

New mixed sodium - alkaline earth thiophosphates

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Alkaline earth phosphates attract interest in material science e. g. due to the possibility of doping them with divalent or trivalent rare earth ions to produce efficient fluorescent materials [1-3]. The analysis of earth alkaline thiophosphates as host lattices is of great importance in order to create new green and yellow luminescent materials.

In this contribution we report on the synthesis, crystal structure, vibrational and solid-state NMR spectra of precursor-compounds, i. e. the thiophosphates $\text{NaM}(\text{PO}_3\text{S})\cdot 9\text{H}_2\text{O}$ with $M=\text{Mg}, \text{Ca}, \text{Sr}$ [4] and Ba.

$\text{NaBa}[\text{PO}_3\text{S}]\cdot 9\text{H}_2\text{O}$ [5] and $\text{NaMg}[\text{PO}_3\text{S}]\cdot 9\text{H}_2\text{O}$ were obtained as single-phase crystalline powders starting from NaOH, PSCl_3 and BaCl_2 . Single-crystals of $\text{NaCa}[\text{PO}_3\text{S}]\cdot 9\text{H}_2\text{O}$ were grown by gel crystallisation.

The structures of the title compounds consist of distorted $[\text{NaO}_6]$ trigonal prisms, non-condensed $[\text{PO}_3\text{S}]$ tetrahedra and $[\text{MO}_9]$ tricapped trigonal prisms ($M=\text{Ca}, \text{Sr}, \text{Ba}$) and crystal water molecules. The nine crystal water molecules coordinate all ions, Na^+ , M^{2+} and $[\text{PO}_3\text{S}]^{3-}$. The sodium ion is six-fold and the calcium ion nine-fold coordinated by crystal water O (Fig. 1). $\text{NaMg}[\text{PO}_3\text{S}]\cdot 9\text{H}_2\text{O}$ adopts a different structure compared with the other members which can be derived from the PbCl_2 structure (cotunnite).

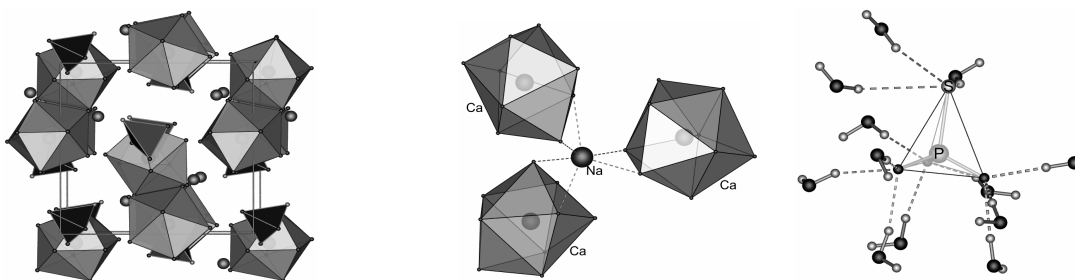


Figure 1. Representation of the unit cell of $\text{NaCa}[\text{PO}_3\text{S}]\cdot 9\text{H}_2\text{O}$ [100] (left), the coordination environments of Ca, Na and the $[\text{PO}_3\text{S}]^{3-}$ tetrahedron (right).

References:

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