The SM8 Universal Solvation Model

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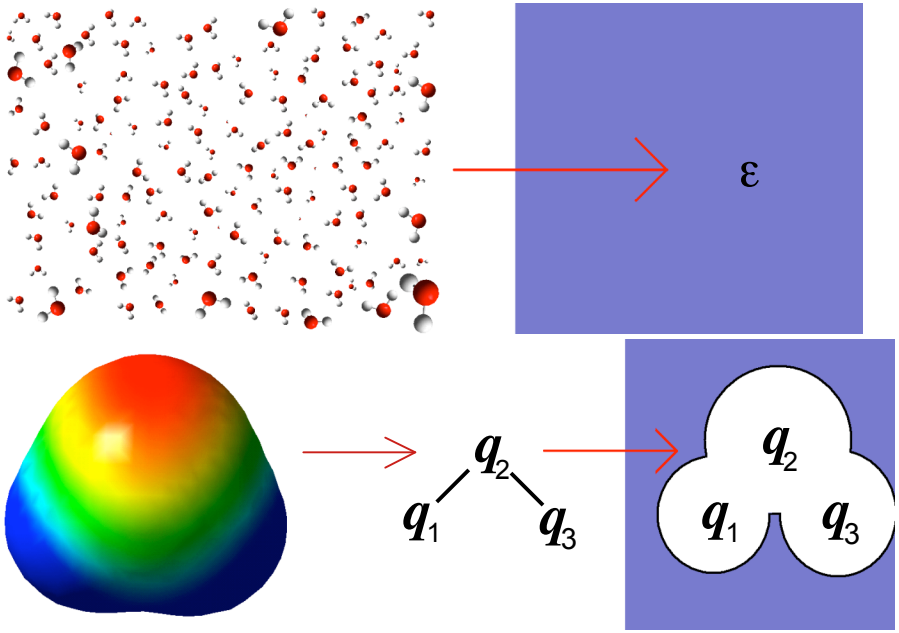
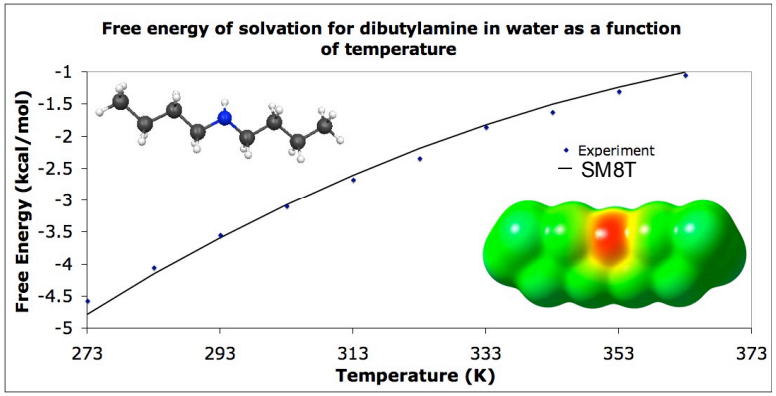
Modeling solute molecules in liquid solutions can be accomplished efficiently using implicit (continuum) solvation models. The recently described* SM8 model is the most accurate continuum model to date and may be applied to compute partition coefficients, acidity constants, redox potentials, solubilities, temperature-dependent absolute free energies of solvation, and solvent effects on solute structure and reactivity in aqueous and non-aqueous solvents and at complex interfaces.



In a continuum model, the actual solvent molecules are replaced by a dielectric medium. The solute charge distribution, which interacts with the medium, may be represented in various ways, e.g., as atomic partial charges.



The SM8T model permits temperature effects on aqueous solvation free energies to be predicted.

Continuum solvation models can be particularly useful for predicting, inter alia, the critically important property of bioavailability for potential drug leads, the distribution properties of environmental pollutants, and the thermodynamics of processes taking place in electrochemical fuel cells.

* Marenich, A. V.; Olson, R. M.; Kelly, C. P.; Cramer, C. J.; Truhlar, D. G. *J. Chem. Theor. Comput.* **2007**, *3*, 2011.

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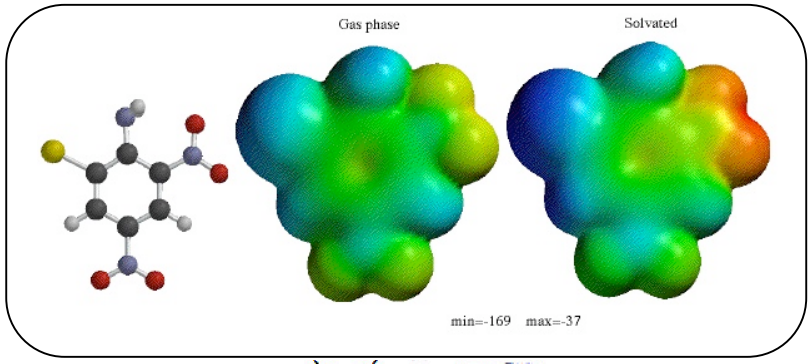
Broader Impacts



SM8 has been incorporated into a number of electronic structure codes, both commercial and freely available, that are very widely distributed in industry, academia, and international research laboratories. Codes incorporating SM8 and other related SM*x* solvation models include AMSOL, GAMESSPLUS, HONDOPLUS, Jaguar®, OMNISOL, and SM*x*GAUSS

Project personnel are trained in theory development and implementation on modern hardware/software combinations.