INFLUENCE OF THE HYDROPHOBIC/HYDROPHILIC INTERPLAY ON THERMODIFFUSION

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ABSTRACT

The hydration of hydrophobic solutes remains still illusive despite the long history of research. Often hydrophobic hydration is explained in terms of a balance between the loss in entropy due to cavity formation to accommodate the hydrophobic molecule and the gain in enthalpy due to attraction between the solute and solvent molecules [1]. This entropic-enthalpic compensation mechanism is often found in the context of biochemical reactions and apparently thermodiffusion is especially sensitive to this balance. We take a closer look into the mechanism by studying systematically hydrophilic and more hydrophobic small molecules as function of temperature and concentration. We elucidate the often found typical temperature dependence of the Soret coefficient of solute molecules in water and relate the empirical parameters with the number and the strength of hydrogen bonds [2]. Using a linear correlation between those parameters, we are able to reduce the number of adjustable parameters to two. We observe a clear correlation of the temperature and concentration dependence of the Soret coefficient with the hydrophilicity, which can be quantitatively described by the logarithm of the 1-octanol/water partition coefficient P, which is a measure for the hydrophilicity/hydrophobicity balance of a solute for numerous systems [3]. It is often used to model the transport of a compound in the environment or to screen for potential pharmaceutical compounds. We give an intuitive picture explaining the correlation between log P and the temperature sensitivity of the Soret coefficient. Finally we discuss a route for a more sophisticated hydrophilicity scale.

REFERENCES

[1] S. Liese et al., *ACS Nano*, **11** 702 (2017).
[2] Niether, D., et al., *Langmuir*, **33,** 8483(2017).
[3] Niether, D., et al., *Physical Chemistry Chemical Physics*, **20,** 1012(2018).