Jahn Teller Transition Phase in $Cu_{0.5}TiO(PO_4)$ Oxyphosphate

Pierre Gravereau[a], Saïd Benmokhtar[b], Jean-Pierre Chaminade[a], Abdelaziz El Jazouli[b], Eric Lebraud[a], Stanislas Péchev[a], *[a]ICMCB-CNRS, University of Bordeaux, Pessac, France. [b]LCMS, Faculté des Sciences Ben M'Sik, Casablanca, Maroc.* E-mail: graver@icmcb-bordeaux.cnrs.fr

In our research interest on titanium oxyphosphates, several compounds $M^{II}_{0.5}TiO(PO_4)$ have been prepared with M^{II} = Mg , Fe , Co , Ni , Cu , Zn. They all belong to the monoclinic $P2_1/c$ structural type determined *"ab initio"* for $Ni_{0.5}TiO(PO_4)$ from X-ray powder diffraction[1].Thermostructural study of $Cu_{0.5}TiO(PO_4)$ shows a phase transition $\alpha \rightarrow \beta$ (~800°C during heating, ~400°C during cooling).

Single crystals of the α phase have been obtained. Its cell presents a Jahn Teller deformation with Cu-O elongation in the (**a,c**) plane: a=7.5612(4) ; b=7.0919(4) ; c=7.4874(4)Å ; β=122.25(6)° ; V=339.55(6)$Å^3$. The single crystal structure confirms and states more precisely the previous powder model (R_1=0.023; wR_2= 0.063).

The β phase has been obtained stabilised at room temperature in a powder mixture α(38%)+β(62%) without impurities. X-ray diffraction pattern of this powder can be indexed in a like α-type $P2_1/c$ monoclinic cell : a=7.1081(10) ; b=7.7384(12) ; c=7.3013(10) Å ; β=119.28(1)° ; V=350.3(1)$Å^3$. As the α-structure is not a good starting model for Rietveld refinement (divergence), an *"ab-initio"* structure determination has been done. The refined structure corresponds to a "rocking" of the Jahn Teller elongation from the (**a,c**) plane to the **b** direction.

[1] Gravereau P., Chaminade J.P., Manoun B., Krimi S., El Jazouli A., *Powder Diffr.* , 1999, **14**, n.1, 10.

Keywords: oxyphosphates, phase transition, Jahn Teller effect