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Figure 1. The room temperature structures of (a)  $Ba_2NiTeO_6$  and  $Ba_2ZnTeO_6$  and (b)  $Ba_2CuTeO_6$ .

Keywords: transition metal oxides, phase transitions, neutron diffraction, magnetism

## MS15-O4 Crystal structure and polymorphism of NaSrVO<sub>4</sub>: the first A<sup>I</sup>B<sup>II</sup>X<sup>V</sup>O<sub>4</sub> larnite related structure from X-ray powder data

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The crystal chemistry of  $A^I B^{II} XO_4$  ( $A^I$  = alkali ion,  $B^{II}$  = alkali-earth ion, X = P, V, As) is very rich and leads to numerous polymorphic phases which belong to 8 different structures types: olivine, arcanite, glaserite, tridymite,  $\alpha$ -K<sub>2</sub>SO<sub>4</sub>,  $\beta$ -Na<sub>2</sub>SO<sub>4</sub> and  $\gamma$ -Na<sub>2</sub>SO<sub>4</sub> [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 lamite/belite structure [3]. The lamite/belite structure has been widely investigated due to its importance for Portland cement and its rich polymorphism [4]. All the materials related to the lamite 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]. Upon doping on the A, B and X sites, some alcaline ions can be incorporated into the structure giving rise to belite [5] and flamite [6].

NaSrVO<sub>4</sub> has been mentioned in the past but with conflicting results and without providing any structural model [3, 7]. 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<sup>I</sup>B<sup>II</sup>X<sup>V</sup>O<sub>4</sub>. 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.

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Keywords: larnite, belite, vanadate, powder diffraction, NaSrVO4