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A QM-CAMD approach to solvent design for optimal reaction rates

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Abstract

The choice of solvent in which to carry out liquid-phase organic reactions often has a large impact on reaction rates and selectivity and is thus a key decision in process design. A systematic methodology for solvent design that does not require any experimental data on the effect of solvents on reaction kinetics is presented. It combines quantum mechanical computations for the reaction rate constant in various solvents with a computer-aided molecular design (CAMD) formulation. A surrogate model is used to derive an integrated design formulation that combines kinetics and other considerations such as phase equilibria, as predicted by group contribution methods. The derivation of the mixed-integer nonlinear formulation is presented step-by-step. In the application of the methodology to a classic S_N2 reaction, the Menschutkin reaction, the reaction rate is used as the key performance objective. The results highlight the trade-offs between different chemical and physical properties such as reaction rate constant, solvent density and solid reactant solubility and lead to the identification of several promising solvents to enhance reaction performance.

Keywords

Quantum mechanics, Computer-Aided Molecular Design, Surrogate model, Phase equilibrium, Kinetics, Group contribution

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