Phonon dispersion curves of SrFCl

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Extensive Raman scattering studies of ionic layered SrFCl crystal have been carried out in the literature. But, to the best of our knowledge there are no measured dispersion curves explaining the vibrational properties of this PbFCl-type compound. Therefore, for a basic understanding of experimental observations in Raman scattering, we have resorted to lattice-dynamical calculations. The long wavelength phonons are computed in the framework using the shell model, which had been applied previously to produce the phonon dispersion relations of BaFCl and BaFBr. This microscopic model includes the long-range Coulomb interactions and the short-range interactions and taking into account the electronic polarizability of constituent ions. The shell model parameters have been obtained in such way that a best fit of the measured Raman frequencies has been achieved in the center of the first Brillouin zone. The values of relevant parameters are critically analyzed. A complete set of transverse and longitudinal phonon branches in each of the three principal directions ($\langle 100 \rangle$, $\langle 001 \rangle$, $\langle 110 \rangle$, $\langle 011 \rangle$, and $\langle 111 \rangle$) have been deduced.