

## MS 1: New Mass Spectrometric Methods and Technical Developments

Time: Monday 10:30–12:30

Location: DO24 1.205

## Invited Talk

MS 1.1 Mon 10:30 DO24 1.205

**Mass spectrometry in planetary sciences** — ●INGO LEYA — Physical Institute, University of Bern, Switzerland

Thanks to recent improvements in mass spectrometry, there is actually a significant progress in our understanding of planet formation and evolution. By way of example, studying meteorites and especially early solar system condensates found in meteorites with secondary ion mass spectrometry, thermal ionization mass spectrometry and/or inductively plasma mass spectrometry a consistent and reliable chronology of the first few million years of the solar system can be obtained. Some of the new results significantly changed our understanding of planetary accretion, differentiation, and evolution. In addition, very important results can be obtained by studying noble gases in planetary bodies and their constituents. Since noble gases are not affected by chemical reactions, their abundances directly trace back to the physical conditions at the beginning of the solar system. Noble gases are depleted in planetary bodies by up to 10 orders of magnitude, therefore small changes and small contributions are relatively easy to detect. By way of example, noble gases are a major tool to detect and study presolar grains, i.e., grains that have been formed in supernova explosions and/or red giant stars earlier and outside of the solar system. However, studying noble gases comes with a price; we need very sophisticated and efficient mass spectrometers and extraction techniques, which very often results in self-made systems and instruments dedicated for special tasks.

MS 1.2 Mon 11:00 DO24 1.205

**MC-ICP-MS vs. IRMS: Advantages and Limits in Case of Isotopic Enriched Silicon** — ●AXEL PRAMANN<sup>1</sup>, JANINE NOORDMANN<sup>1</sup>, OLAF RIENITZ<sup>1</sup>, HELMUT BECKERS<sup>2</sup>, and HELGE WILLNER<sup>2</sup> — <sup>1</sup>Physikalisch-Technische Bundesanstalt (PTB), Bundesallee 100, 38116 Braunschweig, Germany — <sup>2</sup>Bergische Universität Wuppertal, Gausstr. 20, 42097 Wuppertal, Germany

The scheduled redefinition of the Si unit kilogram is connected to the determination of the Avogadro constant with smallest associated uncertainty.[1] Mass Spectrometry on the highest metrological level is used to measure the molar mass of a silicon material enriched in <sup>28</sup>Si.[2] We report on the advantages and improvements using high resolution multicollector-ICP-MS to measure that material. A new advancement of an analytical approach of mass bias correction in isotope ratio measurement, resulted in a strong reduction of the uncertainty associated with M down to a relative uncertainty of  $6.1 \times 10^{-9}$ . The uncertainty budget and main features of the new theory for correction (K) factor determination are given. For calibration purposes of an isotope ratio gas mass spectrometer (IRMS) this Si material was converted into silicon tetrafluoride and further investigated with respect to the isotopic composition of silicon. The limits and improvements compared to the complementary MC-ICP-MS method are presented.

[1] B. Andreas et al., *Metrologia*, 48, S1 (2011).

[2] A. Pramann, O. Rienitz, D. Schiel, J. Schlote, B. Güttler, and S. Valkiers, *Metrologia* 48, S20 (2011).

MS 1.3 Mon 11:15 DO24 1.205

**Performance Results of a Mobile High-Resolution MR-TOF Mass Spectrometer for in-situ Analytical Mass Spectrometry** — ●WAYNE LIPPERT<sup>1</sup>, JOHANNES LANG<sup>1</sup>, SAMUEL AYET SAN ANDRÉS<sup>2</sup>, TIMO DICKEL<sup>1,2</sup>, HANS GEISSEL<sup>1,2</sup>, WOLFGANG PLASS<sup>1,2</sup>, CHRISTOPH SCHEIDENBERGER<sup>1,2</sup>, and MIKHAIL YAVOR<sup>3</sup> — <sup>1</sup>Justus-Liebig-Universität Gießen — <sup>2</sup>GSI, Darmstadt — <sup>3</sup>RAS St. Petersburg

A mobile multiple-reflection time-of-flight mass spectrometer (MR-TOF-MS) has been developed which provides a mass resolving power exceeding 250,000 and sub-ppm mass accuracy in a transportable format. Thus it allows resolving isobars and enables accurate determination of the composition and structure of biomolecules. Furthermore the device offers high mass resolving MS/MS capability via selective ion re-trapping and collisional-induced dissociation (CID). An atmospheric pressure interface (API) provides for routine measurements with various atmospheric ion sources. All supply electronics, DAQ and control system are mounted with the spectrometer into a single frame with a total volume of only 0.8m<sup>3</sup>. With the current system many applications like waste water monitoring at hot spots, mass-based classifica-

tion of biomolecules and breath analysis are possible. In addition the mass spectrometer is readily scalable and can be adopted and simplified for even more specific use like in space science for instance. A characterization and first performance results will be shown and the implementation of MS/MS in combination with CID will be discussed.

MS 1.4 Mon 11:30 DO24 1.205

**Ion Sources for systematic Gas Cell studies** — ●ANN-KATHRIN RINK<sup>1</sup>, SAMUEL AYET<sup>2</sup>, TIMO DICKEL<sup>1,2</sup>, JENS EBER<sup>1</sup>, HANS GEISSEL<sup>1,2</sup>, FLORIAN GREINER<sup>1</sup>, EMMA HAETTNER<sup>2</sup>, IVAN MISKUN<sup>3</sup>, WOLFGANG R. PLASS<sup>1,2</sup>, SIVAJI PURUSHOTHAMAN<sup>2</sup>, MORITZ PASCAL REITER<sup>1</sup>, and CHRISTOPH SCHEIDENBERGER<sup>1,2</sup> — <sup>1</sup>Justus-Liebig Universität Gießen — <sup>2</sup>GSI Helmholtzzentrum für Schwerionenforschung — <sup>3</sup>Tomsk Polytechnic University

The FRS Ion Catcher, a test facility for the low energy branch (LEB) of the Super-FRS, has been commissioned and successfully tested. The current setup consists of a gas filled cryogenic stopping cell (CSC) to thermalise exotic nuclei, a diagnostic unit to monitor and transport the stopped and extracted ion beam into the multiple-reflection time-of-flight mass-spectrometer (MR-TOF-MS), where they are identified by precision mass measurements. The MR-TOF-MS can also be used to provide isobarically clean beams for experiments further downstream.

To investigate ion transport and extraction processes of the CSC three different ion sources are in use inside the CSC. A movable radioactiv ion source is mounted to test the ion transport depending on the initial ion position. A multiple target laser ablation ion source is mounted to test the mass and time dependency of the ion transport and extraction. It also provides calibration ions for the MR-TOF-MS. For investigating intensity limitations due to space charge and plasma effects and the cleanliness of the CSC an electrical discharge ion source is installed.

MS 1.5 Mon 11:45 DO24 1.205

**RF-Quadrupol-Strahlweiche des MR-TOF-Isobarenseparators für das TITAN-Experiment** — ●FLORIAN GREINER<sup>1</sup>, DEVIN SHORT<sup>1,3</sup>, CHRISTIAN JESCH<sup>1</sup>, TIMO DICKEL<sup>1,2</sup>, WOLFGANG PLASS<sup>1,2</sup>, SAMUEL AYET SAN ANDRÉS<sup>2</sup>, ALEXANDER BUERS<sup>1</sup>, HANS GEISSEL<sup>1,2</sup>, JOHANNES LANG<sup>1</sup>, WAYNE LIPPERT<sup>1</sup>, CHRISTOPH SCHEIDENBERGER<sup>1,2</sup> and MIKHAIL YAVOR<sup>4</sup> — <sup>1</sup>JLU Gießen — <sup>2</sup>GSI, Darmstadt — <sup>3</sup>TRIUMF, Vancouver, Kanada — <sup>4</sup>Inst. for Analytical Instrum., Russian Academy of Sci., St. Petersburg, Russland

Eine Möglichkeit zur Erzeugung exotischer Nuklide ist die ISOL-Methode. Neben einer hohen Anzahl an gewünschten, werden aber auch viele unerwünschte Nuklide erzeugt. Daher wird eine effiziente Separationsmethode benötigt. Typischerweise wird ein magnetischer Separator verwendet, welcher jedoch keine Isobarenseparation ermöglicht. Da die TITAN-Anlage an TRIUMF (Vancouver) stark von isobarenreinen Strahlen profitieren wird, wurde ein spezieller Isobarenseparator auf Basis eines MR-TOF-MS entwickelt. Dieser weist ein wesentlich höheres Massenaufklärungsvermögen als Magnetseparatoren auf. Um den Isobarenseparator in die Strahlführung bei TITAN einzubinden, ist eine spezielle Strahlweiche nötig. Wichtige Anforderungen sind das schnelle Umschalten ( $\sim 100\mu\text{s}$ ) zwischen verschiedenen Ein- und Ausgängen und die Möglichkeit sie direkt in ein gasgefülltes System einzubinden. Es konnte erstmals eine solche Strahlweiche erfolgreich getestet werden. Mit ihr ist es ebenfalls möglich Ionen aus mehreren Quellen zu unterschiedlichen Detektoren zu leiten. Die Strahlweiche ist an jeder Niederenergie-Strahlführung universell einsetzbar.

MS 1.6 Mon 12:00 DO24 1.205

**Optimierungen und Anwendungen des kompakten Lasermassenspektrometers LAMPAS 3 zur Charakterisierung von Aerosolpartikeln** — ●KLAUS-PETER HINZ, ALOIS FENDT and BERNHARD SPENGLER — Institut für Anorganische und Analytische Chemie, Universität Giessen, Schubertstrasse 60, 35392 Giessen

Die schnelle und detaillierte Analyse von Aerosolpartikeln der Umgebungsluft ist von zentraler Bedeutung bei der Beurteilung von Umwelt- und Gesundheitsrisiken. Mit dem kompakten, on-line Lasermassenspektrometer LAMPAS 3 [1] steht ein Messsystem zur Verfügung, das eine schnelle und aussagekräftige vor-Ort-Analyse einzelner Partikel ermöglicht. Die Partikel werden dazu ohne störende Beeinflussung direkt in die Ionenquelle eines Flugzeitmassenspektrometers eingelassen.

Nach der Partikeldetektion und der Bestimmung der Partikelgröße erfolgt die zeitlich abgestimmte Laserdesorption/Ionisation (LDI) der Partikel mittels eines UV-Laserpulses. Die simultane Detektion der erzeugten positiv und negativ geladenen Ionen ermöglicht die umfassende chemische Charakterisierung der Einzelpartikel. Die Ergebnisse der instrumentellen Optimierung des LAMPAS 3-Systems und seine Leistungsfähigkeit werden anhand verschiedener Labor- und Feldmessungen vorgestellt. [1] K.-P. Hinz, E. Gelhausen, K.-C. Schäfer, Z. Takats, B. Spengler. *Anal. Bioanal. Chem.* (2011) 401:3165-3172.

MS 1.7 Mon 12:15 DO24 1.205

**Unexpected Ions in the ICPMS: Abundance and Impact of Doubly Charged Molecular Argide ( $\text{M}\text{Ar}^{2+}$ ) Ions** — •BODO HATTENDORF, BIANCA GUSMINI, LADINA DORTA, MARKUS REIHER, and DETLEF GÜNTHER — ETH Zurich, Laboratory of Inorganic Chemistry, Wolfgang Pauli Str. 10, 8093 Zurich, Switzerland

Doubly charged molecular ions containing argon in mass spectra from an inductively coupled plasma mass spectrometer were recently detected using a highly sensitive sector field instrument (NU Plasma

HR). Their presence was previously unexpected as only molecular ions with high binding energies were suspected to survive the high temperature, high density atmospheric ICP ion source. Quantum mechanical calculations indicate that such species can be formed via association of a doubly charged elemental ion to a neutral argon atom and their bond energy can reach values of up to 0.3 eV. Doubly charged atomic ions are present in the ICP at varying degree for elements with low 2nd ionization energy as alkaline earth or rare earth elements amongst others. Due to the fact that formation rates are in the  $10^{-5}$  range, relative to the corresponding elemental ions, their influence on quantification should remain small. Significant impact can, however, occur in isotope ratio analyses, when aiming at accuracy in the 10 ppm range. Critical contributions may be observed for Sr isotope ratios, where  $^{86}\text{Sr}^+$ ,  $^{87}\text{Sr}^+$  and  $^{88}\text{Sr}^+$  cannot be resolved from  $^{132}\text{Ba}^{40}\text{Ar}^{2+}$ ,  $^{134}\text{Ba}^{40}\text{Ar}^{2+}$  and  $^{136}\text{Ba}^{40}\text{Ar}^{2+}$  respectively or S isotopes where  $^{32}\text{S}^+$  and  $^{33}\text{S}^+$  cannot be distinguished from  $^{24}\text{Mg}^{40}\text{Ar}^{2+}$  and  $^{26}\text{Mg}^{40}\text{Ar}^{2+}$ . Additionally interesting was the fact that the corresponding singly charged molecular ions are by about 10 times less abundant, despite the more than 10 times higher concentration of the atomic ions within the ICP source.