Thermodiffusion of Binary Molecular Liquids - the Thermophobicity Concept

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Thermodiffusion relates to diffusive mass transport in fluid mixtures that is driven by a temperature gradient. The strength of the effect is measured by the Soret coefficient. Based on a database of ten compounds, for which the Soret coefficients of almost all possible equimolar mixtures had been determined, we have developed a phenomenological description of thermodiffusion that is based on thermophobicities of the pure compounds, which are related to the heats of transport [1]. The same model turned out to hold also for an extended database of 23 substances and 77 out of 253 possible binary mixtures [2]. The substances can be ordered according to their thermophobicity (their tendency to migrate to the cold side), with cis-decalin being the most thermophobic and hexane the most thermophilic one. Based on the determined thermophobicities and the (isothermal) activity coefficients, which are equilibrium properties, the Soret coefficient of any binary mixture of substances that are linked to the existing data base can be calculated. We have also analyzed the composition dependence of the Soret coefficients and the heats of transport for 22 selected binary mixtures. Both the interpretation of the heats of transport in equimolar mixtures as pure component thermophobicities and the composition dependence of the Soret coefficient can be understood on the basis of the thermodiffusion theory developed by Morozov [Phys. Rev. E 79, 031204 (2009)], according to which the composition dependence is caused by the excess volume of mixing.

References

[1]Hartmann et al., Phys. Rev. Lett. 109 (2012) 065901
[2] S. Hartmann et al., J. Chem. Phys. 141 (2014) 134503