

Molecular Modeling of High and Low Temperature Molten Salts: Melting Points and Other Key Thermophysical Properties

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High temperature alkali nitrate molten salts are being considered for use as a heat storage and transfer media in solar thermal power generation. Low temperature molten salts ("ionic liquids") are also being examined for use in heat transfer applications as well as in a variety of other fields. In both cases, it is important to know how key thermodynamic and transport properties vary with temperature, pressure, dissolved species concentration and chemical structure. It is also essential to know melting points of these species. In this paper, we report results of molecular modeling studies in which these properties are predicted over a wide range of conditions. In particular, we compute melting points, thermal conductivities, viscosities densities and heat capacities, and make comparison with available experimental data.