Transferable Deformation-Dipole Model for Ionic Materials

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A model for the ionic interactions in polyvalent metal halides was originally built for chloro-aluminate clusters using an analysis of data on static and dynamic structure of their molecular monomers [for a review see M. P. Tosi, Phys. Chem. Liquids **43**, 409 (2005)]. Recently, by continuing the deformation-dipole model calculations, the transferability of the halogen parameters was tested through the calculation of the structure of alkali halides and alkaline-earth halides. In this work we test the usefulness of the deformation-dipole model in the study of ionic materials by examining the transferability of the overlap parameters for the halogen ions across families of halide compounds. Following a comparative discussion of alkali and alkaline-earth halide monomers near equilibrium, results on alkaline-earth halides are given. By using the transferable ionic potential model we also calculate the equilibrium structure of the molecular clusters, as well as the vibrational frequencies of ACl_4 compounds (where A = U, Np, Pu, Am and Th).

Key words: Ionic Models; Ionic Clusters; Molten Salts.