PROGRAMME

28th ICP-MS Anwender*innen-treffen 2022

September 5-8, 2022

Montanuniversität Leoben, Austria

MONTAN UNIVERSITÄT LEOBEN

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Programme

Abstracts

Welcoming Words

Liebe ICP-MS - Anwender*innen!

Wir freuen uns sehr, Sie zum 28. ICP-MS ANWENDER*INNEN TREFFEN UND 14. SYMPOSIUM MASSENSPEKTROMETRISCHE VERFAHREN DER ELEMENTSPURENANALYSE (kurz: ICP-MS AW*T2022) in Leoben, Österreich, begrüßen zu dürfen.

Nachdem wir 2001 das ICP-MS Anwendertreffen in Wien und 2012 das ICP-MS Anwendertreffen in Tulln, Österreich, ausrichten durften, sind wir nun wiederum ca. 10 Jahre später sehr dankbar, das ICP-MS AW*T als Präsenzevent zu veranstalten.

In dieser Zeit, in der persönliche Treffen und Tagungen eine Besonderheit geworden sind, blicken wir auf eine Woche im Zeichen des wissenschaftlichen Austauschs im Bereich der Element-, Isotopen-, und Speziesanalytik. Dies beinhaltet neben wissenschaftlichen Vorträgen und Posterbeiträgen sowie der Firmenausstellung ein Angebot an Workshops und Short Courses von Kolleg*innen und Gerätehersteller*innen.

Neben dem wissenschaftlichen Programm werden Ihnen ein abwechslungsreiches Rahmenprogramm bieten, um einerseits die Montanstadt Leoben in der Erzbergregion vorzustellen, sowie ausreichend Raum für persönliche Gespräche und Interaktion zu ermöglichen – in gemütlich steirischer Atmosphäre.

Ohne den großzügigen Support unserer Sponsor*innen wäre es uns nicht möglich, diese Veranstaltung mit dem entsprechenden Rahmenprogramm zu gestalten. Ein ganz großer Dank gilt daher allen unseren Sponsor*innen!

Viele freiwillige Helfer*innen unserer Universität haben im Vorfeld daran mitgearbeitet, diese Tagung erfolgreich vorzubereiten. Vielleicht ist nicht alles bis ins kleinste Detail perfekt, aber mit Herz vom Tagungsteam getragen.

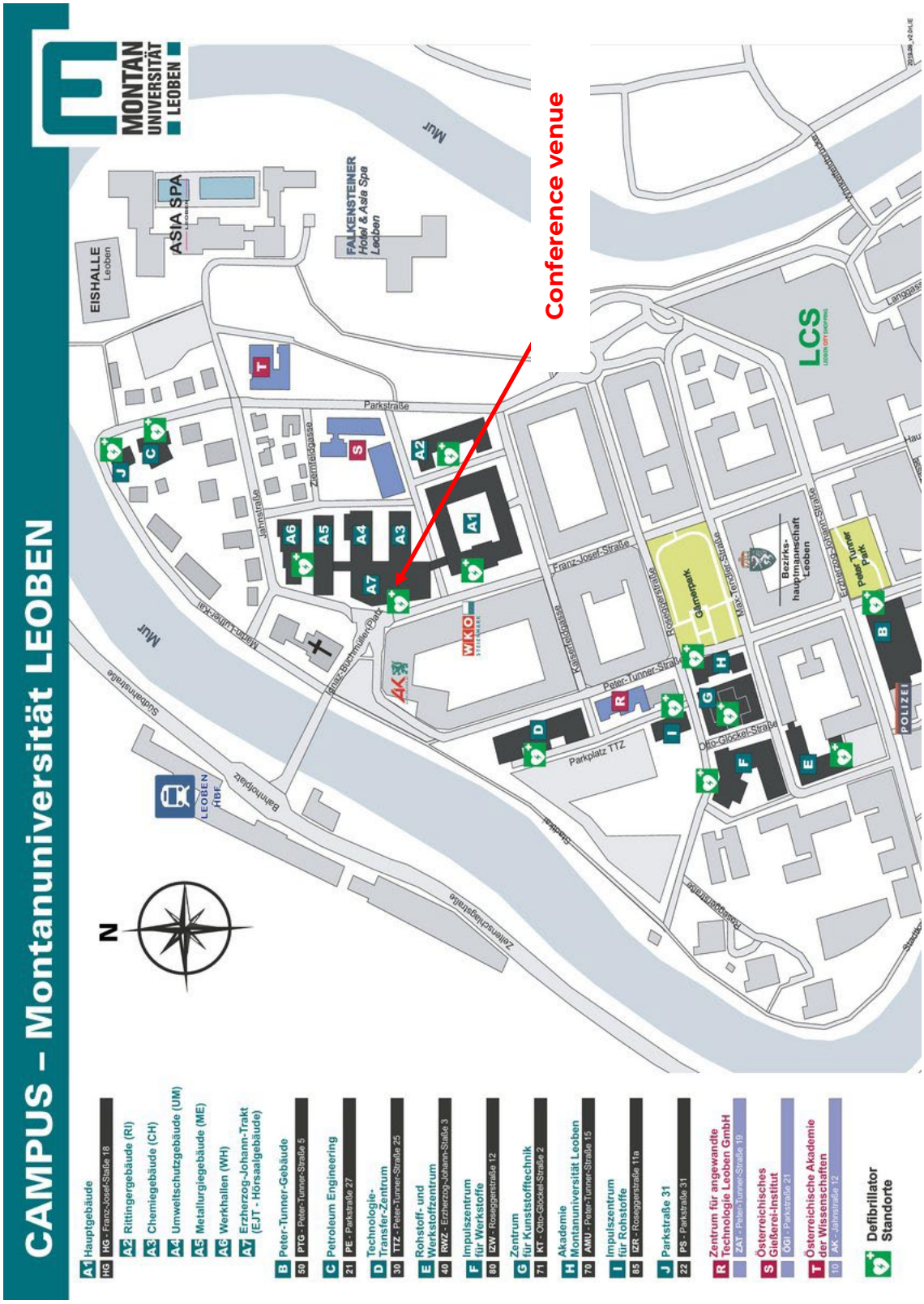
Schlussendlich lebt eine Tagung aber von Ihnen, den Teilnehmer*innen. Wir freuen uns auf eine schöne Tagung in wertschätzender und entspannter Atmosphäre und sind gespannt auf Neuheiten, Entwicklungen und all das, was aus den Begegnungen, Gesprächen und Diskussionen entsteht.

Im Namen des gesamten Organisations- und Tagungsteams,

Glück auf,
Johanna Irrgeher

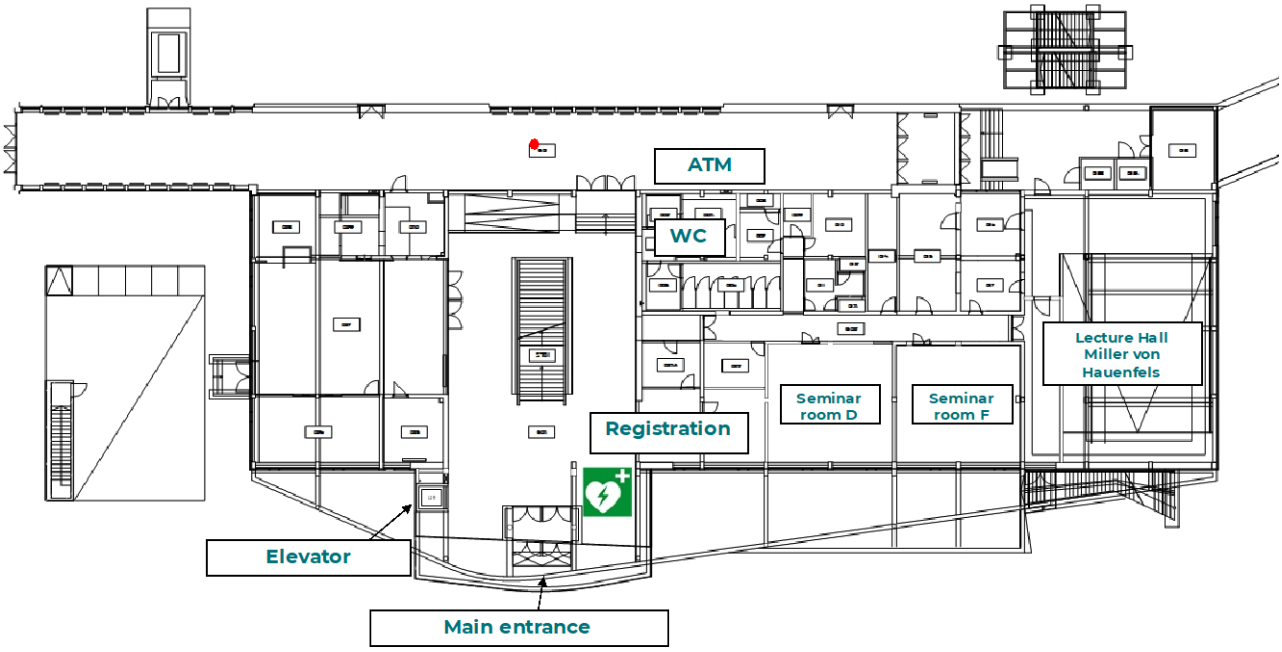
28. ICP-MS ANWENDER*INNEN TREFFEN UND
14. SYMPOSIUM MASSENSPEKTROMETRISCHE VERFAHREN
DER ELEMENTSPURENANALYSE

Venue

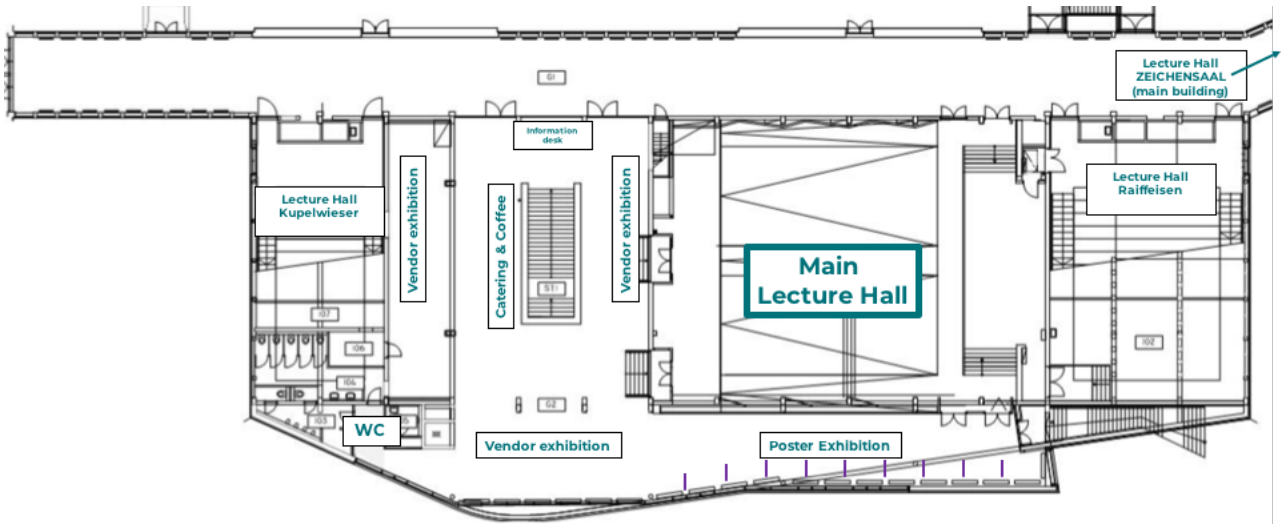

CAMPUS – Montanuniversität LEOBEN
MONTAN UNIVERSITÄT LEOBEN
A1 Hauptgebäude
HG - Franz-Josef-Straße 18
A2 Rittingergebäude (RI)
A3 Chemiegebäude (CH)
A4 Umweltschutzgebäude (UM)
A5 Metallurgiegebäude (ME)
A6 Werkhallen (WH)
A7 Erzherzog-Johann-Trakt (EJT - Hörsaalgebäude)
B Peter-Tunner-Gebäude
PTG - Peter-Tunner-Straße 5
C Petroleum Engineering
PE - Parkstraße 27
D Technologie-Transfer-Zentrum
TTZ - Peter-Tunner-Straße 25
E Rohstoff- und Werkstoffzentrum
RWZ - Erzherzog-Johann-Straße 3
F Impulszentrum für Werkstoffe
IZW - Roseggerstraße 12
G Zentrum für Kunststofftechnik
KT - Otto-Glöckel-Straße 2
H Akademie Montanuniversität Leoben
AMU - Peter-Tunner-Straße 15
I Impulszentrum für Rohstoffe
IZR - Roseggerstraße 11a
J Parkstraße 31
PS - Parkstraße 31
R Zentrum für angewandte Technologie Leoben GmbH
ZAT - Peter-Tunner-Straße 19
S Österreichisches Gießerei-Institut
ÖGI - Parkstraße 21
T Österreichische Akademie der Wissenschaften
AK - Jahnstraße 12
Defibrillator Standorte
Conference venue
N
Mur
EISHALLE Leoben
ASIA SPA
FALKENSTEINER Hotel & Asia Spa Leoben
Parkstraße
Zeiselgasse
Lahnstraße
Franz-Josef-Straße
Kaiserdoppelgasse
Peter-Tunner-Straße
Roseggerstraße
Gänsepark
Max-Tendler-Straße
Otto-Glöckel-Straße
Parkplatz TTZ
Bezirks-hauptmannschaft Leoben
Erzherzog-Johann-Straße
Peter Tunner Park
POLIZEI
LCS
LEOBEN HBF.
Bahnhofplatz
Südbahnstraße
Zeltenschlossstraße
Franz-Buchmüller-Platz
Franz-Josef-Straße
Lamoggasse
Wiesenbachstraße
Roseggerstraße
Stadtbr.
2019-09 - v2.0rLIE

Venue

Ground floor



First floor



General Information

Conference venue:

Montanuniversität Leoben

Franz-Josef-Straße 18

8700 Leoben

Conference telephone & E-mail:

2.9., and 5.-9.9.2022, 8.00 am to 6.00 pm: +43-680-2121145

Emergency number 24/7: +43-664-80898-1204

Contact number for vendors and exhibitors: +43-664-80898-1204

E-mail: icpms-leoben2022@unileoben.ac.at

Conference webpage: https://icpms-leoben2022.at

Registration hours:

Monday, 5.9., 8.00 am – 2.30 pm

Tuesday, 6.9., 8.00 am – 10.00 am

The registration desk can be found at the entrance of the university building.

If you arrive outside of opening hours, contact the conference team and we will be happy to help.

Fotos / Recordings

Von dieser Veranstaltung werden Fotoaufnahmen angefertigt. Wenn Sie nicht fotografiert werden möchten, können Sie direkt den*die Fotograf*In ansprechen. Das digitale Aufzeichnen von Vorträgen während der Tagung ist nicht gestattet.

Photographs will be made of this event. If you do not wish to be photographed or filmed, you can contact the photographer directly. The recording of lectures during the conference is not permitted.

More information will be provided on the conference webpage!

Acknowledgements

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DAAS Deutscher Arbeitskreis für Analytische Spektroskopie

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DGMS Deutsche Gesellschaft für Massenspektrometrie

LACTAN Chemikalien und Laborgeräte

Springer ANALYTICAL & BIOANALYTICAL CHEMISTRY

SPETEC

TELEDYNE CETAC TECHNOLOGIES Everywhereyoulook

AJB INSTRUMENTATION

TOFWERK

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- KATHRIN THIELE
- CHRISTOPH WALKNER
- SARA WIDHALM

Invited Speakers

Jörg Bettmer ist derzeit Professor für Analytische Chemie an der Universität Oviedo, Spanien. Sein Chemie-Studium absolvierte er an der Universität Münster mit anschließender Diplom- und Doktorarbeit unter der Anleitung von Professor Cammann. Seine Dissertation wurde 1996 mit dem A.M.S.El.-Preis ausgezeichnet. Im Jahr 2000 begann er bei Professor Heumann an der Universität Mainz als wissenschaftlicher Assistent und erhielt die „Venia legendi" in Analytischer Chemie im Jahr 2004. Seine Arbeiten wurden 2007 mit dem Bunsen-Kirchhoff-Preis und dem Mattauch-Herzog-Preis ausgezeichnet. Im selben Jahr wechselte er an die Universität von Oviedo und forscht seitdem an der ICP-MS Analyse von Elementspezies, Nanopartikeln und individuellen Zellen.

Lukas Brunnbauer received his BSc and MSc in Technical Chemistry from the TU Wien. He started his PhD in 2018 in cooperation with Infineon Austria AG in the research group "Surface Analytics, Trace Analytics and Chemometrics" headed by Prof. Dr. Andreas Limbeck at TU Wien where he focused mainly on polymer analysis using a tandem LA-ICP-MS/LIBS setup. During his PhD he spent 4 months as a guest researcher at Applied Spectra, Inc, CA, USA working on fs-LIBS. He finished his PhD in 2021 and is now a Post-Doc at TU Wien focusing on the application of LA-ICP-MS and LIBS to various fields of materials science.

Sergei Boulyga received his PhD from the Institute of Radiation Physics and Chemistry in Belarus. With a research fellowship from the Alexander von Humboldt-foundation, he conducted postdoctoral research at Research Center Jülich, Germany. In 2003, he received the Bunsen–Kirchhoff Award for Analytical Spectroscopy. Later on Sergei was employed as a visiting scientist and project leader at Universities in Mainz, Germany and BOKU Vienna, Austria. He completed his habilitation (venia docendi) in Inorganic Analytical Chemistry in 2008. Since 2007, he has been working at the International Atomic Energy Agency. Sergei's research focuses on mass spectrometric trace and isotope analysis.

David Clases ist ein analytischer Chemiker und forscht an Methoden zur Charakterisierung von Mikro- und Nanostrukturen mittels ICP-MS im Kontext der Umwelt- und Lebenswissenschaften. Unter anderem interessiert er sich für den Einsatz funktionaler Nanostrukturen zur Verbesserung analytischer Verfahren. Er studierte Chemie an der Universität Münster und promovierte 2017, bevor er als Stipendiat der Deutschen Forschungsgesellschaft an die University of Technology Sydney ging. Dort wurde er 2020 Dozent und baute seine eigene Gruppe und unabhängiges Forschungsprogramm auf. Seit 2021 ist er Assistenzprofessor für Analytische Chemie am Institut für Chemie der Universität Graz.

Raquel Gonzalez de Vega ist analytische Chemikerin und promovierte 2017 in der Gruppe von Prof. Sanz Medel an der Universität Oviedo (Spanien). Während ihrer Promotion unternahm sie zwei Forschungsaufenthalte an der Universität Münster und wurde anschließend ein Postdoc an der Technischen Universität in Sydney (UTS), wo sie ab 2020 als Dozentin tätig war. Seit 2021 forscht sie am Institut für Chemie der Universität Graz und konzentriert sich auf die Methodenentwicklung und Anwendung der ICP-MS-basierten Kopplungstechniken für die Element-Speziation und Bildgebung. Sie setzt funktionale Nanomaterialien ein, um die ICP-MS am Schnittpunkt von Metallomics und Proteomics einzusetzen.

Invited Speakers

Carsten Engelhard is an Associate Professor of Analytical Chemistry and the Department Chair of the Department of Chemistry and Biology at the University of Siegen. He received his Dr. rer. nat. degree in 2007 from the University of Münster, Germany, and was a post-doctoral fellow at Indiana University, from 2008 to 2010 under the guidance of Prof. G.M. Hieftje. Carsten has 10 years of experience in ultratrace elemental analysis, mass spectrometry, instrumentation, surface analysis, and nanoparticle detection. He has published more than 70 peer-reviewed articles in this field and successfully supervised seven PhDs.

Jörg Feldmann has the chair of analytical chemistry at the University of Graz (Austria) since 2020. He has been educated at the University of Essen as Chemist and did his Master thesis in Geochemistry at Chamber of Mines in South Africa, before he graduated with a PhD in environmental analytical chemistry in 1995. Then he was a Feodor Lynen Fellow (Alexander von Humboldt Foundation) at University of British Columbia and senior postdoc University of Alberta (Canada) in environmental and clinical chemistry. Subsequently, he spent 23 years as a professor for environmental chemistry and director of TESLA (trace element speciation laboratory) at the University of Aberdeen, Scotland, UK.

He is an elected fellow of the Scottish Academy of Science and Society (Royal Society of Edinburgh) and a fellow of the RSC. He has written more than 300 peer reviewed papers (Scholar citations >20,000) and received numerous prizes such as the European Award for Plasma Spectrochemistry (2015) and the RSC Interdisciplinary Prize and Medal (2016), Engagement with the Industry Award (2020) Under his supervision, more than 40 PhD students have graduated. His main interest is in the development of new methodology, mainly using elemental and molecular mass spectrometry and its application for the elements, arsenic, mercury, selenium and lately zinc and fluorine.

More infos: chemie.uni-graz.at/en/analytical-chemistry/research/tesla

Lisa Fischer ist analytische Chemikerin in der Arbeitsgruppe von Prof. Hann am Institut für Analytische Chemie an der BOKU Wien, wo sie 2011 ihre Dissertation abschloss. Forschungsaufenthalte während des Doktoratsstudiums und als Erwin-Schrödinger-Post-Doc-Stipendiatin führten sie an die Rutgers State University in NJ und die UCSC Santa Cruz, Ca (Institute of Marine Sciences). Ihre Forschungsschwerpunkte sind die Entwicklung von automatisierten Anreicherungsmethoden für die Element-Ultraspurenanalytik von Oberflächen- und Grundwasser sowie die Speziesanalytik.

Stephan Hann is Professor of analytical chemistry and Head of the Institute of Analytical Chemistry at the University of Natural Resources and Life Sciences (BOKU) in Vienna, Austria. He obtained his PhD in analytical chemistry in 2001 from the Technical University of Vienna. In the same year, he took a position as University Assistant at BOKU where he established his research group and obtained his Habilitation on the field of elemental speciation analysis in 2005. His main areas of research are separation sciences, elemental and molecular mass spectrometry, environmental analysis, metabolomics, elemental ultra-trace and speciation analysis, authenticity of food and beverages as well as uncertainty of measurement. He has published more than 180 SCI-papers. He is head of the advisory board of the BOKU Core Facility Mass Spectrometry, PI and faculty member of the Doctoral School AgriGenomics, PI and associated faculty member of the PhD Program BioToP, key researcher of the Austrian COMET Centres "Centre of Industrial Biotechnology (acib)" and "Austrian Competence Centre for Feed and Food Quality (FFoQSI)". Additionally, Stephan Hann is board member of Austrian Society of Analytical Chemistry and an Austrian delegate in the Division of Chemistry and the Environment of the European Chemical Society.

Invited Speakers

Uwe Karst studierte Chemie an der Universität Münster und promovierte 1993 in Analytischer Chemie bei Karl Cammann auf dem Gebiet der Immunoassays. Nach einem Aufenthalt als Postdoktorand bei Robert E. Sievers an der University of Colorado in Boulder 1993/1994 baute er seine eigene Arbeitsgruppe in Münster auf und habilitierte sich 1998. Im Jahr 2001 übernahm er den Lehrstuhl für Chemische Analytik an der Universität Twente, bevor er 2005 seine derzeitige Position als Lehrstuhlinhaber an der Universität Münster antrat.

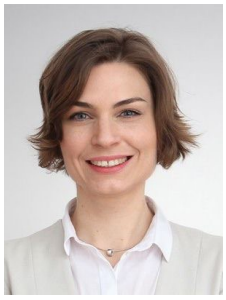
Seine Forschungsinteressen erstrecken sich über analytische Kopplungstechniken und Massenspektrometrie, darunter die online-Kombination aus Elektrochemie und Massenspektrometrie, die Speziationsanalytik und multimodale chemische Bildgebungstechniken. Seine Arbeitsgruppe fokussiert sich hierbei zumeist auf die Entwicklung von Methoden zur Lösung biomedizinischer Probleme, aber auch auf umweltwissenschaftliche und materialwissenschaftliche Fragestellungen. Uwe Karst ist Autor von über 350 Publikationen in wissenschaftlichen Zeitschriften mit Peer Review-System und Betreuer von bisher 86 abgeschlossenen Promotionen. Mit seinem Team organisierte er zahlreiche internationale Tagungen in Münster, darunter das International Symposium on Metallomics 2011 oder die European Winter Conference on Plasma Spectrochemistry 2015.

Daniel Pröfrock studied Chemistry and Environmental Sciences. In 2001, he started his PhD thesis at the GKSS research centre (previously named HZG, now Helmholtz-Zentrum-Hereon) in the group of Prof. Andreas Prange. In 2005, he obtained his PhD degree (summa cum laude) from the Leuphana University Lüneburg (Germany). He continued his work as a post-doctoral fellow, before he became a permanent research scientist at the HZG Institute of Coastal Research in 2007. Currently he is leading the Department Inorganic Environmental Chemistry, which is part of the Institute of Coastal Environmental Chemistry.

Daniels main interests are focused on the determination, speciation and isotopic analysis of (trace) elements in environmental samples within complex interdisciplinary scientific topics via ICP - mass spectrometry (ICP-MS) and other complementary detection techniques such as ESI and MALDI-MS including the development of new speciation approaches and hyphenated techniques. His current research is focused on the analysis of transport processes of contaminants at the interface of aquatic and marine environments using non-traditional stable isotope systems as well as the development of suitable tools for the analysis of new emerging contaminants and their effects.

Daniel is author and co-author of more than 60 papers and 3 book chapters as well as more than 150 contributions (oral and posters) to national and international conferences. In 2011, he received the Bunsen-Kirchhoff Preis from the Gesellschaft Deutscher Chemiker (GDCh) for his contribution within the field of miniaturized hyphenated techniques with element and molecule specific detection and their application for the analysis of heteroelement containing bio molecules. Since 2008, he offers also lectures and seminars focusing on instrumental analytical chemistry at the University of Hamburg.

Invited Speakers



Anastassiya Tchaikovsky ist technische Chemikerin mit Forschungsschwerpunkt Element- und Isotopenanalytik. Auf diesem Gebiet hat sie 15 Jahre Erfahrung. Sie hat bei der Internationalen Atomenergiebehörde (IAEA) im Bereich Nukleare Forensik angefangen. Nach sechs Jahren wollte sie sich die Methoden Isotopenanalytik, Laserablation und Unsicherheitsberechnungen aneignen und hat die Möglichkeit bekommen, ihre Dissertation bei Prof. Thomas Prohaska an der Universität für Bodenkultur (BOKU) im Bereich Herkunftsbestimmung von Lebensmitteln zu machen. Es folgte ein Postdoc auf der Universität Wien mit Fokus auf Speziesanalytik, wo sie Workpackageleiterin in einem EMPIR Projekt war. Nach einem einjährigen Abstecher in die Pharmaindustrie kehrte sie wieder in die Forschung zurück. Aktuell arbeitet sie als Postdoc an der BOKU. Hier kombiniert sie analytische und mathematische Methoden, um neue Erkenntnisse über biologische und geochemische Prozesse zu gewinnen.

Cornel Venzago ist Analytischer Chemiker und leitet das Kompetenzcluster für Element- und Molekülspektroskopie der RD&I (Research, Development and Innovation) bei Evonik Industries. Mit nahezu 40 Jahren Erfahrung in der Analytik wirkt er als Experte für Analytical Sciences in der Evonik, benannt als Senior Research Principal. Sein Portfolio umfasst die Elementanalytik in allen Varianten (ICP-MS, -OES, AAS, IC, titrimetrische und gravimetrische Methoden, Photometrie, CHNSO-Elementaranalysen, GDMS, XRD, XRF, XPS, NMR, IR, Raman). Sein Steckenpferd ist die Ultraspurenanalytik als Festkörperanalytik mit GDMS und seinen Quantifizierungsmethoden sowie nasschemisch mit ICP-MS mit den dazu angewandten verschiedensten Probenvorbereitungstechniken. Seit 2021 ist er im Vorstand des Deutschen Arbeitskreises für Analytische Spektroskopie (DAAS) der GdCh und seit 2014 Dozent bei der GdCh-Frühjahresschule des Arbeitskreises Industrielle Analytik.

Jochen Vogl studied chemistry at the Universities of Regensburg and Mainz in Germany with a focus on speciation analysis with on-line IDMS in his doctoral thesis (1997). He then worked for two years on reference measurements applying IDMS at the IRMM (now JRC Geel) in Belgium. Since January 2000, he is in charge of the field Isotope Analysis at the Bundesanstalt für Materialforschung und -prüfung (BAM) in Berlin, Germany. His main working fields are the application of IDMS for reference measurements, isotope ratio analysis, isotope and matrix reference materials, elemental mass spectrometry in general and metrology in chemistry.

Martin Wende studierte Chemie an den Universitäten von Dortmund und Bordeaux. Nach seiner Promotion am Institut für Analytische Chemie der Universität Leipzig im Arbeitskreis von Prof. Dr. Broekaert arbeitete er als Applikationschemiker für ICP-MS und ICP-OES bei PerkinElmer in Rodgau. Anschließend wechselte er 2002 zur BASF SE als Laborleiter der Elementanalytik. In der BASF konnte er langjährige Analytik- und Managementerfahrung in unterschiedlichen Positionen im In- und Ausland sammeln.

2015 übernahm er dann als Senior Research Manager im Kompetenzzentrum Analytik der BASF SE die Leitung der Elementanalytik. Neben der Weiterentwicklung von Analysenmethoden und Probenvorbereitungsverfahren beschäftigte er sich schon früh mit dem Thema Laborautomatisierung und Analytik 4.0.

Seit 2015 ist er im Vorstand des Deutschen Arbeitskreises für Analytische Spektroskopie (DAAS) und seit 2019 Vorstandsvorsitzender des DAAS sowie seit 2020 stellvertretender Vorstandsvorsitzender der GDCh-Fachgruppe Analytische Chemie.

Information for Presenters

Information for Oral Presenters

Projection and Technical Settings

Presenters should provide PowerPoint presentations in 16:9 format. Presentations need to be uploaded on the day before the talk is scheduled via an owncloud upload link. Please follow the instructions provided by email. Please use the following naming: ContributionCode-Name.ppt (Example: A.06.CL-Wagner.ppt).

You may want to carry a USB stick (compatible with Windows) as a back-up in case there is any technical problem.

Speaking Time

Invited lecture (IL): 16 min plus 4 min for discussion

Contributed lecture (CL): 12 min plus 3 min for discussion

Student lecture (SL): 12 min plus 3 min for discussion

Information for Poster Presenters

Schedule for Display, Mounting and Removal

We ask that you hang up posters in the exhibition area immediately upon arrival. The posters will be on display throughout the conference.

Please indicate on the poster board if you agree that photos of your poster are taken or not. A sign will be provided.

Please note that posters not removed until Thursday, September 8, 2.00 pm, will be taken down and will not be stored or sent to the authors after the meeting.

Poster Board Number

You can find your poster board number in the programme.

Presence at Posters

In order to be eligible for poster awards and enable discussion and interaction with other participants, it is mandatory for the poster presenter to be present at your poster board during the poster session on Tuesday, September 6, 3:30-6:00 pm.

Scientific Programme

Monday, September 5th	
08:15-09:00	**REGISTRATION** Montanuniversität Leoben Franz-Josef-Strasse 18 8700 Leoben
09:00-12:15	**SHORT COURSES**
10:30-12:15	**SC1 Single Event ICP-MS: Basics, Applications and Potential / Single Event ICP-MS: Grundlagen, Applikationen und Potential** *David Clases (Universität Graz, AT)* *Room: Hörsaal Kupelwieser*
09:00-10:30	**SC2 Be certain with measurement uncertainties / Sicherheit bei Messunsicherheiten** *Thomas Prohaska (Montanuniversität Leoben, AT)* *Room: Miller von Hauenfels*
10:30-12:00	**SC3 Sample digestions for spectroscopic analysis – What do we need to know about our samples? / Probenaufschlüsse für die spektroskopische Analyse – Was müssen wir über unsere Proben wissen?** *Thomas Meisel (Montanuniversität Leoben, AT)* *Room: Hörsaal Raiffeisen*
09:00-12:15	**SC4 Hyphenated technique for Speciation in Environmental and Life Sciences /Kopplungstechniken für Speziationsanalyse in Umwelt- und Lebenswissenschaften** *Daniel Pröfrock (HEREON Geesthacht, DE)* *Room: Seminarraum F*
12:15-13:15	**LUNCH-SEMINAR (Gernot Hudin & Jörg Hansmann, Agilent)** *Room: Miller von Hauenfels*
13:15-14:30	**OPENING CEREMONY** *Room: Erzherzog-Johann-Hörsaal (EHJ)*
13:15-13:45	**Welcoming Words** *Johanna Irrgeher*
13:45-14:30	**Opening Lecture** Geschichte des ICP-MS Anwender*innentreffens *Jörg Bettmer and Daniel Pröfrock (Sprecher der Fachgruppe Element-Massenspektrometrie der DGMS)*

Scientific Programme

14:30-15:30	**SESSION A: ISOTOPE RATIO ANALYSIS** *Chair: Thomas Prohaska*
14:30-14:50	**A.01.IL Analytical Services for Safeguards at SGAS** *Sergey Boulyga*
14:50-15:10	**A.02.IL Challenges of origin determination of food using isotopic and elemental patterns** *Anastassiya Tchaikovsky*
15:10-15:25	**A.03.SL Internal quantification of 99-technetium in aqueous samples by means of isobaric dilution analysis** *Maximilian Horstmann*
15:25-15:40	**A.04.SL Data processing tool for automated calculation of isotope ratios from transient signals – IsoCor** *Dariya Tukhmetova*
15:40-16:10	**Coffee Break**
16:10-17:00	**SESSION A: ISOTOPE RATIO ANALYSIS** *Chair: Anika Retzmann*
16:10-16:30	**A.05.IL Isotope Reference Materials – Basic principles and examples** *Jochen Vogl*
16:30-16:45	**A.06.CL Simultaneous assessment of Sr and Pb bioavailability and isotope ratio variations in soils: selective sampling by diffusive gradients in thin films (DGT)** *Stefan Wagner*
16:45-17:00	**A.07.CL Tackling spectral interferences of Fe and Ni in MC-ICP-(CRC)-MS isotope ratio analysis** *Stepan M. Chernonozhkin*
17:00-17:30	**GESCHICHTE DER MASSENSPEKTROMETRIE IN ÖSTERREICH** *Chair: Johanna Irrgeher*
17:00-17:30	**X.01.CL Ein österreichischer Beitrag zur Entwicklung der Massenspektrometrie im 20. Jahrhundert: Hugo Bondy (1900-1985)** *Michael Schober*
17:30-21:00	**ICEBREAKER & EXHIBITION OPENING (Drinks & Fingerfood)**

Scientific Programme

Tuesday, September 6th	
08:30-10:35	**SESSION B: ENVIRONMENTAL AND BIOMEDICAL ANALYSIS** *Chair: Anastassiya Tchaikovsky*
08:30-08:50	**B.01.IL More than trace elements – New applications for ICP-MS to investigate the chemical Anthropocene** *Daniel Pröfrock*
08:50-09:05	**B.02.SL Europium and Samarium Anomalies in Windisch and Aarau** *Chiara Fabbretti*
09:05-09:20	**B.03.SL *In situ* solute imaging of labile alloy elements and pH during tungsten and lead hunting shot weathering in soil using DGT-LA-ICPMS and planar optodes** *Christina Hummel*
09:20-09:35	**B.04.SL Erschließung der „urban Mine" – Entwicklung einer Aufschlussmethode für Leiterplatinen zur Bestimmung der Metallgehälter mittels ICP-MS/MS** *Ole Klein*
09:35-09:50	**B.05.SL Mineral raw material supply chain transparency and traceability: Does provenance matter in the supply chain?** *Valentina Dietrich*
09:50-10:05	**B.06.CL Analyse Seltener Erden in geologischen Proben und hochreinen SEE-Oxiden mit der Multi-Quadrupol-ICP-MS** *Michael Petrich*
10:05-10:20	**B.07.CL Prepared for ICP-MS – How to treat your sample before analysis** *Christian Trampitsch*
10:20-10:35	**B.08.CL ICP-MS-basierte Elementanalytik zur Entwicklung neuer Probenahmetechniken für die Mikroplastikanalytik** *Tristan Zimmermann*
11:00-12:30	**HANDS-ON WORKSHOPS**
11:00-12:30	**PerkinElmer – Hands-On ICP-MS/MS Nexion5000** *Tina Klein und Jörg Michel* *Room: ICP-MS Laboratory Chair of General and Analytical Chemistry*
11:00-12:30	**Agilent – Vorstellung MassHunter 5.x: Neue Features, Neue Optionen; Tipps & Tricks für die ICP-MS aus der Sicht eines Technikers** *Nicole Eichner and Peter Schützner* *Room: Hörsaal Kupelwieser*
11:00-12:00	**NU Instruments/Ametek – TOF-ICP-MS** *Lukas Schlatt* *Room: Seminarraum F*

Scientific Programme

12:30-13:30	**LUNCH-SEMINARS**
12:30-13:30	**Thermo Fisher Scientific – Spurenelementanalytik zwischen Umweltsicherheit und emissionsfreier Mobilität** *Daniel Kutscher* *Room: Miller von Hauenfels*
12:30-13:30	**Karl Andreas Jensen – Practical approaches to use reaction gases in ICP-MS/MS** *Karl Andreas Jensen* *Room: Zeichensaal*
13:30-13:50	**SESSION B: ENVIRONMENTAL AND BIOMEDICAL ANALYSIS** *Chair: Carsten Engelhard*
13:30-13:50	**B.09.IL Trace- and ultra-trace analysis of natural waters** *Lisa Fischer*
13:50-14:05	**B.10.SL Analytik von Meerwasserproben aus Offshore Windparks mittels ICP-MS unter Verwendung des Aufkonzentrierungssystems seaFAST®** *Dominik Wippermann*
14:05-14:20	**B.11.SL Aufbereitung von Meerwasserproben für die Messung der Metallgehalte mittels seaFAST ICP-MS: Einfluss von Filtrationsmethode und Lagerung auf die Ergebnisse** *Anna Przibilla*
14:20-14:35	**B12.SL Multi-Element-Analytik von Flusswasserproben mit ICP-QQQ-MS: Best-Practice-Methode für das Gewässermonitoring** *Nadine Belkouteb*
14:35-14:50	**B.13.SL Supra-regional monitoring of anthropogenic gadolinium and individual gadolinium species in municipal tap waters** *Marcel Macke*
14:50-15:05	**B.14.SL Impurity profiling of organic by-products of a newly developed Gd-based contrast agent** *Sonja Weishaupt*
15:05-15:20	**B.15.CL Simultane Multielement-Bestimmung in Körperflüssigkeiten mittels Multi Quadrupol ICP-MS** *Jörg Michel*
15:45-18:00	**POSTER SESSION (Coffee & Drinks)**
18:00-19:00	**STADTSPAZIERGANG with SophieTheGuide**
19:00-21:00	**EVENING EVENTS (PerkinElmer / Solutions4Science, Agilent, Thermo Fisher Scientific)**

Scientific Programme

Wednesday, September 7th	
08:00-09:00	**Sitzung der DGMS – FG Elementanalytik** *(non-public)*
09:00-10:35	**SESSION C: INSTRUMENTAL ADVANCES AND SPECIATION** *Chair: David Clases*
09:00-09:20	**C.01.IL New Tools for Chemical Measurement and Characterization of Particles** *Carsten Engelhard*
09:20-09:35	**C.02.SL Going Green by Going Pink: from Ar-ICP to N2-MICAP** *Monique Kuonen*
09:35-09:50	**C.03.SL Characterization of a sample introduction system for plasma spectrometry by computational fluid dynamics** *Elke Fasch*
09:50-10:05	**C.04.CL Exploring the use of nitrous oxide as a cell gas for inductively coupled plasma tandem mass spectrometry measurements** *Shaun Lancaster*
10:05-10:20	**C.05.CL Analysis of Cell Culture Media by means of Triple Quadrupole-ICP-MS: Method Development and Applications** *Joshua Fuchs*
10:20-10:35	**C.06.CL Ein neuartiger Ansatz für die Bestimmung von Schwermetallen in Babynahrung (und anderen Probenmatrizes) mittels ICP-MS** *Daniel Kutscher*
10:35-11:00	**Coffee Break**
11:00-12:00	**SESSION C: INSTRUMENTAL ADVANCES AND SPECIATION** *Chair: Jörg Bettmer*
11:00-11:20	**C.07.IL Digitale Transformation in der Elementanalytik: Probenvorbereitung 4.0** *Martin Wende*
11:20-11:35	**C.08.SL Fluorine-Specific Detection Using ICP-MS Helps to Identify PFAS Degradation Products in non-targeted Analysis** *Steffen Heuckeroth*
11:35-11:50	**C.09.SL Fast and automated separation and quantification of bromine species in enzymatically digested DNA samples via IC-ICP-MS** *Catharina Erbacher*
11:50-12:05	**C.10.CL ICP-MS based metallomics coupled with non-targeted metabolomics as a tool in neurodegeneration studies** *Nikolay Solovyev*
12:00-13:15	**CAREER-LOUNGE (Light Lunch)** *Room: Zeichensaal*

Scientific Programme

13:30-15:20	**SESSION D: LASER-BASED ANALYSIS** *Chair: Stepan M. Chernonozhkin*
13:30-13:50	**D.01.IL Identification and quantification of breast cancer biomarkers by LA-ICP-MS** *Raquel Gonzalez de Vega*
13:50-14:05	**D.02.SL Laser ablation-ICP-MS for the investigation of Gd and Pt pharmaceuticals in liver tumors** *Katharina Kronenberg*
14:05-14:20	**D.03.SL LA-ICP-MS for the quantitative assessment of the gadolinium distribution in sheep bone** *Christine Verlemann*
14:20-14:35	**D.04.SL Searching for what's within: By-product critical elements in minerals from ore deposits** *Viktor Bertrandsson Erlandsson*
14:35-14:50	**D.05.CL Mapping of Hg and Se in biological samples with laser ablation – ICP-MS** *Simone Braeuer*
14:50-15:05	**D.06.CL A multi-method approach for investigating non-metallic inclusions in steel** *Christoph Walkner*
15:05-15:20	**D.07.CL Neue Kombination von LA-ICP-MS mit Standardaddition und IDMS zur SI-rückgeführten Quantifizierung von Spurengehalten in festen Proben** *Lena Michaliszyn*
15:20-15:50	**Coffee Break**
15:50-16:25	**SESSION D: LASER-BASED ANALYSIS** *Chair: Marcus von der Au*
15:50-16:10	**D.08.IL Tandem LA-ICP-MS/LIBS: A versatile tool for the direct analysis of solid samples** *Lukas Brunnbauer*
16:10-16:25	**D.09.CL New Capabilities with TwoVol3 Laser Ablation Cell - Simultaneous LA-ICP-MS and LIBS** *C Derrick Quarles Jr.*
16:30-17:00	**IMPULSVORTRAG ZUR PODIUMSDISKUSSION** *Chair: Johanna Irrgeher and Stephan Hann*
16:30-17:00	**X.02.IL Elemental mass spectrometry: Past, presence and future** *Uwe Karst*
17:00-18:00	**PODIUMSDISKUSSION „Lessons to be learned"** *Chairs: Johanna Irrgeher and Stephan Hann*
18:30-23:00	**CONFERENCE DINNER & EVENING EVENT** *(Leoben Hauptplatz Arkadenhof, Music by Bergkapelle Blas)*

Scientific Programme

Thursday, September 8th	
08:00-09:30	**Guided Laboratory Tours** **Chair of General and Analytical Chemistry** **Montanuniversität Leoben**
09:30-10:55	**SESSION E: SINGLE PARTICLE ANALYSIS** *Chair: Raquel Gonzalez de Vega*
09:30-09:50	**E.01.IL Die Charakterisierung von biogenen Nanomaterialien mittels ICP-MS Techniken** *Jörg Bettmer*
09:50-10:10	**E.02.IL Fundamentals and applications of large bandpass mass filters in hyphenated and single event ICP-MS** *David Clases*
10:10-10:25	**E.03.SL Schnelle Einzelpartikel-ICP-MS mit Nanosekundenzeitauflösung als neue Analysenmethode für Nanomaterialien** *Annika Schardt*
10:25-10:40	**E.04.SL Single particle ICP-MS as new characterisation tool for cement systems: characterisation of early hydration products** *Steffen Hellmann*
10:40-10:55	**E.05.SL MDG-ICP-MS - A Versatile Tool for Quantification in the field of Single Particle ICP-MS via Isotopic Dilution** *Marcus von der Au*
10:55-11:10	**E.06.SL Single-Cell ICP-MS analysis of algal cells using an automation platform and advanced data processing algorithms** *Matthias Elinkmann*
11:10-11:40	**Coffee Break**
11:40-11:55	**E.07.CL Automating ICP-MS analyses for total metals and elemental speciation** *C Derrick Quarles Jr.*
11:55-12:15	**E.08.IL Arsenic speciation in soil: how does climate change can enhance arsenic mobility in Swiss soil** *Jörg Feldmann*
12:15-13:00	**AWARD CEREMONY & CLOSING**
13:00-14:00	**FAREWELL LUNCH**
14:00-17:00	**EXCURSION ERZBERGLAND (3-4 h) or** **STADTSPAZIERGANG with SophieTheGuide (1 h)**

List of Posters

Poster Session Tuesday, September 6th, 15:30-18:00	
P1 ISOTOPE RATIO ANALYSIS	
P1.01.SL	**Assessing analytical methods for high precision Ni isotopic analysis in rhizosphere samples and Ni hyperaccumulating plants** *Alexander V. Epov*
P1.02.CL	**Investigating the differences in $^{87}Sr/^{86}Sr$ isotope ratio measurements between MC-ICP-MS and MC-TIMS in cement reference materials** *Jochen Vogl*
P1.03.CL	**Investigation of the mineral-related differences in $^{87}Sr/^{86}Sr$ isotope ratios of three reference materials (OPC-1, OU-6, CGL ML-3) using sequential extraction – the follow-up study** *Anika Retzmann*
P1.04.SL	**Low-amount Ca isotopic analysis using double-spike MC-TIMS and MC-ICP-MS in biological tissues to study metabolic processes** *Dorothy Walls*
P2 ENVIRONMENTAL AND BIOMEDICAL ANALYSIS	
P2.01.SL	**Determination of technology-critical elements (TCEs) in plants from urban green infrastructures by ICP-MS/MS** *Simone Trimmel*
P2.02.SL	**Investigation of multi-element patterns of plant samples from Viennese green facades as potential filters for technology-critical elements using ICP-MS/MS** *Nagi Lashin and Philipp Spörl*
P2.03.CL	**Metrology for the recycling of Technology Critical Elements to support Europe's circular economy agenda** *Marcus Oelze*
P2.04.SL	**MURmap - Holistic geochemical tracking of elements and their sources in the Mur/Mura River Catchment** *Ulrike Moser*
P2.05.CL	**Quantification of cardiac troponin via lanthanide-labeled peptides using ICP-MS** *Danja Kuhfuß*
P2.06.SL	**Enhancement of protein quantification through lanthanide labels** *Marvin Müller*
P2.07.SL	**Salivary iodine as a status biomarker: a challenge for ICP-MS?** *Tanya Mehra*
P2.08.SL	**Trace element analysis of hair and tissues of calves** *Melissa Rauter*

List of Posters

P3 INSTRUMENTAL ADVANCES AND SPECIATION	
P3.01.SL	**Development and construction of an experimental setup for the production of homogeneous microanalytical reference materials** *Stefan Friedl*
P3.02.CL	**Eine neuartige Torch für die ICP-MS: Eine einfache Lösung für viele Probleme?** *Daniel Kutscher*
P3.03.CL	**Prepared for ICP-MS – What to Consider With Microwave Digestion** *Christian Trampitsch*
P3.04.CL	**TOTALQUANT TECHNIQUE – MORE THAN SEMI-QUANTITATIVE ANALYSIS** *Jörg Michel*
P3.05.CL	**Novel possibilities for interference removal using Multi-Quadrupole ICP-MS** *Helmut Ernstberger*
P3.06.CL	**Determination of Toxic and Other Trace Elements in Baby Foods Using ICP-MS** *Daniel Fliegel*
P3.07.CL	**On the origin of species - sind im Plasma wirklich alle Spezies gleich?** *Anita Röthke*
P3.08.SL	**Development of a method for the fast and sensitive speciation analysis of gadolinium-based contrast agents in tissue** *Torben J. Maas*
P3.09.SL	**Rapid speciation analysis of Cr(VI) and Cr(III) using µLC-ICP-MS** *Jelle Verdonck*
P3.10.SL	**Dimethyl carbonate as new eluent for a fast determination of cobalamins with HPLC-ICPMS** *Martin Walenta*
P4 LASER-BASED ANALYSIS	
P4.01.SL	**Elemental bioimaging of atherosclerotic rabbit arteries to investigate the permeability of the artery wall during disease progression via LA-ICP-MS** *Peter Niehaus*
P4.02.SL	***In situ* mapping of localised aluminium corrosion using diffusive gradients in thin films (DGT) coupled to LA-ICP-MS** *Gulnaz Mukhametzianova*
P4.03.SL	**Development of a Laser Ablation ICP-MS Method for the Analysis of the Element Distribution in rigid Polyvinyl chloride** *Saskia Kerkeling*
P4.04.SL	**Development of a laser ablation cell that allows two degrees of translational freedom for planar surfaces** *Anne Folmer*
P4.05.SL	**Application of ICP-MS to study the evolution of non-metallic inclusions in steelmaking** *Kathrin Thiele*

List of Posters

P5 SINGLE PARTICLE ANALYSIS	
P5.01.SL	**Time-Dependent Uptake of Arsenic Species in the Green Alga *Chlamydomonas reinhardtii*** *Alexander Köhrer*
P5.02.SL	**Erfassung und Verarbeitung von spICP-MS Daten mit Nanosekunden – Zeitauflösung** *Johannes Schmitt*
P5.03.CL	**SP-ICP-MS: Fragestellungen aus der Industrie (Merck KGaA)** *Fiona Engsberg*
P6 DIVERSITY, EQUITY, AND INCLUSION	
P6.01.CL	**Fostering inclusive access to analytical instrumentation** *Johanna Irrgeher and Michael Schober*

Programme at a Glance

ICP-MS AW*T 2022 LEOBEN

ZEIT	MONTAG September 5, 2022
8:15	REGISTRIERUNG
9:00	SHORT COURSES (SC2 & SC4)
10:30	SHORT COURSES (SC1, SC3 & SC4)
12:15	LUNCH-SEMINAR (Agilent)
13:15	ERÖFFNUNG & IMPULSVORTRAG (Geschichte des AW*T - J.Bettmer & D.Pröfrock)
14:30	IL Boulyga
14:50	IL Tchaikovsky
15:10	SL Horstmann
15:25	SL Tukhmetova
15:40	KAFFEEPAUSE
16:10	IL Vogl
16:30	CL Wagner
16:45	CL Chernonozhkin
17:00	VORTRAG ZUR GESCHICHTE DER MASSENSPEKTROMETRIE IN ÖSTERREICH (M. Schober)
17:30	ICE-BREAKER & ERÖFFNUNG DER AUSSTELLUNG
	GERÄTE- UND FIRMENAUSSTELLUNG (DRINKS & FINGERFOOD)
21:00	

ZEIT	DIENSTAG September 6, 2022
8:30	IL Pröfrock
8:50	SL Fabbretti
9:05	SL Hummel
9:20	SL Klein
9:35	SL Dietrich
9:50	CL Petrich
10:05	CL Trampitsch
10:20	CL Zimmermann
11:00	HANDS-ON WORKSHOPS (1 PerkinElmer, 2 Agilent, 3 Nu Instruments) / FIRMENAUSSTELLUNG / POSTERAUSSTELLUNG
12:30	LUNCH-SEMINARE (1 ThermoFisher, 2 Karl Andreas Jensen)
13:30	IL Fischer
13:50	SL Wippermann
14:05	SL Przibilla
14:20	SL Belkouteb
14:35	SL Macke
14:50	SL Weishaupt
15:05	CL Michel
15:30	POSTERSESSION & KAFFEE
18:00	STADTSPAZIERGANG mit SophieTheGuide
19:00	FIRMENEVENTS
21:00	

ZEIT	MITTWOCH September 7, 2022
8:00	Sitzung der DGMS - AG Elementanalytik
9:00	IL Engelhard
9:20	SL Kuonen
9:35	SL Fasch
9:50	CL Lancaster
10:05	CL Fuchs
10:20	CL Kutscher
10:35	KAFFEEPAUSE
11:00	IL Wende (20 min)
11:20	SL Heukeroth
11:35	SL Erbacher
11:50	CL Solovyev
12:00	KARRIERE-LOUNGE (LIGHT LUNCH)
13:30	IL Gonzalez de Vega
13:50	SL Kronenberg
14:05	SL Verlemann
14:20	SL Erlandsson
14:35	CL Braeuer
14:50	CL Walkner
15:05	CL Michaliszyn
15:20	KAFFEEPAUSE
15:50	IL Brunnbauer
16:10	CL Quarles
16:30	IMPULSVORTRAG ZUR PODIUMSDISKUSSION (U. Karst)
17:00	PODIUMSDISKUSSION "Lessons to be learned"
18:30	KONFERENZ - DINNER & ABENDEVENT am LEOBENER HAUPTPLATZ (MUSIK: Bergkapellen Blas)
23:00	

ZEIT	DONNERSTAG September 8, 2022
8:00	LABORFÜHRUNGEN LEHRSTUHL ALLG. u. ANALYT. CHEMIE
9:30	IL Bettmer
9:50	IL Clases
10:10	SL Schardt
10:25	SL Hellmann
10:40	SL von der Au
10:55	SL Elinkmann
11:10	KAFFEEPAUSE
11:45	CL Quarles
	IL Feldmann
12:15	PREISVERLEIHUNG & SCHLUSSWORTE
13:00	FAREWELL - LUNCH
14:00	EXKURSION ERZBERGLAND (3-4 h) oder STADTSPAZIERGANG mit SophieTheGuide (1,5 h)
17:00	

Abstracts

ORAL PRESENTATIONS

Session A: Isotope ratio analysis

A.01.IL

Analytical Services for Safeguards at SGAS

Sergei Boulyga* (1)

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The Office of Analytical Services (SGAS) is a part of the IAEA Department of Safeguards and it is responsible for the analysis of nuclear material and environmental samples, the provision of associated sampling and quality control materials, as well as the coordination of sample shipment logistics, and the Network of Analytical Laboratories (NWAL).

The office contains the Safeguards Analytical Laboratories (SAL), comprised of the Environmental Sample Laboratory (ESL) and the Nuclear Material Laboratory (NML). It also includes the On-Site Laboratory in Rokkasho, Japan, and a Coordination and Support Section (CSS), which is responsible for the planning, coordination and reporting of the analytical service of the NWAL; radiation protection; quality management; training and other technical support.

In this presentation I will provide an overview of analytical services for safeguards, describe SGAS and briefly discuss applied analytical methods, equipment and quality control.

A.02.IL

Challenges of origin determination of food using isotopic and elemental patterns

Anastassiya Tchaikovsky* (1), Andreas Zitek (1,2), Johanna Irrgeher (3), Thomas Prohaska (3), Stephan Hann (1)

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(2) FFoQSI - Austrian Competence Centre for Feed and Food Quality, Safety & Innovation, FFoQSI GmbH, Technopark 1C, 3430 Tulln
(3) Montanuniversität Leoben, Chair General and Analytical Chemistry, Franz Josef-Straße 18, 8700 Leoben, Austria

This presentation proposes an analytical and chemometric workflow for the determination of the geographic origin of food using strontium isotope $n(^{87}Sr)/n(^{86}Sr)$ and elemental patterns. Addressing existing approaches of origin determination of food, we share experience from a large project focusing on fish and sturgeon caviar provenance. We show matrix dependent challenges, which have implication on sample collection and preparation. Furthermore, we present that instrumental isotopic fractionation (IIF) calibration using a matrix-matched standard improves the trueness of $n(^{87}Sr)/n(^{86}Sr)$ isotope amount ratios of solid carbonates measured by LA-MC ICP-MS in comparison to IIF calibration using the liquid standard reference material SRM 987 measured by MC ICP-MS. Having sound data at hand, we need chemometrics to link the sample to its geographic origin. This workflow is particularly challenging in case of aquacultured fish and salted sturgeon caviar as fish feed and salt can alter the environmental signature transferred from water into fish making origin determination difficult to impossible. Therefore, we show a step-by-step chemometric protocol, which allows to determine the environmental signature transferred from water into fish, identify alteration by the production process and correct for it. The presented workflow is equally applicable to other isotopic systems and food commodities.

Acknowledgements: The COMET-K1 competence centre FFoQSI is funded by the Austrian ministries BMVIT, BMDW and the Austrian provinces Niederoesterreich, Upper Austria and Vienna within the scope of COMET - Competence Centers for Excellent Technologies. The programme COMET is handled by the Austrian Research Promotion Agency FFG. The strategic objectives of COMET are: developing new expertise by initiating and supporting long-term research co-operations between science and industry in toplevel research, and establishing and securing the technological leadership of companies. By advancing and bundling existing strengths and by integrating international research expertise Austria is to be strengthened as a research location for the long term.

Abstracts

A.03.SL

Internal quantification of 99-technetium in aqueous samples by means of isobaric dilution analysis

Maximilian Horstmann* (1), C. Derrick Quarles Jr. (2), Steffen Happel (3), Andreas Faust (4) und Uwe Karst (1)

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(4) University of Münster, European Institute for Molecular Imaging, Waldeyerstraße 15, 48149 Münster, Germany

Ever since its discovery in 1937, the importance of technetium as a frequently observed anthropogenic radiocontaminant has constantly increased. Having a half-life of over 211,000 years, its primary isotope ^{99}Tc accounts for the entire natural and, by now, also a much higher anthropogenic occurrence. Besides its formation as a by-product of nuclear fission in both, the military and the energy sector, the isotope is also actively used as a radiotracer for scintigraphic techniques in medical diagnosis. Here, the features of the metastable form, ^{99m}Tc, specifically its short half-life of only six hours and its property to act as a γ-emitter, can be variably exploited to localize neoplastic tissue within the human body. Nowadays, ^{99m}Tc is applied in an estimated 40 million procedures per year, and makes up for about 85% of all diagnostic scans performed in nuclear medicine worldwide.

Monitoring of ^{99}Tc and its quantification in aqueous media holds intrinsic complications as most samples contain expectedly low concentrations coinciding with difficult matrices such as wastewater, blood or urine. Additionally, due to its radioactivity (β^-), elemental standards for ^{99}Tc are not easily available, therefore expensive and hard to handle. Besides, Tc is virtually monoisotopic as other isotopes, even those with equally high half-lives than ^{99}Tc, are even harder to obtain and therefore do not qualify as internal standards.

Abstracts

A.04.SL

Data processing tool for automated calculation of isotope ratios from transient signals - IsoCor

Dariya Tukhmetova* (1), Jan Lisec (1), Jochen Vogl (1), Björn Meermann (1)

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Hyphenation of chromatography and electrokinetic separation methods with multicollector (MC) ICP-MS for isotope analysis is opening new insights into the species-specific behavior of elements. Hyphenated systems enable performing isotope analysis within shorter time, less consumption of reagents and minimized "human error" compared to conventional sample introduction. However, main drawback of such systems is the generation of short transient signals which leads to high uncertainty. Therefore, along with optimization of measurement parameters, a robust data processing strategy is highly needed. The lack of universal tool for the processing of transient signals motivated us to build a versatile application to facilitate isotope ratio measurement.

Our data processing application, IsoCor, was developed using R open-source language (https://www.r-project.org/). The application is available online via https://jali.shinyapps.io/isocor/, works as a standalone tool and doesn't require knowledge of programming language to use. The application performs steps such as baseline correction, peak detection, isotope ratio calculation, mass bias correction and delta calculation.

The feasibility and reliability of the application was tested using three datasets generated with Gas Chromatography, Liquid Chromatography and Capillary Electrophoresis coupled with MC-ICP-MS. The results from IsoCor showed an agreement of one standard deviation with the results from the original publication of the datasets.

IsoCor is a data processing solution to the gap in the isotope analysis with hyphenated systems. IsoCor improves reproducibility and trackability of the results, thus it is helpful for validation and quality control.

Abstracts

A.05.IL

Isotope Reference Materials – Basic principles and examples

Jochen Vogl* (1), Martin Rosner (2), Olaf Rienitz (3) und Marcus Oelze (1)

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(3) Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig, Germany

The variation of isotope ratios is increasingly used to unravel natural and technical questions. In the past, the investigation and interpretation of such variations was the field of a limited number of experts. With new upcoming techniques and research topics in the last decades, such as provenance or food authenticity studies, the number of published isotope data strongly increased. Instrumental developments such as the enhancement of inductively coupled plasma mass spectrometers (ICP-MS) from an instrument for simple quantitative analysis to highly sophisticated isotope ratio machines influenced this process significantly. While in former times only experts in mass spectrometry were able to produce reliable isotope data, nowadays many laboratories, never been in touch with mass spectrometry before, produce isotope data with an ICP-MS. Isotope reference materials (iCRM) are indispensable to enable a reliable method validation or in rare cases even SI-traceability. The fast development and the broad availability of ICP-MS also lead to an expansion of the classical research areas and new elements are under investigation. Irrespective of the investigated element or the knowledge of the user all isotope ratio applications require reference materials either for correction of instrumental isotope fractionation, for method validation or to provide a common accepted basis as needed for delta measurements. This presentation will outline the basic principles and illustrate the urgent need for new iCRMs. Consequently, the production and certification of iCRMs will be discussed and illustrated by examples of already completed certification projects. Finally, plans for future iCRMs to be produced at BAM will be presented.

Abstracts

A.06.CL

Simultaneous assessment of Sr and Pb bioavailability and isotope ratio variations in soils: selective sampling by diffusive gradients in thin films (DGT)

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Stable isotope signatures of Sr and Pb in bioavailable fractions of soil are widely applied as tracers in archaeology, (paleo)ecology, (food) forensics, and environmental science. Yet, the assessment of Sr and Pb bioavailability and their isotope ratios by ICP-MS remains elusive due to the typically low analyte levels along with complex sample matrices obtained by traditional soil extraction methods. Here, the development, validation, and application of a method using diffusive gradients in thin films (DGT) in combination with multi-collector (MC)-ICP-MS for the simultaneous assessment of Sr and Pb concentrations and isotope ratio variations in labile, bioavailable soil fractions is presented. [1] The method is based on novel extraction chromatography membranes with modified crown-ether functionality (TK100 membrane, TrisKem International), providing high selectivity for Sr and Pb at environmentally relevant ranges of pH (3.9-8.2), ionic strength (0.001-0.1 mol L^{-1}), and cation competition (50-160 mg L^{-1} Ca in a synthetic soil solution matrix). Selective three-step elution of TK100 membranes using hydrochloric acid enabled quantitative (≥96 %) matrix separation and adequate (≥75 %) elution recovery without causing significant isotopic fractionation. Application of TK100 DGT in a greenhouse experiment using a range of different soil types (n = 5) and plant species (n = 3) demonstrated the capability of the method to determine bioavailable Sr and Pb isotope signatures as geo-reference in food provenancing in a single sampling step and with low relative combined uncertainty ($u_{c,rel}$ = 0.01-0.03 %).

[1] S. Wagner, J. Santner, J. Irrgeher, M. Puschenreiter, S. Happel, T. Prohaska, Selective Diffusive Gradients in Thin Films (DGT) for the Simultaneous Assessment of Labile Sr and Pb Concentrations and Isotope Ratios in Soils. Analytical Chemistry 2022, 94 (16), 6338-6346

A.07.CL

Tackling spectral interferences of Fe and Ni in MC-ICP-(CRC)-MS isotope ratio analysis

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Since the advent of ICP-MS spectral interferences were recognized as major obstacle for accurate measurements, and multiple approaches to address these were suggested from the early days onwards. Although the multi-collection nature of the detection does not influence the formation of the interferences in ICP-MS *per se*, the tiny magnitude of isotope ratio variations that need to be revealed by MC-ICP-MS requires the principles of evaluating the effect of interferences to be looked at from another angle. For many years, high mass resolution and target element isolation have been regarded as the universal approach for resolving interferences in MC-ICP-MS, but constantly rising interest in novel and complex isotope systems calls to revive the existing alternatives or their combination, such as the use of cold plasma conditions, sample desolvation systems, and MC-ICP-MS units with collision/reaction cell (CRC) or with MS/MS design. The susceptibility of the measured isotope ratios to the interference/analyte ratios is a critical parameter for the design of MC-ICP-(CRC)-MS measurements overall, as it governs the required element/analyte separation factors of the target element isolation protocols and the ability to use various sample introduction systems.

Here our experience in handling spectral interferences for high-precision MC-ICP-MS isotope ratio analysis of Fe and Ni will be presented, including (i) application of high mass resolution, (ii) use of cold plasma conditions to counteract the presence of argide species in plasma, and, finally, (iii) the use of a novel Sapphire MC-ICP-MS (Nu Instruments, Wrexham, UK) unit equipped with a hexapole CRC operated with various collision and reaction gases (He, Ar, H_2, CH_4) for chemical resolution of spectral interferences.

Abstracts

Session B: Environmental and biomedical analysis

B.01.IL

More than trace elements – New applications for ICP-MS to investigate the chemical Anthropocene

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Legacy heavy metal and species contamination still represents a major adverse threat for many aquatic and marine ecosystems within highly populated catchment areas because of their inherent toxicity, vast sources and persistence. Despite the ongoing reduction of emissions of such contaminants into the environment, the coastal zones of the North Sea still belong to the most impacted ecosystems worldwide. In particular, the ongoing evolution of coastal zones into industrialized areas, e.g. due to extensive shipping or the construction of offshore wind parks, offshore PTX or CDR activities within the framework of the ongoing energy transition and CO_2 reduction in Europe even boosted the release of either known, but also of various new contaminants into the marine environment. Nowadays, due to changing industrial processes and product portfolios also other elements such as the REE beside PGEs and TCEs and also new element species indicate an increasing release into the environment beside other threats such as nano materials, micro plastic or organic contaminants. The accurate analysis of such contaminants is in particular of significance for public health concerns beside the overall future sustainable development and management of the coastal zones as required by EU wide legislation. This contribution will highlight some recent examples of ICP-MS based elemental analysis and their application within the context of large scale environmental studies on the interactions of entire river catchments and coastal zones or new approaches for e.g. CO_2 removal. The focus of this lecture will be in particular on the recent possibilities arising from the application of ICP-MS/MS for interference handling as well as on the role of new approaches for routine ultra trace analysis of emerging contaminants at ng/L levels, or its role as complementary technique for emerging research areas such as particle analysis.

Abstracts

B.02.SL

Europium and Samarium Anomalies in Windisch and Aarau

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The increasing use of Rare Earth Elements (REEs) for technological applications will likely lead in increased amounts REEs discharged to the environment, with only poorly understood consequences for the receiving compartments. Results from initial screening studies demonstrated the presence of most of the REEs in wastewater [1] and sewage sludge samples [2] collected for more than 60 wastewater treatment plants in Switzerland. Of special interest is the fraction of REEs which is related to anthropogenic activities and in selected sewage sludge samples high fractions of Ce, Sm, Eu and Gd were associated with anthropogenic activities. Additional sampling campaigns confirmed exceptionally high concentrations of Sm and Eu in sewage sludge collected from the wastewater treatment plants of Windisch and Aarau [1]. In this work, the Sm and Eu anomalies from the Windisch and Aarau WWTPs were studied in further detail. Sewage sludge samples were analyzed by triple-quadrupole inductively coupled mass spectrometer (ICP-MS) and normalized to the Post Archean Australian Shale (PAAS). This revealed that PAAS normalized Eu and Sm concentrations were higher compared to their neighboring (PAAS normalized) REEs, suggesting a substantial anthropogenic contribution of Sm and Eu to the respective wastewaters. A single-particle time-of-flight ICP-MS (sp-ICP-TOFMS) was used to analyze the particulate and dissolved fractions of REEs in influent and effluent wastewater. Low dissolved concentrations of Eu and Sm were found both in the influent and effluent, and no Eu NPs were observed, but Sm NPs were detected.

[1] Vriens, B.; Voegelin, A.; Hug, S. J.; Kaegi, R.; Winkel, L. H. E.; Buser, A. M.; Berg, M. Environ. Sci. Technol. 2017, 51 (19), 10943–10953
[2] Kaegi, R.; Gogos, A.; Voegelin, A.; Hug, S. J.; Winkel, L. H. E.; Buser, A. M.; Berg, M Water Research X 2021, 11, 100092

Abstracts

B.03.SL

Erschließung der „urban Mine“ – Entwicklung einer Aufschlussmethode für Leiterplatinen zur Bestimmung der Metallgehälter mittels ICP-MS/MS

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Technologie-kritische Elemente (TCEs), stellen einen elementarten Bestandteil in der heutigen Hochleistungsindustrie dar. Für viele Elemente der TCEs (u.a. Ga, Ge, In, Nb, Seltene Erden und Ta) ergibt sich neben einer hohen Nachfrage auch ein sehr hohes Versorgungsrisiko. Die Ressourcenknappheit vieler TCEs lässt sich hierbei sehr häufig auf stark gestörte Kreislaufwirtschaften zurückführen. Aufgrund der unzureichenden Wiederverwertung gelten TCEs daher auch als potenzielle neue Schadstoffe, da bisher nur wenig über ihren Eintrag und Verbleib in die Umwelt bekannt ist. Unter diesen Aspekten haben insbesondere End-of-Life Leiterplatinen (PCBs) große Aufmerksamkeit in der Wissenschaft erregt. PCBs zeichnen sich vor allem aufgrund der möglichen Umweltbelastung durch die zunehmenden Elektroschrottströme, aber auch wegen des Potentials der Nutzung von Elektroschrott als sog. „urban Mine“ aus.

Ziel dieser Studie war es die TCE Massenanteile von End-of-Life PCBs mittels ICP-MS/MS zu bestimmen. Hierzu wurde eine geeignete Ausschlussmethode für PCBs und die anschließende ICP-MS/MS Analyse entwickelt. Zur Entwicklung der Ausschlussmethode wurden insgesamt sechs Säuremischungen in sowohl offenen und als auch Mikrowellen-unterstützten Aufschlussansätzen getestet. Zur Validierung wurde das Referenzmaterial (CRM) BAM-M505a (Elektroschrott) verwendet. Unter Verwendung des optimierten Aufschlussprotokolls (mikrowellen-unterstützt, 1 mL HCl, 3 mL HNO_3, 1 mL HBF_4) können alle zertifizierten Elemente, mit Ausnahme von Ag und Cr, des CRMs *BAM-M505a* mit niedrigen Bestimmungsgrenzen (0.10 mg kg^{-1} für Cd bis 130 mg kg^{-1} für Ta) und Wiederfindungsraten zwischen 80 % und 124 % analysiert werden. Für die analysierten PCB-Proben konnten Massenanteile von 0.12 mg kg^{-1} ± 0.05 mg kg^{-1} (Eu) bis 169 g kg^{-1} ± 14 g kg^{-1} (Fe) festgestellt werden. Vergleicht man die so bestimmten Metallgehalte mit den kommerziell geförderten Primärerzen einiger Metalle zeigt sich, dass PCBs zum Teil 5 (Au) oder 10 (Pt) mal höhere Gehalte aufweisen können, was die Effizienz der PCB als urbane Minen deutlich unter Beweis stellt

B.04.SL

***In situ* solute imaging of labile alloy elements and pH during tungsten and lead hunting shot weathering in soil using DGT-LA-ICPMS and planar optodes**

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Hunting ammunition represents a substantial pathway for toxic lead (Pb) to enter terrestrial and aquatic environments. Tungsten (W) ammunition as a 'green alternative' to Pb is considered less toxic and less mobile in soil, but knowledge about its biogeochemical behavior in soil is still limited. Oxidation and dissolution processes of weathering shots consume or release protons and hence locally change soil pH which in turn will affect metal solubility. To study the interplay of small-scale pH changes and corresponding elemental solubility during weathering of alloys in soil we applied non-destructive solute imaging techniques. W and Pb gunshots were incubated in boxes filled with a sandy soil for 10 weeks at a water content of 40%. Hydrogels capable of binding labile alloy elements (Diffusive Gradients in Thin films) were applied *in situ* and analyzed by LA-ICP-MS to generate 2D images of soluble element gradients around the shots. Planar pH optodes were applied to visualize pH distribution. Despite our expectation to find acidification around the W-shots due to the oxidation of metallic W to WO_4^{2-}, we mainly found alkalinization by ~0.5 pH units around W-shots. Alkalinization around Pb-shots was similar, and also constrained to the shot surface, while alloy elements migrated further into soil. Labile Pb concentrations around Pb-shots were 6 times higher than labile W concentrations around W-shots, but Pb mobility in soil was lower than W mobility. Surprisingly, Nickel deriving from the W-shot alloy showed the largest mobility (up to 5 mm from the shot surface) and highest soil solution concentrations, despite comprising only 7% of the W-shot alloy. These results suggest the substantial release of Ni should be considered in risk assessments of W-shots.

B.05.SL

Mineral raw material supply chain transparency and traceability: Does provenance matter in the supply chain?

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Nowadays information about nearly every aspect of our lives can easily be accessed. Surprisingly, one will soon reach the limits of information available regarding the components and conditions of manufacturing our consumer products, especially when it comes to mineral raw materials contained in products we use every day. This project focuses on the aspect of developing various methodical approaches for an analytical proof of origin for natural graphite. Europe's battery producers and other graphite-consuming industries are largely reliant on imported raw materials. The graphite demand is predicted to significantly increase within the next 30 years due to the high forecasted demand in lithium-ion batteries. The analytical proof of origin for graphite aims to differentiate between various origins of the material, in particular from African countries (Mozambique, Madagascar and Zimbabwe), but also from Korea, China, Brasil and others. A meaningful combination of the applied methods allows to decipher geological and mineralogical processes and, in the end, define the source of a material, as unique. Therefore, the following parameters are considered useful and important: 1) Geochemical parameters such as minor and trace element compositions and isotope ratios of carbon and sulphur allow conclusions about depositional processes and environments. 2) Crystallographic parameters (e.g. d-values in XRD and characteristic absorption bands in Raman spectra) allow conclusions about the prevailing metamorphic P-T conditions and 3) Grain morphology as assessed by microscopical work (e.g. SEM and light microscopy) is controlled by crystal growth but also weathering and abrasion, being important indicators of the sample origin. The applied parameters must be easy to reproduce and the analytical methods must be widely available. In case of changes during later geological history (e.g. diagenesis, metamorphism), some geochemical characteristics must be preserved to an extent that the original chemical signature is still recognizable. Major obstacles for a chemical fingerprint are the poor solubility of graphite, the lack of certified reference materials for trace elements and isotopes, and the challenges to ablate fine graphite powders by LA-ICP-MS.

Abstracts

B.06.CL

Analyse Seltener Erden in geologischen Proben und hochreinen SEE-Oxiden mit der Multi-Quadrupol-ICP-MS

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Der Vortrag gibt einen Überblick über die analytischen Herausforderungen bei der Analyse Seltener Erden in alkalischen Schmelzaufschlüssen geologischer Proben und von SEE-Spuren in hochreinen Oxiden der Elemente Ce, Eu, Gd, Nd, Pr.

Neue Wege der Interferenzbeseitigung durch Mass Shift Reaktionen mit O_2 und NH_3 werden aufgezeigt.

Abstracts

B.07.CL

Prepared for ICP-MS – How to treat your sample before analysis

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Although modern spectrometers have gained increasing robustness during the last decades, accurate and effective sample preparation is still the key issue for precise analytical data – errors occurring during sample preparation cannot be compensated later during analysis.

In this presentation we will demonstrate suitability and possibilities of modern sample preparation techniques for subsequent ICP-MS analysis for a variety of different application requirements, covering a wide range of solutions, like analysis of food or environmental samples, pharmaceutical substances, or platinum group metals, to name just a few.

We will also have a closer look on the way from an unknown sample to a safe and effective digestion method, while considering specific requirements for ICP-MS.

See how your analysis can benefit from improving your sample preparation procedures.

Abstracts

B.08.CL

ICP-MS-basierte Elementanalytik zur Entwicklung neuer Probenahmetechniken für die Mikroplastikanalytik

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Mikroplastikpartikel (i.d.R. Partikel zwischen 1 µm und 5 mm Durchmesser) gelten mittlerweile als allgegenwärtiger Schadstoff - nicht nur in der aquatischen Umwelt. Allerdings ergeben sich große analytische Herausforderungen unter anderem bei der Validierung von entsprechenden Probenahmetechniken für z.B. wässrige Proben.

Dieser Beitrag thematisiert die Nutzung von Metall-dotierten Mikroplastikpartikeln zur Validierung eines neuen Probenahmeprotokolls für die Extraktion von Mikroplastikpartikeln aus wässrigen Proben. Das vorgestellte Probenahmesystem basiert auf einer vollständig aus Edelstahl gefertigten Filtrationskaskade mit Sieben unterschiedlicher Maschenweiten. Das System ermöglicht die kontaminationsarme Filtration von großen Wasservolumina (mehrere m^3). Zur Validierung dienten Indium-dotierte Mikroplastikpartikel unterschiedlicher Dichte (Polylactid und Polyethylenterephtalat) in Partikelgrößen zwischen 63 µm – 125 µm und ≤ 63 µm. Die Mikroplastikpartikel wurden sowohl im Rohzustand als auch nach einem Fouling mit einem Biofilm aus typischen phototrophen Wasseralgen verwendet. Als Basis zur korrekten Quantifizierung der Dotierungselemente diente ein Mikrowellen-unterstützter Säureaufschluss sowie die anschließende Analyse der Aufschlusslösungen mittels ICP-MS. Zur Validierung des Aufschlusses wurde sechs Referenzmaterialien unterschiedlicher Polymere verwendet (Polyethylen, Polypropylen, Polyacrylnitril, Styrol-Butadien-Kautschuk und Polyvinylchlorid). Die Wiederfindungen der zertifizierten Elemente (As, Cd, Cr, Hg, Pb, Sb, Sn und Zn) betrugen zwischen 95.9% ± 2.7% und 112% ± 7% in allen untersuchten Referenzmaterialien.

B.09.IL

Trace- and ultra-trace analysis of natural waters

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This work is focused on developing emerging analytical tools based on ICP-MS to cope with the increasing role that hazardous elements and emerging inorganic pollutants play in the aquatic environment. Given the well-known potential dangers posed by toxic elements such as heavy metals for both natural environments and human health, analytical methods capable of accurately monitoring their distribution in natural waters are essential. To address this goal, advanced and robust methodologies capable of selectively and quantitatively analysing these elements at naturally occurring concentrations will be developed to accurately map the distribution of these elements in our environment. The analytical methods investigated will involve ICP-SF-MS operated under clean-lab conditions in combination with on-line matrix-separation and analyte enrichment techniques such as solid-phase extraction and cold vapour technique. This combination will provide an improved and valuable set of analytical methods capable of mapping of elements in the environment at trace- and ultra-trace levels, which is invaluable for our understanding with respect to the environmental fate and eco-toxicological potential. Compartments recently investigated were high mineralized ground waters of important geological fault zones of Austria's territory, rock glacier waters for investigating their role in ground water formation as well as open ocean surface and deep waters of the Southern Ocean (ANT-XXVIII/3 "Eddy pump" cruise).

Abstracts

B.10.SL

Analytik von Meerwasserproben aus Offshore Windparks mittels ICP-MS unter Verwendung des Aufkonzentrierungssystems seaFAST®

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Sowohl durch den immer präsenter werdenden Klimawandel, als auch durch aktuelle politische Entwicklungen, ist die Nachfrage nach erneuerbaren Energien in Europa so groß wie nie zuvor. Offshore Windenergie spielt hierbei eine zentrale Rolle und wird momentan europaweit in Küstenregionen stark ausgebaut. Die harschen Bedingungen, denen die Offshore Windparks ausgesetzt sind machen den Einsatz von Korrosionsschutzsystemen wie z.B. Beschichtungen und/oder Anoden für die Stahlfundamente nötig. Dabei wird das Anodenmaterial über die Lebensdauer einer Windkraftanlage fast vollständig verbraucht. Diese Anoden enthalten je nach Hersteller unterschiedliche Elemente (u.a. Al, Zn, In, Ga, Cd, Pb), deren Freisetzung in die Umwelt (Meerwasser) und deren möglicher Einfluss bei einer Freisetzung nicht abschließend geklärt ist. Durch die Analyse von Meerwasserproben aus Offshore Windparks auf spezielle Tracer-Elemente (z.B. In und Ga) soll ein möglicher Eintrag in die Meeresumwelt untersucht und charakterisiert werden. Zur Untersuchung dieser und anderer Elemente wurde eine Methode zur Meerwasseranalytik weiter optimiert: Durch die Verwendung des seaFAST® Systems (Elemental Scientific, Nebraska) kann die gefilterte (<0.45 µm) und angesäuerte Meerwasserprobe direkt gemessen werden, wobei sowohl die nötige Matrix-Abtrennung, wie auch die Aufkonzentrierung automatisch und online ablaufen. Gekoppelt an ein ICP-MS (Agilent 7900, Agilent Technologies, Japan), unter Verwendung eines He/H_2 Gemisches in der Reaktionszelle, lassen sich bei einem Probenvolumen von 7 mL und einer Messzeit von 12 min 36 Elemente quantifizieren (u.a. Mn, Fe, Co, Ni, Zn, Cd, In, seltene Erden, Pb), wobei niedrigste Bestimmungsgrenzen routinemäßig erzielt werden können (0.001 ng L^{-1} für In oder 0.23 ng L^{-1} für Ga). Proben aus dem Jahr 2022 aus Offshore Windparks der Nordsee zeigten Konzentrationen im Bereich von 0.01 ng L^{-1} bis 0.11 ng L^{-1} für In und 2.92 ng L^{-1} bis 4.32 ng L^{-1} für Ga.

Abstracts

B.11.SL

Aufbereitung von Meerwasserproben für die Messung der Metallgehalte mittels sea*FAST* ICP-MS: Einfluss von Filtrationsmethode und Lagerung auf die Ergebnisse

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Meerwasserproben werden für die Metallanalytik in der Regel schiffsgestützt mit metallfreien Wasserschöpfern (GoFlo, Niskin-Flasche) genommen. Die Proben müssen zeitnah nach der Probenahme filtriert werden, um auszuschließen, dass die Konzentration der gelösten Metalle in den Proben nachträglich durch Adsorption/Desorption oder biologische Prozesse verändert wird. Bei der zumeist genutzten Druckfiltration werden auf dem Schiff neben einem sauberen Arbeitsplatz (z.B. Cleanbench) auch Gasflaschen, sowie Platz und Zeit für gleichzeitig oder nacheinander laufende Filtrationsreplikate benötigt. Eine interessante Alternative bieten DigiFILTER (SCP Science, 0.45 µm Teflonmembran), die direkt mit den sog. DigiTUBEs (SCP Science, 50 mL) für Probe und Filtrat verschraubt werden. Hier können in einem geschlossenen System auf kleinem Raum bis zu 10 Proben zeitgleich filtriert werden. Die DigiTUBES passen in die gängigen Autosampler des ICP-MS, sodass entsprechende Kontaminationsrisiken beim Umfüllen von Proben vermieden und die Handhabung auf dem Schiff und im Labor erleichtert wird.

Der Vergleich der Blindwerte bisher genutzter Polycarbonatfilter (Whatman Nucleopore, 0.4 µm) mit denen vorgereinigter DigiFILTER (0.1% w/w HCl, 2 Tage) hat gezeigt, dass mit beiden Methoden vergleichbare Bestimmungsgrenzen erreicht werden (Cu 8-10 ng/L, Pb 3 ng/L) und die DigiFILTER für einige Elemente geringere Blindwerte aufweisen (z.B. Fe 61 ng/L statt 250 ng/L, Mn 5 ng/L statt 26 ng/L). Erste Ergebnisse zeigen außerdem, dass Filtrationsreplikate bei der Digifiltration geringere Standardabweichungen aufweisen als bei der Druckfiltration. Durch die Etablierung der Digifiltration für Meerwasserproben in einer mobilen Cleanbench vor Ort kann die Lagerung und der Transport großer unfiltrierter, nicht stabilisierter Probenvolumina vermieden werden. Im Rahmen dieser Studie wurden die Meerwasserproben und Blindwerte am ICP-MS mit Hilfe eines sea*FAST* Systems (Elemental Scientific) gemessen. Dieses trennt online automatisiert die Salzmatrix ab und reichert die Analyten an. Die Bestimmungsgrenze der Messung lässt sich so im Vergleich zur direkten Messung mittels ICP-MS deutlich reduzieren (z.B. Mn 0,5 ng/L, Fe 24 ng/L, Cu 1,3 ng/L, Zn 5 ng/L, Pb 0,18 ng/L). Wenn trotz der Erleichterungen durch die Digifiltration keine Filtration an Bord möglich ist (z.B. fehlende Cleanbench), werden Meerwasserproben gekühlt oder gefroren ins Labor transportiert. Dabei

besteht allerdings das Risiko, dass in gekühlten Proben weiterhin biologische Prozesse, Adsorption und Desorption den Anteil von gebundenen und gelösten Metallen verändern. Beim Einfrieren von Wasserproben platzen zudem biologische Zellen auf, sodass Metalle freigegeben werden, die eigentlich der partikulären Phase zuzuordnen wären. Daher wurde zusätzlich untersucht, ob die Lagerungsdauer und -art einen signifikanten Einfluss auf die Konzentrationen von z.B. gelöstem Mn, Fe, Cu, Pb in Meerwasser haben. Abhängig von den Möglichkeiten an Bord ermöglichen die vorhandenen Daten eine Abwägung, ob die Filtration vor Ort oder der Transport der Meerwasserproben ins Labor den besseren Ansatz bietet.

Abstracts

B.12.SL

Multi-Element-Analytik von Flusswasserproben mit ICP-QQQ-MS: Best-Practice-Methode für das Gewässermonitoring

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Ein Best-Practice-Vorschlag für Flusswasser wurde erarbeitet, um bisher getrennte Methoden zur Analyse von 68 Elementen in einem einzigen Analysenlauf zu vereinigen. Damit kann die Zahl der vorzuhaltenden Methoden reduziert und die Anzahl der Analyten von Spuren- bis Mengenelementen entsprechend des jeweiligen Einzugsgebietes angepasst werden, um vorhandene Lücken im Verständnis geochemischer Stoffkreisläufe in Flüssen zu schließen. Unsere Methode erlaubt die Quantifizierung von 68 aus ursprünglich 71 Zielelementen mittels Triple Quadrupol Massenspektrometrie mit induktiv gekoppeltem Plasma (ICP-QQQ-MS) in der gelösten Fraktion (< 0,45 µm). Multi-Element-Analysen bergen mit jedem hinzugefügten Analyten neue Herausforderungen (spektralen und nicht spektralen Ursprungs). Folgende Schwerpunkte wurden deshalb während der Methodenentwicklung adressiert: Analyt-Stabilisierung, Multi-Element-Referenzmaterialien, Mischung von Kalibrationsstandards, Verschleppungseffekte, bester Analysemodus zur Interferenzeliminierung, analytischer Hintergrund, Analyt-Analyt- und Analyt-Matrix-Wechselwirkungen. Die Methode wurde auf Basis zertifizierter Referenzmaterialien, (dotierter) Flusswasserproben, Multi-Element-Standards und „worst-case"-Matrices entwickelt und erfolgreich an Realproben validiert. Dabei wurden 65 von 68 Elementen in Proben aus zwölf verschiedenen Flüssen (n=140: u.a. Rhein, Mosel, Elbe, Donau) über der jeweiligen Bestimmungsgrenze quantifiziert. Im nächsten Schritt wird die Methode für die zeitnahe Gewässerüberwachung und für die Matrix „Gesamtwasserprobe" (unfiltriert) in Kombination mit einem optimierten Mikrowellen-Aufschluss angepasst, sodass erweiterte Stoffbilanzen von Flussgebieten erstellt werden können und ein multi-dimensionaler geochemischer Fingerabdruck von Flusswasserproben ermittelt werden kann.

B.13.SL

Supra-regional monitoring of anthropogenic gadolinium and individual gadolinium species in municipal tap waters

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Gadolinium-based contrast agents (GBCAs) are administered in approximately 40% of all magnetic resonance imaging examinations to improve image contrast. After intravenous administration, the highly polar and inert Gd complexes are excreted unmetabolized within a few hours and due to their chemical nature, they also pass through wastewater treatment plants almost unaffected. In Germany alone, up to 4 tons of Gd are discharged into the environment every year, leading to anthropogenic Gd anomalies in surface and drinking waters. Due to its persistence, anthropogenic Gd can be used as a sensitive tracer for other polar microcontaminants and to monitor hydrological processes, but the fate and long-term behavior of GBCAs in aquatic systems is largely unknown.

The amount of anthropogenic Gd versus its geogenic background can be determined by reference shale-normalized patterns of the rare earth elements (REE). Inductively coupled plasma-mass spectrometry (ICP-MS) has proven to be a valuable tool for this purpose. However, total metal analysis by ICP-MS does not provide any species-related information and therefore, chromatographic hyphenations must be employed to explore speciation analysis, e.g., based on ion-exchange chromatography (IC).

With this work, we present the large-scale Gd monitoring of tap water samples, which have been collected in the 30 largest cities in the German state of North Rhine-Westphalia. REE patterns and individual Gd species were determined using a single platform system for total metal analysis and syringe-driven chromatography. A high-throughput IC-ICP-MS method was employed for speciation analysis, offering a rapid GBCA screening in less than two minutes and species-specific detection limits in the lowest ng/L range. Quantitative results indicate varying GBCA distributions and Gd levels between 1 and 100 ng/L that depend on geographical criteria and the local drinking water supply situation.

B.14.SL

Impurity profiling of organic by-products of a newly developed Gd-based contrast agent

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As medicinal products, paramagnetic Gd(III)-based MRI contrast agents (GBCAs) are subject to the European Medicines Agency guidance requiring the identification and quantification of impurities that exceed a content threshold of 0.05 mass%. For this purpose, a new high-performance liquid chromatography-inductively coupled plasma-mass spectrometry (HPLC-ICP-MS) method was developed for quantitative impurity profiling of Gd-containing by-products, with significantly improved limits of quantification (LOQ) compared with HPLC-UV analysis.

For the quantification of organic by-products, a HPLC-UV system and a HPLC-ICP-MS system were used. A reversed phase (RP)-HPLC column with a phenyl-modified stationary phase was used to separate the analytes. To identify the by-products, a HPLC-electrospray ionisation-high-resolution mass spectrometry (ESI-HRMS) system with an Orbitrap mass analyzer was used.

With a value of 15 nmol/L, the HPLC-ICP-MS technique achieves a LOQ that is lower by a factor of 10 than the LOQ for HPLC-UV determination. Furthermore, by detecting the ^{158}Gd signal, the elemental analysis allows species independent quantification of Gd-containing compounds via external calibration with a Gd-containing standard substance. Thereby, the detected ^{158}Gd signal intensity of the by-products depends on the number of complexed Gd atoms, which can be derived from the characteristic isotopic patterns of Gd-containing compounds. For this purpose, a complementary HPLC-ESI-HRMS investigation was carried out, which was also used to identify the by-products. In summary, this study shows that the HPLC-ICP-MS method is a powerful complement to the routinely used HPLC-UV methodology for the quantitative impurity profiling of GBCAs.

Abstracts

B.15.CL

Simultane Multielement-Bestimmung in Körperflüssigkeiten mittels Multi Quadrupol ICP-MS

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Der Vortrag gibt einen Überblick über hochproduktive Routinemethoden für ICPMS, die eine simultane und ökonomische Analyse von bis zu 28 Analyten in Urin, Serum und Vollblut unter Verwendung eines Multiquadrupol - ICP-MS ermöglichen. Aspekte der Probenvorbereitung, der Ausgestaltung der Methoden mit Einsatz unterschiedlicher Ion-Guide Modi, von MSMS- und Mass-Shift Modi mit O2 und NH3, sowie elektronischer Verdünnung werden dargestellt.

Abstracts

Session C: Instrumental advances and speciation

C.01.IL

New Tools for Chemical Measurement and Characterization of Particles

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In this presentation, recent advances in plasma spectrochemistry for the detection of nanoparticles and microplastics will be reviewed and some contributions from our laboratory to this field will be presented. In the first part, recent developments in inductively coupled plasma mass spectrometry (ICP-MS) instrumentation for nanomaterials characterization in complex mixtures will be reviewed. The current state-of-the-art in single-particle (sp) ICP-MS instrumentation for the detection and characterization of single nanoparticles (NP) as well as remaining challenges will be discussed. While millisecond dwell times were used in the advent of spICP-MS, the use of microsecond dwell times helped to improve nanoparticle data quality and particle size detection limits. Further to this development, we could show that a custom-built high-speed data acquisition unit with microsecond time resolution (µsDAQ) can be used to successfully address issues of split-particle events and particle coincidence, to study the temporal profile of individual ion clouds, and to extend the linear dynamic range by compensating for dead time related count losses. Our next generation DAQ for spICP-MS features nanosecond time resolution. First results of a proof-of-concept study will be discussed. In the second part of the presentation, we turn to a cooler plasma source, which proved useful in ambient desorption/ionization mass spectrometry (ADI-MS). Specifically, the use of molecular mass spectrometry with a home-built flowing atmospheric-pressure afterglow (FAPA) source (which was first developed in the Hieftje laboratory [1-2]) for the direct analysis of microplastics will be discussed. Microplastics (MPs) are typically characterized by Raman spectroscopy and pyrolysis/thermal desorption coupled to gas chromatography, respectively. In this work, the FAPA source is coupled to a high-resolution mass spectrometer (HR-MS) and used to probe selected microplastics directly on a sample target without a preceding separation step. Characteristic mass spectra from polystyrene (PS), polypropylene (PP), polyethylene (PE), and polycarbonate (PC) MPs were obtained and multivariate statistical data analysis tools were used to process the raw data. FAPA-HRMS analysis in combination with principal component analysis is considered an interesting tool for microplastics analysis.

[1] F.J. Andrade, J.T. Shelley, W.C. Wetzel, M.R. Webb, G. Gamez, S.J. Ray, G.M. Hieftje, Anal. Chem., 80, 2646-2653 (2008).

[2] F.J. Andrade, J.T. Shelley, W.C. Wetzel, M.R. Webb, G. Gamez, S.J. Ray, G.M. Hieftje, Anal. Chem., 80, 2654-2663 (2008).

Abstracts

C.02.SL

Going Green by Going Pink: from Ar-ICP to N_2-MICAP

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Despite being the most widely used ion sources for element and isotope analyses by mass spectrometry (MS), the argon inductively coupled plasma (ICP) suffers from multiple drawbacks, such as the need for a complex power generator design, high running cost and the occurrence of Ar-based spectral inter-ferences. The recently introduced microwave inductively coupled atmospheric pressure plasma source (MICAP, Radom Corp) [1] can be sustained by nitrogen, which is more cost effective, environmentally friendlier and the nitrogen-based molecular ions in most cases do not create as severe overlaps with isotopes of interest.[2,3] However, as nitrogen has different physical and chemical properties as argon, the characteristics of the nitrogen sustained MICAP were investigated by coupling it to a commercial quadrupole-based ICPMS instrument (ELAN 6100^{PLUS}, PerkinElmer) and using pneumatic nebulization. The influence of forward power and nebulizer gas flow rate was evaluated and revealed that the N_2-MICAP source can reach similar sensitivities as the Ar-ICP, while similar metal oxide ratios indicate that a comparable gas temperature can be obtained. To study to which extent the use of N_2 as plasma gas affects the gas dynamics during the extraction of the plasma into the MS, different configurations of the vacuum interface were investigated. These modifications, however, caused no distinct changes in the analyte ion transmission, indicating that the supersonic expansion of a N_2 and an Ar plasma do not differ substantially.

[1] J. Jevtic, A. Menon, and V. Pikelja, Plasma Generator Using Dielectric Resonator, PCT/US2014/024306, 2014

[2] M. Schild *et al.*, Replacing the Argon ICP: Nitrogen Microwave Inductively Coupled Atmospheric-Pressure Plasma (MICAP) for Mass Spectrometry, *Anal. Chem.*, vol. 90, no. 22, 2018

[3] C. Neff, P. Becker, B. Hattendorf, and D. Günther, LA-ICP-MS using a nitrogen plasma source, *J. Anal. At. Spectrom.*, vol. 36, no. 8 , 2021

C.03.SL

Characterization of a sample introduction system for plasma spectrometry by computational fluid dynamics

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Physical properties (e.g. density, viscosity, and surface tension) of finely dispersed liquids in gases as well as the transport of liquid and gas through the nozzle and the spray chamber affect the characteristics of a sample introduction system. The quality of an aerosol is governed by key parameters such as particle size, particle velocity and aerosol concentration. These parameters are important to predict the performance behavior of plasmas in analytical measurements. In order to better understand the influence of the spray chamber and to possibly improve the design and size of spray chambers, a CFD (computational fluid dynamics) approach is used in a parameter study of the dispersed flow in a Scott-type spray chamber equipped with a micro-uptake glass concentric nebulizer. Calculations are carried out at different temperatures and flow conditions in the spray chamber. The numerical simulations provide insight in aerosol transport and modification processes (*i.e.* impacts, droplet breakup and coalescence, evaporation, decay of turbulence etc.) that are experimentally nearly inaccessible. Nebulizer characteristics, such as the aerosol size distribution generated by the nebulizer itself (primary aerosols), the aerosol size distribution at the outlet of the Scott spray chamber (tertiary aerosols), and velocity distributions are obtained experimentally by PDA (phase Doppler anemometry) and PIV (particle image velocimetry) measurements. Using these experimental data as input parameters, the numerical results provide an approximation of the transport phenomena occurring inside the chamber and confirm the tendency that only a small amount of droplets is able to reach the plasma relative to the injected liquid. Considering different conditions in the spray chamber, it can be seen that chamber cooling leads to a better performance of the sample introduction system as the solvent plasma load is reduced. Analyte transport measurements show that as the spray chamber temperature increases, the mass of the transported solvent increases and thus also the solvent plasma load, but not necessarily the mass of the analyte to that extent. Hence, the analyte transport efficiency remains almost unchanged in the temperature range investigated.

Abstracts

C.04.CL

Exploring the use of nitrous oxide as a cell gas for inductively coupled plasma tandem mass spectrometry measurements

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Overcoming spectral interferences in inductively coupled plasma mass spectrometry (ICP-MS) measurements is of utmost importance when striving to achieve reliable data. One widely utilised method is to employ the use of a reaction cell gas to mass-shift either the analyte or the interfering species to obtain interference free determinations at the shifted mass of the analyte or on-mass. Amongst others, ammonia (NH_3) and oxygen (O_2) have been used as reaction gas to resolve interferences via the formation of molecular species in the reaction cell. However, NH_3 is a corrosive and toxic gas that is not universally compatible with every gas cell and O_2 only has a selective range of elements that react readily enough to benefit from mass-shift.

Nitrous oxide (N_2O) is an alternative reaction gas to form oxide species. N_2O has a much higher reactivity than O_2 and leads to increased sensitivity when used in ICP-MS. However, due to its high reactivity, a tendency to form new spectral interferences from other matrix components historically rendered N_2O unfavourable for ICP-MS measurements. With the advent of tandem mass spectrometry (MS/MS), formations of new interferences are no longer as problematic, as the additional quadrupole provides a mass-filter that only allows the target mass-to-charge ratio enter the reaction cell. Thus, N_2O becomes a more viable option and is recently gaining traction within the community.

Here, the use of N_2O has been explored as an alternative cell gas for ICP-MS/MS measurements. The comparison of reaction gases for selected elements of interest will be discussed.

C.05.CL

Analysis of Cell Culture Media by means of Triple Quadrupole-ICP-MS: Method Development and Applications

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In recent years, the biopharmaceutical market for producing modern protein therapeutics by cell culture processes has seen an increasing interest in the formulation of the utilized cell culture media (CCM). Historically used serum-based media have been replaced by chemically defined media. This led to beneficial effects on lot-to-lot variability, higher titers, and overall quality of the products. Main constituents of CCM are amino acids, carbohydrates, inorganic salts, vitamins, lipids, and trace elements (TE). Especially, the latter have experienced greatest attention, as it is reported, to affect the cellular metabolism and thus exhibiting influence on the overall protein expression or glycosylation, for example.

A CCM with its up to 100 different components represents a highly complex matrix leading to various possible polyatomic and spectral interferences on the respective mass-to-charge ratios of the analyte of interest. Thus, high resolution (HR-)ICP-MS instruments would be the instrument of choice for TE analysis. Yet, some TE are only present at lowest concentration levels within the final preparation of the medium, falling below the detection limits of HR-ICP-MS instruments. The use of an Agilent 8900 Triple Quadrupole ICP-MS (TQ-ICP-MS) offers the required sensitivity and collision/reaction cell technology as well as meeting regulatory requirements needed for analyses within the good manufacturing practice guidelines.

Hereby, the applicability of the TQ method is demonstrated by examples from the method development process, e.g. the applicability of different mass shift or collision modi as well as their optimization is shown. Furthermore, it will be discussed how changes in sample matrices affect mass shift modi. Finally, the key aspects of TE determination in cell culture media will be presented by recent projects studying the uptake of TE by cells and the coincidental TE depletion within the actual cell culture process.

[1] C. Grinnell, L. Bareford, T.E. Matthews, T. Brantley, B. Moore, D. Kolwyck, Elemental metal variance in cell culture raw materials for process risk profiling, *Biotechnol Progress* 2020, **36**, 5, doi: 10.1002/btpr.3004

Abstracts

C.06.CL

Ein neuartiger Ansatz für die Bestimmung von Schwermetallen in Babynahrung (und anderen Probenmatrizes) mittels ICP-MS

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Lebensmittel sowie Nahrungsergänzungsmittel enthalten essenzielle Nährstoffe und müssen auf potenziell toxische Verunreinigungen getestet werden. Für die Elementspurenanalyse wird häufig ICP-MS eingesetzt, in den meisten Laboratorien bevorzugt Single-Quadrupol Geräte. Obwohl Triple-Quadrupol-ICP-MS-Systeme bauartbedingt viele potenziell kritische Interferenzen besser auflösen können, und vielfach niedrigere Nachweisgrenzen erreichen, sind sie im Routinebetrieb oft nicht die erste Wahl, da aufgrund der Verwendung einer Vielzahl von reaktiven Gasen potenzielle Einschränkungen des Probendurchsatzes erwartet werden. Unter den häufig eingesetzten Gasen (auch im Single Quadrupol Bereich) spielen Helium (als inertes Kollisionsgas) sowie Wasserstoff und Sauerstoff (als reaktive Gase) wichtige Rollen. Die Verwendung von Sauerstoff als einziges reaktives Gas, in Kombination mit einem Triple Quadrupol Gerät, ist jedoch eine Möglichkeit, eine überlegene Interferenzentfernung mit kurzen Probenumschlagszeiten für eine vollständige Multielementanalyse zu kombinieren. Diese neuartige Methode, basierend auf dem Einsatz von Sauerstoff als einzigem Reaktionsgas, wird in dieser Präsentation umfangreich für die Analyse von Babynahrung vorgestellt. Die vollständige Eliminierung von kritischen Interferenzen wurde dabei durch die Messergebnisse, sowie separat durchgeführte Aufstockungsexperimente, bestätigt. Die Probenumschlagszeit wurde durch die Verwendung eines Ventilsystems weiter reduziert. Speziell für die hochtoxischen Elemente wie Arsen und Cadmium, aber auch für eine Vielzahl weiterer Elemente ergeben sich durch die neue Methode bessere Nachweisgrenzen, ohne das die Nachweisgrenzen für typische Haupt und Spurenelemente signifikant beeinflusst werden. Gleichzeitig sind ein hoher dynamischer Bereich und eine empfindliche Detektion aller Elemente von Interesse sichergestellt. Lange Sequenzen mit ununterbrochener Analysendauer von über >10 Stunden demonstrieren die Robustheit der Methode und unterstreichen einmal mehr die Fähigkeit, die Anforderungen von Hochdurchsatzlaboren zu erfüllen. In dieser Präsentation werden die Messergebnisse für eine Vielzahl von im Handel erhältlicher Babynahrungen sowie geeigneten zertifizierten Referenzmaterialien vorgestellt. Gleichzeitig ist die neuartige Methode flexibel für weitere Probenmatrizes einsetzbar, wie zum Beispiel für Proben aus dem Umweltbereich, sowie industrielle Applikationen. Der in dieser Studie vorgeschlagene neuartige Analysemodus mit Triple-Quadrupol-ICP-MS kombiniert das Beste aus zwei Welten, die Analysegeschwindigkeit eines Single Quadrupol-ICP-MS-Systems mit den zusätzlichen Interferenzeliminierung eines Triple-Quadrupol-ICP-MS.

Abstracts

C.07.IL

Digitale Transformation in der Elementanalytik: Probenvorbereitung 4.0

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Digitalisierung und Automatisierung von Laborprozessen gewinnen zunehmend an Bedeutung in der chemischen Industrie. Was ist heute schon möglich und wie könnte die Zukunft aussehen? In der zentralen Elementanalytik der BASF in Ludwigshafen werden seit vielen Jahren Roboteranlagen für die vollautomatisierte Bestimmung von Elementen eingesetzt. Dabei handelt es sich ausschließlich um Eigenentwicklungen der BASF Forschung, da auf dem Markt vergleichbare Systeme nicht verfügbar sind.

Am häufigsten genutzt werden Probenvorbereitungssysteme für einen mehrstufigen offenen Aufschluss in Gegenwart von verschiedenen Säuren und Säuremischungen. Nach dem Aufschluss wird die Aufschlusslösung für die Messung vorbereitet und anschließend in ein ICP-OES zur Bestimmung der Elemente überführt. Die Ergebnisse der Analyse werden direkt vom Analysengerät ins LIMS übertragen und können von dort weiterverarbeitet, dem Auftraggeber online zur Verfügung gestellt und archiviert werden. Intelligente Automatisierungslösungen helfen, die Arbeitssicherheit zu verbessern, die Produktivität zu steigern und sind gleichzeitig eine wichtige Voraussetzung für die Erzeugung von aussagekräftigen Datensätzen. Diese analytischen Daten zusammen mit den richtigen Metadaten sind die Grundlage für sinnvolles Data Mining.

Wie sehen die Herausforderungen für die Zukunft aus? Wie müssen die neuen Konzepte zur Automatisierung daran angepasst werden? Für die gestiegenen Anforderungen an die Bestimmungsgrenzen reichen immer öfter die der ICP-OES nicht mehr aus und erfordern schon heute den Einsatz eines offline ICP-MS. Auch hat sich die Komplexität der Anforderungen geändert: Durch zielgerichtetere Forschung und optimierte Qualitätskontrolle geht die Anzahl der großen Probenserien immer mehr zurück und wir bewegen uns in Richtung „Losgröße 1“. Die Anlagen von morgen müssen daher deutlich flexibler sein als ihre Vorgänger.

C.08.SL

Fluorine-Specific Detection Using ICP-MS Helps to Identify PFAS Degradation Products in non-targeted Analysis

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Although several per- and polyfluoroalkyl substances (PFAS) have been banned and classified as substances of very high concern by the European Chemicals Agency, similar chemicals remain widely used compounds to date. Even though more than 4700 PFASs may occur in the environment, only 40–50 substances are routinely determined in targeted analysis by electrospray ionisation (ESI)-MS/MS. Non-targeted analysis using high-resolution (HR) molecular mass spectrometry suffers from a lack of data mining algorithms for identification and often low ionisation efficiency of the compounds. Here, we demonstrate the usefulness of a hard ionization source (ICP-MS/MS) as a fluorine-specific detector in combination with ESI-MS for the identification of fluorine containing compounds. Simultaneous hyphenation of HPLC-ICP-MS/MS with HR-ESI-MS is applied to evaluate biodegradation products of organofluorine compounds by sewage sludge. The data was analysed in a non-target approach using MZmine. Due to the fluorine-specific detection by ICP-MS/MS, more than 5000 features of the ESI-MS were reduced to 15 features. Of these, one was identified as a PFAS degradation product of fluorotelomer alcohol (8:2 FTOH) without using targeted analysis. The feasibility of the detection of organofluorine metabolites using a fluorine-specific detection was demonstrated using a model compound and can thus be applied to new experiments and unknown organofluorine containing samples in the future. [1]

[1] Fluorine-Specific Detection Using ICP-MS Helps to Identify PFAS Degradation Products in Nontargeted Analysis, S. Heuckeroth, T. N. Nxumalo, A.Raab, J. Feldmann, *Anal. Chem.* 2021 93 (16), 6335-6341

C.09.SL

Fast and automated separation and quantification of bromine species in enzymatically digested DNA samples *via* IC-ICP-MS

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In recent years, there has been a rising interest in utilizing DNA in material sciences, leading to the question of whether DNA is able to transfer electrical charges. Charge transport along DNA could potentially be implemented in nanotechnological applications like molecular wires. Therefore, a fast and automated separation and quantification method for bromide and the artificial nucleoside 5-bromo-2'-deoxyuridine (5-BrdU) *via* hyphenation of ion exchange chromatography (IC) and inductively coupled plasma mass spectrometry (ICP-MS) is presented in this study. The analysis of these two species is relevant to monitor the transfer of electrons along metal-mediated DNA base pairs. Here, electrons are injected into the base stack using a photosensitive electron donor. The electron acceptor 5-BrdU, which is implemented into the sequence downwards the DNA strand, releases bromide upon one electron reduction after occured electron transfer along the DNA. Concentrations of 5-BrdU and bromide in enzymatically digested DNA samples can therefore be used as a marker for the efficiency of electron transfer along the DNA helix. The developed separation and quantification method utilizes an automated IC system, which enables time-efficient external calibration by inline dilution of a stock solution. Due to the fast separation of the two bromine species in less than 90 s, the developed method is suitable for screening applications with a multitude of samples. Despite isobaric interferences and a low degree of ionization for bromine detection *via* ICP-MS, the method has a limit of detection of 30 ng/L, which is approximately an order of magnitude lower than a comparable method using reversed phase high performance liquid chromatography and ICP-MS.

C.10.CL

ICP-MS based metallomics coupled with non-targeted metabolomics as a tool in neurodegeneration studies

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Background ICP-MS-based hyphenated techniques are approved tools for the study of trace element metabolism and their role in human health and disease. Amyotrophic lateral sclerosis (ALS) is a progressive neurodegenerative disease of motor neurons. There are some indications of the role of redox-active metal and metalloid selenium (Se) chemical species in ALS pathology.

Methods Iron (Fe), copper (Cu), and manganese (Mn) redox speciation as well Se speciation were assessed in cerebrospinal fluid (CSF), which is the medium in direct contact with the brain parenchyma. In the same set of samples, we performed non-targeted metabolomics using Fourier transform ion cyclotron resonance mass spectrometry after solid-phase microextraction. We analyzed CSF samples of 7 ALS cases with disease-related mutations (ATXN2, C9ORF72, FUS, SOD1, and TARDBP), and 13 matched controls.

Results New possible interactions between metabolomic and metallomic parameters were studied in the CSF of the ALS individuals. Non-targeted metabolomics showed reduced steroids, including sex hormones, as well as copper and manganese species were found to be the most relevant features for ALS patients. Some associations between iron species and steroid metabolism were noticed.

Conclusion A potential impairment of sex hormone pathways in the ALS-affected brain, as reflected in the CSF was detected. This study demonstrates the fruitfulness of the combined use of ICP-MS-based speciation analysis and non-targeted metabolomics for neurological research.

Abstracts

Session D: Laser-based analysis

D.01.IL

Identification and quantification of breast cancer biomarkers by LA-ICP-MS

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The abundance and location of various marker molecules and elements can be used as indicator to interrogate the health of biological systems. The accurate and precise identification and quantification of trace elements and molecules can be challenging but as well very rewarding regarding potential insight into the underlying mechanisms of the origin, understanding and progression of diseases.

Elemental bioimaging by means of laser ablation coupled to inductively coupled plasma mass spectrometry (LA-ICP-MS) is a powerful technique for the investigation of elemental distributions in tissue sections since it provides high spatial resolution, excellent sensitivity and the possibility of quantitative imaging. The potential of LA has been expanded beyond the sole analysis of elements and targeting proteins that lack heteroatoms is now possible with the integration of immunoasshistochemsitry to the LA workflow.

In this work, an immunohistochemistry (IHC)-assisted LA-ICP-MS method was successfully developed and optimised using lanthanide tagged monoclonal antibodies as proxies to determine spatial distributions and concentrations of two breast cancer biomarkers (MMP-11 and CD45) in metastatic, non-metastatic and healthy breast tissues. To improve repeatability and standardisation, a SEC-ICP-MS/MS method with on-line isotope dilution analysis was applied to determine labelling degrees of antibodies. The levels of metal labels were calibrated as proxies for protein concentrations in precisely manufactured mould-prepared gelatine-based standards.

Altogether, this work features the most recent tools in Metallomics and presents novel approaches for standardisation and data processing. The high sensitivity and resolution of LA-ICP-MS enhanced visualisation of the tumour microenvironment and provided a nuanced vista for improved interpretation of protein expression and application of statistical models to objectively contrast differences between various cohorts.

Abstracts

D.02.SL

Laser ablation-ICP-MS for the investigation of Gd and Pt pharmaceuticals in liver tumors

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Liver cancer is the sixth most occurring cancer type worldwide. Symptoms and signs of liver cancer usually appear late in the course of the disease, which is often medicated by the antitumor agent cisplatin. Due to the late diagnosis, survival rates are poor and therefore, often palliative therapies are chosen. Hence, an early and reliable diagnosis of liver carcinomas and tumor stages plays an important role in suggesting appropriate therapies and increasing survival rates. In this context, magnetic resonance imaging combined with liver-specific contrast agents significantly improves the detection and characterization of liver lesions.

This study aims to determine cisplatin and the liver-specific gadolinium-based contrast agent gadoxetic acid in liver lesions. Rats with liver tumors were administered with gadoxetic acid as well as cisplatin and sacrificed 15 minutes after injection. The resection of tumor tissue with surrounding liver tissue allows the direct comparison of gadolinium, platinum, and other endogenous elements in both tissue types. A 213 nm laser ablation (LA) system hyphenated to inductively coupled plasma-mass spectrometry (ICP-MS) revealed quantitative and spatially resolved element information in the tissue thin sections. Element distributions were correlated with different pathological tissue types, which were examined by hematoxylin and eosin staining. Furthermore, gadolinium and platinum were quantified in regions of interest, providing information on how the uptake of gadoxetic acid and cisplatin varies in different tumor regions and stages. Liver lesions and tumors show decreased gadolinium and iron concentrations, indicating the expected low uptake of gadoxetic acid and the absence of iron-storing hepatocytes. In contrast, the copper content reveals accumulations while cisplatin is distributed heterogeneously in the various tissue types.

D.03.SL

LA-ICP-MS for the quantitative assessment of the gadolinium distribution in sheep bone

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The aim of the study was to determine the localisation of gadolinium in different areas of the bone after the administration of a gadolinium-based contrast agent (GBCA). An elemental bioimaging method based on laser ablation - inductively coupled plasma - mass spectrometry (LA-ICP-MS) was developed for this purpose. An external calibration with gelatin standards was used to quantify gadolinium in the tissue thin sections. The endogenous elements calcium, sulphur, zinc and iron were detected to depict the structure of the bone. As an overview of a larger sample area, an image with a spot size of 25 µm was acquired. Based on these images, areas of interest were selected and analysed at a higher resolution.

The investigated samples originate from a sheep study. The healthy animals received a single clinical dose of a macrocyclic or a linear GBCA or saline. Ten weeks later, they were sacrificed and the femur was harvested. Thin sections were prepared and mounted on quartz slides prior to analysis.

Gadolinium deposits were mainly found in spatial proximity with blood-bearing structures. Correlations of the distribution of gadolinium with those of zinc, iron and calcium were seen. This is an indication of possible transmetallation of gadolinium and subsequent incorporation into the hydroxyapatite phase of the bone. Furthermore, higher gadolinium concentrations were found after administration of a linear GBCA.

D.04.SL

Searching for what's within: By-product critical elements in minerals from ore deposits

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Trace element compositions of minerals have been extensively used to characterize and better understand the geological processes that lead to mineral formation. The need of new critical element resources is rapidly increasing and ore deposits e.g. mined for classical base metals are being targeted as possible sources. Trace element analysis using LA-ICP-MS is a powerful tool in constraining the specific phases that contain elevated concentrations of critical elements in ore deposits. Ore deposits often portray several formation stages that may result in multiple generations of minerals and zonation within one mineral. Laser ablation ICP-MS enables precise in situ measurements of the different generations. We analyze minerals from diverse localities and ore deposit types to understand what critical elements are present in the main ore minerals. Additionally, we are also looking into investigating the potential of old mine tailings serving as a source for critical elements.

Our work is primarily focused on Zn-Cu-Fe sulfide minerals from different ore deposit types and utilizes a ESI NWR213 Nd:YAG laser ablation system coupled to an Agilent 8800 triple quadrupole ICP-MS. The typical suite of masses includes: ^{34}S, ^{51}V, ^{52}Cr, ^{55}Mn, ^{57}Fe, ^{59}Co, ^{60}Ni, ^{63}Cu, ^{65}Cu, ^{67}Zn, ^{71}Ga, ^{72}Ge, ^{73}Ge ^{74}Ge, ^{75}As, ^{82}Se, ^{95}Mo, ^{107}Ag, ^{111}Cd, ^{115}In, ^{118}Sn, ^{121}Sb, ^{125}Te, ^{197}Au, ^{201}Hg, ^{205}Tl, ^{208}Pb and ^{209}Bi. Although spot analyses are the most typical approach, LA-ICP-MS trace element mapping is a potent approach to visualize the trace element distribution in minerals. The analyses show that sulfides from: (1) several carbonate-hosted deposits have elevated concentrations of Ga and Ge, with a large generational variation; (2) sediment-hosted Co deposits contain Co-rich phases besides the cobalt-sulfides themselves; (3) the Polish Kupferschiefer contains the copper sulfide djurleite with elevated Re.

D.05.CL

Mapping of Hg and Se in biological samples with laser ablation – ICP-MS

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Over the last years, mapping of element distributions in biological samples via laser ablation coupled to inductively coupled plasma mass spectrometry (LA-ICP-MS) has substantially evolved towards higher speed, sensitivity, spatial resolution and improved quantification strategies. However, some elements, like Hg and Se, still show a significantly longer single pulse response (SPR) duration, resulting in longer measurement times [1] or poor image quality, if the instrument settings are not properly adjusted to the longer SPRs. In addition, Hg is generally known as one of the more "difficult" elements to investigate, because it is prone to effects like evaporation or adsorption.

In the presented work, the influence of different instrumental parameters on the SPR profile of Hg and Se was systematically investigated, to find the best possible setup for quasi-simultaneous measurements of Hg and Se with LA-ICP-MS. Further, the protocol for the preparation of gelatin standards for external quantification was assessed and optimized. The final method was applied to thin sections of porcini mushrooms (*Boletus edulis* and closely related species), which are known to accumulate large amounts of Hg as well as Se, and to an in-house mushroom reference material.

With the optimized instrumental setup, SPRs of around 50 ms were obtained for Hg and Se (peak width at 10% of the maximum peak height, laser spot size of 20 µm diameter). Although this is still considerably longer than for most other elements, it is more than a five-fold improvement compared to a standard setup. Concerning the quantification strategy, the addition of L-cysteine to the gelatin matrix substantially improved the figures of merit of the calibration for both elements, leading to limits of detection of 0.006 and 0.3 µg g^{-1} for Hg and Se, respectively, at a pixel size of 20 µm. The investigation of mushroom samples revealed that the peripheral tissues of caps and stipes contained 2-6 times higher concentrations of Hg and Se than the adjacent context tissues. Over all, this work highlights the immense potential of an optimized LA-ICP-MS setup for the quantitative investigation of the distribution of Hg and Se in biological tissues with high speed, spatial resolution (5 µm pixel size and lower) and sensitivity.

[1] M. Debeljak, J. T. Van Elteren, K. Vogel-Mikuš, Development of a 2D laser ablation inductively coupled plasma mass spectrometry mapping procedure for mercury in maize (Zea mays L.) root cross-sections, Anal. Chim. Acta, 2013, 787, 155-162

D.06.CL

A multi-method approach for investigating non-metallic inclusions in steel

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Modern high-performance steels have to meet increasingly stringent cleanliness criteria, frequently summarized as "clean steel". These include strict limitation of the number and size of non-metallic inclusions, which negatively affect both the mechanical properties and corrosion resistance of the steel.

The aim of the present study is to elucidate sources and processes leading to the formation of macroscopic (i.e. larger than 100 µm) non-metallic inclusions in steels, potentially enabling further improvements in the production process. For this purpose, macroscopic inclusions in steel ingots were examined using SEM-EDX, LA-ICP-MS and LA-MC-ICP-MS in order to extract a maximum of information from individual inclusions. Thereby, data on morphology, major constituents, trace elements (including rare earth elements) and $^{87}Sr/^{86}Sr$ ratios were obtained. For comparison, these parameters were also determined in potential source materials for inclusions, such as slag, refractory materials and auxiliary materials used in the casting process.

The combination of several complementary measurement principles used in this study allows for a more comprehensive examination of individual inclusions than each of these methods alone. The results show that particles of the refractory lining are the most likely source of the inclusions. Moreover, the composition of these particles appears to be altered by chemical reactions during the casting and in the present case following refining processes like vacuum arc remelting in a tertiary phase of metallurgy.

Abstracts

D.07.CL

Neue Kombination von LA-ICP-MS mit Standardaddition und IDMS zur SI-rückgeführten Quantifizierung von Spurengehalten in festen Proben

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Seit den 1970er Jahren wird die Methode der Laser-Ablation (LA) mit der Massenspektrometrie (MS) kombiniert.[1] Trotz umfangreicher Entwicklungen – auch auf dem Gebiet der quantitativen Anwendungen – sind SI-rückgeführte Messungen noch immer schwierig umzusetzen.[2] Die Kombination der LA-ICP-MS mit dem Prinzip der Isotopenverdünnung (ID) stellt einen vielversprechenden Lösungsansatz dar. Basierend auf dieser Kombination wurde eine neue Technik entwickelt, die SI-rückführbare, quantitative Messungen ermöglicht, ohne matrix-angepasstes Referenzmaterial zu benötigen. Dafür nutzt die LA-ID-ICP-MS ein ebenfalls in der Probe enthaltenes Element mit bekanntem Massenanteil als Referenzelement. Für beide Elemente sind Lösungen in einer Konzentrationsreihe mit veränderten Isotopenverhältnissen notwendig.
Mit der neuen Methode wurde Bor in dem auf Glas basierenden Standardmaterial SRM 612 (NIST) quantifiziert, um die Anwendbarkeit zu überprüfen. Der ermittelte Borgehalt von (33,3 ± 3,7) µg/g war reproduzierbar und im Rahmen der Messunsicherheit (k = 2) nicht vom Informationswert (32 µg/g [3]) zu unterscheiden. Mit der bereits etablierten LA-ICP-MS Methode [4] wurde eine etwa doppelt so hohe Messunsicherheit erhalten, was für kritische Anwendungen den Mehraufwand rechtfertigt.

[1] A. L. Gray, The Analyst, 1985, 110, 551
[2] D. Pozebon et al., JAAS, 2014, 29, 2204–2228
[3] NIST, Certificate of Analysis - SRM 612, 2012
[4] L. Michaliszyn et al., JAAS, 2020, 35, 126–135

Abstracts

D.08.IL

Tandem LA-ICP-MS/LIBS: A versatile tool for the direct analysis of solid samples

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Laser Ablation – Inductively Coupled Plasma – Mass Spectrometry (LA-ICP-MS) and Laser Induced Breakdown Spectroscopy (LIBS) are both well-established analytical techniques that have been developed and improved individually over the last decades. They both use the principle of laser ablation (LA) for sampling, replacing the necessity of sample digestion for the analysis. LIBS collects chemical information by detecting the light emitted from the plasma caused by LA. LA-ICP-MS on the other hand makes use of the generated sample aerosol produced by LA which is transported to the ICP-MS for further analysis. Even though, both techniques are considered stand-alone techniques used for elemental analysis, they offer complementary information and their simultaneous application in a tandem setup can be highly beneficial for applications in many different fields. While LA-ICP-MS excels in sensitivity and provides isotopic information, LIBS provides simultaneous multi-element detection of all elements of the periodic table (including elements non-accessible with ICP-MS: H, C, N, O, F, …). Additionally, both techniques enable spatially resolved measurements.

This contribution aims to provide a short introduction to both techniques and the tandem setup indicating the advantages and limitations they have to offer. Additionally, application examples from selected fields (materials science, environmental biological samples, …) are presented which highlight the benefits of a tandem LA-ICP-MS/LIBS measurement setup.

D.09.CL

New Capabilities with TwoVol3 Laser Ablation Cell - Simultaneous LA-ICP-MS and LIBS

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The TwoVol3 (TV3) was recently introduced as Elemental Scientific Lasers newest ablation cell which is ideal for high-resolution, high-speed LA-ICP-MS elemental images. The TwoVol3 is a redesigned two volume sample chamber that offers two different operation modes, imaging or analytical, which are interchangeable cups that can be swapped in < 5 minutes of time. The imaging cup provides washout times that are in the 1-50 ms time frame, whereas, the analytical cup is for more traditional LA applications or imaging that doesn't require the extremely fast washout times. Laser induced breakdown spectroscopy (LIBS) is the newest capability that is now possible with the TV3. LIBS offers the added advantage of measuring elements that can be difficult or impossible to detect by ICP-MS, such as H, O, and F. In addition, when performing imaging experiments the ICP-MS (quadrupole based) can be dedicated to the 5-10 elements of interest, while LIBS can collect information about everything else (e.g., major elements such as Ca, Na, Mg, K, etc.).

High-speed simultaneous LA-ICP-MS and LIBS images were collected on shark's teeth species (sand tiger, tiger, and hammerhead). Quantitative spatial fluorine distribution via LIBS was determined to be mainly in the enamel of the shark's tooth. Comparing to traditional techniques for F distribution, EDS can take up to 4 h to do a single line scan whereas LIBS can do a single line scan in seconds. For example, a 350 mm^2 area, utilizing a 50 µm laser spot size, can be mapped in minutes. This new methodology allows for much larger data sets to be explored, with elemental data sets that were not possible previously.

Abstracts

Session E: Single particle analysis

E.01.IL

Die Charakterisierung von biogenen Nanomaterialien mittels ICP-MS Techniken

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Zielsetzung: Selen gehört zu den essentiellen Spurenelementen. Unter den verschiedenen Se-Spezies zeigten bislang insbesondere Nanopartikel aufgrund ihrer hohen Bioverfügbarkeit bei gleichzeitig niedriger Toxizität vielversprechende antibakterielle und antikarzinogene Eigenschaften. Zur Charakterisierung biogener Selen-Nanopartikel wird in diesem Beitrag ein Überblick über Techniken gegeben, die im Bezug zur ICP-MS stehen.

Methoden: Neben dem erwähnten Überblick werden eigene Arbeiten vorgestellt, die grundlegend auf der ICP-MS in verschiedenen Konfigurationen basieren: „single particle“ ICP-MS und HPLC-ICP-MS. Durch Verwendung eines ICP-TQ-MS wird die selektive Detektion von ^{80}Se über die Bildung von $^{80}Se^{16}O^{+}$ erreicht. Erhaltene Daten über Nanopartikel werden mit komplementären Techniken wie TEM überprüft.

Ergebnisse: Recht wenige Arbeiten über die Anwendung spezieller ICP-MS Methoden zur Untersuchung biogener Nanomaterialien sind bislang bekannt. Unsere Studien konnten beispielsweise aufzeigen, dass Hefezellen Selen-haltige Nanopartikel in einer breiten Größenverteilung (ca. 4 - 250 nm Durchmesser) enthalten [1], während in verschiedenen Pilzproben keine Nanopartikel detektiert werden konnten, die kleiner als 40 - 50 nm waren.

Schlussfolgerung: Durch die Wahl geeigneter ICP-MS Methoden können übereinstimmende Resultate mit der TEM für die Charakterisierung von Selen-Nanopartikel in verschiedenen Organismen erhalten werden.

[1] R. Álvarez-Fernández García et al. (2020) Addressing the presence of biogenic selenium nanoparticles in yeast cells: analytical strategies based on ICP-TQ-MS. Analyst 145: 1457-1465.

Abstracts

E.02.IL

Fundamentals and applications of large bandpass mass filters in hyphenated and single event ICP-MS

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Analytical Chemistry is increasingly becoming an indispensable joint between life- and environmental sciences, medicine, and nanotechnology. As an interdisciplinary science, it is capable of providing novel and innovative perspectives on current pressing matters that are connected to medical research, industrial applications but also to changing environments. Specifically, inductively coupled plasma – mass spectrometry (ICP-MS) is now a mature technology that allows far more than the sole determination of element concentrations in aqueous samples. ICP-MS offers unique detection modes and signal acquisition strategies for characterisations of individual nanomaterials and cells and further provides elegant solutions for elemental speciation and bioimaging via its associated hyphenated techniques. However, the analysis of complex matrices, small sample volumes and trace concentrations often require dedicated methodologies to achieve high accuracies, to improve limits of detection, enhance spatial resolutions and to establish accurate models.

We recently published a series of studies demonstrating the capabilities and advantages of quadrupoles operated with altered mass bandwidths to push limits in speciation analysis, bioimaging and single event ICP-MS [1-4]. This presentation will detail the concepts, fundamentals and applications of large bandpass mass filters and demonstrate how dedicated methods improve figures of merit in single event ICP-MS for the characterisation of small and complex nanomaterials. Furthermore, we will demonstrate how this method may be exploited to improve spatial resolution and limits of analysis in elemental bioimaging via laser ablation (LA)-ICP-MS targeting metal-coded antibodies and endogenous elements in heterogeneous biological tissues. Finally, we will showcase how increased mass bandwidths contribute to enhanced detection power in elemental speciation analysis via liquid chromatography (LC)-ICP-MS analysing Gd-based contrast agents in the aqueous environment of Australia.

[1] D. Clases, R. Gonzalez de Vega, S. Funke, T.E. Lockwood, M. Westerhausen, R.V. Taudte, P.A. Adlard, P. Doble, J. Anal. At. Spectrom. 35 (**2020**) 728–735.
[2] M. Horstmann, R. Gonzalez de Vega, D.P. Bishop, U. Karst, P. Doble, D. Clases, J. Anal. At. Spectrom. 36 (**2021**) 767–775.
[3] S. Meyer, R.G. De Vega, X. Xu, Z. Du, P.A. Doble, D. Clases, Anal. Chem. 92 (**2020**) 15007–15016
[4] R. Gonzalez de Vega, T. Lockwood, X. Xu, C. Gonzalez de Vega, J. Scholz, M. Horstmann, P. Doble, D. Clases, *accepted for publication* (**2022**)

Abstracts

E.03.SL

Schnelle Einzelpartikel-ICP-MS mit Nanosekundenzeitauflösung als neue Analysenmethode für Nanomaterialien

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Im Laufe des letzten Jahrzehnts hat sich die Einzelpartikel-Massenspektrometrie mit induktiv-gekoppeltem Plasma (engl. *single particle inductively coupled plasma mass spectrometry*, spICPMS) als eine leistungsstarke Methode zur Analyse von Nanomaterialien etabliert. Ursprünglich wurde spICPMS mit einer Zeitauflösung im Millisekundenbereich für transiente Messungen von kolloidalen Suspensionen verwendet, um die Detektion von individuellen Partikeln zu ermöglichen. Seit einigen Jahren konnten die größenbezogenen Nachweisgrenzen durch den Einsatz von Mikrosekundenzeitauflösung gesenkt werden.

In dieser Studie präsentieren wir unseren Beitrag zur Weiterentwicklung von spICPMS mit einer neu entwickelten Datenaufnahmeeinheit mit Nanosekundenzeitauflösung (engl. *nanosecond data acquisition unit*, nsDAQ) und einem darauf abgestimmten Datenverarbeitungsansatz. Das neue System ermöglicht die Detektion von nur 7 nm großen Goldnanopartikeln (AuNP) mit einem kommerziellen ICPQuadrupol-MS und konnte in vorläufigen Tests zur Partikelanzahlbestimmung von monodispersen AuNP Suspensionen verwendet werden.

Die nsDAQ nimmt das Detektorsignal mit einer Integrationszeit von ca. 4 ns auf. Die von uns entwickelte Datenverarbeitungsmethode für diesen neuen Typ transienter Daten basiert auf der Bestimmung der zeitlichen Distanz zwischen zwei Detektor-Events, welche als *event gap* (EG, Event-Lücke) bezeichnet wird. Es hat sich gezeigt, dass der inverse mittlere Logarithmus der EG einer Partikelsignalverteilung linear proportional zur ursprünglichen Partikelgröße ist und somit in Zukunft eine neue, ergänzende Möglichkeit zur Größenkalibrierung von Nanomaterialien darstellen kann.

Abstracts

E.04.SL

Single particle ICP-MS as new characterisation tool for cement systems: characterisation of early hydration products

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Single particle (sp)ICP-MS is a powerful tool to characterise nanoparticles and colloids in aqueous suspensions with respect to their size, concentration and elemental composition. However, analysing suspensions containing water reactive particles is still challenging. For instance, Calcium-Silicate-Hydrates (C-S-H) develop during the early stages of cement hydration, showing variable particle size and Ca/Si ratios according to the original cement/water mix and influencing cement rheology to an unknown extent. To stop this hydration process and to investigate these products on the nano-scale, alcohol-based suspensions may be applied. In this work, we present for the first time a spICP-MS (*ICP-MS/MS 8900* Agilent Technologies) method developed for particle characterisation in ethanol suspensions. Several certified reference materials presenting variable particle sizes (10–1000 nm), particle concentration and elemental composition (i.e., Al, Au, Ca, Mg, Fe, S and Si) were investigated and used for method validation. To avoid agglomeration, all suspensions were sonicated systematically in a temperature controlled sonification bath. Ethanol induced polyatomic interferences were selectively overcome via optimized gas modes (e.g., H_2, H_2+O_2, O_2 or NH_3) for each target element. Data post-processing, based on the particle detection threshold approach for separating ionic/dissolved from particle signals [1], was performed using a self-written python code. Overall, this new method allows the direct quantification of reactive phases developed in all sorts of fast nucleation or mineral formation processes. Such an approach broadens ongoing and future research fields of social relevance such as the role of C-S-H phases in the sorption/transport of radionuclides from deep geological nuclear storage sites, or the use of calcinated clays as an alternative for reducing the CO_2 footprint of Ordinary Portland Cement production.

[1] H. E. Pace et al., Determining transport efficiency for the purpose of counting and sizing nanoparticles via single particle inductively coupled plasma mass spectrometry, Anal Chem, 83(24):9361–9, 2011, doi: 10.1021/ac201952t.

E.05.SL

MDG-ICP-MS - A Versatile Tool for Quantification in the field of Single Particle ICP-MS via Isotopic Dilution

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In recent years, the release of nanoparticles into the environment has increased significantly, not least due to their rapidly growing market share. Due to the strongly differing properties of nanoparticles compared to bulk materials, the detection and evaluation of nanoparticles in the environment is an important issue for environmental analytics.

An established method for the detection of type and size of nanoparticles is single particle ICP-MS. Here, they are introduced as a suspension into the plasma of the mass spectrometer and the particles are recorded as "events". In addition to the influence of the matrix, which can lead to ion suppression and thus to underestimation in addition to superposition of the event signal, calibration with ionic standards is also non-trivial. Here, the transport efficiency plays a major role, as it has an influence on the signal intensity for ionic standards as well as on the frequency of detected events for particles.

To circumvent these two challenges an isotope dilution (ID) method comprising a microdroplet generator (MDG) as the introduction system coupled on-line with an ICP-ToF-MS was used in this work. For ID, ICP-ToF-MS has the advantage that isotopic patterns can be measured in individual particles.

Using platinum nanoparticles as proof-of-concept application, it was shown that it is possible to correctly determine the size of the particles on basis of the known volume of the droplets generated by the MDG applying isotope dilution. With this method, the determination of the transport efficiency as well as external calibration becomes redundant. This makes the developed method very fast and robust and due to the ICP-ToF-MS applicable to a plethora of nanoparticles.

E.06.SL

Single-Cell ICP-MS analysis of algal cells using an automation platform and advanced data processing algorithms

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The elemental analysis of single biological cells by means of inductively coupled plasma-mass spectrometry (scICP-MS) is gathering increased attention and popularity. Similar to optical flow cytometry, specialized low flow sample introduction systems facilitate operation with small sample volumes and cell concentrations. Moreover, low dead volume and minimal carry-over as well as precise flow control improve ICP-MS performance. Following analysis, comprehensible and autonomous algorithms are beneficial to process scICP-MS data reliably.

In this work, a triple quadrupole ICP-MS was used in oxygen mode to study the response of *C. reinhardtii* green algae to changes in the nutritional iron status. Automation was carried out via a microliter flow platform for single-cell ICP-MS instruments. Data evaluation was performed by a set of both established and novel algorithms focused in a single Java-based tool.

Single-cell analysis confirmed the change in the nutritional iron status. Other elements, such as magnesium, did not reflect evident changes in the chlorophyll content, indicating a redistribution within the cell. The copper content was observed to increase under iron-depleted conditions, suggesting an induction of Cu-based enzymes that facilitate the iron uptake by the cell.

In conclusion, it could be emphasized that a combination of different algorithmic approaches improved the data evaluation process by making it more robust and autonomous from arbitrary user input.

E.07.CL

Automating ICP-MS analyses for total metals and elemental speciation

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Inductively coupled plasma-mass spectrometry (ICP-MS) is the principal workhorse for trace elemental analysis. Thanks to advanced engineering the instruments have become more robust with better sensitivity. However, an often-overlooked aspect is the automation required for a truly high-throughput ICP-MS method. Coupling high-end automation or hyphenated techniques is important to take full advantage of the ICP-MS's capabilities. This automation can take different shapes, from simple automation up to advanced systems.

The prepFAST IC is an advanced system which incorporates an autosampler with inline autocalibration and sample preparation functions, and the added ability to do chromatography all within a single platform system. When combined with an ICP-MS, this system can be operated in total metals mode or in chromatography mode without any user intervention. Switching between methods is fully automated, including the data processing, which is all powered by Xceleri software. To demonstrate these capabilities, total arsenic and arsenic speciation methods were used to evaluate proficiency testing urine samples from the New York Department of Health and the Centre de Toxicologie du Québec (CTQ).

E.03.IL

Arsenic speciation in soil: how does climate change can enhance arsenic mobility in Swiss soil

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The mobility of arsenic is depending on its speciation. Arsenic is known to be methylated and thiolated in soil porewaters. In this study the effect of climate change, i.e., higher precipitation and enhanced temperature, on arsenic speciation [1]. Hypothesis: mobility of arsenic in the soil as well as its volatilization will increase at higher temperature.

We used two different type of soils; one affected by mining and one natural soil from Switzerland. Microcosm analysis at two different temperatures and flooded and non-flooded were set up and soil porewater as well as its headspace was sampled at different times and analysed for arsenic speciation in addition to classical soil redox elements. Arsenic speciation methods needed to be developed to guarantee the integrity of its speciation, when methylated and thiolated arsenic species are investigated. We used different type of HPLC-ICPMS and aimed to determine all arsenic species in a non-targeted approach. Furthermore, the volatile arsenic species were trapped on $AgNO_3$ impregnated silica tubes. The oxidized arsines could be quantified and speciated again with using HPLC-ICPMS.

Results: Temperature increase of 5°C leads to a faster release of arsenic from flooded soils. Methylated arsenic appeared earlier and at a higher concentrations with higher temperature, although higher thiolation of arsenic was observed at higher temperature. The rate of biovolatilisation of arsenic increased 4-folds at higher temperature in acidic soils. Conclusion: The anticipated environmental perturbation from climate change will have a significant effect on the biogeochemical cycle of the toxic element arsenic.

[1] V. Mueller, T. Chaves-Capilla, J. Feldmann, A. Mestrot. Science of the Total Environment, 838, 156049 (2022)

Abstracts

Session X: Special lectures

X.01.CL

Ein österreichischer Beitrag zur Entwicklung der Massenspektrometrie im 20. Jahrhundert: Hugo Bondy (1900-1985)

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Die Entwicklung der Massenspektrometrie seit Anfang des 20. Jahrhunderts hat die analytische Chemie revolutioniert. Viele wichtige Beiträge sind allerdings im Laufe der Geschichte in Vergessenheit geraten. So wurde das erste doppelfokussierende Massenspektrometer im Jahr 1933 nach den theoretischen Überlegungen von Walter Bartky und Arthur Jeffrey Dempster durch Hugo Bondy und seinen Kollegen an der Universität Wien erbaut. Jedoch geriet dieser wissenschaftliche Beitrag in Vergessenheit und wurde durch das doppelfokussierende Sektorfeld-Massenspektrometer nach der Geometrie von Josef Mattauch und Richard Herzog aus dem Jahr 1934 überlagert, welche bis zum heutigen Tag Anwendung findet.

Das Ziel dieser Präsentation ist es die Entstehung und Entwicklung des ersten doppelfokussierenden Massenspektrometers und die Biographie der Erbauer im Kontext der damaligen Zeit vorzustellen. Für die Rekonstruktion der Ereignisse wurde eine geschichtswissenschaftliche Recherchearbeit in verschiedenen österreichischen Archiven und Bibliotheken durchgeführt und die wissenschaftlichen Veröffentlichungen der Erbauer evaluiert. Der Fokus liegt einerseits auf der Funktionalität des Massenspektrometers und andererseits auf der Biographie von Hugo Bondy mit seinem Ausschluss vom regulären Wissenschaftsbetrieb aufgrund seiner jüdischen Herkunft.

Die Auseinandersetzung mit den wissenschaftlichen Beiträgen von Bondy und seinen Kollegen ermöglicht es, ein originales Design eines Massenspektrometers erneut kennenzulernen und zu verstehen. Die Biographie von Hugo Bondy verschafft einmalige Einblicke in die außergewöhnliche Situation eines Wissenschaftlers in Österreich während des 20. Jahrhunderts. Beide Aspekte zusammen illustrieren die Mechanismen von wissenschaftlichen Entdeckungen und Institutionen in einer Forschungsgemeinschaft, welche bis heute relevant sind.

Abstracts

X.02.IL

Elemental mass spectrometry: Past, presence and future

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Elemental mass spectrometry, particularly inductively coupled plasma-mass spectrometry (ICP-MS), has evolved into one of the most powerful analytical tools, which are currently available. While total elemental analysis by ICP-MS allows the simultaneous multielemental analysis at concentations down to the ultratrace level already since decades, the combination of ICP-MS with dedicated sample introduction and separation techniques is in the current focus of our scientific community.

Speciation analysis, based on the combination of analytical separation techniques with ICP-MS and complementary electrospray ionization (ESI) MS, offers fascinating possibilities to better understand the role of metal species in biology, medicine and the environment. However, what can we do to improve its frequency of use and its impact to science and society?

Elemental bioimaging based on laser ablation (LA)-ICP-MS offers, in comparison to molecular mass spectrometric imaging (MSI) techniques such as matrix-assisted laser desorption/ionization mass spectrometry (MALDI-MS), far superior options for quantification, as well as similar spatial resolution. What can we do to increase the use of LA-ICP-MS at least to the current levels of MALDI-MSI?

Single cell ICP-MS with the goal to address the natural elemental distribution at the individual cell level or to undergo single cell immunohistochemical labelling experiments will (and partly already do) allow to better understand the composition of individual cells. How can we make sure that relevant biological information arises from these experiments and that the respective methods are competitive to other developing and established methods outside of the elemental mass spectrometry world?

The focus of this presentation will be directed towards strategical, technical and applicational aspects of hyphenated techniques based on ICP-MS.

Abstracts

POSTER PRESENTATIONS

P1 Isotope ratio analysis

P1.1.SL

Assessing analytical methods for high precision Ni isotopic analysis in rhizosphere samples and Ni hyperaccumulating plants

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This contribution compiles the results for the "Mobilisation of Nickel by hyperaccumulating plants" FWF project (P 34719). In this project between the University of Natural Resources and Life Sciences, Tulln and the Montanuniversität, the focus is to investigate Ni solubilisation processes in the rhizosphere of Ni hyperaccumulating plants. One of the ways this is achieved is by studying Ni isotope ratio variations between soil and plants. Ni is a bio-essential trace element, which was observed to show mass dependent isotope fractionation in geological as well as biological processes. Soil solutions, iron oxides and clay minerals were reported to be more enriched in the heavier Ni isotopes compared to their respective parent bedrock [1,2]. However, the range of Ni isotope fractionation in biological processes was observed to be significantly larger compared to abiotic processes [3,4]. As such, studies of Ni isotope composition ($\delta^{60}Ni/^{58}Ni$ and $\delta^{62}Ni/^{58}Ni$) in soil and plant materials may be critical to understand processes in the rhizosphere, elucidating interactions in the plant soil microbe system. However, routine measurements of Ni isotope ratios are currently hampered by complex sample preparation procedures such as laborious Ni/matrix separation and difficulty to obtain isotope ratio results with low measurement uncertainties with multi collector inductively coupled plasma mass spectrometry (MC-ICP-MS). In this contribution, we refine the measurement procedures of Ni isotope ratio measurements with the use of a novel MC-ICP-CRC-MS and special attention to the digestion and chromatographic isolation protocols, methods of overcoming spectral interferences and correction of instrumental isotope fractionation.

[1] Estrade et al., 2015, EPSL, 423, p. 24-35 ; [2] Ratié et al., 2015, ChemGeol, 402, p. 68-76 ; [3] Zelano et al., 2020, Plant Soil 454, p. 225–243 ; [4] Wasylenki, et al., 2015, ChemGeol, 400, p. 56-64

P1.2.CL

Investigating the differences in $^{87}Sr/^{86}Sr$ isotope ratio measurements between MC-ICP-MS and MC-TIMS in cement reference materials

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Thirteen laboratories participated in an international interlaboratory comparison for the determination of $^{87}Sr/^{86}Sr$ isotope ratios in four cement reference materials (RM) using the conventional method for $^{87}Sr/^{86}Sr$ isotope ratios analyses. Sample dissolution and Sr isolation via ion exchange chromatography were required since the cement samples were distributed as powders. Analytical preparation included the use of various digestion methods including mixed mineral acids, microwave/acid, bomb/acid digestion or borate fusion, followed by Sr separation using ion exchange chromatography. In this study, we evaluated whether any statistically significant differences were attributable to instrumental differences (i.e., MC-ICP-MS and MC-TIMS), or to laboratory-specific techniques (different sample preparation techniques, Sr isolation and the procedures for correcting the data outputs). To evaluate these effects, consensus values for cement RMs and associated standard uncertainties were estimated by fitting a linear, Gaussian mixed effects model using the R function "lmer" defined in package "lme4". No statistically significant effects (SSE) attributable to instrumental differences regardless of whether the materials are considered together or separately were evident. There were SSE attributable to differences between laboratories for three cement RMs when the individual cements were considered separately. Since consideration or disregard for such differences does not induce significant changes in the estimate of the consensus values for the $^{87}Sr/^{86}Sr$ isotope ratios in cement RMs, these effects can safely be neglected when calculating the best estimates for the true values of $^{87}Sr/^{86}Sr$ isotope ratios in these RMs.

Abstracts

P1.3.CL

Investigation of the mineral-related differences in $^{87}Sr/^{86}Sr$ isotope ratios of three reference materials (OPC-1, OU-6, CGL ML-3) using sequential extraction – the follow-up study

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The BAM organized an interlaboratory comparison for the characterization of $^{87}Sr/^{86}Sr$ isotope ratios of three reference materials: Limestone (IAG/CGL ML-3), Ordinary Portland Cement (IAG OPC-1) and Penrhyn Slate (IAG OU-6). The reported $^{87}Sr/^{86}Sr$ isotopic ratios for OPC-1 and OU-6 showed deviations that were sevenfold and threefold higher than those of CGL ML-3, respectively. Possible reasons for this could be inhomogeneity of the powered material or incomplete dissolution due to differences in the 87/86 isotope ratios of different mineral phases. In this follow-up study, the $^{87}Sr/^{86}Sr$ isotope ratios of the mineral phases dissolved by sequential extraction were investigated: (i) Performance of successive leaching using 1 mol L^{-1} HNO_3,[1] aqua regia and HNO_3-HCl-HBF_4 (5 : 2 : 1). (ii) Isolation of Sr using Sr spec resin. (iii) Determination of $^{87}Sr/^{86}Sr$ isotope ratios using MC ICP-MS and internal normalization to $^{86}Sr/^{88}Sr$ = 0.1194. In case of the OPC-1, more than 80 % of the certified Sr content was extracted using 1 mol L^{-1} HNO_3 – likely easily dissolvable di- and tricalciumsilicate and carbonate.[1] Further, more than 10 % of the certified Sr content was found in the HNO_3-HCl-HBF_4 digest – likely silicates. These two leached fractions showed significantly different $^{87}Sr/^{86}Sr$ isotope ratios. In case of OU-6, less than 5 % of the certified Sr content was extracted using 1 mol L^{-1} HNO_3, whereas about 50 % of the certified Sr content was found in the aqua regia soluble fraction. Further, about 40 % of the certified Sr content was found in the HNO_3-HCl-HBF_4 digest. These three leached fractions showed significantly different $^{87}Sr/^{86}Sr$ isotope ratios. Consequently, incomplete digestion of either one of these mineral fractions can lead to bias in the measured $^{87}Sr/^{86}Sr$ isotopic signature of these two reference materials.

[1] A. Kazlagić, F. Russo, J. Vogl, P. Sturm, D. Stephan, G. Gluth, Development of a sample preparation procedure for Sr isotope analysis of Portland cements, Analytical and Bioanalytical Chemistry volume, 414, 2022.

P1.4.SL

Low-amount Ca isotopic analysis using double-spike MC-TIMS and MC-ICP-MS in biological tissues to study metabolic processes

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Calcium (Ca) is an essential mineral in the body. Ca dysregulation can result in serious health issues related to the bone mineral balance, but is also a sign for Alzheimer's disease or mitochondrial dysfunction. Therefore, a reliable and efficient method of monitoring changes in Ca metabolism can help to provide early diagnosis. One approach is the study of the change in stable Ca isotope compositions in biological tissues that occur during Ca metabolism. This is due to the kinetics underlying metabolic processes that involve Ca are mass dependent and will redistribute the abundances of naturally occurring, stable Ca isotopes. High-precision isotopic analysis of the Ca pools in the body can provide unique insight into the disruption of Ca metabolism and subsequently be used as a diagnostic marker for various diseases. The extent of natural variations of stable Ca isotopes in the human metabolism is limited with a relative natural variation of about 2-4 ‰ of $\delta(^{44}Ca/^{40}Ca)$. Reliable measurement of Ca isotopic composition has remained challenging, especially considering low Ca levels and significant procedural blanks. In this study, small amounts of Ca (≈1 µg) were isolated from a diverse set of biological matrices using a procedure optimized for low procedural blanks (<10 ng) and separation from matrix elements and isobaric interferences such as Mg, K, Ti, and Fe [1]. A ^{42}Ca–^{48}Ca double spike (DS) was applied to correct for potential isotopic fractionation during sample purification and measurement procedures using MC TIMS. In addition, the potential of a MC-ICP-MS with collision cell was explored for accurate Ca isotope ratio measurements. Data reduction of the measured Ca isotope ratios was performed using in-house developed software solving the DS algorithm. The measurement procedure enabled measurement of the Ca isotopic compositions in biological material concerning mice, including food, water, bone, and kidneys.

[1] Retzmann et.al. Analytical and Bioanalytical Chemistry, pages 675–689, 2021.

Abstracts

P2 Environmental and biomedical analysis

P2.1.SL

Determination of technology-critical elements (TCEs) in plants from urban green infrastructures by ICP-MS/MS

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TCEs are a group of elements increasingly used in high-tech applications. There is substantial knowledge missing regarding quantities released, environmental cycles and potential health hazards. The FWF-funded project TecEUS (P 33099-N; www.teceus.at) aims to assess the levels of selected TCEs in plant samples from green facades and gardens from the urban spheres of Vienna in the context of public health. This poster shows an analytical methodology for the determination of 52 elements including TCEs with ICP-MS/MS, validated with 7 plant CRMs. Closed-vessel microwave digestion was optimized using HNO_3, H_2O_2 and HBF_4. Mass fractions of elements with spectral interferences (e.g. Fe, Ge and REEs) were successfully analysed in mass-shift mode with N_2O as reaction gas.

*LOD*s range from 5 fg g^{-1} (Tb in GBW10015 Spinach Leaves) to 11 ng g^{-1} (Ca in GBW10015 Spinach Leaves). Recoveries range from 80 to 120% and are within the uncertainty of the certified values. This work presents a completed table of mass fractions in all 7 CRM materials for 52 elements with a large range of mass fractions, which provide a valuable basis in future studies. First results from urban plant samples show increasing mass fractions of most investigated elements with decreasing sampling height on green facades, indicating accumulation in urban road dust. Significant differences in elemental accumulation patterns between the investigated species were found, presumably linked to characteristic surface properties of leaves. These results form the basis for a prospective larger-scale dynamic scenario modelling.

P2.2.SL

Investigation of multi-element patterns of plant samples from Viennese green facades as potential filters for technology-critical elements using ICP-MS/MS

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Technology-critical elements (TCEs) such as Ga, Ge, Te and rare earth elements, are playing an increasingly important role in modern technologies. Even though it can be assumed that their increasing use in recent decades has led to elevated concentrations in the environment, limited knowledge is available about how this level of use affects our environment. The FWF-funded project TecEUS (P 33099-N; www.teceus.at) investigates green facades in Vienna to understand the filter capacity of urban greening for technology-critical elements.

Leaf samples of 8 different plant species were taken from 2 green facades in Vienna during 4 seasons. The samples were either washed or treated as unwashed replicates in order to monitor surface dust. After drying, they were brought into solution using microwave-assisted digestion with HNO_3, H_2O_2 and HBF_4. The samples were analysed for 48 elements focusing on TCEs bz means of ICP-MS/MS applying N_2O as reaction gas for elements with interferences. A first trend map of the facades comparing the mass fractions of selected elements in leaf samples depending on species and building height is presented.

P2.3.CL

Metrology for the recycling of Technology Critical Elements to support Europe's circular economy agenda

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Technology critical elements (TCE) are key materials for high-tech products such as smartphones, notebooks and monitors. Their demand is expected to increase exponentially due to the shift towards greener economy through the deployment of renewable energy and electro mobility solutions (European Green Deal). This and the lack of TCE production within the EU, puts the market under pressure and leads to increasing prices. The need to secure TCE supply has become even more pressing under the current health crisis and it is a major objective of the Covid-19 Recovery Plan aimed at reinforcing Europe's resilience and autonomy. A sustainable solution is effective recycling and finally a circular economy. However, the analysis of waste streams is difficult and requires suitable SI traceable analytical solutions to allow for comparability of measurement results throughout the recycling process. The required reference materials (RMs) certified for TCE in the corresponding waste or secondary raw materials and specific documentary standards for TCE to comply with ISO/IEC 17025 requirements, however, are lacking. Furthermore, waste from the so-called "urban mine" is extremely heterogeneous making the estimation of its TCE content difficult. Currently, there is a lack of knowledge at the European level about the TCE stocks and flows in the urban mine. Given the high volume of waste generated and received, fast reliable analytical methods as well as sampling and sample preparation strategies are needed to determine the economic value of the waste and of the final product and to develop and improve recycling procedures.

Within this project we focus on TCEs (Co, Ga, Ge, In, Ta, Nd, Pr, Dy, Gd, La, Au, Pt, Pd, Rh), which have been selected from the list of critical elements for Europe established by the EU in 2020. The overall objective of the project is to provide the reliable and SI traceable determination of TCE in urban waste material at µg/g levels to increase the efficiency and accuracy of TCE recycling. This will be realized by developing validated SI-traceable reference methods, developing traceable and validated RMs for the TCEs, validating the use of the routine methods and RMs for real world applications and facilitating the take up of the technology and measurement infrastructure developed in the project by the measurement supply chain, standards developing organizations and end users.

P2.4.SL

MURmap - Holistic geochemical tracking of elements and their sources in the Mur/Mura River Catchment

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In the project MURmap, new scientific knowledge of the environmental geochemistry of conventional and modern inorganic pollutants is obtained on a European river catchment on the example of the Mur/Mura River. In the following, a holistic approach towards cross-border geochemical elemental and isotopic tracking of the fluvial system and its tributaries will be carried out. The project aims at the determination of (1) natural geochemical background of the catchment area, (2) historical and recent anthropogenic sources of chemical elements, (3) interaction of chemical elements between solid and liquid phases in different physical and chemical water conditions, (4) individual particles as carriers of specific pollutants, (5) differences in the elemental composition of water and sediments in high, medium and low water regime (6) the potential contamination and baseline levels of emerging modern high-technology pollutants, (7) chemical and isotopic composition (based on XRF and MC ICP-MS) of drainage systems, including drainage waters and drainage sediments and (8) at the establishment of sampling, analytical and data curation protocols for such a complex dataset. The obtained data and information will be (9) merged into an easily understandable set of ecological indicators and maps. In three campaigns (May 2022, August 2022 and February 2023) water samples, suspended particulate matter, and alluvial and stream sediment samples are taken and processed to comprehensively characterize the Mur catchment area. First sample analyses taken in 2022 at selected sites show already a wide-ranging occurrence and variation in elements and are discussed along with geological background data and historical usage within the area.

P2.5.CL

Quantification of cardiac troponin via lanthanide-labeled peptides using ICP-MS

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Cardiac troponin (cTn) is now established as one of the most important biomarkers for the diagnosis of acute myocardial infarction (MI) and other cardiovascular diseases (CVDs). cTn levels of patients are usually in the low µg/L range and below, which makes quantification challenging. To ensure a fast and reliable diagnosis, accurate measurements of cTn concentrations are crucial. In current clinical practice, cTn is measured with high sensitivity ELISAs which can detect levels as low as 1 ng/L. However, these tests often give rise to discordant results, therefore standardization is necessary.
The goal of this work was to develop a reference measurement procedure for cardiac troponin I (cTnI). The method was based on proteolytic peptides which were tagged with a lanthanide enabling its quantification using an inductively coupled plasma mass spectrometer (ICP-MS). An immunoaffinity enrichment step was used to achieve lower limits of quantification (LOQs).
The ICP-MS was not sensitive enough to quantify the peptides via their integral sulfur, from methionine and cysteine. Therefore a lanthanide-DOTA-maleimide (2,2',2''-(10-(2-((2-(2,5-dioxo-2,5-dihydro-1H-pyrrol-1-yl)ethyl)amino)-2-oxoethyl)-1,4,7,10-tetraazacyclododecane-1,4,7-triyl)triacetic acid) complex was bound to the sulfur and used to quantify the peptides via the coordinated metal. Synthetic cTnI specific peptides containing the tag were measured as low as 25 nmol/L, which corresponds to 600 µg/L cTnI. Recombinant cTnI was tagged with the complex and was enzymatically digested by GluC to yield specific peptides. These were separated using reversed phase-liquid chromatography and detected with ICP-MS. To reach even lower LOQs, protein G functionalized magnetic beads with anti-cTnI antibodies were used for immunoaffinity enrichment. Enrichment from a PBS sample showed that samples as low as 10 µg/L of cTnI could be detected. In serum detection limits are higher due to matrix effects. The method is still undergoing further development as including the reduction of background noise levels.
This project 18HLT10 CardioMet has received funding from the EMPIR programme co-financed by the Participating States and from the European Union's Horizon 2020 research and innovation programme.

P2.6.SL

Enhancement of protein quantification through lanthanide labels

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The ability to quantify the concentration of specific proteins is now essential for many applications but is especially important in the field of laboratory medicine. Knowledge of these concentrations in the bloodstream or other body fluids can help in the diagnoses, treatment, and in monitoring the progress of certain diseases (Prognosis). Mass spectrometric detection has recently gained more attention due to its lower limits of quantifications (LOQs), lower cross reactivity and higher accuracy compared to other methods. The most common approach when using mass spectrometric detection is to use a specific enzyme to digest the protein of interest and search for proteotypic peptides for quantification. However, to obtain this high accuracy the peptides must be fully released from the protein, which can often result in long (> 24 hours) digestion times.

In our work, we have studied an alternative protein quantification method based on mass spectrometric detection without the prior necessity for protein digestion. This was achieved by first chromatographically separating the target protein using high performance liquid chromatography and then detecting and quantifying its constituent heteroatoms with an ICP-MS. For metallo proteins, such as hemoglobin (iron) and superoxide dismutase (copper), this approach was easier than for non-metal containing proteins, which could only be quantified using sulfur. However, quantification of sulfur suffered from a higher background and a lower sensitivity compared to the metals.

To achieve better sensitivity different lanthanide labels were attached to the cysteines in the protein. This way, LOQs were enhanced 100 fold into the range of low µg/L range for cardiac troponin. For very low protein levels, an enrichment step was also required to reach clinically relevant LOQs. In our poster we will present an approach using immunoaffinity enrichment in combination with lanthanide labeling to improve the sensitivity of the measurement of non-metal containing proteins in clinical samples.

P2.7.SL

Salivary iodine as a status biomarker: a challenge for ICP-MS?

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Background

The study gives a brief presentation of how saliva can be used as a prospective biomarker of iodine status. Iodine is transported to saliva by active transport due to the expression of sodium iodide symporters (NIS) in salivary gland, which makes saliva a potentially relevant medium for assessing body iodine status. ICP-MS seems to be a technique of choice but it faces challenges while working with saliva because of the low sensitivity of iodine due to high ionization potential and matrix effects. This leads to increase in RSD (Relative Standard Deviation) and detection limits. Other limitations which also exists are the large amount of saliva sample required for the reliable ICP-MS analysis.

Methods

This study involves the use of ICP for the quantification of iodine in saliva. This entailed the selection of sample preparation, including relevant internal standards for quantification, with a prospect of testing the method on a small cohort of volunteers.

Results

Sample dilution, composition of diluent, internal standards and plasma parameters were optimized for ICP-MS quantification of iodine in the saliva. LODs and LOQs as well as the potential effects of matrix elements (sodium, potassium etc.) were evaluated. Preliminary method validation was performed through standard addition.

Conclusion

Saliva can be considered as an effective individual biomarker. In the future, the proposed method can be tested in the cohort of volunteers for highlighting the individual iodine status and also can be validated by analyzing relevant reference materials of biological fluids.

P2.8.SL

Trace element analysis of hair and tissues of calves

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Trace elements are compounds that are present in nature in low concentrations. Essential trace elements can have many physical functions in humans and animals, including a normal metabolism, growth, as well as development. They are also necessary for an effective immune function and healthy reproduction [1].

Trace elements are stored in tissues like liver, kidney or muscles and also in hair [2]. Although trace element concentrations can be measured well in tissues, it would be easier and less invasive to determine the trace element status via the hair when analyzing a living animal. However, this would require a correlation between the trace element content in hair and that in organs. The aim of this project is to investigate whether there is such a correlation in cattle. For this purpose, samples of liver, kidney, muscle, serum and hair (from the shoulder and the ears) were taken from 100 calves. Since trace element levels can vary depending on environmental and feeding conditions, the calves which were selected for the project lived under the same conditions for at least three months. The samples were washed (hair) or freeze-dried (tissues) and then digested with nitric acid. The concentrations of 38 elements were determined with ICPMS. The first results will be presented at the ICP-MS Anwender*innen Treffen.

Abstracts

P3 Instrumental advances and speciation

P3.1.SL

Development and construction of an experimental setup for the production of homogeneous microanalytical reference materials

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The aim of the project is to develop a manufacturing method for the production of homogeneous glass reference materials extended to calibration standards for particularly challenging matrices (metals, silicates with high silica content, various oxides etc.) synthesized from natural rocks powders or custom tailored with defined matrix, elemental and isotopic composition. Synthetic micro-analytical glasses are currently only available for a very limited series of materials with a limited petrographic range (mainly basalts) and melting point often not with the necessary quality (e.g. homogeneity) or not with the desired composition.

These microanalytical reference materials must meet the following criteria: (1) a matrix that is as similar as possible to the sample to be analysed; (2) a homogeneous distribution of specific isotope ratios and trace element mass fractions in the µm range and (3) the possibility to prepare precisely a priori defined element and isotopic compositions.

Therefore, a high-temperature reactor was developed, which can be operated both under vacuum, a protective gas atmosphere using inert gases or a precisely adjustable atmosphere. The furnace structure is made of stainless steel and does not require any additional insulation panels. This should reduce the risk of contamination from the furnace chamber.

The reactor can operate in a temperature range of 500 – 2500 °C. Because of a very flexible design, it is possible to use different heat sources and crucible systems. Through the use of inductive heating, a movement and thus a thorough mixing of the melt can also be achieved. The possibility of changing the angle of the axis of rotation enables the melt to be mixed without an additional stirrer in order to avoid possible contamination.

As additional major asset, the rapid cooling of the melt for a vitreous solidification can be carried out directly during the heating process.

P3.2.CL

Eine neuartige Torch für die ICP-MS: Eine einfache Lösung für viele Probleme?

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Die Torch (oder Fackel) eines ICP-MS-Systems ist eine der wichtigsten Komponenten, um einen sicheren und zuverlässigen Betrieb zu gewährleisten. Sie steht in direktem Kontakt mit dem Plasma und dem vom Zerstäuber erzeugten Probenaerosol, und ist dadurch hohen Temperaturen, intensiver UV-Emission und korrosiven Dämpfen ausgesetzt. Im Rahmen der routinemäßigen Wartung des ICP-MS-Systems muss die Torch regelmäßig inspiziert, gereinigt und möglicherweise ausgetauscht werden.

Während für den Injektor unterschiedliche Materialien verwendet werden (z.B. Platin oder Saphir), wird die Torch üblicherweise aus hochreinem Quarz hergestellt. Im Laufe der Zeit, und besonders wenn sie anspruchsvollen Probentypen ausgesetzt ist, kann das Material spröde und instabil werden, was letztendlich einen Austausch erfordert.

In Laboratorien, die stark matrixhaltige Proben wie Brackwasser, stark saure Proben oder organische Lösungsmittel (z. B. Rohöl oder raffinierte Produkte) analysieren, können dadurch Probleme auftreten und zu den Betriebskosten beitragen, oder sogar ein Grund für ungeplante Ausfallzeiten sein.

Gleichzeitig kann die Torch, obwohl er aus hochreinem Quarz besteht, zu Untergründen beitragen, speziell für schwierige Elemente, und ganz besonders für Silizium.

Um diese Herausforderungen zu meistern, wurde die neuartige PLUS Torch entwickelt, die mit allen Geräten der Thermo Scientific™ iCAP™ Qnova™ Series ICP-MS kompatibel ist. Die PLUS Torch besteht aus einem hochreinen und leistungsstarken keramischen Material, das eine deutlich verbesserte Messstabilität und eine längere Lebensdauer bei geringerem Wartungsaufwand bietet.

Diese Präsentation wird einen Überblick über Möglichkeiten bieten, die durch einen Austausch der Standardtorch gegen eine PLUS Torch möglich sind. Dies erfolgt anhand von Beispielen aus der Routineanalytik, beginnend mit der Analyse von Acetonitril, einem wichtigen Lösungsmittel mit einer Vielzahl von Anwendungen im industriellen Bereich. Gleichzeitig werden auch die Vorteile bei der Analyse von schwierigen Analyten, wie Silizium, Schwefel, Phosphor oder Chlor, gezeigt.

P3.3.CL

Prepared for ICP-MS – What to Consider With Microwave Digestion

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Although modern spectrometers increased their robustness in the past, accurate and effective sample preparation is still the key for correct analytical data – errors resulting from sample preparation cannot be compensated later during analysis.

In the meantime, microwave digestion techniques have undergone a similar evolution, developing from simple, but error-prone systems into a valuable tool for the daily analytical workflow. However, even if microwave digestion is widely established nowadays, many users are still struggling during their daily digestion tasks.

In this poster we are going to summarize extensive sample preparation knowledge from decades of experience and tips & tricks how to streamline the path from an unknown sample to a safe and effective digestion method, while considering specific requirements for ICP-MS.

P3.4.CL

TOTALQUANT TECHNIQUE – MORE THAN SEMI-QUANTITATIVE ANALYSIS

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This poster is to describe TotalQuant (TQ) principles, features, and applications for a better understanding of this specific type of analysis.

These applications include semi-quantitative analysis, quantitative analysis, fingerprinting and quick survey scan fully integrated in Syngistix™ software for NexION ICP-MS.

P3.5.CL

Novel possibilities for interference removal using Multi-Quadrupole ICP-MS

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When the first commercial ICP mass spectrometer (ICP-MS) was introduced in 1983, it was of general opinion that this new technology freed analysts from worries about interferences.

Now, many years later, we have a good understanding about interferences and over the years, new techniques and technologies have been developed to reduce or eliminate them.

In this poster the removal of spectral interferences with Multi-Quadrupole technology of the NexION 5000 ICP-MS will be discussed.

P3.6.CL

Determination of Toxic and Other Trace Elements in Baby Foods Using ICP-MS

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Commercial baby foods are the main source of nutrients and energy for many children around the globe, and therefore, the quality and safety of baby foods are extremely important during these crucial developmental stages. This work describes a procedure for the analysis of toxic elements and trace elements in baby foods following U.S. FDA EAM 4.7 using PerkinElmer's Titan™ MPS microwave digestion system for sample digestion and the PerkinElmer's NexION 2000 ICP-MS.

P3.7.CL

On the origin of species - sind im Plasma wirklich alle Spezies gleich?

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Allgemein wird angenommen, dass sich verschiedene anorganische Spezies ein und desselben Elementes im Plasma eines ICP-MS oder -OES nicht signifikant in ihrer Detektorantwort unterscheiden. [1] Meistens werden nur Effekte durch unterschiedliche Proben-Matrices als relevant betrachtet. [2,3] Bei der Gehaltsbestimmung mehrerer hochreiner Palladiumstandards mittels ICP-OES wurden unerklärliche Diskrepanzen von bis zu 1.5 % beobachtet. Diese blieben selbst bei Verdünnung zur Messung mittels ICP-MS bestehen, obwohl die Matrix spätestens hier als angepasst bzw. für alle untersuchten Standards als gleich betrachtet werden konnte. Diese Beobachtung deutet darauf hin, dass sogar die Historie einer Palladium-Spezies durchaus eine Rolle spielt. Die ursprüngliche Form, z. B. als Chlorokomplex im Gegensatz zu Nitrat, sowie das Lösungsmittel, das zum Auflösen des Metalls benutzt wurde, mit anderen Worten der Ursprung der Spezies, beeinflussen ICP-Messergebnisse auch noch in sehr verdünnten Lösungen. Erst nach vollständiger Zerstörung der Spezies durch Mikrowellen-unterstützten Aufschluss bei 200 °C, Eindampfen zur Trockne und erneutem Aufnehmen in Säure konnte kein Einfluss der ursprünglichen Spezies mehr gemessen und der Palladiummassenanteil sicher bestimmt werden. Das Ergebnis der Palladium-Gehaltsbestimmung wurde ergänzend mit einer plasma-unabhängigen Methode, der komplexometrischen Titration, verifiziert.

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[2] J. W. Olesik and S. Jiao, J. Anal. At. Spectrom. 32, 951-966, 2017.
[3] S. H. Tan and G. Horlick, J. Anal. At. Spectrom. 2, 745-763, 1987.

P3.8.SL

Development of a method for the fast and sensitive speciation analysis of gadolinium-based contrast agents in tissue

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Gadolinium-based contrast agents (GBCAs) have been used in magnetic resonance imaging (MRI) for more than three decades, and the highly stable complexes are generally considered safe. However, there is an increased risk of side effects associated with Gd depositions inside the human body, and the retention behavior of gadolinium after GBCA administration is not yet fully understood. The aim of this study was to develop a method for the rapid and highly sensitive speciation analysis of GBCAs and other Gd species in various tissue samples.

A bead mill was used for sample preparation to allow for the homogenization of tissues of different hardness. The homogenate was then centrifuged to obtain the water-soluble fraction as the supernatant. Different membrane materials of centrifugal filters were compared regarding the subsequent removal of interfering matrix components from the supernatant. The stability and recovery of the GBCAs during this sample preparation procedure were evaluated by spiking samples of calf's liver, which acts as a model tissue, with the investigated GBCA prior to the homogenization step. Different classes of GBCAs were tested in these spiking experiments to elucidate ligand-dependent effects. For the subsequent analysis of the samples, an automated single platform system for total metal analysis and syringe-driven chromatography was utilized. Contrary to previously published methods, an anion-exchange chromatography (IC) method combined with inductively coupled plasma-mass spectrometry (ICP-MS) was employed for the speciation analysis of gadolinium. This approach offers a fast separation of species and detection limits in the sub nmol L^{-1}-range. Total gadolinium and individual species were quantified for every fraction of the sample preparation process by external calibration utilizing the auto-dilution function of the instrumental setup.

P3.9.SL

Rapid speciation analysis of Cr(VI) and Cr(III) using µLC-ICP-MS

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Chromium (Cr) is a transition element that exists in oxidation states ranging from - 2 to +6. The common stable ones in the environment are trivalent Cr(III) and hexavalent Cr(VI) chromium. Cr(III) is an important micronutrient for the human body, while Cr(VI) is highly toxic and carcinogenic. The environmental concentrations of both oxidation states are low. Due to the differences in toxicity between Cr(VI) and Cr(III) compounds, speciation of Cr is very important. Therefore, an improved sensitive and robust method for the simultaneous determination of Cr(III) and Cr(VI) in water samples has been developed. The method uses a hyphenated micro liquid chromatography (µLC) system coupled to inductively coupled plasma mass spectrometry (ICP-MS). The optimised method incorporates a pH adjusted EDTA complexation step to stabilise Cr(VI) and Cr(III). The µLC system uses an anion exchange micro-sized column to separate the Cr species. Cr(III) and Cr(VI) were separated with different retention times at 170 and 230 sec, respectively. The method was optimized and validated by spiking Cr(III) and Cr(VI) in various water samples. Furthermore, the method was validated using a drinking water proficiency testing material sample. The developed method can be used for rapid routine determination of chromium species with high precision and reliability.

P3.10.SL

Dimethyl carbonate as new eluent for a fast determination of cobalamins with HPLC-ICPMS

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Vitamin B_{12} (various forms of cobalamin) is one of the essential vitamins for humans and therefore has to be part of our daily nutrition. However, it is mainly found in meat, seafood and dairy products, which increases the risk of a deficiency through a vegan lifestyle. Mushrooms are often mentioned as a possible alternative vitamin B_{12} source. Until now, cobalamins were usually only determined via spectrophotometry or electrospray ionization mass spectrometry, after derivatization to cyano-cobalamin. [1]

To get information about all individual biologically active cobalamin species, we developed a fast method using high performance liquid chromatography (HPLC) coupled to an inductively coupled plasma mass spectrometer (ICPMS). Already published methods are rather time consuming and use an organic solvent gradient to separate the compounds. [2] This results in the need of a special torch for the ICPMS or the addition of oxygen to the plasma. To evade these needs, we used dimethyl carbonate (DMC) as an eluent, which provided a faster elution, favored the sensitivity of the ICPMS detection and can be used with a standard ICPMS setup. [3] A reversed-phase column with an ammonium acetate buffer and DMC were used to separate the inorganic Co(II), cyano-cobalamin, hydroxo-cobalamin, 5'-deoxyladenosyl-cobalamin and methyl-cobalamin in less than 6 minutes. The optimized method was then applied to the extracts of different mushroom samples to determine the concentrations of the different cobalamins.

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P4 Laser-based analysis

P4.1.SL

Elemental bioimaging of atherosclerotic rabbit arteries to investigate the permeability of the artery wall during disease progression via LA-ICP-MS

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Laser ablation – inductively coupled plasma – mass spectrometry (LA-ICP-MS) has been established as a valuable tool for elemental bioimaging in a variety of samples. In the presented work, a LA-ICP-MS-based method was developed to investigate changes in the permeability of artery walls during progressing atherosclerosis using gadolinium-labeled albumin. The results were expected to show an advancing distribution of Gd into the inner parts of the artery wall as well as an increase in calcium and magnesium hotspots the further the disease progresses. To verify this, frozen samples of aortas and iliac arteries were collected from a rabbit study. In this study, accelerated formation of atherosclerotic plaques was induced in the animals via cholesterol-rich diet as well as surgical injury of the endothelium over a period of 49 days. Artery samples were collected at different points throughout the study, with each of the animals being injected with gadolinium-labeled albumin prior to sacrificing. The samples were embedded in cryomatrix, cryosectioned and then mounted onto quartz glass slides for investigation via LA-ICP-MS.

For quantification, matrix-matched gelatin standards were produced for gadolinium, calcium and magnesium, respectively. They were analyzed with LA-ICP-MS together with the artery samples using external calibration. Phosphorus was additionally recorded to depict the biological structure. The resulting bioimages confirm that with progressing disease, an increased amount of Gd is present within the inner layers of the artery walls, thus indicating an increasing permeability for the albumin. Hotspots of calcium and magnesium further indicate the existence of calcifications within the arteries.

P4.2.SL

***In situ* mapping of localised aluminium corrosion using diffusive gradients in thin films (DGT) coupled to LA-ICP-MS**

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The combination of passive solute sampling by diffusive gradients in thin films (DGT) and spatially resolved chemical analysis by LA-ICP-MS allows for non-destructive visualisation and quantification (mapping) of elemental mobilisation processes *in situ*. Traditionally, DGT LA-ICP-MS was being used for environmental studies, but recent developments opened the door for studying corrosion processes in materials science [1]. This study presents a novel application of DGT LA-ICP-MS for *in situ* mapping of corrosion processes, with a focus on localised pitting corrosion of aluminium (Al) workpieces, primarily formed of Al (*w* = 99.5 %) and further including traces of constituent elements such as Fe (*w* = 0.375 %), Zn (*w* = 0.0046 %), and Cu (*w* = 0.0014 %). Since pitting corrosion initiates the formation of microcracks and cavities in Al metal, which can act as a starter for fatigue cracks and lead to metal failure, it's important to better understand the corrosion processes of Al workpieces. Polyacrylamide- and polyurethane-based DGT binding gels with homogeneously distributed iminodiacetate (Chelex 100) and TiO_2 (Metsorb) binding phases were evaluated and applied to the Al samples and immersed for 24- and 72 hours in a NaCl solution (*w* = 1.5%, pH = 4.5). The DGT gels were analysed by LA-ICP-MS and quantification of corrosive metal fluxes was accomplished by linear calibration using DGT gel standards with known analyte mass loadings. The first results of this study showed that DGT LA-ICP-MS enables *in situ* mapping of spatiotemporal patterns of localised multi-elemental (Al, Fe, Cu, Zn) metal solubilisation and release accompanied by different corrosion processes. The method has a high potential for application in materials science, providing quantitative information on the spatiotemporal reaction dynamics of corrosion processes.

[1] S. Wagner et al., *In situ* spatiotemporal solute imaging of metal corrosion on the example of magnesium, Analytica Chimica Acta, 2022, vol. 1212, p. 339910.

P4.3.SL

Development of a Laser Ablation ICP-MS Method for the Analysis of the Element Distribution in rigid Polyvinyl chloride

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Polyvinyl chloride (PVC) contains various stabilizers (e. g. calcium and zinc soaps) and additives (e. g. magnesium hydroxide, calcium carbonate, and titanium dioxide) that introduce elements such as magnesium (Mg), aluminum (Al), calcium (Ca), titanium (Ti), and zinc (Zn) into the material. These components impact the weather resistance of PVC profiles. A matrix adapted laser ablation inductively coupled plasma mass spectrometry (LA-ICP-MS) is developed to investigate the influence of three-dimensional element distribution on degradation.

An ArF excimer laser (193 nm) and a triple quadrupole ICP-MS were used for the investigation. To reduce polyatomic interference, the ICP-MS measurements were conducted in MS/MS mode using helium as collision gas. The laser's fluence and frequency were optimized to the analyzed PVC matrix to achieve high intensity and the lowest relative standard deviation (RSD) for Mg, Al, Ca, Ti, and Zn. The ablation was performed in the form of a line over a length of 1 cm with a laser spot diameter of 25 µm on a window profile. To generate the depth profiles, the material was ablated five times in succession on each line. For statistical validation, the precision of the instrument was determined by repeated measurements conducted in close proximity on the profile. A total of five depth profiles were measured. The median was formed because it is less sensitive to variations. From the five measurements, the RSD of the medians was calculated for each ablation line.

The influence of the position of the sampling area was analyzed by variation of measurement position on the same profile. Five test specimens were selected at different locations on the PVC profile. The measurement and calculation were analogous to the procedure described for the system precision.

A fluence of 2.5 J/cm^2 and a frequency of 30 Hz were determined as ideal values. The RSD of the system precision was below 3.5 % for all elements and all ablation lines. Compared to the first ablation layer, the RSD decreased with increasing layer depth. The RSD between the different specimens cut from one profile was below 5 % for all elements except for the first ablation of zinc (RSD of 15 %).

An LA-ICP-MS method for analyzing element distributions adapted to PVC was developed and statistically validated. The method is used to investigate the accelerated aging of artificially weathered profiles.

P4.4.CL

Development of a laser ablation cell that allows two degrees of translational freedom for planar surfaces

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Objectives – LA-ICP-MS is an outstanding method for spatially resolved investigation of the elemental distribution of surface dimensions up to 100 x 100 mm. When working with larger samples, LA-ICP-MS is associated with time-consuming sample preparation, including sample destruction, which is a result of limited ablation cell size. However, a destruction-free analysis of larger sample material is desirable for various reasons, including eliminating contamination from sample preparation tools, residual sawdust, loss of functionality, etc. Due to current cell spatial restraints, analysis of surfaces wider than 100 x 100 mm without sample destruction remains an unrealized LA-ICP-MS feature, therefore, a non-destructive solution with increased sample surface accessibility was developed. **Approach/Design/Methodology** – Conventional LA cells are airtight, enclosed polymer containers with two carrier-gas ports and a window providing laser beam access. These conventional cells are limited in volume to account for low carrier gas flow rates (economical evaluation), short wash-out times of ablated material, and high flow speeds to increase the yield of ablated material. Increasing the volume of a cell to allow the analysis of larger samples would diminish these features. To remove this limitation, our approach uses the sample's planar surface as part of the cell's structure, forming the "floor". The cell itself becomes a cup, rather than a container. A conventional, standard cylindrical cell design was chosen, and computational fluid dynamics (CFD) were calculated using SolidWorks 2018. Based on this standard design, several cell versions with varied inner volumes and shapes and differing carrier gas port positions were developed to optimize CFD results regarding turbulence and flow direction. These versions were printed in ABS with the CreatBot F430. The window's position remained constant. To avoid ablated material loss, the sealing on the cell's "floor", the cell's open side against the sample surface, was ensured with a Hermetic sealing of silicone and a polyester microfiber to facilitate sample mobility under the cell. The Hermetic sealing was maintained with the introduction of the microfiber layer.The resulting cells were then tested with an Nd: YAG laser (*LSX-213, Teledyne CETAC*) on the ICP-MS (*8900 ICP-MS Triple Quad, Agilent Technologies*). The results, wash-out time, and signal intensity at varied flow rates were recorded and compared with those of the conventional cell. To facilitate a consistent testing environment, an Aluminum-Matrix-Composite (AMC) disc was used as the sample for all measurements. **Findings** – The developed LA cells have presented the possibility of enabling laser ablation on planar surfaces without surface spatial restraints and while maintaining low gas flow volumes. The cells showed results comparable to the manufacturer's standard ablation cell.

P4.5.SL

Application of ICP-MS to study the evolution of non-metallic inclusions in steelmaking

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The presence of microscopic particles, so-called non-metallic inclusions (NMI), cannot be entirely avoided during steelmaking. These NMIs usually negatively affect the mechanical properties of the final steel product or already cause problems during processing in the steel plant. Tracing techniques are applied to track the particle evolution to improve the detailed understanding of inclusion behavior over different process steps. One approach is to deliberately add rare earth elements (REE) to the melt and thus mark the inclusions. Another method determines and compares the natural REE fingerprint of inclusions and their potential sources. In the case of the REE pattern matches, the investigated auxiliary is supposed to contribute to the formation of the examined inclusion. Accurate analysis of the low REE concentrations by ICP-MS and LA-ICP-MS is essential for both concepts. The present study explains the principle and relevance of both approaches to meet the continuously increasing demands regarding steel quality.

Abstracts

P5 Single particle analysis

P5.1.SL

Time-Dependent Uptake of Arsenic Species in the Green Alga *Chlamydomonas reinhardtii*

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Arsenic is a well-known pollutant, especially in water. Its compounds may originate from both natural and anthropogenic sources. In general, arsenic species can be divided into organic and inorganic species. While organic compounds are generally assumed to be less toxic, adverse effects of both types to mammalian as well as plant cells and tissues have been reported. Therefore, research on the metabolism and bioavailability of arsenic species is required. In this study, the time-dependent uptake of both organic and inorganic arsenic species in the model organism *Chlamydomonas reinhardtii* (*C. reinhardtii*), a type of green algae, is observed using single cell ICP-MS (sc-ICP-MS). In sc-ICP-MS, cells in suspension are directly introduced into the plasma, allowing for the analysis of thousands of cells within minutes. During this process, all compounds in these cells are atomised and ionised. Thereby, individual cells each form a distinct ion cloud, resulting in signal spikes upon arrival at the detector. By using sufficiently low dwell times, ionic background signals and cell events can be differentiated. Statistical relevance is achieved by rapid analysis of these large cell numbers. As the distribution of elemental contents of an entire population is measured, cell heterogeneity is highlighted. Here, *C. reinhardtii* was incubated with different organic and inorganic arsenic species. Afterwards, cell number concentrations were determined using flow cytometry, and cells were immediately introduced into ICP-MS. Incubations with different arsenic species were evaluated and compared after varying incubation times. The analytes showed different time dependencies in their uptake behaviour, confirming previously reported differences in biological availability. In summary, sc-ICP-MS provides an easy-to-use, fast, and reliable method for the determination of elemental contents in whole algal cell populations. To analyse the biological availability of various toxicologically relevant compounds, incubation experiments with *C. reinhardtii* algae can be employed, and time-dependencies of the species uptake can be monitored using sc-ICP-MS.

P5.2.SL

Erfassung und Verarbeitung von spICP-MS Daten mit Nanosekunden – Zeitauflösung

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Ziel dieser Arbeit war die Entwicklung eines Datenaufnahmesystems für die Einzelpartikel-Massenspektrometrie mit induktiv-gekoppeltem Plasma (engl. *single particle inductively coupled plasma mass spectrometry*, spICPMS) mit Nanosekunden-Zeitauflösung, sowie der nötigen Algorithmen zur anschließenden Datenverarbeitung. Die Hardware wurde durch eine Feld-Programmierbare Gatter-Anordnung (FPGA) und dedizierte integrierte Schaltkreise zur hochaufgelösten zeitlichen Erfassung (d.h. mit einer Abtastrate von ca. 4 ns) der Signale des angeschlossenen Sekundärelektronenvervielfachers realisiert. Zusätzlich wurden eine Steuerungssoftware für die Hardware und eine Datenverarbeitungssoftware basierend auf C++ entwickelt. Die Datenaufnahmeeinheit mit Nanosekunden-Zeitauflösung (engl. *nanosecond data acquisition unit*, nsDAQ) wurde erfolgreich anhand der Analyse von suspendierten Goldnanopartikeln getestet und es wurde gezeigt, dass die hochaufgelöste Datenerfassung neue Erkenntnisse über den zeitlichen Abstand zwischen der Detektion einzelner Ionen in einer Ionenwolke liefert, welche im Plasma generiert wurde. Die hochfrequente Zeitauflösung ermöglicht eine niedrigere größenbasierte Nachweisgrenze für Goldnanopartikel im Vergleich zu anderen spICP-MS-Methoden mit einfachen Quadrupol-Massenanalysatoren, welche Integrationszeiten von wenigen Mikrosekunden verwenden.[1] Mithilfe der nsDAQ konnten die erfassten Signale von 7 nm AuNP deutlich vom Untergrundsignal unterschieden werden. Die zusätzlichen Informationen über den zeitlichen Abstand zwischen den detektierten Ionen aus Partikeln könnten in Zukunft die Charakterisierung von Nanomaterialien durch spICPMS komplementieren und erweitern.

[1] I. Strenge and C. Engelhard, Capabilities of fast data acquisition with microsecond time resolution in inductively coupled plasma mass spectrometry and identification of signal artifacts from millisecond dwell times during detection of single gold nanoparticles, J. Anal. At. Spectrom., 2016, 31, 135

P5.3.CL

SP-ICP-MS: Fragestellungen aus der Industrie (Merck KGaA)

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Die *Single Particle* - induktiv gekoppelte Plasmamassenspektrometrie (SP-ICP-MS) ermöglicht es Partikelgrößen und Konzentrationen von (Nano-)Partikeln in Suspensionen zu bestimmen. Da in Analysen von nur wenigen Minuten sowohl die Größe als auch die Anzahl der Partikel elementselektiv und höchstempfindlich bestimmt werden können, bietet die Technik Potential als moderne Analysemethode zur routinetauglichen Bestimmung verschiedener Partikelcharakteristika an. Hierbei ist die Vergleichbarkeit der gewonnen Informationen sowie die Routinetauglichkeit von zentraler Bedeutung

In diesem Beitrag soll anhand aktueller Studien aus dem industriellen Umfeld exemplarisch gezeigt werden, welchen Einfluss die Probenvorbereitung, die Bestimmung der Transporteffizient, die Kalibrierung sowie die Auswertung auf das Analysenergebnis haben können. Eine der größten Herausforderungen ist die Übertragung der aktuellen Erkenntnisse aus der Forschung auf industrielle Fragestellungen mit komplexen Matrizes. Hierbei wurden neben Partikelstandards insbesondere kosmetische Produkte, wie Lippenstifte und Lidschatten, sowie die darin enthaltenen Perlglanzpigmente untersucht. Bei den Analyten handelte es sich um Mischoxide, beispielsweise TiO_2 und Fe_2O_3. Für diese Analysen wurde ein modernes, schnell scannendes Quadrupole-ICP-Massenspektrometer (NexIon 2000, PerkinElmer) mit *Dwell Times* von bis zu 10 µs eingesetzt. Im speziellen soll dargestellt werden, welchen Einfluss die Kalibrierart und die Methode zur Bestimmung der Transporteffizienz auf das Analysenergebnis haben können, wie gut die Reproduzierbarkeit der bestimmten Partikelcharakteristika für o.g. Proben ist und wie sich z.B. der Einsatz von Ultraschall bei der Probenvorbereitung auf die Partikelgröße und -anzahlkonzentration auswirken, wobei hier der Nachweis immer kleinerer Partikelgrößen durch optimierte Methoden weiterhin berücksichtig wurde.

[1] F. Laborda, J. Jimenez-Lamana, E. Bolea, J. R. Castillo, *J. Anal. At. Spectrom.*, 2013, **28**, 1220.
[2] H.E. Pace, N. J. Rogers, C. Jarolimek, V. A. Coleman, C. P. Higgins, J. F. Ranville, *Anal. Chem.*, 2011, **83**, 9361.

Abstracts

P6 Diversity and inclusion

P6.1.CL

Fostering inclusive access to analytical instrumentation

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Chemistry should be for everyone, which includes accessibility and operability of analytical instrumentation, such as software but also hardware (e.g. mass spectrometers …). Within this project, we aim at evaluating support strategies for promoting accessibility and operability of disabled scientists to analytical instrumentation.

The primary objective of the project to improve accessibility to analytical instrumentation (both related to software and hardware) will be evaluated by the actual stakeholders with disabilities as the direct target group. Their judgement will be used to evaluate on the success of the project directly.

With current instrumental setups and lab infrastructure, ranging from simple benchtop instruments to more sophisticated analytical equipment, accessibility is often limited or access to critical parts of instrumentation are difficult to impossible to reach considering people having disabilities.

We developed a questionnaire to investigate the situation of people with conscious and unconscious disabilities in the laboratory, specifically regarding analytical instruments. The results of this survey should benefit challenged people to ease their access to this infrastructure and to create a more inclusive and diverse workplace in chemistry laboratories. As a consequence, the results will be presented to laboratory suppliers and instrument manufactures for consideration. The questionnaire is open for every interested person and supports the contribution of staff experience and opinion concerning disabilities in the laboratory. The questionnaire is fully anonymous and no personal data is provided to the authors.

Please support us by taking the survey: https://icpms-leoben2022.at/inclusion-in-lab