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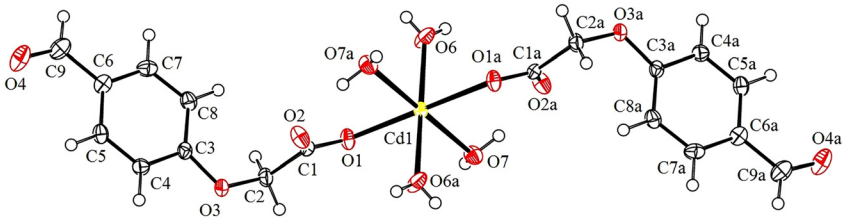
Crystal structure of tetraaqua-(2-(4-formylphenoxy)acetato-k^1*O*)cadmium(II), $C_{18}H_{22}O_{12}Cd$



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Abstract

$C_{18}H_{22}O_{12}Cd$, monoclinic, $P2_1/c$ (no. 14), a = 13.3069(9) Å, b = 9.9041(6) Å, c = 8.1580(5) Å, β = 96.244(10)°, V = 1031.57(12) Å^3, Z = 2, $R_{gt}(F)$ = 0.0216, $wR_{ref}(F^2)$ = 0.0522, T = 200 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.

Source of material

An amount of 0.180 g 4-formylphenoxyacetic acid (1.0 mmol) and 0.040 g NaOH (1.0 mmol) were dissolved into 15 ml ethanol-water (v:v = 2:1) solution with stirring at room temperature. After the solution was stirred for 1.0 h, 5 ml water solution of 0.150 g cadmium nitrate tetrahydrate (0.5 mmol) was added. The mixture was stirred for 6 h at 70 °C. The colorless crystals of the title compound were obtained through slow evaporation in 25 days.

Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	0.14 × 0.12 × 0.09 mm
Wavelength:	Mo Kα radiation (0.71073 Å)
μ:	1.12 mm^{-1}
Diffractometer, scan mode:	SuperNova, ω
θ_{max}, completeness:	25.0°, 99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	3892, 1801, 0.022
Criterion for I_{obs}, $N(hkl)_{gt}$:	I_{obs} > 2 σ(I_{obs}), 1577
$N(param)_{refined}$:	158
Programs:	Bruker [1], Olex2 [2], Shelx [3], Diamond [4]

Experimental details

The hydrogen atoms were positioned geometrically. Their U_{iso} values were set to 1.2U_{eq} or 1.5U_{eq} of the parent atoms.

Comment

Over the past decades, transition metal complexes show rich coordination pattern [5, 6] and properties in some fields [7–10]. The Co(II), Mn(II) and Cu(II) complexes using 4-formylphenoxylate as ligand have been reported by Das [11]. Our group has been studying the synthesis, structure and properties of related metal complexes [12–15].

In the title complex, the fundamental unit contains a Cd(II) ion, two 4-formylphenoxyacetic acid ligands and four coordinated water molecules. The asymmetric unit is one half of the complex (see the figure). The Cd(II) ion is six-coordinated with two O atoms from two 4-formylphenoxyacetate ligands and four O atoms from four coordinated

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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}
Cd1	0.000000	0.500000	0.500000	0.01528 (10)
O1	0.07432 (11)	0.44096 (15)	0.28565 (19)	0.0204 (4)
O2	0.15987 (13)	0.63688 (15)	0.29804 (19)	0.0255 (4)
O3	0.21540 (11)	0.58490 (15)	0.01171 (19)	0.0211 (4)
O4	0.70560 (13)	0.68907 (17)	0.1859 (2)	0.0360 (4)
O6	0.08108 (15)	0.32591 (17)	0.6719 (2)	0.0301 (5)
H6A	0.058 (3)	0.252 (2)	0.702 (4)	0.080 (12)*
H6B	0.137 (2)	0.325 (3)	0.712 (3)	0.021 (8)*
O7	−0.14666 (13)	0.37704 (18)	0.3833 (2)	0.0237 (4)
H7A	−0.162 (2)	0.355 (3)	0.472 (4)	0.039 (9)*
H7B	−0.147 (3)	0.316 (3)	0.324 (4)	0.055 (11)*
C1	0.12889 (17)	0.5257 (2)	0.2318 (3)	0.0171 (5)
C2	0.1559 (2)	0.4854 (2)	0.0689 (3)	0.0216 (6)
H2A	0.195250	0.401643	0.089148	0.026*
H2B	0.091495	0.469000	−0.020538	0.026*
C3	0.32133 (16)	0.5884 (2)	0.0797 (3)	0.0173 (5)
C4	0.37323 (17)	0.6804 (2)	0.0022 (3)	0.0198 (5)
H4	0.335054	0.735801	−0.085369	0.024*
C5	0.48019 (16)	0.6888 (2)	0.0549 (3)	0.0200 (5)
H5	0.514450	0.749270	0.001815	0.024*
C6	0.53824 (17)	0.6075 (2)	0.1876 (3)	0.0198 (5)
C7	0.4858 (2)	0.5183 (2)	0.2654 (3)	0.0235 (6)
H7	0.524256	0.464421	0.354519	0.028*
C8	0.3773 (2)	0.5071 (2)	0.2139 (3)	0.0219 (6)
H8	0.342965	0.447125	0.267520	0.026*
C9	0.65201 (19)	0.6129 (2)	0.2431 (3)	0.0281 (6)
H9	0.686527	0.553633	0.328890	0.034*

water molecules, forming a distorted octahedral coordination geometry. The Cd1–O bond distance are 2.3136(16) Å (O1, O1a), 2.2913(17) Å (O6, O6a) and 2.2695(17) Å (O7, O7a), respectively. The sum of bond angles around Cd1 (O7–Cd1–O6a 86.92(6)°, O6a–Cd1–O7a 93.08(6)°, O7a–Cd1–O6 86.92(6)°, O6–Cd1–O7 93.08(6)°) is 360. The complex molecules form 1D chained structure by hydrogen bonds.

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