

*Crystal structure and polymorphism of a new larnite vanadate: NaSrVO₄*Gwilherm Nenert¹, Paul O'Meara², Thomas Degen¹¹PANalytical B. V., Almelo, Netherlands, ²PANalytical B. V., Cambridge, United Kingdom

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The crystal chemistry of AIBIXO₄ (AI = alkali ion, BII = alkali-earth ion, X = P, V, As) is very rich and leads to numerous polymorphic phases which belong to numerous structures types, such as olivine, arcanite, glaserite, tridymite, α-K₂SO₄, β-Na₂SO₄ and γ-Na₂SO₄ [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].

Within the rich crystal chemistry of this family, no structural data have demonstrated the occurrence of the larnite/belite structure [1]. The larnite/belite structure has been widely investigated due to its importance for Portland cement and its rich polymorphism [2]. All the materials related to the larnite structural type have the general formula AE₂MO₄ (AE = Ca, Sr, Eu; Ba; M = Si, Ge, Ti) [3]. Upon doping on the AE and M sites, some alkaline ions, such as Na, K, or of phosphor, can be incorporated into the structure giving rise

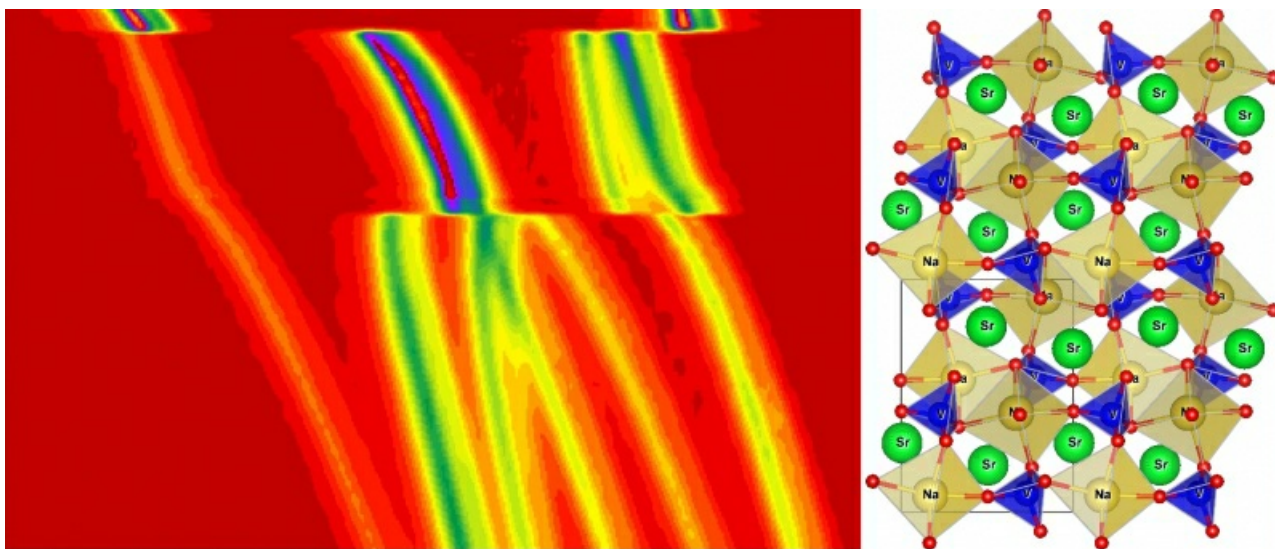
to flamite.

NaSrVO₄ has been mentioned in the past but with conflicting results and without providing any structural model. 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 AIBIXVO₄. 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.

[1] Isupov, V. A. (2002) *Ferroelectrics*, 274, 203-283.

[2] Taylor, H. F. W. (1990) *Cement Chemistry*, Academic Press.

[3] Catti, M. et al. (1983). *Acta Crystallogr., Sect. B: Struct. Sci.*, 39, 674-679; Deganello, S. (1973). *Acta Cryst. B* 29,2593-2597 ; Felsche J. (1971). *Die Naturwissenschaften*, 58, 218-219; Midgley, C. M. (1952). *Acta Cryst.* 5, 307-312.



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