MS 7: New Methods, Technical Development II

Time: Thursday 14:45–15:30 Location: HS 2 Chemie

MS 7.1 Thu 14:45 HS 2 Chemie

Optimizing ToF-SIMS Analysis Conditions for Detecting Antibiotics in Frozen Hydrated Samples — •Michael Bäumer, Thorsten Adolphs, Richard Erling Peterson, Bonnie June Tyler, and Heinrich Franz Arlinghaus — University of Münster, Münster, Germany

In order for most biological specimens to be analyzed with ToF-SIMS, either the water must be removed via a process such as freeze-drying or the samples must be frozen and analyzed under cryogenic conditions. Cryogenic preparation and analysis of biological samples preserves the 3-dimensional structure of tissues and biofilms and can prevent migration artifacts that occur during freeze-drying. However, ToF-SIMS analysis of frozen aqueous sample systems results in a spectrum of pure and non-pure water ice cluster ions, extending to high masses, which can interfere with detection of biomolecules. Furthermore, metastable decay of the cluster ions in the time-of-flight analyzer can lead to a high background that raises the detection limit for target analytes. In this study, we have investigated the influence of a range of analytical parameters, including primary ion species, cluster size, analysis temperature and analyzer voltages, on the spectrum of water ice mixed with typical biological sample preparation additives such as dextran, ammonium formate, acetic acid and the antibiotic ciprofloxacin. The aim of this work is to optimize analysis conditions in order to improve the detection limit for antibiotic compounds. We also provide an outlook on further reduction of background signals by the destruction of water ice clusters using a 157 nm excimer laser.

MS 7.2 Thu 15:00 HS 2 Chemie

Status of the MR-ToF MS for JetRIS for laser spectroscopy of heavy actinides at GSI/HIM — •J. Weyrich[1,2,3], M. Block[1,2,3], A. Brizard[4], C. Helmel[2,3], D. Münzberg[1,2,3], P. Fischer[5], S. Raeder[1,2], D. Rodríguez[7], M. Schlaich[6], L. Schweikhard[5], K. Wendt[3], and F. Wienholtz[6] — [1]GSI, Darmstadt, DE — [2]Helmholtz-Institut, Mainz, DE — [3]JGU, Mainz, DE — [4]GANIL, Caen, France — [5]Universität Greifswald, Greifswald, DE — [6]Technische Universität, Darmstadt, DE — [7]Universidad de Granada

Research on heavy and superheavy elements enhances our understanding of the nuclear structure, as these elements exist just due to nuclear shell effects. These elements are radioactive, with short half-lives, and produced only in limited quantities. As a result, techniques like Resonant Ionization Spectroscopy (RIS) play a crucial role in studying atomic spectra to determine atomic and nuclear properties. The in-gas Jet Resonant Ionization Spectroscopy (JetRIS) experiment at GSI in Darmstadt, Germany, allows spectroscopy of heavy elements on minute amounts and with a spectral resolution of down to 260 MHz. JetRIS currently utilizes α-decay detection to selectively measure isotopes achieving low to zero background. However, this method is not suitable for long-lived isotopes or those without an α-decay branch. Thus, a Multi-Reflection Time-of-Flight Mass Spectrometer (MR-ToF MS) [DOI: 10.1016/j.ijms.2023.117166] will be integrated into the JetRIS setup enabling ion detection through mass-to-charge ratio separation. This contribution will discuss the MR-ToF MS setup, its commissioning status, and the latest experimental results.

MS 7.3 Thu 15:15 HS 2 Chemie

TOFControl, a data acquisition and analysis software system for multiple-reflection time-of-flight mass spectrometry (MR-TOF-MS) — •Makar Simonov and Julian Bergmann for the FRS Ion Catcher-Collaboration — Justus-Liebig-Universität Gießen, Gießen, Germany

TOFControl is a software system that was developed to perform high-accuracy measurements utilizing MR-TOF-MS techniques in analytical chemistry at the Justus-Liebig University (JLU), Giessen, Germany and in accelerator-based physics research centers at GSI, Darmstadt, Germany and TRIUMF, Vancouver, Canada. The software allows to control timing settings and data acquisition hardware, monitor and optimise measurement performance. In addition, it is equipped with various tools for the interpretation and evaluation of mass spectra including data adjustment, peak detection, and recognition procedures.

In this talk, an overview of the TOFControl functionality for the acquisition and analysis of mass spectrometry data will be given. Several examples illustrating the software's capabilities to perform filtering, identification, and mass measurement of atomic and molecular ions will be provided.