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Crystal and Molecular Structures of Tetraaqua(di-*para*-oxybenzoato)iron(II) Tetrahydrate

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Abstract—The new complex $[(p\text{-HOC}_6H_4CO_2)_2Fe(H_2O)_4] \cdot 4H_2O$ is synthesized and studied by X-ray diffraction analysis. The Fe(II) cation is coordinated by two *para*-hydroxybenzoate anions through the monodentate mode. Four oxygen atoms of the water molecules complete the coordination polyhedron of the central atom to an octahedron. Four molecules of water of crystallization “cross-link” the monomers to form a polymeric structure.

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INTRODUCTION

The simplest representative of aromatic hydroxyacids, *para*-hydroxybenzoic acid (p-HOC_6H_4COOH), is met in soils [1], sea water [2], various organs of plants, grape leaves and berries [3], and sweet beet [4] and is introduced into food products as a preserving agent [5]. This acid composes a number of pharmaceuticals that stimulate inotropic effects of human heart and is active against arrhythmia [6].

Based on the aforesaid, it seems interesting to synthesize and study by X-ray diffraction analysis complexes of hydroxybenzoic acid with microelements, namely, with iron(II), which is in the composition of hemoglobin.

EXPERIMENTAL

Single crystals of $HOC_6H_4COO)_2Fe(H_2O)_4] \cdot 4H_2O$ (**I**) for X-ray diffraction analysis was prepared by the reaction of aqueous solutions of iron(II) sulfate and sodium p-hydroxybenzoate taken in a ratio of 1 : 2. The mixture of the solutions heated to boiling was cooled to room temperature. After several days, brown crystals of **I** precipitated from the mixture.

The X-ray diffraction analysis was carried out on an Enraf-Nonius CAD-4 automated diffractometer.

The crystals are orthorhombic: $a = 7.758(3)$, $b = 11.225(5)$, $c = 24.152(5)$ Å, $V = 2099(1)$ Å^3, $M = 464$, $\rho_{\text{calcd}} = 1.498$ g/cm^3, $Z = 4$, space group *Pcab*, $R = 0.027$, $T = 295$ K.

The intensities of 2835 independent reflections were measured for the crystal 0.14 × 0.18 × 0.21 mm in size ($\text{Mo}K_\alpha$ radiation, $\lambda = 0.71073$ Å, $\theta = 9.92°–18.12°$, $\mu = 10.73$ mm^{-1}).

The structure of complex **I** was determined by the heavy atom method [7]. The coordinates of atoms are given in Table 1 (the values of the thermal parameters

Table 1. Coordinates of atoms ($\times 10^4$) in structure **I**

Atom	*x*	*y*	*z*
Fe	500	500	0
O(1)	9659(7)	4627(5)	831(2)
O(2)	8987(8)	2702(4)	830(3)
O(3)	9225(9)	3745(3)	3416(3)
O(4)	2271(5)	5828(4)	116(4)
O(5)	8409(7)	4519(4)	869(2)
C(1)	9325(8)	3675(7)	1092(4)
C(2)	9268(9)	3679(6)	1698(5)
C(3)	8519(9)	2749(7)	2561(4)
C(4)	8449(8)	2753(8)	2554(5)
C(5)	9216(8)	3688(9)	2861(4)
C(6)	10012(11)	4629(7)	2563(4)
C(7)	1002(1)	4632(8)	2005(4)

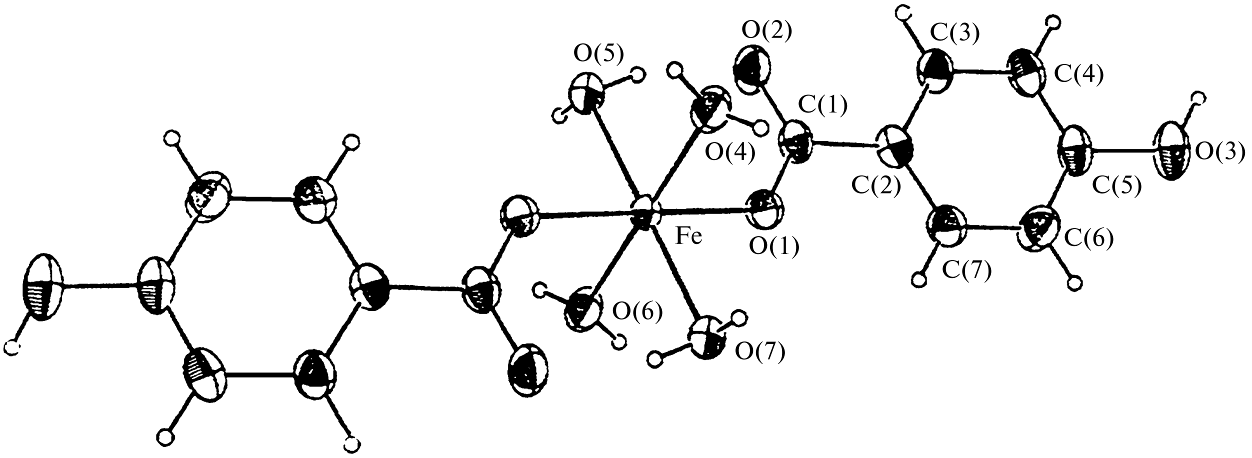

Fig. 1. Structure of $[(p\text{-HOC}_6\text{H}_4\text{CO}_2)_2\text{Fe(H}_2\text{O)}_4] \cdot 4\text{H}_2\text{O}$.

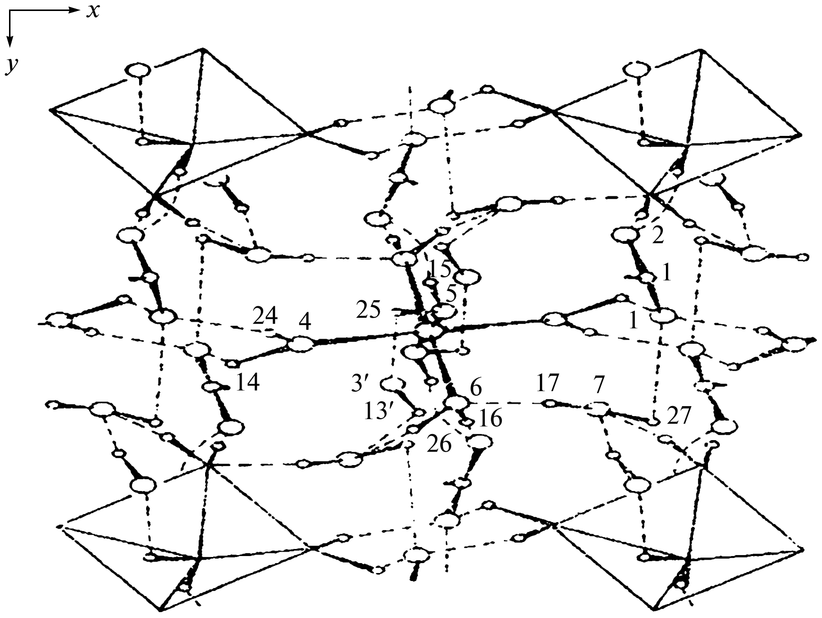

Fig. 2. Projection of the fragment of the structure of complex **I** on the plane [001].

Table 2. Selected bond lengths and bond angles in structure **I**

Bond	*d*, Å	Bond	*d*, Å	Bond	*d*, Å
Fe–O(1)	2.162(5)	O(1)–C(1)	1.243(2)	C(2)–C(3)	1.40(1)
		O(2)–C(1)	1.268(5)	C(3)–C(4)	1.36(1)
Fe–O(4)	2.284(3)	O(3)–C(5)	1.352(2)	C(4)–C(5)	1.40(1)
Fe–O(5)	2.287(5)	C(1)–C(2)	1.472(4)	C(5)–C(6)	1.41(1)
		O(3)–H(13)	1.02(3)	C(6)–C(7)	1.37(1)
Angle	ω, deg	Angle	ω,deg	Angle	ω, deg
O(1)FeO(4)	92.41(2)	C(1)C(2)C(3)	121.67(4)	C(2)C(3)C(4)	122.25(7)
O(1)FeO(7)	90.02(2)	C(1)C(2)C(7)	121.12(3)	C(3)C(2)C(1)	119.81(7)
O(7)FeO(6)	89.87(3)	O(3)C(5)C(4)	122.54(7)	C(5)C(6)C(7)	119.34(4)
O(1)C(1)O(2)	121.72(3)	O(3)C(5)C(6)	118.65(4)	C(6)C(7)C(2)	122.81(3)
O(2 C(1)C(2)	119.16(3)	C(3)C(2)C(7)	118.19(4)		

are available from the authors). Selected bond lengths and bond angles are listed in Table 2.

RESULTS AND DISCUSSION

In the centrosymmetric molecule of complex **I** (Fig. 1), the Fe^{2+} ion is coordinated by four oxygen atoms of the water molecules [8]. The iron atom is completed to the octahedral coordination by two oxygen atoms of the carboxylate groups of two monodentate *para*-hydroxybenzoate anions. Four molecules of water of crystallization “cross-link” the monomers to form the polymeric structure (Fig. 2).

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