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VARIOUS ASPECTS OF THE DYNAMICS OF ATOMS IN FLUOROPEROVSKITES

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Many properties of crystals are related to their atom dynamics. Owing to the weak polarisabilities of their atoms, the dynamical properties of the fluoroperovskites AMF_3 are very well represented by rigid-ion models. This dynamical aspect is illustrated in the three following cases :

1. **Debye Waller calculation** . From a rigid ion model, it is possible to calculate the harmonic contribution of the mean square amplitudes of atoms in crystals. The comparison between experimental and calculated values can give fruitful information about anharmonicity. In this paper, such calculations are illustrated through the temperature dependence of the ionic mean square amplitudes near a displacive phase transition in $RbCaF_3$ (M. Rousseau, C. Ridou and A. Bulou Solid State Commun. 41, 951, 1982) and near the melting point in $KZnF_3$ in which ionic conductivity was expected (C. Ridou, M. Rousseau, B. Pernot and J. Bouillot, J. Phys. C, 19, 4847 (1986)).

2. **Heat capacity calculation** . The heat capacity of crystals is affected by structural, rotational, magnetic or electronic transitions. The lattice contribution can be estimated from the phonon density of states. The comparison between experimental and calculated temperature dependence of heat capacity performed in $KZnF_3$, which provides a good stable matrix without any phase transformation, is presented (R. Burriel, J. Bartholome, D. Gonzalez, R. Navarro, C. Ridou, M. Rousseau and A. Bulou, J. Phys. C, in press).

3. **Vibronic contribution of luminescence spectra** . Fluorides doped with metal ions (Ni^{2+}, Co^{2+}, V^{2+}) constitute a broad family of compounds utilizable as solid-state laser sources. In this context we show that the emission band at 20 000 cm^{-1} in $KZnF_3$:Ni at 10 K may be calculated as a summation of several phonon contributions within a linear coupling approximation (R. Russi, G.A. Barbosa, M. Rousseau and J.Y. Gesland, J. Phys. 45, 1773, 1984).