A Structural Model for Mixed-Nitrate Ionic Glasses

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We propose and evaluate a structural model for mixed K-Ca nitrate melts and glasses, which invokes the presence of strongly bound $Ca_2(NO_3)_7$ groups surrounded by K ions that can transport charge by relatively free jumps. To this purpose we first construct ionic models for the pure ANO_3 compounds (with A = alkali metal ion), by searching for suitable $A^{+Z}\cdot(NO_3)^{-Z}$ interionic potentials in the space of interionic-law parameters with the help of known models for alkali chlorides. The available evidence mainly consists of infrared-active mode frequencies, and is compatible with two alternative types of interionic parameters. A choice between them is made on the basis of the fact that the NO_3 group has a flat triangular shape and can execute torsional oscillations giving rise to a low-frequency Raman-active mode in the melt. This interionic force model is then combined with a similar model for $Ca(NO_3)_2$ to evaluate the structural properties of a $3KNO_3\cdot 2Ca(NO_3)_2$ unit, which is the constituent of the well-known glassformer CKN. We expect that the present model should be representative of other mixed alkali-divalent ion nitrate systems in the range of concentration where glass formation is observed.

Key words: Ionic Glasses; Molten Salts.