Poster Presentation

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Structure Determination of New Phases K1.65V1.78W0.22O2(AsO4)2 and K2V2O2(AsO4)2

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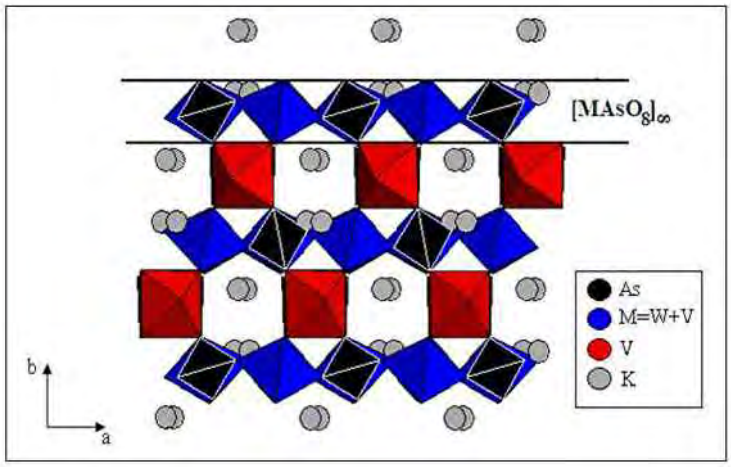
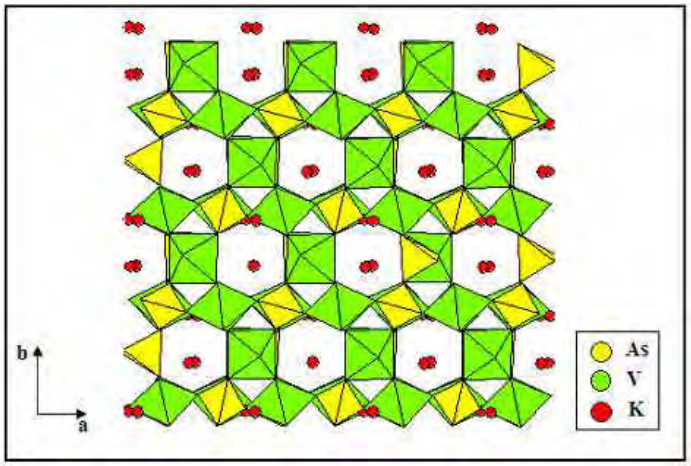
Two new phases K1.65V1.78W0.22O2(AsO4)2 and K2V2O2(AsO4)2 [1,2] belonging to KTiOPO4 family (KTP) [3] have been synthesized and characterized by single crystal X-ray diffraction. The structure of K1.65V1.78W0.22O2(AsO4)2 shows an irregular MO6 octahedra (M=78%V+22%W) with two abnormal short bonds M—O (1.774 (7) Å) and (1.824 (8) Å) which suggest that the non linear optical property could be more important. In order to show the influence of the tungsten and vanadium on the distortion of the MO6 octahedra, we substituted the tungsten by the vanadium element. The single-crystal K2V2O2(AsO4)2 consists of common VO6 octahedra with one short bond V—O (1.652(2) Å) . We used SUPERFLIP and JANA 2006 programs [4, 5] to resolve and refine these structures. The refinement by JANA 2006 led to the reliability factors: (R =0.048, Rw = 0.064) for K1.65V1.78W0.22O2(AsO4)2, and (R =0.028, Rw = 0.034) for K2V2O2(AsO4). Structure of K1.65V1.78W0.22O2(AsO4)2 Structure of K2V2O2(AsO4)2 Space group: Pc21n Space group: Pc21n Cell parameters: Cell parameters: a = 6.5322 (7) Å a = 6.5368 (2) Å b = 10.7228 (9) Å b = 10.7228 (5) Å c = 13.0782 (5) Å c = 13.0666 (4) Å

[1] *S. Belkhiri, M. Kars and D. Mezaoui, Acta Cryst E65 (2009) i69,* ***[2]*** *S. Belkhiri, D. Mezaoui and T. Roisnel, Acta Cryst E68 (2012) i54,* ***[3]*** *G. D. Stucky, M. L. F. Phillips and T. E. Gier, Chem. Mater 1(5) (1989) 492-509*





Keywords: Arsenate-Tungsto-Vanadate, KTiOPO4 family (KTP), non linear optical property