

STRUCTURAL PHASE TRANSITIONS IN Rb₂KFeF₆ AND Rb₂KYF₆ ELPASOLITES

A. Tressaud*, S. Khairoun, J. P. Chaminade, J. Grannec

Laboratoire de Chimie du Solide du CNRS, Université de Bordeaux I, 33405 Talence Cédex (France)

and M. Couzi

Laboratoire de Spectroscopie Infrarouge, Université de Bordeaux I, 33405 Talence Cédex (France)

The elpasolite-type compounds Rb₂KFeF₆ and Rb₂KYF₆ undergo a structural phase transition at 175 K and 398 K, respectively, from a high-temperature cubic phase (Fm3m) to a tetragonal - or pseudo-tetragonal - distorted low-temperature phase. These transitions have been studied on powdered samples and on single crystals using DSC, X-ray diffraction and Raman scattering techniques. The group to sub-group relations are proposed, which lead to the "family tree" of the elpasolite series.

Rb₂KYF₆ : the space group of the low-temperature phase of Rb₂KYF₆ is either P12₁/n1 or P112₁/n. It can be assumed that the transition is of first order¹ although it is apparently continuous. This transition, which is probably of the "triggered"-type, is induced by an order-disorder process. In the cubic phase of Rb₂KYF₆, the orientational disorder of the YF₆ octahedra may be coupled with a positional disorder of the Rb⁺ cations in CN = 12.

Rb₂KFeF₆ : on the basis of both group-theory considerations and experimental data, it may be assumed that P4/m, P2/m, P112₁/n and P1 space groups are candidates for the low-temperature phase of Rb₂KFeF₆. On the basis of the present data, the strong first-order character of this transition does not allow any further hypothesis on the involved transition mechanism.