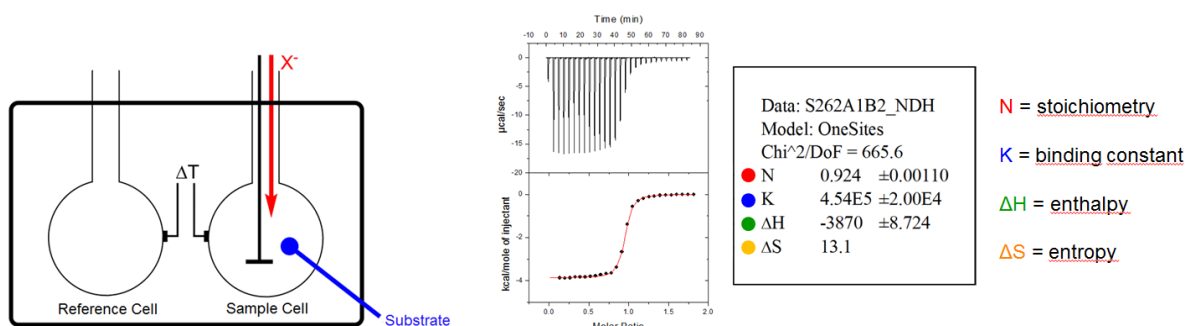


Isothermal Calorimetric Titration (ITC) in Supramolecular Chemistry: Role of Entropy, Counterions, Solvent and Temperature

Compounds in solution interact with each other and of course with the solvent itself. In supramolecular chemistry the focus addresses the strongly interacting parts of compounds and investigates the origin of these non-covalent interactions. Despite the strength of these interactions they readily break up in solution due to thermal collisions, leading to a rapid interchange of molecular relationships in solution.

In order to determine the strength of non-covalent interaction, isothermal titration calorimetry (ITC) measurements can be carried out. To a solution of the Host molecules a defined quantity of the Guest is added and the heat response, based on the interaction, can be observed. This allows the direct determination of the binding constant K , the enthalpy ΔH as well as the binding stoichiometry N . From these variables, the free enthalpy ΔG and the entropy ΔS can be calculated.

In this course you will get an introduction into ITC as well as its capabilities in supramolecular chemistry. You will get hands on experience and a feeling for the abilities and limitations of this Method.



Scheme: (left) Schematic of an ITC instrument; (right) typical ITC-Experiment and its evaluation.