CRYSTAL STRUCTURE OF ADIPATE ZINC DIHYDRATE

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Figure 1. ORTEP plot of a portion of the structure of adipate zinc dihydrate drawn at the 50% probability level. Selected bond distance and angles: Zn1-Ow = 2.007(3), Zn1-O1 = 2.120(3), Zn1-O2 = 2.246(3), O1-C1 = 1.260(5), O2-C1 = 1.248(4) Å; Ow-Zn1-Ow^a = 100.5(2), Ow-Zn1-O1 = 90.5(1), Ow^a-Zn1-O1 = 103.0(1), O1-Zn1-O1^a = 159.0(2), Ow-Zn1-O2 = 148.7(1), Ow^a-Zn1-O2 = 95.1(1), O1-Zn1-O2 = 59.5(1), O1^a-Zn1-O2 = 103.8(1), O2-Zn1-O2^a = 84.9(1)°. Symmetry code: a = -x, y, 1/2-z.

Comment

The two carboxylate groups in adipic acid have been employed as building blocks to form coordination polymers [1-3]. In $[\text{Zn}(\text{O}_2\text{CC}_4\text{H}_8\text{CO}_2)(\text{H}_2\text{O})_2]_n$, the zinc atom is located on a twofold symmetry axis and is six-coordinated in a distorted octahedral geometry defined by two water molecules and two carboxylate groups derived from two symmetry related bis-bidentate adipate ligands (Figure 1). The adipate ligand acts as a bridging ligand by connecting adjacent two zinc(II) atoms to form an infinite one-dimensional zigzag chain, which, through H-bonding between hydrate oxygens and carboxylate oxygens, are assembled into a two-dimensional structure along *c*-axis (Figure 2). Further H-bonding along the *b*-axis, *i.e.* between layers, results in the formation of a three-dimensional structure (Figure 3). The structure is very similar to the three-dimensional structure formed by zinc(II) and terephthalic acid [4].

Figure 2. ORTEP plot showing two-dimensional structure in adipate zinc dihydrate connected by H-bonds, viewed along the *c*-axis.

Figure 3. ORTEP plot showing three-dimensional structure of adipate zinc dihydrate connected by H-bonds viewed along the *b*-axis.

Experimental

Adipic acid (0.16g, 1.0mmol) was added to a solution of $\text{Zn}(\text{NO}_3)_2$ (10 cm³ of 0.4 mol L⁻¹). The pH was adjusted to 5~6 by adding NaOH solution. After most of the acid was dissolved, the mixture was filtered and set aside at room temperature. Colorless single crystals suitable for X-ray diffraction were obtained in a few days.

Table 1. Crystal data for adipate zinc dihydrate complex

Empirical formula	$\text{C}_6\text{H}_{12}\text{O}_6\text{Zn}$	Formula weight	245.53
Space group	<i>C2/c</i>	Diffractometer	Enraf-Nonius CAD4
<i>a</i> , Å	16.373(3) Å	<i>b</i> , Å	5.426(1)
<i>c</i> , Å	10.755(2)	β , °	97.89(3)
<i>V</i> , Å ³	946.5(3)	<i>Z</i>	4
<i>D</i> _{calc} , g cm ⁻³	1.723	μ (Mo- <i>K</i> α), mm ⁻¹	2.591
<i>F</i> (000)	504	θ range, °	2.5–26.0
<i>T</i> , °C	25	Trans. Factors (ω -scans)	0.796–0.998 [5]
Reflections collected	961	Independent reflections	928 (<i>R</i> _{int} 0.023)
Reflections with $I > 2\sigma(I)$	784	No. parameters refined	68
<i>R</i> (all data)	0.053	Final <i>R</i> [$I > 2\sigma(I)$]	0.041
<i>wR</i> (all data)	0.087	Goodness-of-fit on <i>F</i> ²	1.06
Weighting scheme	$1/[\sigma^2(F_o^2) + (0.0339P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$		
Diff. hole and peak, eÅ ⁻³	-0.30 to 0.36	CCDC deposition no	176388
Programs	SHELXS-97 [6], SHELXL-97 [7], ORTEP [8]		

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