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LATTICE DYNAMICS AND STRUCTURAL PHASE TRANSITIONS IN THE $AM^{II}F_3$ AND $AM^{III}F_4$ FLUORIDES

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Perovskite fluorides $AM^{II}F_3$ ($RbCaF_3$, $KCaF_3$) and perovskite-type layer fluorides $AM^{III}F_4$ ($RbAlF_4$, $KAlF_4$, $TlAlF_4$) exhibit a large variety of structural phase transitions where MF_6 octahedra are concerned, the MF_6 octahedra being linked together in a three-dimensional array for the first family and in a two-dimensional one for the second. These fluorides are well adapted systems to study the lattice instabilities and particularly the incidence of dimensionality on the structural phase transitions.

The ability to grow in our laboratory large single crystals of fluoride has enabled us to investigate lattice dynamic properties of these materials using ultrasonic methods, Raman scattering and inelastic neutron scattering. The phonon dispersion curves have been measured; they are well described using a rigid ion model which is convenient for the fluorides considering the small polarizability of fluorine ions and the ionic character of fluorine bonds. This model was successfully applied to account for the dynamics of several fluoroperovskites ($RbCaF_3$, $KMnF_3$ ...) giving the magnitude of short range interactions (M. Rousseau, J. Nouet R. Almairac, J. Phys. 38, 1423, 1977). These data have been used to describe the phonon spectra of the tetrafluoroaluminates though the structure is less symmetric. Several parameters of the model have been adjusted for $RbAlF_4$ which exhibits the aristotype structure and undergoes transitions by octahedra tilts (A. Bulou, J. Nouet, J. Phys. C, 15, 183, 1982). The extension to $KAlF_4$ helps to explain the mechanism of its shear transformation typical of a layered structure (J.M. Launay et al. J. Phys. 46, 771, 1985). This model has also been used to investigate the structural transformations of $TlAlF_4$ (A. Bulou, M. Rousseau, J. Nouet, to be published).

Such studies performed on fluoroperovskites and tetrafluoroaluminates make it possible to obtain the variation of short range F-F interactions in a wide range of interionic distances. The knowledge of these data is very useful not only for the studies of crystallized fluorides but also for amorphous fluorides.