

Estimation of the Chemical Potential and the Activity of NaCl in Molten DyCl₃-NaCl by Molecular Dynamics Simulation

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Molecular dynamics simulations of molten DyCl₃-NaCl were carried out at liquidus temperatures of the phase diagram. The chemical potential and the activity of NaCl was successfully estimated with the method proposed by Powles et al., which requires only positional data of the ions at the temperatures in question.

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