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Crystal structure of bis(2-(2-((2,6-dichlorophenyl)amino)phenyl)acetato- $\kappa^2 O, O'$)-(1,10-phenanthroline- $\kappa^2 N, N'$)zinc(II), $C_{40}H_{28}Cl_4N_4O_4Zn$

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.42 × 0.38 × 0.26 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	1.01 mm ⁻¹
Diffractometer, scan mode:	SuperNova, ω
$\theta_{\max}$, completeness:	25.5°, 98%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	7005, 3329, 0.048
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1966
$N(\text{param})_{\text{refined}}$:	240
Programs:	CrysAlis ^{PRO} [1], SHELX [2, 3]

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

Atom	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Zn1	1.0000	0.26895(6)	1.2500	0.0470(3)
Cl1	0.73219(5)	0.35914(12)	0.71525(12)	0.0754(5)
Cl2	0.84789(5)	0.09311(11)	1.07578(11)	0.0707(4)
O1	1.00073(13)	0.3776(3)	1.0914(3)	0.0767(12)
O2	0.92965(12)	0.3169(3)	1.1175(3)	0.0626(10)
N1	1.02997(13)	0.1428(3)	1.1774(3)	0.0425(9)
N2	0.83447(13)	0.2720(3)	0.9023(3)	0.0497(10)
H2	0.8519	0.2944	0.9764	0.060*
C1	0.9515(2)	0.3733(4)	1.0582(4)	0.0496(13)
C2	0.91497(15)	0.4339(3)	0.9460(3)	0.0427(12)
H2A	0.8842	0.4592	0.9641	0.051*
H2B	0.9345	0.4935	0.9325	0.051*
C3	0.89525(16)	0.3699(3)	0.8277(4)	0.0403(11)
C4	0.91605(18)	0.3899(4)	0.7346(4)	0.0518(13)
H4	0.9432	0.4390	0.7483	0.062*
C5	0.8968(2)	0.3374(4)	0.6209(5)	0.0674(16)
H5	0.9102	0.3529	0.5581	0.081*
C6	0.8583(2)	0.2632(4)	0.6027(4)	0.0621(15)
H6	0.8458	0.2270	0.5276	0.075*
C7	0.83759(17)	0.2411(4)	0.6955(4)	0.0553(14)
H7	0.8114	0.1902	0.6822	0.066*
C8	0.85598(17)	0.2950(4)	0.8087(4)	0.0428(12)
C9	0.78783(18)	0.2164(4)	0.8849(4)	0.0468(13)
C10	0.73801(19)	0.2442(4)	0.7985(4)	0.0532(13)
C11	0.6925(2)	0.1869(5)	0.7809(5)	0.0710(17)
H11	0.6600	0.2066	0.7203	0.085*
C12	0.6947(2)	0.1003(5)	0.8526(6)	0.0746(18)
H12	0.6639	0.0609	0.8395	0.090*
C13	0.7422(2)	0.0721(4)	0.9431(5)	0.0628(14)

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Abstract

$C_{40}H_{28}Cl_4N_4O_4Zn$, monoclinic, $C2/c$ (no. 19), $a = 26.573(4)$ Å, $b = 12.898(2)$ Å, $c = 11.4503(17)$ Å, $\beta = 110.837(12)^\circ$, $V = 3667.8(10)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0631$, $wR_{\text{ref}}(F^2) = 0.1100$, $T = 293(2)$ K.

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The molecular structure of the title complex is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

A mixture of $Zn(OAc)_2 \cdot 2 H_2O$ (22 mg, 0.1 mmol), 1,10-phenanthroline (0.1 mmol, 18 mg), and 2-(2-((2,6-dichlorophenyl)amino)phenyl)acetic acid (H2dpa) (0.1 mmol,

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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}
H13	0.7435	0.0152	0.9940	0.075*
C14	0.78830(18)	0.1286(4)	0.9586(4)	0.0511(13)
C15	1.01730(15)	0.0496(4)	1.2141(4)	0.0404(11)
C16	1.03460(16)	−0.0444(4)	1.1796(4)	0.0449(12)
C17	1.06833(17)	−0.0396(4)	1.1096(4)	0.0569(14)
H17	1.0817	−0.1001	1.0874	0.068*
C18	1.08143(18)	0.0544(5)	1.0742(4)	0.0634(15)
H18	1.1036	0.0587	1.0271	0.076*
C19	1.06111(17)	0.1446(4)	1.1095(4)	0.0552(14)
H19	1.0699	0.2084	1.0842	0.066*
C20	1.01663(17)	−0.1390(4)	1.2170(4)	0.0570(14)
H20	1.0281	−0.2019	1.1954	0.068*

891 mg), was dissolved in 9 mL H₂O. The solution was heated in a 23 mL Teflon-lined autoclave under autogenous pressure at 373 K for 4 days. After cooling to room temperature colorless crystals formed.

Experimental details

Coordinates of hydrogen atoms were added using various restraints. Their *U*_{iso} values were set to 1.2*U*_{eq} of the parent atoms.

Comment

The design and construction of MOFs is based on organic ligands, which are different in size, exibility, coordination ability and so on [4]. In most situations, *N*-containing ligands are electrically neutral, while carboxylate ligands are negatively charged in these compounds. Among organic aromatic carboxylates, the 2-(2-(2,6-dichlorophenylamino)phenyl)acetate can yield predetermined networks [5–8]. On the other hand, 1,10-phenanthroline serves as co-ligand [9–11].

In the title complex, there is one half of a Zn(II), one Hdpa, and one half of the 1,10-phenanthroline ligand in the asymmetric unit (cf. the figure). Zn1 is six-coordinated with a distorted octahedral geometry by four O atoms from the Hdpa ligands, and two N atoms from one 1,10-phenanthroline ligand. The Zn–N bond length is 2.108(4) Å; and the Zn–O ones are in the range of 2.041(3) to 2.298(4) Å, respectively. The bond angles of O–Zn–O are in the range of 59.36(12)° to 144.6(2)°. All geometric parameters are comparable to related ones [12, 13]. There is a hydrogen bond between each O2 oxygen atom and the NH group of the organic ligands: d(N⋯O): 2.893(5) Å and N–H⋯O is 145.7 Å.

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