CRYSTAL STRUCTURE AND POLYMORPHISM OF $NaSrVO_4$: THE FIRST $A^IB^{II}X^VO_4$ LARNITE RELATED STRUCTURE FROM X-RAY POWDER DATA

Gwilherm Nénert[a], P. O'Meara[b], T. Degen[a]

[a] *PANalytical B. V., Lelyweg 1, 7602 EA, Almelo, The Netherlands*
[b] *PANalytical Ltd., 7310 Ground Floor, Beach Drive Water-beach Cambridge CB25 9AY United Kingdom*
gwilherm.nenert@panalytical.com

The crystal chemistry of $A^IB^{II}XO_4$ (A^I = alkali ion, B^{II} = alkali-earth ion, X = P, V, As) is very rich and leads to numerous polymorphic phases which belong to several structures types: olivine, arcanite, glaserite, tridymite, α-K_2SO_4, β-Na_2SO_4 and γ-Na_2SO_4 [1]. Among the various families (X = P, V, As); the phosphates have been the most widely investigated. Besides the purely interest from a crystal chemistry point of view, the research activities related to this family of materials is driven mainly due to their ferroelectric and ferroelastic properties and possible applications as phosphors for LEDs [1,2].
Within the rich crystal chemistry of this family, no structural data have demonstrated the occurrence of the larnite/belite structure [3]. The larnite/belite structure has been widely investigated due to its importance for Portland cement and its rich polymorphism [4]. All the materials related to the larnite structural type have the general formula $A^{II}B^{II}X^{IV}O_4$ (A, B = Ca, Sr, Eu; Ba; X = Si, Ge, Ti) [4,5].
$NaSrVO_4$ has been mentioned in the past but with conflicting results and without providing any structural model [3, 6]. These contradicting results and the absence of report on the crystal structure motivated us to reinvestigate this material. We present here its crystal structure, as determined and refined from laboratory powder X-ray diffraction data. This is the first crystal structure reported among the larnite/belite structural type exhibiting the chemistry $A^IB^{II}X^VO_4$. Similarly to other larnite structures, we observe a rich polymorphism in the temperature range 25 – 900°C and we report one polymorph which was not previously reported in the larnite family [7].

[1] V. A. Isupov, *Ferroelectrics*, **2002** *274:1*, 203-283.
[2] S. Choi, *et al. Optical Letters,* **2013** *38*, 1346-1348.
[3] S. Drai, *et al.*, **1974**. *Journal of Solid State Chemistry*, *10*, 95-101
[4] H. F. W. Taylor, **1990** *Cement Chemistry*, Academic Press.
[5] M. Catti, *et al.* **1983**. *Acta Crystallogr., Sect. B: Struct. Sci.*, *39*, 674-679; S. Deganello, **1973**. *Acta Cryst. B 29*,2593-2597 ; J. Felsche **1971**. *Die Naturwissenschaften*, *58*, 218-219; C. M. Midgley **1952**. *Acta Cryst. 5*, 307-312.
[6] R. Klement, P. Kresse **1961**. *Zeitschrift für anorganische und allgemeine Chemie*, *310*, 53-68.
[7] G. Nénert, P. O'Meara, T. Degen, Phys Chem Minerals (2017). doi:10.1007/s00269-017-0873-6, http://rdcu.be/o4B6