	0.3209	0.2507	0.050*
C42	0.5560(3)	0.42831(14)	0.05210(9)	0.0355(4)
C43	0.4028(3)	0.41592(15)	0.01432(11)	0.0448(5)
H43	0.3360	0.3593	0.0237	0.054*
C44	0.6524(3)	0.51369(16)	0.03709(11)	0.0450(5)
H44	0.7550	0.5238	0.0618	0.054*

so on, play crucial role in the design and construction of desirable frameworks with interesting properties [7–10]. In addition, N-containing auxiliary ligands are known to be ideal connectors between metal atoms for the propagation of coordination networks.

The asymmetric unit of the title structure contains one Zn(II) ion, two half of a 1,4-di(pyridin-4-yl)benzene and one 2-(2-(2,6-dichlorophenylamino)phenyl)acetate anion to construct a new coordination polymer. The zinc atom is five-coordinated [ZnN₂O₃] by three oxygen atoms from 2-(2-(2,6-dichlorophenylamino)phenyl)acetate ligands and by two nitrogen atoms from two 1,4-di(pyridin-4-yl)benzene ligands. The Zn–O bond lengths are 1.9506(17)–2.271(2) Å. The Zn–N bond lengths range from 2.0548(17)–2.1187(16) Å. The bond angles of O–Zn–O are in the range of 58.35(7)° to 115.23(8)°. The Cl–C bond lengths range from 1.717(4)–1.735(3) Å. All the oxygen atoms of the carboxylic group participate in the

hydrogen bonding, contributing to packing stability. Thus these weak interactions result in the infinite three dimensional architecture.

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