

# Structure and Thermodynamic Properties of Molten Rare Earth-Alkali Chloride Mixtures

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The dependence of the enthalpy of mixing on the structure of molten rare earth-alkali chloride mixtures has been investigated by molecular dynamics simulation. The experimental enthalpy of the mixing with its negative and its dependence on the cation size was qualitatively reproduced. It became clear that the enthalpy of mixing depends on the structural features of short and medium range.

*Key words:* Molten Salt; Molecular Dynamics; Enthalpy of Mixing; Rare Earth-alkali Chloride Mixture.