MS16- Understanding of functional materials

Chairs: Dr. Oleg Siidra, Dr. Claire Colin

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Synthesis structure determination of béta-$K_{0.399}V_{2.623}W_{0.377}O_{7.5}$ with mixed occupation of vanadium and tungsten elements

Djillali Mezaoui[1], Sabrina Belkhiri[2], Olivier Perez[3]

1. U.S.T.H.B, Laboratoire des Sciences des Matériaux, Faculté de chimie, Alger, Algeria
2. Université de Boumerdès, Laboratoire Sciences des Matériaux, L.S.M, Boumerdès, Algeria
3. Laboratoire de cristallographie et Sciences des matériaux, CRISMAT, UMR 6508 CNRS, CAEN, France

email: mezaoui_dji@yahoo.fr

The title compound vanadium-tungsten mixed oxide bronze $K_{0.399}V_{2.623}W_{0.377}O_{7.5}$ was prepared by solid state reaction at 700°C in an evacuated silica ampoule. The single crystal $K_{0.399}V_{2.623}W_{0.377}O_{7.5}$ crystallizes in the monoclinic system, C 2/m (n°12) space group, with cell parameters a = 15.7123 (3) Å, b = 3.6796 (6) Å, c = 10.2092 (2) Å and b = 108.994° (4) .This phase is isostructural to b-$K_xV_2O_5$ called: Bannermanite family with x ranging between 0.19 and 0.4.

The idea of this work is to incorporate the vanadium and the tungsten in the same site in order to distort the octahedral polyhedra occupied by the transition metals M (M : vanadium and tungsten elements). The irregular octahedral site is based on the presence of long (M−O) and short bonds (M=O) formed between the transition metal and the oxygen. On the other side, the distortion involves a polarization along the short and long bonds, which can be the origin to improve the electronic delocalization and the no linear optical property. In this context, in 2009 and 2012 we synthesized two single crystals $K_{1.65}V_{1.78}W_{0.22}As_2O_{10}$ (Acta Cryst. (2009). E65, i69) and $K_2V_2As_2O_{10}$ (Acta Cryst. (2012). E68, i54) isostructural to $KTiPO_5$. The comparison between the MO_6 octahedra (M: 78% of vanadium and 22% of tungsten) of $K_{1.65}V_{1.78}W_{0.22}As_2O_{10}$ and VO_6 octahedra of $K_2V_2As_2O_{10}$, showed clearly a strong distortion in “M” site due to the mixed occupation of vanadium and tungsten simultaneously. Furthermore the mixed occupation creates two short bonds, which can have a strong impact on the no linear optical property.

We are interested in the mixed occupation of vanadium and tungsten to improve the physical properties specially the electronic conduction and the no linear optical property, and explain these physical behavior by the structural arrangement of the atoms. In this context, the electrical conductivity measurement as function of various temperatures ranging (between 400 and 625 K) and frequency (100 - 10^5 Hz) showed a semi-conductor behavior for $K_{0.399}V_{2.623}W_{0.377}O_{7.5}$. The flexibility of the investigated structure gives the possibility to substitute the potassium ion by another alkaline ion with small size as lithium, in order to create a new material used as a rechargeable electrode in the lithium batteries.

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