

Theoretical Approaches to the Ludwig-Soret Effect in Liquid Mixtures

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In a liquid mixture subject to a temperature gradient, thermal diffusion (the Ludwig-Soret effect) leads to the formation of a composition profile in the steady state that is still difficult to predict with theoretical methods. In this work we investigate the Soret effect in liquid mixtures in the context of non-equilibrium steady state statistical mechanics. Extending the work of Attard [1] to liquid mixtures, we discuss which aspects of the phenomenon may be described by time-reversal invariant probability distributions and which aspects require the inclusion of dynamical (odd under time reversal) contributions. The configurational part of the probability distribution is time invariant and contains the effects of the molecular interactions and the thermodynamic state on the composition profile; it is expected to yield the dominant contributions to the Soret effect in many liquid mixtures. We relate this configurational part to our earlier derived probability distributions for two-chamber lattice models and show by comparison with experimental data that this is indeed the case. In contrast, the isotope effect observed in liquid mixtures of deuterium substituted cyclohexane and benzene [2] cannot be described in this way. We discuss briefly how one might include collision effects in probability distributions in order to estimate the isotope effect.

[1] P. Attard, J. Chem. Phys. **121**, 7076 (2004); **124**, 224103 (2006).

[2] C. Debuschewitz and W. Köhler, Phys. Rev. Lett. **87**, 055901 (2001)