

MS 5: Molecules, Clusters, Decay and Reactions

Time: Tuesday 16:30–17:45

Location: DO24 1.205

Invited Talk

MS 5.1 Tue 16:30 DO24 1.205

Quantitative Elemental and Molecular Mass Spectrometry for Biological Application — SEBASTIAN BECK, GUNNAR SCHWARZ, RENEE BECKER, DAVID BENDA, VIOLETTE FROCHAUX, KATHLEEN SCHWARZ, KATRIN BRÜCKNER, and MICHAEL LINSCHIED — Humboldt-Universität zu Berlin, Dept. of Chemistry

When chromatographic techniques such as high pressure chromatography (HPLC) and electrophoresis were coupled directly to ICP-MS, elemental MS began to attract attention in biological research, since particularly heavy metals play an important role in biology and ICPS MS is one of the most precise methods in quantitative mass spectrometry. Thus, the analysis of metals and synthetic metal tags came into focus. Recently, we introduced metal tags carrying lanthanoids ("MeCAT") to quantify biopolymers using ICP-MS. Then, we investigated the fragmentation of MeCAT labeled peptide molecular ions and found characteristic fragments, which are formed upon infrared multiphoton dissociation. Hence, it should be possible to screen for MeCAT peptides in mixtures and distinguish between the different metals without the need for an element specific mass spectrometer. Most recently we extended the application range of the tagging technique to DNA oligomers allowing the detection and quantification of specific DNA sequences at very low levels. In this presentation the design of the techniques and the required instrumentation will be discussed. Then, strategies for application in biological mass spectrometry will be presented. Finally, the scope and limitations of this approach will be discussed in the light of most recent developments.

MS 5.2 Tue 17:00 DO24 1.205

Desorption and evaporation sources with photoionizable organic molecules beyond 24 kDa for their suitability for matter wave interferometers — UGUR SEZER¹, LUKAS FELIX², PHILIPP SCHMID¹, MARCEL MAYOR^{2,3}, and MARKUS ARNDT¹ — ¹University of Vienna, Faculty of Physics, QuNaBioS, VCQ Vienna, Austria — ²Department of Chemistry, University of Basel, Basel, Switzerland — ³Karlsruhe Institute of Technology (KIT), Institute of Nanotechnology, Karlsruhe, Germany

With new matter-wave interferometers substantial progress has been made in testing the quantum superposition in a domain of higher complexity. In order to push the limits of matter wave interferometry towards even higher masses, the production of a neutral and slow molecular beam of complex and massive molecules is essential. In this work we present a series of experiments characterizing different laser desorption sources in combination with photoionization (157 and 266 nm). A major result of these studies is the intact volatilization and successful single-photon ionization of organic molecules beyond 24 kDa. Using organic molecules between 7 and 13 kDa we investigate the mass dependence of the photoionization efficiency and of the desorption process. We present mass spectra, velocity distributions, photoionization efficiencies and fragmentation rates of large tailor-made perfluoroalkyl-functionalized molecules as well as more thermolabile biomolecules and

we discuss the suitability of each of the desorption/evaporation sources for matter wave interferometry.

MS 5.3 Tue 17:15 DO24 1.205

Wie invasiv ist der Electrospray-Ionisationsprozess? — ANDREAS HARTMANN¹, MEIJIE CHENG^{1,2}, MICHAEL STEPPERT¹ und CLEMENS WALTHER¹ — ¹Leibniz Universität Hannover, Institut für Radioökologie und Strahlenschutz, Herrenhäuser Str. 2, 30419 Hannover — ²Karlsruher Institut für Technologie, Institut für Nukleare Entsorgung, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen

Die nano-Electrospray-Ionisations Flugzeit Massenspektrometrie kann zum direkten Nachweis in Lösung vorkommender Spezies eingesetzt werden. Mit dieser sanften Ionisationsmethode lassen sich dabei die relativen Anteile geladener Spezies in Lösung abbilden. Dazu wird mit Hilfe einer Spraykapillare, welche sich auf einem hohen positiven Potential befindet, aus einer Lösung ein so genanntes Electrospray erzeugt, in dessen Tröpfchen sich positiv geladene Ionen befinden. Diese werden ins Vakuum überführt und massenspektrometrisch untersucht. Aufgrund der großen positiven Spannung, herrschen in der Kapillare oxidierende Bedingungen. In kürzlich erfolgten Messungen an Mischungen aus Molybdän und Eisen, wurden beide Metalle trotz der oxidierenden Bedingungen zum Teil in ihren reduzierten Formen detektiert (Mo(V) bzw. Fe(II)). Um einen Einfluss der Methode auf den Oxidationszustand der in Lösung vorkommenden Ionen auszuschließen, werden Eisenlösungen mit definierten Fe(II)/Fe(III)-Verhältnissen im stark sauren Bereich bei verschiedenen Säurestärken untersucht.

MS 5.4 Tue 17:30 DO24 1.205

Novel setup for the investigation of metal-cluster-ligand complexes in the gas phase — DANIEL NEUWIRTH, KATHRIN LANGE, JAN ECKHARD, BRADLEY VISSER, MARTIN TSCHURL, ULRICH BOESL, and UELI HEIZ — Lehrstuhl für Physikalische Chemie & Catalysis Research Center, Chemistry Department, Technische Universität München, Lichtenbergstraße 4, 85748 Garching bei München, Germany

Many properties, like reactivity, of metal clusters are different from those of the bulk material. While gold is noble under most circumstances the reactivity of gold clusters depends highly upon charge and size. Furthermore noble metal clusters can catalyze various reactions. Our goal is to study metal clusters with organic ligands acting as tracer molecules in the gas phase.

Therefore, a state of the art cluster source was combined with a pulsed gas inlet. The formed cluster-ligand complexes can then be characterized by time-of-flight mass spectrometry or further investigated by different spectroscopic methods.

In a second part of the experiment it is planned to store cluster-ligand complexes within an ion trap. The trapped complexes can then interact with reactant gases present in the trap. Therefore a ring electrode trap is currently added to the experiment.