CRYSTAL STRUCTURE OF ZINC(II) 4,4'-OXYBIS(BENZOATE)

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Figure 1. ORTEP plot of the title complex at the 50% probability level. Selected bond distances and angles: Zn1—O1 = 1.971(3), Zn1—O2A = 1.978(3), Zn1—O3B = 1.953(3), Zn1—O4C = 1.945(3) Å; O1—Zn1—O2A = 105.7(1), O1—Zn1—O3B = 114.1(1), O1—Zn1—O4C = 103.3(1), O2A—Zn1—O3B = 107.8(1), O2A—Zn1—O4C = 110.0(1), O3B—Zn1—O4C = 115.4(2)°. Symmetry transformation: $a = 1 - x, -y, 1 - z$; $b = 3/2 - x, y - 1/2, 1/2 - z$, $c = x - 3/2, 1/2 - y, 1/2 + z$.

COMMENT

Metal-organic frameworks based on rigid linear dicarboxylate linkers have attracted considerable attention because of their intrinsic aesthetic appeal and potentially exploitable properties [1]. More recently, rigid angular dicarboxylate linkers with a 120° angle [2] and a 90° angle [3] between two functional groups have been used to construct discrete nanometer-sized polygons and nanoscopic rectangles, respectively. We believe that other angular dicarboxylate ligands would be also ideal for building extended coordination polymers, as demonstrated by 4,4'-oxybis(benzoate), with a 118° angle between the two benzoate groups (Figure 1). The slightly distorted tetrahedral geometry of Zn(II) atom is completed by four oxygen atoms derived from four different 4,4'-oxybis(benzoate) ligands, with similar Zn—O distances shorter than those found in bis(4,4'-bipyridine)zinc(II) succinate [4]. Each 4,4'-oxybis(benzoate) ligand coordinates four zinc(II) atoms through its two carboxylate groups in a bis-bidentate fashion leading to a three-dimensional framework (Figure 2).

EXPERIMENTAL

The title compound was obtained from a hydrothermal synthesis by reacting zinc nitrate, 4,4'-oxybis(benzoic) acid and sodium hydroxide in a 1:1:2 molar ratio at 180°C for 60 hours. CH analysis: C 52.29, H 2.51%. Calc. for $C_{14}H_8O_5Zn$: C 52.40, H 2.45%.

Table 1. Crystal data for zinc(II) 4,4'-oxybis(benzoate)

Empirical formula	C ₁₄ H ₈ O ₅ Zn	Formula weight	321.57
Crystal system	Monoclinic	Space group	<i>P</i> 2 ₁ / <i>c</i>
Unit cell dimensions	<i>a</i> = 7.355(3) Å <i>b</i> = 16.034(5) Å <i>c</i> = 10.575(8) Å	β	102.64(2)°
<i>Z</i>	4	Volume	1216.9(11) Å ³
μ , mm ⁻¹	2.034	<i>T</i>	293 K
θ range	2.4 – 27.0°	<i>D</i> _{exptl} , g cm ⁻³	1.755
Independent reflections	2664 (<i>R</i> _{int} = 0.040)	<i>F</i> (000)	648
Goodness-of-fit on <i>F</i> ²	1.04	Reflections with <i>I</i> > 2 σ (<i>I</i>)	1965
<i>R</i> (all data)	0.124	Parameters refined	182
Weighting scheme, <i>w</i>	[$\sigma^2 + (0.078P)^2 + 0.8449P$] ⁻¹ where $P = (F_o^2 + 2F_c^2)/3$	Final <i>R</i> [<i>I</i> > 2 σ (<i>I</i>)]	0.050
Programs	ORTEP-II [5], SHELX-97 [6]	Diff. hole and peak	-0.46 – 0.42 eÅ ⁻³
		CCDC deposition no.	185137

Figure 2. Perspective view of the structure along *a* axis.**ACKNOWLEDGMENTS**

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