The Thermophobicity Concept in Thermodiffusion - Expanding the Matrix

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Although the Soret effect of binary liquid mixtures is difficult to predict, it shows some phenomenological regularities. Components with a very large positive Soret coefficient in some mixture have, as a rule, also positive Soret coefficients when mixed with other compounds, and vice versa. Despite this tendency, there is no obvious route to determine the Soret coefficient of a mixture of components A and B from known Soret coefficients of the mixtures of A with C and B with C. In an early publication [Phys. Rev. Lett. 109 (2012) 065901] it was shown for ten different components with 41 out of 45 possible mixtures that, as expected, a simple additive rule does not hold for the Soret coefficients. After factoring out the so-called thermodynamic factors, the remaining heats of transport of equimolar mixtures do indeed follow an additive law to a good approximation. This additivity allowed us to determine single-component heats of transport that can be interpreted as thermophobicities, which are a measure of the tendency of a given substance to migrate towards the cold side in a temperature gradient. Later, the database was expanded and the model was applied to arbitrary concentrations. Nevertheless, the matrix of tested binary mixtures was in parts still sparsely populated [J. Chem. Phys. 141 (2014) 134503]. In our recent work [Pur, J. Chem. Phys. 152 (2020) 054501] we have expanded the database to 24 compound with 107 out of 276 possible combinations measured. Besides many new own measurements, we have also included a number of literature data. In particular the homologous series of n-alkanes is now closely tied to the remaining substances, and their thermophobicities are directly related to their chain length: the longer the chain the larger the thermophobicity. In our contribution we will discuss the development of the thermophobicity concept and its relation to the pseudo-isotope effect.