

Dienstag, 17.01.2012

Hörsaal D, Chemie Zentralbau, 17:15 Uhr

Sprecher: **Detlef Schröder**
***Tschechische Akademie der
Wissenschaften Prag***

Thema: **On-line monitoring of chemical
reactions by ESI-MS**
**Or: Mass spectrometry going
towards the condensed phase**

Abstract: Electrospray ionization (ESI) is a powerful method in mass spectrometry (MS) which can be applied to a rather large variety of samples and involves ion generation directly from solution. From the beginning of ESI-MS arose the question, to which extent the ions observed in ESI mass spectra are related with the species present in solution. In the rich literature about this topic, some authors claim a 1:1 sampling of the solution properties, whereas others conclude that the species observed in the gas phase have nothing in common with their counterparts present in solution.

In the course of the HORIZOMS project supported by the *European Research Council*, we set out to address this problem in an empirical manner by the deliberate investigation of (seemingly) simple systems for which complementary condensed-phase data is available. The lecture addresses solutions of simple metal salts MX_n in aqueous and organic solvents as well as the monitoring of catalytic reactions using ESI-MS. In combination, this approach permits several qualitative and also some quantitative correlations between condensed-phase properties and ion abundances in ESI mass spectra.

In selected cases, even a direct modeling of the MS data by condensed-phase concept is possible, as demonstrated in the Figure which shows the ESI-MS results for anion recognition by a supramolecular host (data points) and a thermodynamic modeling based on solution chemistry.

Organisation: I. Fischer

Kontakt: Prof. Dr. Tobias Brixner, Institut für Physikalische und Theoretische Chemie,
brixner@phys-chemie.uni-wuerzburg.de

Weitere Informationen unter
<http://www.phys-chemie.uni-wuerzburg.de>