





Figure 1. Formation of the biclinic parallelepiped. (a): orthorhombic parallelepiped, (b):monoclinic parallelepiped, (c): biclinic parallelepiped.

Keywords: crystal system, space group, formulae, kaolinite

MS15-P23 Crystal Structure of a New Coordination Polymer

Hamadene Malika¹, Benhacine Mohamed El-Amin¹, Bouacida Sofiane², Merazig Hocine²

1. Laboratoire de Cristallographie-Thermodynamique, Faculté de Chimie, U.S.T.H.B, Alger, Algérie

 Unité de Recherche de Chimie de l'Environnement et Moléculaire Structurale, Faculté des Sciences Exactes, Université des frères Mentouri, Constantine 1, 25000, Algérie

email: hamadene.m21@gmail.com

The oxalate dianion is one of the most studied ligands. capable of bridging two or more metal centres and creating inorganic polymers based on the assembly of metal polyhedra with a wide variety of one-, two - or three dimensional extended structures. Among the oxalate-based compounds M with the general formula $AM(C_2O_4)_2$.n (H₂O) (A= alkali metal and , M= trivalent element), only a few crystal structures involving sodium metal have been reported in the literature with M=Yb [1]<. As a continuation of work on mixed oxalate-based compounds with a tri- or bivalent element [2] a new diaquasodium(I)]-µ-oxalato-k⁴ catena-poly[[01,02:01,02 -[diaquairon(III)]-µ -oxalato-k⁴O1,O2:O1',O2'], [NaFe(C₂O₄),(H₂O₄], has been prepared and its crystal structure elucidated by single-crystal X-Ray diffraction analysis [3]. The compound crystallizes in the non centrosymmetrical space group $I4_1$ (Z = 4). The asymmetric unit contains one Na(I) atom and one Fe(III) atom lying on a fourfold symmetry axis, one oxalate ligand and two aqua ligands. Each metal atom is surrounded by two chelating oxalate ligands and two equivalent water molecules, in a cis arrangement. The structure consists of infinite one-dimensional chains of NaO₄(H₂OW2)₂ alternating FeO₄(H₂OW1)₂ and octahedra, bridged by oxalate ligands, parallel to the [100] and [010] directions, respectively (Fig. 1). Because of the cis configuration and the µ2-coordination mode of the oxalate ligands, the chains run in a zigzag manner. This arrangement facilitates the formation of hydrogen bonds between neighboring chains involving the H_oO and oxalate ligands, leading to a two-dimensional framework. The resulting framework exhibits tunnels parallel to the c axis with an elliptic cross-section as shown in Fig. 1. The structure of this new one dimensional coordination polymer is shown to be unique among the $A^{I}M^{III}(C_{2}O_{4})_{2}(H_{2}O)_{n}$ series. The thermal decomposition behavior has been studied by TG and DTA and gave as a final product the well-known ternary oxide NaFeO₂ [1] Chapelet-Arab B., Duvieubourg, L., Nowogrocki G., Abraham F., Grandjean S. (2006). J. Solid State Chem. 179, 4029 [2] Kherfi H., Hamadène M., Guehria A., Dahaoui S. & LecomteC. (2011). Acta Cryst. C67, m85 (2013). Acta Cryst. E69, m493 [3]Benhacine M.A., Hamadène M., Bouacida S., Mérazig H. (2016). Acta Cryst. C72, 243

Keywords: absolute structure, one-dimensional chains, new structural type