Development of a Generalized Group Contribution Approach for Solubility Prediction of Organic Molecules Using SAFT-γ Mie Approach

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The applications and importance of prediction of solubility of organic molecules spans across a large sector of the chemical and pharmaceutical industries. The diverse and wide range of molecules for which such predictions are needed also have a wide range of other physicochemical properties.. A successful method to predict solubility of solutes in solvents for such a variety of compounds needs to be very versatile in terms of the types of molecules it can describe, while being accurate over broad ranges of conditions. Group contribution approaches can be very powerful techniques in this context. In the SAFT-γ Mie group-contribution approach [1] a heteronuclear model is implemented and an accurate expression for the Helmholtz free energy change due to association is obtained for pure components. The physicochemical properties of molecules of interest are described by appropriate summation of the contributions of the groups they contain. Each of the groups is characterised based on the fluid phase behaviour and properties of simple molecules, and the parameters characterizing the groups are then transferred to more-complex molecules. The robustness of the underlying physics allows the treatment of a broad collection of compounds, including associating ones, and provides the ability to describe a wide array of physicochemical properties with a single set of interactions. Although the group-contribution method enables many molecules to be treated with a small number of constituting groups, the power of the approach is truly demonstrated when the solubility of large and complex multifunctional pharmaceutical molecules is predicted based only on experimental data that were obtained for small and simple molecules. Here we provide a wide range of examples of the prediction of solubility of organic molecules ranging from asymmetric alkanes mixtures to lovastatin in various solvents.

References

[1] V. Papaioannou, T. Lafitte, C. Avendaño, C. S. Adjiman, G. Jackson, E. A. Müller, and A. Galindo, J. Chem. Phys., 2014, 140, 054107.