Phase Transition and Structures of the Phosphate $Zn_{0.50}Ti_2(PO_4)_3$

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Compounds of general formula $M^{II}_{0.5}M^{IV}(PO_4)_3$ with M^{II} = Mg, Mn, Fe, Co, Cu, Cd, Ca, Sr, Pb and M^{IV}= Ti, Zr crystallize with either a Nasicon-type structure or a $Sc_2(WO_4)_3$- type structure, depending on the size of the M^{II} element [1]. Temperature dependent XRD study of $Zn_{0.5}Ti_2(PO_4)_3$ reveals a reversible $\alpha \rightarrow \beta$ phase transition around ~400°C.

Single crystals of the α phase have been obtained with cell parameters, a=14.652(2)Å, b=8.602(1)Å, c=16.930(2)Å, β=125.89(1)° and V=1728.7(1)Å^3. The single crystal structure was solved in the non standard space group $P2_1/a$ (referring to the $Fe_2(MoO_4)_3$ study [2]) with R_1=0.059 and wR_2= 0.090.

Diffraction data of the β phase were collected at 500°C on a Philips PW 1050 equipped with an Anton Paar furnace. X-ray diffraction pattern of this powder can be indexed in the $P2_1/n$ monoclinic cell: a=11.918(5)Å; b=8.610(4)Å, c=8.506(4)Å; β=90.37(3)°; V=873.8(1)Å^3 referring to the $Sc_2(WO_4)_3$ study [1]. This structure type was confirmed by Rietveld refinement (R_B= 0.043, R_{wp}=0.076, R_P=0.053). The α phase can be considered as a superstructure of the β one with an ordering of zinc atoms and vacancies along b direction.

[1] Jouannaux A.,Verbaere A., Piffard Y., Fitch A. N., Kinoshita M., *Eur. J. Solid State Inorg. Chem*., 1991, **28**, 683. [2] Chen H. Y., *Mat. Res. Bull.,* 1979, **14**, 1583.

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