COSMO-RS Method for Predicting Thermodynamics Properties

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Abstract

The conductor-like screening model for real solvents (COSMO-RS) combines unimolecular quantum mechanical calculations with statistical thermodynamics methods to account for molecular interactions, thus enabling predictions of thermodynamic parameters for multicomponent solvent systems and novel solutes without system-specific experimental data. It has been widely used in chemical engineering thermodynamics, pharmaceutical research, as well as environmental research. In this talk, I will introduce the basics of this method and provide input examples for associated software. I will also talk about one application of this method in solvent selection for the separation of lignin-derived monomers.