

Structure and Dynamic Properties of Molten Lanthanum Tribromide

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The structure of molten LaBr_3 was investigated by X-ray diffraction and molecular dynamics simulations. It was found that the short range structure of molten LaBr_3 is very similar to that of molten LaCl_3 , except for some structural features such as interionic distances based on the difference of anion sizes. In the MD simulation, the shear viscosity of molten LaBr_3 was estimated from the structurally-optimized MD calculations.

Key words: Molten Salt; Rare Earth Halide; X-ray Diffraction; Molecular Dynamics.

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