General valence force field and molecular dynamic parameters for cubic lanthanide hexachloro-elpasolite crystals

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A normal coordinate analysis has been carried out for the series Cs2NaLnCl6, where Ln represent a trivalent lan thanide cation such as Pr+ 3, Sm+3, Eu+3, Tb+ 3, Ho+3and Tm+3by using a general valence force field (GVFF). A convenient parametrization has been developed to obtain symmetrized F-matrix elements which are able to reproduce both the experimental frequencies and the expected poten tial energy distribution for these systems. It is shown that these force fields may be of great interest to calculate vibronic intensities for these complex ions, when a molecular model is adopted. The force fields developed throughout this work have been used to calculate mean amplitudes of vibrations, mean square perpendicular amplitudes and Bastiansen-Morino shrinkage effects at 0 and 298 K.