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Crystal structure of poly[aqua- μ_2 -4,4'-bipyridine- $\kappa^2 N:N'$]- μ_2 -bis(2-(2-((2,6-dichlorophenyl)amino)phenyl)acetato- $\kappa^2 O,O'$)zinc(II)], $C_{38}H_{28}Cl_4N_4O_4Zn$

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.43 × 0.32 × 0.29 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	1.02 mm ⁻¹
Diffractometer, scan mode:	Xcalibur, ϕ and ω
$\theta_{\max}$, completeness:	25.5°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	10765, 3370, 0.028
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 2461
$N(\text{param})_{\text{refined}}$:	231
Programs:	CrysAlis ^{PRO} [1], SHELX [2, 3]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Zn1	0.0000	0.06395(10)	0.2500	0.0782(4)
Cl1	0.23415(4)	0.2524(2)	0.25344(12)	0.0886(5)
Cl2	0.11808(5)	0.0513(3)	−0.00205(13)	0.1082(7)
O1	0.06757(11)	0.1538(7)	0.2136(4)	0.119(2)
O2	0.03476(11)	0.2183(6)	0.3352(3)	0.0936(13)
N1	−0.00512(14)	−0.1270(5)	0.3556(3)	0.0788(13)
N2	0.14857(11)	0.2136(5)	0.1774(3)	0.0557(9)
H2	0.1479	0.1551	0.2297	0.067*
C1	0.06619(13)	0.2243(6)	0.2913(4)	0.0606(13)
C2	0.10244(14)	0.3121(7)	0.3370(4)	0.0628(12)
H2A	0.0944	0.3695	0.3949	0.075*
H2B	0.1220	0.2255	0.3564	0.075*
C3	0.12241(12)	0.4393(5)	0.2751(4)	0.0552(11)
C4	0.12000(16)	0.6125(7)	0.2963(5)	0.0836(18)
H4	0.1048	0.6479	0.3472	0.100*
C5	0.1397(2)	0.7328(7)	0.2433(7)	0.121(3)
H5	0.1377	0.8482	0.2583	0.145*
C6	0.16203(19)	0.6818(8)	0.1695(7)	0.125(3)
H6	0.1759	0.7624	0.1348	0.150*
C7	0.16437(16)	0.5103(7)	0.1451(5)	0.089(2)
H7	0.1788	0.4774	0.0924	0.107*
C8	0.14542(12)	0.3884(5)	0.1984(4)	0.0543(11)
C9	0.17836(13)	0.1491(5)	0.1199(3)	0.0544(11)
C10	0.16852(15)	0.0669(7)	0.0337(4)	0.0671(13)
C11	0.19659(18)	−0.0061(8)	−0.0230(4)	0.0819(16)
H11	0.1886	−0.0607	−0.0801	0.098*
C12	0.23605(19)	0.0020(8)	0.0051(5)	0.0831(17)
H12	0.2551	−0.0476	−0.0330	0.100*
C13	0.24806(15)	0.0826(7)	0.0890(5)	0.0740(16)
H13	0.2752	0.0885	0.1077	0.089*

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Abstract

$C_{38}H_{28}Cl_4N_4O_4Zn$, monoclinic, $C2/c$ (no. 19), $a = 33.2980(15)$ Å, $b = 7.8254(3)$ Å, $c = 13.8939(9)$ Å, $\beta = 92.506(5)^\circ$, $V = 3616.9(3)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0702$, $wR_{\text{ref}}(F^2) = 0.1774$, $T = 293(2)$ K.

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Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

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Table 2 (continued)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
C14	0.21935(13)	0.1554(6)	0.1461(4)	0.0598(12)
C15	0.02167(15)	−0.1460(6)	0.4266(4)	0.0649(13)
H15	0.0400	−0.0579	0.4386	0.078*
C16	0.02431(14)	−0.2874(6)	0.4842(3)	0.0612(12)
H16	0.0440	−0.2920	0.5338	0.073*
C17	−0.00126(14)	−0.4219(6)	0.4704(3)	0.0569(11)
C18	−0.0311(2)	−0.3983(9)	0.4007(6)	0.136(4)
H18	−0.0506	−0.4819	0.3896	0.164*
C19	−0.0321(3)	−0.2496(10)	0.3472(7)	0.148(4)
H19	−0.0533	−0.2351	0.3021	0.178*

Source of material

A mixture of Zn(OAc)₂·2H₂O (22 mg, 0.1 mmol), 4,4'-bipyridine (0.1 mmol, 0.0156 g), and 2-(2-(6-dichlorophenylamino)phenyl)acetic acid (H2dpac) (0.1 mmol, 891 mg), was dissolved in 9 mL H₂O. The solution was heated in a 23 mL autoclave under autogenous pressure at 383 K for four days. After cooling to room temperature colorless crystals formed.

Experimental details

Hydrogen atoms were positioned using a riding model. Their *U*_{iso} values were set to 1.2*U*_{eq} of the parent atoms.

Comment

The design and construction of metal-organic frameworks (MOFs) and coordination polymers are of interest due to their interesting properties [4–6]. In most situations, *N*-containing ligands are electrically neutral, while carboxylate ligands are negatively charged [7–9]. On the other hand, 4,4'-bipyridine serves as bridging ligand [10–12].

In the title complex, there is one half of a Zn(II) ion, one Hdpac ligand, and one half of the 4,4'-bipyridine ligand in the asymmetric unit (cf. the figure). The zinc atom Zn1 is six-coordinated with a distorted octahedral geometry by four O atoms from the Hdpac ligands, and two N atoms from two 4,4'-bipyridine ligands. The Zn–N bond length is 2.104(4) Å; and the Zn–O ones are in the range of 2.022(4) to 2.430(3) Å, respectively. The C(9)–C(14)–Cl(1) angle is 118.7(3)°, the C(13)–C(14)–Cl(1) angle is 119.6(4)°, the C(11)–C(10)–Cl(2) angle is 118.9(4)°, the C(9)–C(10)–Cl(2) angle is 118.2(3)°. The bond angles of O–Zn–O are in the range of 55.72(13)° to 146.4(2)°. All geometric parameters are comparable to related ones [12, 13]. The hydrogen bond between the carboxylate oxygen and the NH group is in the normal range: d(N...O): 2.815(4).

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