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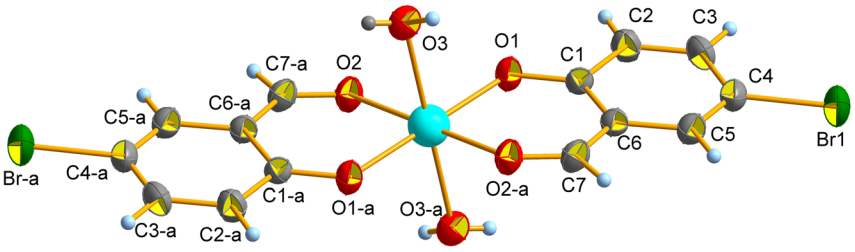
The crystal structure of diaqua-bis(4-bromo-2-formylphenoxy)zinc(II), $C_{14}H_{12}Br_2O_6Zn$



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Abstract

$C_{14}H_{12}Br_2O_6Zn$, monoclinic, $C2/c$ (no. 15), a = 29.43(2) Å, b = 4.774(4) Å, c = 11.658(9) Å, β = 103.194(7)°, V = 1595(2) Å^3, Z = 4, R_{gt} (F) = 0.0235, wR_{ref} (F^2) = 0.0647, T = 296(2) K.

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The molecular structure 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.

1 Source of material

5-Bromosalicylaldehyde (402 mg, 2 mmol) and zinc acetate (183 mg, 1 mmol) were added to ethanol (10 mL) and refluxed for 1 h to obtain the complex. The pure zinc complex can be obtained by removing solvent, washing with little cold ethanol and recrystallizing in ethanol (326 mg, 70% yield). The crystals of the title compound were obtained by slow evaporation within a week.

Table 1: Data collection and handling.

Crystal:	block
Size:	0.46 × 0.39 × 0.31 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	6.58 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
θ_{max}, completeness:	25.0°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	6951, 1406, 0.033
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 1282
$N(param)_{refined}$:	112
Programs:	Bruker [1], SHELX [2, 3]

2 Experimental details

All hydrogen atoms were identified in difference Fourier syntheses. The U_{iso} values of the methyl groups were set to $1.5U_{eq}$(C) and the U_{iso} values of all other hydrogen atons were set to $1.2U_{eq}$(C).

3 Comment

Zinc complexes have a wide range of biological activities. It can be used with drugs for the treatment of Alzheimer's disease, as well as antibacterial, anticonvulsant, antidiabetic, anti-inflammatory and antiproliferative-antitumor [4–8].

Herein, a new bis(4-bromo-2-formylphenoxy)zinc dihydrate compound was synthesized and characterized by single-crystal X-ray diffraction [1–3]. In the crystal, the complex exhibits crystallographic C_i symmetry with the Zn(II) atom located on an inversion center. Two 5-bromosalicylaldehyde anions are chelated through their phenolate O(1) and carbonyl O(2) oxygen atoms in trans-position

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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	0.000000	0.000000	0.000000	0.02945 (16)
Br1	0.22301 (2)	0.41307 (10)	−0.15865 (3)	0.06235 (18)
O1	0.05905 (6)	0.2199 (4)	0.05857 (16)	0.0335 (4)
O2	−0.03340 (7)	0.2070 (4)	0.11757 (16)	0.0337 (4)
C1	0.09456 (9)	0.2460 (5)	0.0101 (2)	0.0283 (5)
O3	0.02383 (8)	−0.3061 (4)	0.13883 (18)	0.0374 (5)
H3A	0.040732	−0.430456	0.115160	0.056*
C4	0.17177 (10)	0.3396 (7)	−0.0903 (3)	0.0391 (7)
C6	0.10011 (9)	0.0945 (5)	−0.0909 (2)	0.0292 (6)
C5	0.13898 (10)	0.1455 (6)	−0.1397 (2)	0.0365 (6)
H5	0.142333	0.046330	−0.205909	0.044*
C7	0.06901 (10)	−0.1242 (6)	−0.1452 (2)	0.0338 (6)
H7	0.076727	−0.213798	−0.209017	0.041*
C3	0.16772 (10)	0.4840 (7)	0.0104 (3)	0.0410 (7)
H3	0.190588	0.612163	0.044764	0.049*
C2	0.13029 (10)	0.4385 (6)	0.0590 (3)	0.0380 (7)
H2	0.128237	0.537199	0.126435	0.046*
H3B	0.0048 (15)	−0.384 (10)	0.151 (4)	0.070 (15)*

to the metal ion and occupied on the equatorial plane. At the same time, the planes of the two 5-bromo-salicylaldehyde anions are parallel to each other. A slightly distorted octahedral coordination geometry of Zn(II) is furnished by the oxygen atoms of two water molecules in axial positions. The geometry of the metal center is similar to those of the earlier reported zinc(II) complexes with substituted salicylaldehyde ligands [9–13].

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Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

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