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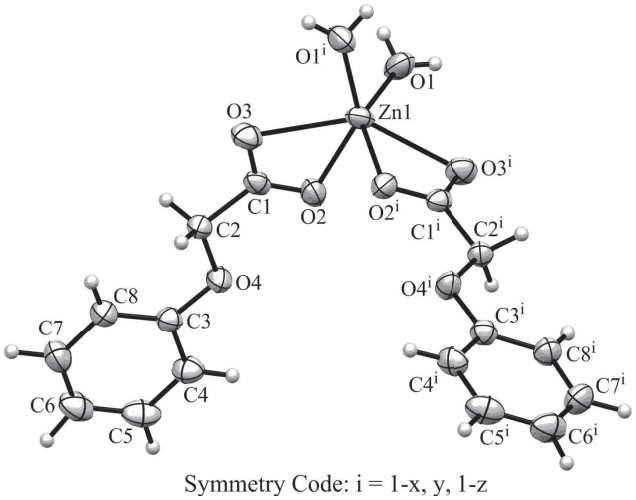
Crystal structure of diaquabis(phenoxyacetato-κ²*O*,*O*′)-zinc(II), $C_{16}H_{18}O_8Zn$



Symmetry Code: i = 1-x, y, 1-z

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Abstract

$C_{16}H_{18}O_8Zn$, Monoclinic, *C*2, $a = 11.612(2)$ Å, $b = 5.2119(11)$ Å, $c = 13.762(3)$ Å, $\beta = 101.151(3)°$, $V = 817.2(3)$ Å^3, $Z = 2$, $R_{gt}(F) = 0.0248$, $wR_{ref}(F^2) = 0.0790$, $T = 296(2)$ K.

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Source of material

An aqueous solution (8 mL) of phenoxyacetic acid (270 mg, 1.8 mmol), $NaHCO_3$ (150 mg, 1.8 mmol) was added into an aqueous solution (2 mL) dissolving $Zn(NO_3)_2{\cdot}6H_2O$ (360 mg, 1.2 mmol). To the mixture a methanolic solution of imidazole (60 mg, 0.8 mmol) was added, resulting a colorless solution. Colorless block crystals were obtained after two weeks (yield 140 mg, 38.5%), in which imidazole molecules were not included.

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Table 1: Data collection and handling.

Crystal:	Colorless, block, size 0.19×0.21×0.25 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	15.46 cm^{-1}
Diffractometer, scan mode:	CCD area detector, φ and ω scans
$2\theta_{max}$:	56.72°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	2570, 1714
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 1670
$N(param)_{refined}$:	150
Programs:	SHELX [9]

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

Atom	Site	*x*	*y*	*z*	U_{iso}
H(1A)	4*c*	0.141(4)	0.53(1)	0.429(3)	0.08(2)
H(1B)	4*c*	0.042(4)	0.607(9)	0.407(3)	0.05(1)
H(2A)	4*c*	−0.284(3)	−0.166(7)	0.283(2)	0.038(9)
H(2B)	4*c*	−0.266(3)	−0.352(7)	0.375(2)	0.038(9)
H(4)	4*c*	−0.083(3)	−0.75(1)	0.176(2)	0.039(8)
H(5)	4*c*	−0.183(4)	−1.05(1)	0.065(3)	0.07(1)
H(6)	4*c*	−0.377(4)	−1.10(1)	0.043(3)	0.07(1)
H(7)	4*c*	−0.489(3)	−0.82(1)	0.125(3)	0.06(1)
H(8)	4*c*	−0.388(3)	−0.53(1)	0.237(3)	0.06(1)

Experimental details

All the hydrogen atoms were found from the Fourier difference map.

Discussion

The rigid aromatic carboxylic acids have been extensively used to construct metal complexes with fascinating topological structures [1, 2]. On the other hand, flexible aromatic carboxylic ligands have not been much studied due to their varied geometries and conformations [3, 4]. Phenoxyacetic acid (pa) and its derivatives, a class of flexible aromatic carboxylic ligands, have been applied in agriculture such as herbicides, etc. [5]. In recent, they have been used as ligands to build carboxylic complexes [6–8]. In this paper, we report the synthesis, crystal structure of a phenoxyacetic acid (pa) complex, $[Zn(pa)_2(H_2O)_2]$.

Table 3: Atomic displacement parameters (Å^2).

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Zn(1)	2*b*	0.0	0.22814(2)	0.5	0.0422(2)	0.0201(2)	0.0342(2)	0.0	−0.0000(1)	0.0
O(1)	4*c*	0.0759(2)	0.4871(5)	0.4270(2)	0.037(1)	0.034(1)	0.072(2)	0.0086(9)	0.012(1)	0.015(1)
O(2)	4*c*	−0.0379(2)	−0.0557(4)	0.3883(2)	0.0321(9)	0.032(1)	0.042(1)	−0.0057(8)	−0.0004(8)	0.0041(8)
O(3)	4*c*	−0.1914(2)	0.0855(4)	0.4417(2)	0.049(1)	0.032(1)	0.039(1)	−0.0012(9)	0.0033(9)	−0.0098(8)
C(1)	4*c*	−0.1453(2)	−0.0661(5)	0.3895(2)	0.037(1)	0.023(1)	0.027(1)	−0.003(1)	−0.002(1)	0.0032(8)
C(2)	4*c*	−0.2252(2)	−0.260(1)	0.3299(2)	0.029(1)	0.027(1)	0.0317(9)	0.001(2)	0.0032(8)	−0.004(2)
O(4)	4*c*	−0.1612(2)	−0.4269(4)	0.2790(1)	0.0281(9)	0.033(1)	0.045(1)	−0.0010(8)	0.0062(8)	−0.0127(8)
C(3)	4*c*	−0.2268(2)	−0.6004(6)	0.2172(2)	0.033(1)	0.027(1)	0.030(1)	0.000(1)	0.005(1)	−0.0018(9)
C(4)	4*c*	−0.1641(2)	−0.760(1)	0.1649(2)	0.042(1)	0.034(2)	0.040(1)	0.003(2)	0.014(1)	−0.004(2)
C(5)	4*c*	−0.2231(3)	−0.9403(7)	0.1001(2)	0.068(2)	0.035(2)	0.036(1)	0.005(1)	0.016(1)	−0.007(1)
C(6)	4*c*	−0.3429(3)	−0.9620(7)	0.0863(2)	0.064(2)	0.037(2)	0.038(1)	−0.005(2)	−0.004(1)	−0.008(1)
C(7)	4*c*	−0.4044(3)	−0.807(1)	0.1389(2)	0.041(1)	0.041(3)	0.050(1)	−0.008(2)	−0.004(1)	−0.005(2)
C(8)	4*c*	−0.3475(2)	−0.6255(6)	0.2044(2)	0.034(1)	0.034(2)	0.042(1)	0.000(1)	0.004(1)	−0.006(1)

The asymmetric unit of the title complex consists of one half of a Zn^{2+} ion, one pa^- ligand, and a water ligand. Each Zn^{2+} ion is six coordinated in a distorted triprism geometry with four oxygen atoms of two pa^- ligands, and the other two oxygen atoms of two water molecules. Each pa^- ligand adopts chelating mode to coordinate with the Zn^{2+} ion by using the carboxylate group. The oxyacetate group is almost parallel to the phenyl ring, with the torsion angle of C1–C2–O4–C3 being −175.9(2)°. Each water molecule is hydrogen bonded with two different carboxyl groups from the two $[Zn(pa)_2(H_2O)_2]$ molecules (O1–H1A$\cdots$O3 = 2.719(3), O1–H1B$\cdots$O2 = 2.727(3) Å). Thus, each $[Zn(pa_2(H_2O)_2]$ complex is hydrogen bonded with six neighboring complexes to form a 2-D hydrogen bonding sheet.

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