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THE STRUCTURE DETERMINATION OF A NEW MIXED MONOARSENATE $K_2V_2O_2(AsO_4)_2$

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Abstract : In two years later we synthetized a new compound $K_{1.65}V_{1.78}W_{0.22}O_2(AsO_4)_2$ [1] belonging to $KTiOPO_4$ family (KTP) [2]. The structure of KTiOPO4 is known by the presence of an irregular octahedron with one short bond (1.653 (5) Å to 1.851 (5) Å)) [3] which the most responsible of the non linear optical property. In the case of our compound ($K_{1.65}V_{1.78}W_{0.22}O_2(AsO_4)_2$), the structure shows an irregular MO_6 octahedra (M=V+W) with two abnormal short bonds M—O (1.774 (7) Å) and(1.824 (8) Å) whichsuggest that the non linear optical property could be more important in this compound, because the most physical related to structural studies showed that the non linear optical property is due to the short bond in the octahedral polyhedral [3]. We are interested on $K_{1.65}V_{1.78}W_{0.22}O_2(AsO_4)_2$ for these two short bonds, we substituted the tungsten by the vanadium element in order to show the influence of the tungsten and vanadium on the distortion of the MO6 octahedra. We synthetized and studied the structure of new single-crystal $K_2V_2O_2(AsO_4)_2$ [4] isotype to $KVOPO_4$ [5], we describe here the structure of $K_2V_2O_2(AsO_4)_2$. The program used to resolve this structure is Superflip [6] and we realized the refinement of the structure by Jana 2006 program [7].

Keywords : Arsenate, KTiOPO4 family, non linear optical property