A Molecular Dynamics Simulation of the Molten Ternary System (Li, K, Cs)Cl

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The self-exchange velocity (SEV) of neighboring unlike ions, has been evaluated by molecular dynamics simulations of molten CsCl, (Li, K)Cl and (Li, K, Cs)Cl at 673 K. From the increase of the SEV's in the same order as the internal mobilities it is conjectured that there is a strong correlation between these two properties. The pair correlation functions, and the self-diffusion coefficients and the SEV's of Li^+, K^+, and Cs^+ with reference to Cl^- have also been calculated. The results allow to conclude that the self-exchange velocity of the cations become $v_{Cs} < v_K < v_{Li}$ at x_{Cs} =0.1 and $v_{Li} < v_K < v_{Cs}$ at $x_{Cs} > 0.4$. The sequence of the self-diffusion coefficients agrees with that of the SEV's. The results enable to conclude that it is possible to enrich Cs at up to x_{Cs} ≈ 0.3 - 0.4 in the molten LiCl-KCl eutectic system.

Key words: Chemla Effect; Internal Cation Mobility; Molten Ternary System; Molecular Dynamics Simulation; Self-exchange Velocity; Self-Diffusion Coefficient.