

Modeling solvation effects on protonation equilibria

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Solvation effects play an important role for equilibrium constants, particularly if the ionization states of reactants change in a polar environment in comparison to the gas phase. In this module you will learn (1) how computational models for predicting chemical equilibria can be built by performing quantum-chemical calculations, (2) to apply such computations to protonation equilibria on the example of predicting differences of pK_a values between various compounds, (3) how the presence of water can be incorporated in electronic structure calculations, (4) how and why results vary between gas phase and an aqueous environment, and (5) inasmuch the predictions depend on the chosen level of theory or model detail.

The practical course requires developing some familiarity with workstations equipped with the Linux operating system. You will learn to construct virtual molecular models on the computer using a hierarchy of techniques, to prepare input files for the computations and to work with and interpret the resulting outputs. Such workflows composed of a variety of software packages are typical examples for working with computational models in practice. The interpretation of the results requires some understanding of the connection between molecular energetics from electronic structure calculations and statistical thermodynamics in order to finally arrive at measurable quantities. You will develop the necessary skills for coupling abstract theoretical models and real-world experiments.