

2020 Winter Conference Short Courses

2020 Winter Conference Short Courses

Friday, January 10 - Monday, January 13, 2020

Saturday, January 18, 2020

Tucson, Arizona

Schedule

Analysis by Plasma Spectrochemistry

SA-01 Practical Guide to ICP-MS for Toxicology, Saturday, January 11, 8 am, Frederick Strathmann, NMS Labs, 3701 Welsh Rd, Willow Grove, PA 19090, frederick.strathmann@nmslabs.com

SA-02 Environmental Isotope Geochemistry: Plasma Spectrochemistry as an Essential Tool, Michael E. Ketterer, Saturday, January 11, 8 am, Department of Chemistry and Biochemistry, Northern Arizona University, Box 5698, Flagstaff, AZ 86011-5698, michael.ketterer@nau.edu

SA-03 Speciation Analysis: Complementarity of Elemental, Isotopic and Molecular Mass Spectrometry in Environmental and Life Sciences. Monday, January 13, 7 pm, Joanna Szpunar, Laboratoire de Chimie Analytique Bio-inorganique et Environnement, CNRS UMR 5254-IPREM, Hélioparc, 2, Av. Président Angot, 64053 Pau, France, joanna.szpunar@univ-pau.fr

SA-04 Arsenic and Mercury Speciation in Biological Samples, Saturday, January 11, 7 pm, Jörg Feldmann, University of Aberdeen, College of Physical Sciences, Department of Chemistry, Trace Element Speciation Laboratory, Aberdeen AB24 3UE Scotland, United Kingdom, j.feldmann@abdn.ac.uk

SA-05 Clinical ICP-MS: Inorganic Chemical Exposure Evaluations for Clinical Diagnosis, Biomonitoring and Emergency Response. Sunday, January 12, 1 pm, Robert Jones, rljones@cdc.gov, Cynthia Ward, dmo9@cdc.gov, Jeff Jarrett, CDC, Inorganic and Radiation Analytical Toxicology Branch, 4770 Buford Hwy, Mailstop F-50, Atlanta, GA 30341-3724

SA-06 Antibody Labeling for ICP-MS Applications, Saturday, January 11, 8 am, Norbert Jakubowski, BAM, Federal Institute for Materials Research (retired), 12498 Berlin, Germany, norbi.jakubowski@gmail.com

SA-07 ICPMS for the Characterization of Nanomaterials: Focusing on the Human Exposure to Nanoproducts, Saturday, January 11, 7 pm, Petra Krystek, Vrije University (VU) Amsterdam, Amsterdam, The Netherlands, petra.krystek@vu.nl

SA-08 USP <232> and <233> and ICH-Q3D: Next Steps and Compliance, Saturday, January 11, 1 pm, Nancy Lewen, BMS (retired), New Brunswick, NJ 08903, gnlewen@optonline.net

SA-09 Analysis of Petroleum and Petroleum Products, Monday, January 13, 7 pm, José Luis Todolí, Department of Analytical Chemistry, Nutrition and Food Sciences, University of Alicante, PO Box 99, 03080 Alicante, Spain, jose.todoli@ua.es

SA-10 Single Particle and Single Cell ICP-MS Theory and Applications, Sunday, January 12, 8 am, Chady Stephan, PerkinElmer, 501 Rowntree Dairy Rd, Woodbridge, ON L4L 8H1, Canada, chady.stephan@perkinelmer.com, and Ruth Merrifield, ruth.merrifield@perkinelmer.com

SA-11 Speciation Analyses for Environmental, Forensic, Biomedical, and Industrial Applications. Olivier Donard, Sunday, January 12, 1 pm, MARSS-IPREM, University of Pau, Pau, France, olivier.donard@univ-pau.fr

SA-12 Chemical Imaging by Plasma Spectrochemistry, Saturday, January 11, 7 pm, Davide Bleiner, Empa, Überlandstrasse 129, CH 8600 Dübendorf, Switzerland, davide.bleiner@empa.ch

SA-13 Tracing Element Metabolism in Animals and Humans Using Stable Isotope Techniques, Monday, January 13, 7 pm, Thomas Walczyk, Department of Chemistry, National University of Singapore, Science Drive 4, Singapore 117543, walczyk@nus.edu.sg

Spectrochemical Instrumentation

SI-01 Calibration, Optimization, and Interferences in Plasma Spectrochemical Analysis, Sunday, January 12, 8 am, José A.C. Broekaert, Department of Chemistry, University of Hamburg, Martin-Luther-King-Platz 6, D-20146 Hamburg, Germany, jose.broekaert@chemie.uni-hamburg.de

SI-02 Quantifying Complex Nanoparticles: Direct Coupling of Field Flow Fractionation with Inductively Coupled Plasma Mass Spectrometry, Saturday, January 11, 8 am, James F. Ranville, Colorado School of Mines, Department of Chemistry and Geochemistry, Golden, CO 80401, jranvill@mines.edu

SI-03 High-Resolution ICP-MS, Sunday, January 12, 7 pm, Norbert Jakubowski, BAM, Federal Institute for Materials Research (retired), 12498 Berlin, Germany, norbi.jakubowski@gmail.com

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SI-04 Opportunities, Challenges, and Application of Glow Discharge Techniques, Sunday, January 12, 7 pm, Volker Hoffmann, Leibniz Institute for Solid State and Materials, Research Dresden, PO Box 27 00 16, D-01171 Dresden, Germany, v.hoffmann@ifw-dresden.de; Jorge Pisonero, Universidad de Oviedo, Oviedo, Spain, pisonerojorge@univovi.es

SI-05 Time-of-Flight and Distance-of-Flight Mass Spectrometry for Atomic Analyses, Sunday, January 12, 8 am, Steven J. Ray, SUNY-Buffalo, Department of Chemistry, Buffalo, NY 14280, sray2@buffalo.edu; and Alexander Gundlach-Graham, Department of Chemistry and Applied Biosciences, ETH Zurich, Switzerland, graham@inorg.chem.ethz.ch

SI-06 ICP-MS I: Introduction, Saturday, January 11, 1 pm, John Olesik, Ohio State University, School of Earth Sciences, 125 S. Oval Mall, 026 Mendenhall Labs, Columbus, OH 43210-1002, olesik.2@osu.edu

SI-07 ICP-MS II: Advanced Topics, Sunday, January 12, 1 pm, John Olesik, Ohio State University, School of Earth Sciences, 125 S. Oval Mall, 026 Mendenhall Labs, Columbus, OH 43210-1002, olesik.2@osu.edu

SI-08 Theory and Practical Use of Reaction Cells and Collision Cells for ICP-MS, Monday, January 13, 7 pm, John Olesik, Ohio State University, School of Earth Sciences 125 S. Oval Mall, 026 Mendenhall Labs, Columbus, OH 43210-1002, olesik.2@osu.edu

SI-09 Interferences in ICP Spectroscopy, Sunday, January 12, 1 pm, José Luis Todolí, Department of Analytical Chemistry, Nutrition and Food Sciences, University of Alicante, PO Box 99, 03080 Alicante, Spain, jose.todoli@ua.es

SI-10 Identification and Correction of Interferences in Practical ICP-OES, Saturday, January 11, 7 pm, Deborah Bradshaw, Atomic Spectroscopy Consulting, PO Box 536307, Orlando, FL 32853-6307, bradshawdk@cs.com

SI-11 Identification and Correction of Interferences in Practical ICP-MS, Sunday, January 12, 7 pm, Deborah Bradshaw, Atomic Spectroscopy Consulting, PO Box 536307, Orlando, FL 32853-6307, bradshawdk@cs.com

SI-12 Direct Analysis with Ambient Mass Spectrometry: Chemical Analysis of Things as They Are, Sunday, January 12, 8 am, Jacob Shelley and Brian T. Molnar, Rensselaer Polytechnic Institute, Department of Chemistry and Chemical Biology, Troy, NY 12180, shellj@rpi.edu, and

SI-13 Atmospheric-Pressure Glow Discharge and Liquid-Based Plasmas for Spectrochemical Analysis, Sunday, January 12, 1 pm, Steven J. Ray, and Andrew Schwartz, SUNY-Buffalo, Department of Chemistry, Buffalo, NY 14280, sray2@buffalo.edu

SI-14 New Calibration Strategies in Spectrochemical Analysis, Sunday, January 12, 1 pm, George L. Donati, Wake Forest University, Department of Chemistry, Winston-Salem, NC 27109, donatigl@wfu.edu

SI-15 Flow Injection Analysis for Increased Productivity with ICP Spectrometry, Diane Beauchemin, Sunday, January 12, 7 pm, Queen's University, Department of Chemistry, 90 Bader Lane, Kingston, ON K7L 3N6, Canada, diane.beauchemin@queensu.ca

Sample Introduction Approaches

SS-01 A Practical Guide to Nebulizers and the Part They Play in Modern Sample Introduction, Saturday, January 11, 1 pm, Gerhard Meyer, Promerus LLC, 9921 Brecksville Rd., Breckville, OH 44141, gary.meyer@promerus.com

SS-02 Laser Ablation Mass Spectrometry I, Friday, January 10 1 pm, Bodo Hattendorf, bodo@inorg.chem.ethz.ch, and Detlef Günther, guenther@inorg.chem.ethz.ch, Department of Chemistry and Applied Biosciences, ETH Zurich, Vladimir-Prelog-Weg 1 8093 Zurich, Switzerland

SS-03 Laser Ablation Mass Spectrometry II, Friday, January 10, 7 pm, Detlef Günther, guenther@inorg.chem.ethz.ch, Bodo Hattendorf, bodo@inorg.chem.ethz.ch, Laboratory of Inorganic Chemistry, Department of Chemistry and Applied Biosciences, ETH Zurich, Vladimir-Prelog-Weg 1 8093 Zurich, Switzerland

SS-04 Latest Advances in Laser Ablation-Based Chemical Analysis and Emerging Applications: LIBS, LA-ICP-(OES/MS), and Tandem LA – LIBS, Monday, January 13, 7 pm, Jhanis Gonzalez, Applied Spectra, Inc., 46661 Fremont Blvd, Fremont, CA 94538, jhanis@appliedspectra.com, jjgonzalez@lbl.gov; Rick Russo, Lawrence Berkeley National Laboratory, 1 Cyclotron Rd, Berkeley, CA 94720, rerusso@lbl.gov

SS-05 Application of a Microdroplet Generator in Plasma Spectrochemistry, Jutta Tentschert, Saturday, January 11, 8 am, German Federal Institute for Risk Assessment (BfR), Department of Chemical and Product Safety (BfR), 10589 Berlin, Germany, jutta.tentschert@bfr.bund.de; Daniel Rosenkranz, BAM Federal Institute for Materials Research and Testing, Unter den Eichen 87, 12205 Berlin, Germany, daniel.rosenkranz@bfr.bund.de

SS-06 Microplasma for Chemical Analysis. Sunday, January 12, 7 pm, Vassili Karanassios, University of Waterloo, Department of Chemistry and Waterloo Institute for Nanotechnology, Waterloo, ON N2L 3G1, Canada, vkaranassios@uwaterloo.ca

SS-07 Laser-Induced Breakdown Spectroscopy (LIBS), Saturday, January 11, 7 pm, Vassilia Zorba, Laser Technologies Group, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, vzorba@lbl.gov

Plasma Spectrochemical Techniques

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ST-01 On-the-Job and Soft Skills for Technology Developers (Things You Were Not Taught in School), Saturday, January 11, 8 am & 1 pm, Andrew T. Zander, Consultant, Gerson Lehman Group, 1632 Hickory Ave, Torrance, CA 90503, atzander1027@gmail.com

ST-02 Isotopic Measurements Using ICP-MS, Monday, January 13, 7 pm, Frank Vanhaecke, Ghent University, Department of Analytical Chemistry, Campus Sterre, Krijgslaan 281 - S12, 9000 Ghent, Belgium, frank.vanhaecke@ugent.be, and Nancho Garcia Alonso, University of Oviedo, Oviedo, Spain, jiga@uniovi.es

ST-03 Isotope Dilution for Accurate, Precise and SI Traceable Measurements, Sunday, January 12, 8 am, Lu Yang, National Research Council Canada, 1200 Montreal Rd., Ottawa, Ontario, K1A 0R6, Canada, lu.yang@nrc-cnrc.gc.ca

ST-04 Isotopic Analysis of Heavy Elements for Environmental, Forensic, Biomedical and Industrial Applications, Saturday, January 11, 7 pm, Olivier Donard, MARSS-IPREM, University of Pau, Pau, France, olivier.donard@univ-pau.fr

ST-05 Isotope Fractionation Correction Methods for Accurate Isotope Amount Ratio Measurements by MC-ICP-MS, Saturday, January 11, 8 am, Lu Yang, National Research Council Canada, 1200 Montreal Rd., Ottawa, ON, K1A 0R6, Canada, lu.yang@nrc-cnrc.gc.ca

ST-06 Contamination Control for Elemental Analysis, Sunday, January 12, 1 pm, Brad McKelvey, Seastar Chemicals Inc., 10005 McDonald Park Rd., Sidney, BC V8L 5Y2, Canada, bmckelvey@seastarchemicals.com

ST-07 Launching or Modifying Your Laboratory for Trace Analyses, Saturday, January 11, 1 pm, Ela Bakowska, Elba Elemental Consulting, PO Box 1050, Corning, NY 14830, ela@bakowska.com, bakowskae@corning.com

ST-08 IUPAC Commission on Isotopic Abundances and Atomic Weights (CIAAW): Tables of Isotopic Composition of the Elements and Standard Atomic Weights and Their Relevance for the Plasma Spectrochemist, Sunday, January 12, 8 am, Johanna Irrgeher, Montanuniversität Leoben, Department of General, Analytical and Physical Chemistry, Chair of General and Analytical Chemistry, Isotope Research Group; Franz Josef-Strasse 18, 8700 Leoben, Austria, johanna.irrgeher@boku.ac.at, johanna.irrgeher@unileoben.ac.at

ST-09 Microwave-Assisted Sample Preparation for Trace Elemental Analysis: Think Blank and Go Green, Sunday, January 12, 8 am, Joaquim A. Nóbrega, Federal University of São Carlos, Department of Chemistry, São Carlos, SP, Brazil, djan@terra.com.br

ST-10 Plasma Diagnostics: Fundamentals, Measurements, and Applications, Sunday, January 12, 7 pm, Igor B. Gornushkin, BAM, Federal Institute for Materials Research and Testing, Berlin, Germany, igor.gornushkin@bam.de

ST-11 Triple Quad (QXQ) ICP-MS, Sunday, January 12, 1 pm, R. Steven Pappas, and Nathalie Gonzalez-Jimenez, Centers for Disease Control & Prevention, 4770 Buford Hwy NE, MS F44, Atlanta, GA 30341-3717, rpappas@cdc.gov

ST-12 Quadrupole, Triple Quad, and Sector Field ICP-MS, ETV-AAS, ICP-AES/ICP-OES Method Development Problem Solving, Saturday, January 11, 1 pm, R. Steven Pappas and Mark R. Fresquez, Centers for Disease Control and Prevention, 4770 Buford Hwy NE, MS F-44, Atlanta, GA 30341-3717, rpappas@cdc.gov

ST-13 Sample Preparation Problem Solving for Atomic Mass Spectrometry, Saturday, January 18, 8 am, R. Steven Pappas and Naudia Gray, Centers for Disease Control and Prevention, 4770 Buford Hwy NE, MS F44, Bldg 110, Atlanta, GA 30341-3717, rpappas@cdc.gov

ST-14 Validation Assessment and ISO/IEC 17025: An Interactive Session, Sunday, January 12, 1 pm, Rob Ritsema, RR Quality Consultancy, Amersfoort, The Netherlands; robritsema@gmail.com; Petra Krystek, VU Amsterdam, The Netherlands, petra.krystek@vu.nl

ST-15 Uncertainty of Measurements: Practical Approaches to Determine Measurement Uncertainty Budgets, Sunday, January 12, 7 pm, Thomas Prohaska, Chair General and Analytical Chemistry, Montanuniversität Leoben, Franz Josef-Strasse 18, 8700 Leoben, Austria, thomas.prohaska@unileoben.ac.at

ST-16 Nanomaterials: Regulations, Standards, Measurement Advances and Remaining Challenges, Monday, January 13, 7 pm, Heidi Goenaga-Infante, LGC Limited, Queens Road, Teddington, Middlesex TW11 OLY, UK, heidi.goenaga-infante@lgcgroup.com

ST-17 Metrology Concepts in Plasma Spectrochemistry, Saturday, January 11, 7 pm, Zoltán Mester, National Research Council of Canada (NRC), 1200 Montreal Rd, Building M-58, Ottawa, ON K1A 0R6, Canada, zoltan.mester@nrc-cnrc.gc.ca

Manufacturer's Workshop

Schedule by Date and Time

Friday, January 10, 1 pm

SS-02 Laser Ablation Mass Spectrometry I, Bodo Hattendorf, bodo@inorg.chem.ethz.ch, and Detlef Günther, guenther@inorg.chem.ethz.ch, Department of Chemistry and Applied Biosciences, ETH Zurich, Vladimir-Prelog-Weg 1 8093 Zurich, Switzerland

Friday, January 10, 7 pm

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SS-03 Laser Ablation Mass Spectrometry II, Detlef Günther, guenther@inorg.chem.ethz.ch, Bodo Hattendorf, bodo@inorg.chem.ethz.ch, Laboratory of Inorganic Chemistry, Department of Chemistry and Applied Biosciences, ETH Zurich, Vladimir-Prelog-Weg 1 8093 Zurich, Switzerland

Saturday, January 11, 8 am

SA-01 Practical Guide to ICP-MS for Toxicology, Frederick Strathmann, NMS Labs, 3701 Welsh Rd, Willow Grove, PA 19090, frederick.strathmann@nmslabs.com

SA-02 Environmental Isotope Geochemistry: Plasma Spectrochemistry as an Essential Tool, Michael E. Ketterer, Department of Chemistry and Biochemistry, Northern Arizona University, Box 5698, Flagstaff, AZ 86011-5698, michael.ketterer@nau.edu

SA-06 Antibody Labeling for ICP-MS Applications, Norbert Jakobowski, BAM, Federal Institute for Materials Research (retired), 12498 Berlin, Germany, norbi.jakubowski@gmail.com

SI-02 Quantifying Complex Nanoparticles: Direct Coupling of Field Flow Fractionation with Single Particle Inductively Coupled Plasma Mass Spectrometry, James F. Ranville, Colorado School of Mines, Department of Chemistry and Geochemistry, Golden, CO 80401, jranvill@mines.edu

SS-05 Application of a Microdroplet Generator in Plasma Spectrochemistry, Jutta Tentschert, German Federal Institute for Risk Assessment (BfR), Department of Chemical and Product Safety (BfR), 10589 Berlin, Germany, jutta.tentschert@bfr.bund.de; Daniel Rosenkranz, BAM Federal Institute for Materials Research and Testing, Unter den Eichen 87, 12205 Berlin, Germany, daniel.rosenkranz@bfr.bund.de

ST-01 On-the-Job and Soft Skills-- for Technology Developers (Things You Were Not Taught in School), Andrew T. Zander, Consultant, Gerson Lehman Group, 1632 Hickory Ave, Torrance, CA 90503, atzander1027@gmail.com

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ST-01 On-the-Job and Soft Skills for Technology Developers (Things You Were Not Taught in School), Andrew T. Zander, Consultant, Gerson Lehman Group, 1632 Hickory Ave, Torrance, CA 90503, atzander1027@gmail.com

ST-07 Launching or Modifying Your Laboratory for Trace Analyses, Ela Bakowska, Elba Elemental Consulting, PO Box 1050, Corning, NY 14830, ela@bakowska.com

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SA-07 ICPMS for the Characterization of Nanomaterials: Focusing on the Human Exposure to Nanoparticles, Petra Krystek, Vrije University (VU) Amsterdam, Amsterdam, The Netherlands, petra.krystek@vu.nl

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SI-01 Calibration, Optimization, and Interferences in Plasma Spectrochemical Analysis, José A.C. Broekaert, Department of Chemistry, University of Hamburg, Martin-Luther-King-Platz 6, D-20146 Hamburg, Germany, jose.broekaert@chemie.uni-hamburg.de

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ST-06 Contamination Control for Elemental Analysis, Brad McKelvey, Seastar Chemicals Inc., 10005 McDonald Park Rd., Sidney, BC V8L 5Y2, Canada, bmckelvey@seastarchemicals.com

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ST-14 Validation Assessment and ISO/IEC 17025: An Interactive Session, Rob Ritsema, RR Quality Consultancy, Amersfoort, The Netherlands, robritsema@gmail.com; Petra Krystek, VU Amsterdam, The Netherlands, petra.krystek@vu.nl

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SS-06 Microplasma for Chemical Analysis, Vassili Karanassios, University of Waterloo, Department of Chemistry and Waterloo Institute for Nanotechnology, Waterloo, ON N2L 3G1, Canada, vkaranassios@uwaterloo.ca

ST-10 Plasma Diagnostics: Fundamentals, Measurements, and Applications, Igor B. Gornushkin, BAM, Federal

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Institute for Materials Research and Testing, Berlin, Germany, igor.gornushkin@bam.de

ST-15 Uncertainty of Measurements: Practical Approaches to Determine Measurement Uncertainty Budgets

Thomas Prohaska, General and Analytical Chemistry, Montanuniversitaet Leoben, Franz Josef-Strasse 18, 8700 Leoben, Austria, thomas.prohaska@unileoben.ac.at

Monday, January 13, 7 pm

SA-03 Speciation Analysis: Complementarity of Elemental, Isotopic and Molecular Mass Spectrometry in Environmental and Life Sciences.

Joanna Szpunar, Laboratoire de Chimie Analytique Bio-inorganique et Environnement, CNRS UMR 5254-IPREM, Hélioparc, 2, Av. Président Angot, 64053 Pau, France, joanna.szpunar@univ-pau.fr

SA-09 Analysis of Petroleum and Petroleum Products, José Luis Todolí, Department of Analytical Chemistry, Nutrition and Food Sciences, University of Alicante, PO Box 99, 03080 Alicante, Spain, jose.todoli@ua.es

SA-13 Tracing Element Metabolism in Animals and Humans Using Stable Isotope Techniques, Thomas Walczyk, Department of Chemistry, National University of Singapore, Science Drive 4, Singapore 117543, walczyk@nus.edu.sg

SI-08 Theory and Practical Use of Reaction Cells and Collision Cells for ICP-MS, John Olesik, Ohio State University, School of Earth Sciences 125 S. Oval Mall, 026 Mendenhall Labs, Columbus, OH 43210-1002, olesik.2@osu.edu

SS-04 Latest Advances in Laser Ablation-Based Chemical Analysis and Emerging Applications: LIBS, LA-ICP-(OES/MS), and Tandem LA – LIBS, Jhanis Gonzalez, Applied Spectra, Inc., 46661 Fremont Blvd, Fremont, CA 94538, jhanis@appliedspectra.com, jjgonzalez@lbl.gov; Rick Russo, Lawrence Berkeley National Laboratory, 1 Cyclotron Rd, Berkeley, CA 94720, rerusso@lbl.gov

ST-02 Isotopic Measurements Using ICP-MS, Frank Vanhaecke, Ghent University, Department of Analytical Chemistry, Campus Sterre, Krijgslaan 281 - S12, 9000 Ghent, Belgium, frank.vanhaecke@ugent.be, and Nancho Garcia Alonso, University of Oviedo, Oviedo, Spain, jiga@uniovi.es

ST-16 Nanomaterials: Regulations, Standards, Measurement Advances and Remaining Challenges, Heidi Goenaga-Infante, LGC Limited, Queens Road, Teddington, Middlesex TW11 OLY, UK, heidi.goenaga-infante@lgcgroup.com

Saturday, January 18, 8 am

ST-13 Sample Preparation Problem Solving for Atomic Mass Spectrometry

R. Steven Pappas and Naudia Gray, Centers for Disease Control and Prevention, 4770 Buford Hwy NE, MS F44, Bldg 110, Atlanta, GA 30341-3717, rpappas@cdc.gov

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Descriptive Abstracts

Analysis by Plasma Spectrochemistry

SA-01 Practical Guide to ICP-MS for Toxicology, Saturday, January 11, 8 am, Frederick Strathmann, NMS Labs, 3701 Welsh Rd, Willow Grove, PA 19090, frederick.strathmann@nmslabs.com, and Christian Law, ARUP Laboratories, 500 Chipeta Way, Salt Lake City, UT 84108

Topics to be covered will be part of a practical focus on the clinical utility of using ICP-MS in clinical and forensic testing laboratories. Tales from the front line will be given by a board certified Clinical and Toxicological Chemist, a supervisor from a high volume reference laboratory, a supervisor from a low volume reference laboratory, and a scientist tasked with making all approaches work. Discussions on specific tools for high volume testing, low volume testing, and validation needs for less common matrices will be discussed. Lastly, novel and future applications of ICP-MS in clinical and forensic testing will be highlighted. The course is designed for laboratory supervisors, laboratory technologists, researchers, and medical directors.

Keywords: ICP-MS, toxicology, workflow, quality control, test menu design, clinical presentation

Frederick Strathmann is currently Vice President of Quality Assurance at NMS Labs. Previously, he was medical director of Toxicology at ARUP Laboratories and an assistant professor of Pathology at the University of Utah where he oversaw clinical testing for the Trace and Toxic Elements and Clinical Toxicology Laboratories. He received his MS and PhD in

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Pathology and Laboratory Medicine from the University of Rochester, completed a clinical chemistry fellowship at the University of Washington in Seattle, and is board certified in Clinical chemistry and Toxicological chemistry by the American Board of Clinical Chemistry.

Christian Law is the current Technical Supervisor of the Trace and Toxic Elements Laboratory at ARUP Laboratories. He received his Bachelors of Science in Medical Laboratory Science at the University of Utah. Afterward he began his career at ARUP Laboratories as a generalist in the University of Utah Hospital Clinical Laboratory. He has progressed through several positions of increasing responsibility over his tenure at ARUP, including the technical supervisor of the Molecular Amplified Detection Laboratory for seven years before moving to his current area of responsibility.

Stephanie Stripp is the current Supervisor of the Metals Department at NMS Labs. She received her BS in chemistry with a concentration in Forensic Sciences from The College of New Jersey. Soon after, she began her career as an analyst in the Special Chemistry (Drug Screen) Department before transferring to the Metals Department as Technical Team Leader. She has had the pleasure of working on numerous projects with other departments throughout the laboratory and recently celebrated her 10-year anniversary with NMS Labs.

Riley Murphy is currently the Technical Director of the Metals Department at NMS Labs. He received his BS in chemistry at the University of Vermont in Burlington and his PhD in physical chemistry at Temple University in Philadelphia. He started his tenure at NMS Labs as an analyst and moved through several R&D positions within the metals department before landing in his current role.

SA-02 Environmental Isotope Geochemistry: Plasma Spectrochemistry as an Essential Tool, Michael E. Ketterer, Saturday, January 11, 8 am, Department of Chemistry and Biochemistry, Northern Arizona University, Box 5698, Flagstaff, AZ 86011-5698, michael.ketterer@nau.edu

The majority of the chemical elements possess multiple isotopes. Natural or synthetic variation of isotope compositions are widely used in geochemistry and the environmental sciences for gaining insight into the sources, transport and fate of these elements in the natural and human-affected environment. This course provides a broad overview of the isotope geosciences, with emphasis on sources of these variations, and the use of plasma spectrochemistry to generate the requisite data. Applications to environmental/geochemical studies of important elements such as Pb, Sr, Nd, U, and Pu will be discussed, using examples from the literature.

Keywords: Isotopes, environmental sciences, geochemistry, ICPMS, source/transport/fate processes

Michael E. Ketterer obtained his primary and secondary education in Buffalo, NY, and received a B.S. in Chemistry from University of Notre Dame in 1980. He pursued graduate studies in electron transfer and interfacial chemistry at the University of Colorado under the direction of Prof. Carl A. Koval, receiving a Ph.D. in 1985. After brief employment as an industrial electrochemist, he worked from 1987-1993 at the US Environmental Protection Agency's forensic laboratory, and was Assistant Professor at John Carroll University from 1993-1998. Mike has since taught at Northern Arizona University (1998-2013) and Metropolitan State University of Denver (2013-2018), and is presently Professor Emeritus at Northern Arizona University. His research interests include plasma spectrochemistry, an interest that began when he first used an Elan 250 in 1988, and applications of isotope measurements in the environmental geosciences. Mike has published ~90 peer-reviewed papers in his career, is a prolific collaborator, and has traveled and lectured worldwide in pursuit of his scientific interests. As an Emeritus, Mike is pursuing consulting and *pro bono* work, teaches part-time at University of Denver, and focuses on assistance to communities affected by legacy Cold War-era nuclear contamination.



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SA-03 Speciation Analysis: Complementarity of Elemental, Isotopic and Molecular Mass Spectrometry in Environmental and Life Sciences. Monday, January 13, 7 pm, Joanna Szpunar, Laboratoire de Chimie Analytique Bio-inorganique et Environnement, CNRS UMR 5254-IPREM, Hélioparc, 2, Av. Président Angot, 64053 Pau, France, joanna.szpunar@univ-pau.fr

The development of trace inorganic analysis was a response to the increasing concerns about the role of chemical elements, even when present at low concentrations, in the environment and living organisms. The classical approach providing information on the total element concentration in a bulk sample has been giving way to finer approaches including trace element spatial (imaging), isotope or molecular resolution (speciation). In recent years, each of these approaches has grown into a separate field with a number of specific applications. The short course lecture will address the complementarity of elemental, isotopic and molecular information to study the status, pathways and transformations of trace elements in biota. The topics discussed will include:

- Speciation analysis and coupled techniques: the concept of elemental speciation, the occurrence and classification of metal and metalloid species, the techniques used, the criteria of choice of a method for speciation analysis;
- ICP MS detection in chromatography; ICP MS-assisted proteomics;
- Electrospray MS in speciation analysis (*de novo* identification of organometallic species, characterization of metal complexes with peptides and proteins);
- Complementarity of ICP and MALDI MS in bioimaging;
- The potential of stable isotope labels and isotope ratio determination Selected case studies.

Keywords: ICP-MS, speciation, coupled techniques, metal isotopes

Joanna Szpunar is research engineer at the French National Research Council (CNRS) in Pau, France. She has a broad experience in the field of bioinorganic speciation analysis with a focus on the identification and quantification of trace elements in biological systems and in the chemistry of metal-biomolecule interactions. She is the author or co-author of a book and more than 130 scientific publications in peer-reviewed international journals. Her works have received more than 5500 citations (h-factor 51). Dr. Szpunar (fellow of RSC) has given 30 invited lectures and is a member Advisory Boards of *JAAS*, *Metallomics* and *Brazilian Journal of Analytical Chemistry*. The investigations carried out under her supervision and/or with her active participation resulted in the identification of molecular targets of metals in biological systems including, among others, Bi-binding proteins in *Helicobacter pylori*, Cd-metallothionein complexes in kidney cell lines upon exposure to CdS nanoparticles, I-containing protein in algae as well as selenoproteins in bacteria and plants. Her research involves several collaboration projects (University of Zaragoza (Spain), Italian National Institute of Health, University of Vigo (Spain), University of Santiago de Compostela (Spain), University of Naples (Italy), the Norwegian University of Life Sciences, Hong Kong University, and Mahidol University (Thailand) laboratories. She has supervised six PhD theses and several post-doctoral fellows.

Dr. Szpunar was the chairperson of the European Winter Conference on Plasma Spectrochemistry in 2013. She was awarded the Agilent Plasma Award 2017 for her innovative contributions in the field of metallomics and bioorganic speciation and her support of the plasma spectrochemistry and inorganic mass spectrometry community.

SA-04 Arsenic and Mercury Speciation in Biological Samples, Saturday, January 11, 7 pm, Jörg Feldmann, University of Aberdeen, College of Physical Sciences, Department of Chemistry, Trace Element Speciation Laboratory, Aberdeen AB24 3UE Scotland, United Kingdom, j.feldmann@abdn.ac.uk

This course is divided into three parts. Part 1 shows how speciation analysis is done when only an element-selective detector is available. In particular identification strategies of known and unknown species using HPLC-ICP-MS will be elaborated. Part 2 introduces electrospray mass spectrometry and discusses the advantages and limitation of this technique for complex sample matrices. Part 3 focuses on quantitative aspects in element speciation analysis when chromatographic separations are used.

Keywords: Electrospray MS, ICP-MS, food analysis, arsenic, arsenosugars, mercury, phytochelators, plant physiology

Jörg Feldmann received his PhD at University of Essen (Germany) in 1995; he studied volatile metal and metalloids in the environment by using GC-ICP-MS. He was Feodor Lynen Postdoc (Alexander von Humboldt) at University of British Columbia, Canada in 1995-1997 when he investigated complimentary use of GC-MS and GC-ICP-MS for volatile tin, antimony and bismuth compounds. Since 1997 he was a Lecturer at University of Aberdeen, Scotland and became full Professor in 2003. He has published more than 100 papers in peer-reviewed journals mainly about arsenic speciation. His focus is on the determination of the arsenosugar metabolism by seaweed-eating sheep and the transport and biotransformation of arsenic in plants and the pro and cons of ES-MS and ICP-MS and the online combination of both MS techniques

SA-05 Clinical ICP-MS: Inorganic Chemical Exposure Evaluations for Clinical Diagnosis, Biomonitoring and Emergency Response. Sunday, January 12, 1 pm, Robert Jones, rljones@cdc.gov, Cynthia Ward, dmo9@cdc.gov, Jeff

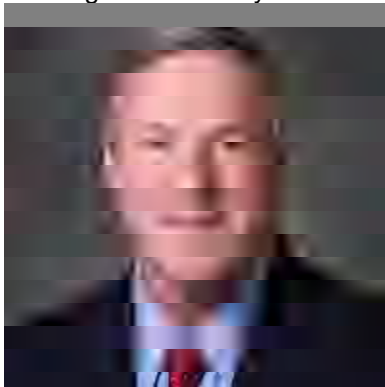
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Jarrett, CDC, Inorganic and Radiation Analytical Toxicology Branch, 4770 Buford Highway, Mailstop F-50, Atlanta, GA 30341-3724

Successful application of inductively coupled plasma mass spectrometry (ICP-MS) is dependent upon correctly addressing numerous pre-analytical, analytical, and post-analytical issues. This workshop will address key issues including matrix selection, contamination control, sample collection/processing/transport, short and long-term quality control, method validation, quality assurance, CLIA regulations, and human subject issues (IRB). Topics will also include discussion of laboratory environment/infrastructure, considerations for automation of sample processing and analysis, and considerations for Biomonitoring versus clinical diagnosis and emergency response preparedness.

Keywords: Clinical ICP-MS, matrix, method validation, biomonitoring, clinical diagnosis, quality control, emergency response

Robert L. Jones is Chief of the Inorganic and Radiation Analytical Toxicology Branch. His responsibilities include the planning, implementation, oversight, and completion of laboratory programs related to public health that involves possible exposures to non-radioactive and radioactive elements or their isotopes. These programs involve research and development of a wide variety of analytical methods to enable the Centers for Disease Control and Prevention to assay and monitor the exposure of populations to toxic or essential elemental or radioactive exposures. In addition, the laboratory group responds to Epidemiological (EPI) Aids, "emergency responses", and is involved with inorganic and radiological laboratory terrorism preparedness.



Cynthia Ward is Chief of the Speciation and Lot Screening Laboratories. Her responsibilities include the planning, implementation, oversight, and completion of programs implementation, oversight, and completion of laboratory speciation programs related to public health that involves possible exposures to non-radioactive elements or elemental species. These programs involve research and development of a wide variety of analytical methods to enable the Centers for Disease Control and Prevention to assay and monitor the exposure of populations to toxic or essential elemental exposures. Her other responsibilities include the implementation and laboratory aspects of multiple local, state, regional, national and international studies or investigations.



SA-06 Antibody Labeling for ICP-MS Applications, Saturday, January 11, 8 am, Norbert Jakubowski, BAM, Federal Institute for Materials Research (retired), 12498 Berlin, Germany, norbi.jakubowski@gmail.com

Keywords: Metal tags, antibody labels, ICP-MS

SA-07 ICPMS for the Characterization of Nanomaterials: Focusing on the Human Exposure to Nanoproducts, Saturday, January 11, 7 pm, Petra Krystek, Vrije University (VU) Amsterdam, Amsterdam, The Netherlands,

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petra.krystek@vu.nl

This course will provide an overview about the role of ICPMS in the characterization of (engineered) nanomaterials, and the analysis of (contact) matrices from human exposure scenarios to nanoproducts as well as in assessments regarding occupational exposure. The stepwise procedures from sampling, sample pre-treatment and measurements by ICPMS will be discussed while aspects of validation and quality control will be involved too. In these cases, ICPMS is used for elemental identification and quantification. The possibilities by single particle (sp) ICPMS will be shown as well.

The knowledge on exposure and possible toxicity of nanotechnological products is still limited, resulting in a great relevance of human risk assessments while exposure can occur by inhalation, ingestion, injection and/or skin contact. For answering these questions, integrated approaches based on the use of ICPMS including hyphenation to asymmetric flow field flow fractionation (AF4), for example, and other complementary techniques are needed. An overview about the selection criteria of matrices and analytical procedures by ICPMS will be given. Examples with body fluids, saliva, tissues (organs) and skin will be discussed more closely. This course will be held as an interactive session.

Keywords: Nanoparticles, exposure, consumer products, ICPMS, analytical approaches

Petra Krystek received her PhD in 1999 at the University of Mainz, Germany. She has more than 20 years experience in the field of ICPMS. Her research is application focused, especially regarding to ultra-trace, speciation and nano-analysis mainly in the field of health and environmental aspects. She worked at research institutes like the National Institute for Public Health and the Environment (RIVM) in the Netherlands as well as in industries as Thermo and Philips. Since 2009 she has been a visiting scientist at the Department Environment & Health at the Vrije Universiteit (VU) Amsterdam, The Netherlands. Since 2003 she has been a lead assessor and freelance assessor in inorganic analytical chemistry at the Dutch Accreditation Council (RvA) for auditing laboratories in the Netherlands, which are accredited according to ISO/IEC 17025. Petra has published over 60 peer reviewed articles and book chapters, and she is a regularly invited lecturer and speaker at international symposia and organized many workshops. She is also member of the editorial board of the journal *Chemosphere* and associate member of the analytical chemistry division of IUPAC. Within her international network she is an expert in the working group for ICP spectrometry of the European Pharmacopoeia Commission (EDQM).



SA-08 USP <232> and <233> and ICH-Q3D: Next Steps and Compliance, Saturday, January 11, 1 pm, Nancy Lewen, BMS (retired), New Brunswick, NJ 08903, gnlewen@optonline.net

As ICH and USP take steps to finalize requirements that require compliance with elemental impurity limits, the pharmaceutical industry will need to be able to demonstrate that compliance. This course will cover the USP and ICH requirements for testing pharmaceuticals for element impurities, how to develop/validate methods, the concepts of risk assessment and risk –based approaches, and helpful hints on analytical work and documentation.

Keywords: Elemental impurities, pharmaceuticals, ICH-Q3D, USP, <232>, <233>

Nancy Lewen has over 26 years' experience in the pharmaceutical industry and was the supervisor of the Atomic Spectroscopy Laboratory in Analytical R&D at Bristol-Myers Squibb until she retired in 2018. Nancy has served as a USP volunteer for over 10 years, having chaired the Elemental Impurities Advisory Panel and the <191>--Identity Tests sub-committee. She has also served on the Spectroscopy and Water sub-committees. Her work focuses heavily on the use of the techniques of atomic spectroscopy to solve analytical problems in the pharmaceutical industry, and also includes the use of XRF for use as a rapid screening technique for process development work.

Nancy has written papers and lectured on the subject of pharmaceutical applications of atomic spectroscopy, and has

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taught several short courses on that subject, as well. Nancy is the recipient of the 2008 New Jersey Association of Biomedical Research "Outstanding Women of Science" award, the Bristol-Myers Squibb 2005 Chemistry Leadership Award and the 2014, USP Award for "An Innovative Response to a Public Health Challenge" as a member of the USP Elemental Impurities Advisory Panel.

SA-09 Analysis of Petroleum and Petroleum Products, Monday, January 13, 7 pm, José Luis Todolí, Department of Analytical Chemistry, Nutrition and Food Sciences, University of Alicante, PO Box 99, 03080 Alicante, Spain, jose.todoli@ua.es

This course will provide an overview of the analysis of petroleum and petrochemicals by ICP OES and ICP-MS techniques and, in depth, information on specific applications and challenges. Sample types will include crude oil, distillate fractions, volatile hydrocarbons and solvents, used oils and other materials found in petrochemical processing. Sample preparation and sample introduction will be highlighted. Existing methods, calibration standards, and certified samples will be evaluated, as well as result validation and quality. The advantages of ICP-MS hyphenation with separation techniques will be discussed. Time for class discussion on topics of individual interest will be provided, and advice will be available on carrying out the ICP-OES and ICP-MS analysis of different petroleum products.

Keywords: ICP OES, ICPMS, plasma spectrometry, petroleum, crude oil, metals, organic solvents, sample preparation, sample introduction, HPLC



SA-10 Single Particle and Single Cell ICP-MS Theory and Applications, Sunday, January 12, 8 am, Chady Stephan and Ruth Merrifield, PerkinElmer, 501 Rowntree Dairy Rd, Woodbridge, ON L4L 8H1, Canada, chady.stephan@perkinelmer.com, ruth.merrifield@perkinelmer.com

This course will briefly review the theory of SP-ICP-MS focusing on the state-of-the-art innovations in hardware and software with relation to the latest applications in environmental, forensic and semiconductor sciences. We will introduce the concept of single cell-ICP-MS and discuss the challenges faced when analyzing cells suspensions with an in-depth focus on the necessary hardware and software requirements to quantify accurately the number of particles and/or metal content in individual unicellular organisms. Various applications to human and environmental health applications of this technique will be discussed.

Keywords: Single cell ICP-MS, single particle ICP-MS, bioaccumulation, nanoparticles, environment, cancer, semiconductor, forensic

Chady Stephan holds a Ph.D. in Analytical Chemistry from the Université de Montréal. He worked as a project manager for QSAR risk assessment services before joining PerkinElmer as an Inorganic Product Specialist supporting the various elemental analysis platforms. He then managed the development of various nanotechnology applications that focus on measurement techniques for nano-object characterization using various analytical platforms. He currently leads a multifunctional team composed of marketing, technical marketing, application scientist and strategists focusing on delivering complete market solutions. He is a thought leader in elemental analysis with over 20 peer-reviewed published papers and book chapters. Over the past few years, his main research activities at PerkinElmer have been in developing single-particle ICP-MS and more recently Single Cell ICP-MS.



SA-11 Speciation Analyses For Environmental, Forensic, Biomedical, and Industrial Applications. Olivier Donard, Sunday, January 12, 1 pm, MARSS-IPREM, CNRS UMR 5034 (LCABIE), University of Pau, Pau, France, olivier.donard@univ-pau.fr

Metal speciation is gaining increasing importance in a wide variety of fields, for example, clinical, environmental, nutritional, industrial, and geochemical applications. It is well understood now that the determination of the chemical form of metals is essential for the correct evaluation of their fate, impact, and "risk assessment" in all traditional compartments where inorganic analysis is involved. In the past 20 years considerable effort has been made by academic, regulation and industrial communities to identify, rationalize, and promote simple and effective analytical procedures that will improve our understanding of metal related issues in the environment, nutrition, hygiene and industry. The aim of this course is to detail the status of metal speciation analysis and will consist of the following topics: a. Overview of traditional and classical aspects of sampling, extraction and detection of analyte species. b. Current status of metal species determination strategies (elemental speciation). c. Identification of the areas of growing demand. d. Review, examination and critically assess major developments in sample collection, preservation, preparation, analyte detection and validation. e. Description of analytical speciation procedures using examples from environment, nutrition and industrial applications.

Keywords: Sampling, metal speciation, detection, applications, environment, nutrition, industry

Olivier F.X. Donard is a Research Director at the French CNRS, He is the head of the "Mass Spectrometry Center for Reactivity and Speciation Sciences" and is the codirector of a commercial enterprise (Ultra Traces Analyses Aquitaine - UT2A) dedicated to speciation analysis. He has developed analytical strategies and promoted speciation related issues for a large variety of international environmental organizations (USA EPA, Dutch Ministry of Water and Environment, and French Fisheries IFREMER). He has pioneered several approaches for sample preparation, derivatization, and detection using atomic absorption, atomic fluorescence, ICP-AES and mass spectrometries that facilitate routine "elemental speciation" and is now developing similar approach in isotopic analysis both applied for fundamental research of commercial analytical applications. He is the author of more than 290 international publications in analytical and environmental chemistry He has delivered over 130 plenary and invited lectures at international meetings and more than 500 poster and oral presentations on the topic of atomic spectrometry, speciation and now isotopic signatures applied to a large array of applications. He has an h factor of 50 (ISI Web Sciences). He is the cofounder and an executive member of the "European Virtual Institute of Speciation Analysis - EVISA". He collaborates with instrument and sample preparation manufacturers in order to improve instrument performance and preserve the integrity of the species of interest.

SA-12 Chemical Imaging by Plasma Spectrochemistry, Saturday, January 11, 7 pm, Davide Bleiner, Empa, Überlandstrasse 129, CH 8600 Dübendorf, Switzerland, davide.bleiner@empa.ch

From geosciences to biomedical, to thin films or operando catalysis, the bulk information proves insufficient. Often the requirement to understand how a certain analyte, (e.g., metals, contaminants, functional groups, etc.) distribute across a sample is essential. The term "chemical imaging" thus emerged, adopted from other fields, e.g. Raman, and we will learn the correct terminology, e.g. to distinguish imaging, mapping, hyperspectral, etc. Building on a correct language we will address two main aspects: (i) the data acquisition process, as influenced by instrumentation and operating conditions; (ii) the data reduction and visualization, which has the character of big data problems.

Keywords: Imaging, hyperspectral, spot, laser, ablation, discharge, data, mapping, visualization, artifacts

Davide Bleiner is head of the Advanced Analytical Technologies division at the Swiss Federal Laboratories for Materials & Technology, aka Empa. He has been assistant professor at the University of Bern (2011-15) where he developed a

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plasma-driven X-ray laser, which allows nano-scale spot sizes. He had carried out postdoctoral research at the University of Antwerp (Belgium) focusing on the modeling of laser microanalysis. His PhD degree was earned at the ETH Zurich in 2002 working on short-wavelength laser ablation coupled to time-of-flight for fast transient signal acquisition of fluid inclusions. He teaches currently at the University of Zurich on advanced spectroscopy, laser ablation chemistry and chemometrics.



SA-13 Tracing Element Metabolism in Animals and Humans Using Stable Isotope Techniques, Monday, January 13, 7 pm, Thomas Walczyk, Department of Chemistry, National University of Singapore, Science Drive 4, Singapore 117543, walczyk@nus.edu.sg

Participants will be familiarized in this course with the basic principles and practicalities of tracing element uptake, utilization and excretion from the body in living organisms. This includes a basic introduction to human physiology, metabolism and bioavailability of the most relevant essential elements (iron, zinc, calcium, selenium), theoretical concepts of element tracing in living organisms based on isotope dilution principles, standard methods and protocols to study element metabolism in animals and humans, aspects to consider in the design of such studies, practicalities of sample collection and preparation as well as mass spectrometric analysis and, finally, principles and algorithms for translation of analytical data into physiological information. Participants with a background either in inorganic mass spectrometry or life sciences with an interest to conduct stable isotope studies in animals or humans are encouraged to attend. Expertise in isotope analysis and/or basic physiology is an advantage but not a prerequisite for attending the course

Keywords: Stable isotopes, element metabolism, biomedical research, human studies, animal studies, isotope dilution mass spectrometry

Thomas Walczyk is a chemist by training who earned his PhD degree in isotope sciences/isotope ratio mass spectrometry. For more than 20 years he has been exploring the potential of stable isotope techniques in biomedical research and contributed significantly to the shaping of the field and its recognition as a research domain in inorganic mass spectrometry. After more than a decade at the Laboratory of Human Nutrition at ETH Zurich, he joined the National University of Singapore as a faculty member in 2007, jointly appointed by the Department of Chemistry (Science) and the Department of Biochemistry (Medicine).

Spectrochemical Instrumentation

SI-01 Calibration, Optimization, and Interferences in Plasma Spectrochemical Analysis, Sunday, January 12, 8 am, José A.C. Broekaert, Department of Chemistry, University of Hamburg, Martin-Luther-King-Platz 6, D-20146 Hamburg, Germany, jose.broekaert@chemie.uni-hamburg.de, www.chemie.uni-hamburg.de/ac/broekaert

Calibration and statistical data evaluation in spectrochemical analysis are treated, including calibration with external standards, calibration by standard addition, and the use of internal standards. A discussion of detection/determination limits, signal-to-noise considerations, acquisition of the spectral background and the concept of traceability are covered. Methods for optimization (trial-and-error, Simplex) and chemometrics (data display, multivariate analysis and clustering) will be discussed as are strategies for high-precision analysis. Also topics like matrix induced signal enhancements and depressions are treated. Examples from ICP-AES/MS with solutions, slurry nebulization ICP-AES, ETV-ICP-AES/MS, microwave plasma and glow discharge AES as well as speciation will be given.

Keywords: Calibration, statistical data evaluation, figures of merit, detection limits, optimization, high-precision analysis, interferences, data treatment

José A.C. Broekaert received his Ph.D. in chemistry at University of Gent (Belgium) in 1976; he was an Alexander-von-Humboldt Research Fellow Germany (1977), and a scientist at ISAS - Leibnitz Institut für Analytische Wissenschaften, Dortmund, Germany from 1978 to 1991. He was Associate Professor of Analytical Chemistry at University of Dortmund

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(1991-1998), Professor of Analytical Chemistry at University of Leipzig (1998-2002) and subsequently at University of Hamburg (2002-2014), and he is Emeritus professor at University of Hamburg (since 2014). He was a Visiting Fulbright Research Fellow at Indiana University, Bloomington (1998), and is an Adjunct Professor of Chemistry at Indiana University (since 2004). He is a Fellow of the Society for Applied Spectroscopy (since 2008), and an Ordinary member of the European Academy of Sciences and Arts (since 2014). His research interests include analytical chemistry especially with atomic spectrometric methods.



SI-02 Quantifying Complex Nanoparticles: Direct Coupling of Field Flow Fractionation Inductively Coupled Plasma Mass Spectrometry, Saturday, January 11, 8 am, James F. Ranville, Colorado School of Mines, Department of Chemistry and Geochemistry, Golden, CO 80401, jranvill@mines.edu; Robert Reed, Postnova

This course will outline a novel set of hyphenated analytical methods: field-flow fractionation (FFF) – inductively coupled plasma mass spectrometry and single-particle ICP-MS (spICP-MS). The FFF-ICP-MS technique enables the measurement of the elemental composition across the size distribution of particulate and macromolecular samples. Particle-by-particle analysis of the FFF effluent by spICP-MS provides further particle characterization as well as providing number concentrations. Thus the hyphenation of these two approaches yields size-based element speciation data applicable to a wide range of samples and applications. The course will concentrate on the optimization of the FFF and spICP-MS methods and will illustrate the detailed information that can be derived from the combined instruments. The course will examine the choice of equipment and run conditions for a given sample and data analysis. Commercial instrumentation should be available for demonstration. Conventional on-line and off-line detectors will be compared, and ICP-MS with quadrupole and high-resolution instruments will be used to illustrate practical examples with biological, environmental, geological samples, polymers, engineered nanomaterials, and other sample types.

Keywords: FFF, ICP-MS, nanomaterials, water, soils, sediments, particle sizing, elemental speciation

SI-03 High-Resolution ICP-MS, Sunday, January 12, 7 pm, Norbert Jakubowski, BAM, Federal Institute for Materials Research (retired), 12498 Berlin, Germany, norbi.jakubowski@gmail.com

This course is an introduction to ICP-MS with a double focusing magnetic sector mass analyzer. It offers fundamental background, a thorough discussion of analytical features, and state of the art information on applications. Different types of double focusing instruments also are considered. Specific topics include fundamental aspects of ICP-MS (physical properties of a double focusing instrument, operational characteristics in comparison with quadrupole instruments); analytical characteristics (spectral and non-spectral interferences, figures of merit in low and high resolution modes, blanks and memory effects, HPLC and GC interfaces), and applications (industrial including ultra-pure reagents and alloys, environmental, geological, and biomedical materials).

Keywords: High-resolution ICP-MS, figures of merit, interfaces, applications, ultra-trace analysis

Norbert Jakubowski graduated as “Diplom-Physiker” from the University in Essen/Duisburg and obtained his doctorate (Dr. rer. nat.) in 1991 from the University of Stuttgart/Hohenheim. In 1981 he joined the Institute for Analytical Sciences (ISAS) in Dortmund to work as a research scientist in the laboratory for inorganic analysis. He became the head of the division 1.1 (Inorganic Trace Analysis) of the Federal Institute of Materials Research and Testing in Berlin in 1999, and he retired in 2018. His present activities are mainly focused on analytical chemistry with special interest in development of

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instruments, methods and problem-orientated procedures based on the use of plasma sources (inductively coupled plasma, glow discharge) for elemental mass spectrometry of solid and liquid samples. Key Topics of his research include speciation of P, Pt, Gd; metallomics; bioconjugation of antibodies for clinical assays; bio-imaging; analytical characterization of nanoparticles and their interaction with cells.

SI-04 Opportunities, Challenges, and Application of Glow Discharge Techniques, Sunday, January 12, 7 pm, Volker Hoffmann, Leibniz Institute for Solid State and Materials, Research Dresden, PO Box 27 00 16, D-01171 Dresden, Germany, v.hoffmann@ifw-dresden.de; Jorge Pisonero Castro, Department of Physics, Faculty of Science, University of Oviedo, Oviedo, Spain, pisonerojorge@univovi.es

This course is designed to review the application of GD-OES and -MS in modern material science. Advantages and disadvantages of the technique and different instruments will be discussed from practical point of view. Hard- and software (quantification) will be explained, and applications will be compared with other methods of direct solids elemental analysis. Analytical figures of merit for the two spectrometric methods will be presented. We offer all participants a discussion about their actual analytical problems. Finally, the session will be concluded with a discussion of future trends in instrumentation and applications, as e.g. imaging spectroscopy and ToF-MS.

Keywords: GD-OES, GD-MS, applications, solid-state analysis

Volker Hoffmann graduated as "Diplom-Physiker" from the Technical University in Dresden and obtained his doctorate (Dr. rer. nat.) in 1986. The same year he joined the Central Institute of Solid State Physics and Materials Research in Dresden (now Leibniz Institute of Solid State and Materials Research) to work as a research scientist in the laboratory for spectral analysis, where he became the head in 1996. His present activities are mainly focused on the research and development of glow discharge optical (GD-OES) and mass spectrometry (GD-MS), which are performed in cooperation with different companies and research groups in Europe and USA. In cooperation with LECO Germany and USA, a new radio frequency (rf) technology for the analysis of non-conductors by glow discharge spectroscopy was developed. In the field of GD-MS he worked in joint cooperation together with PTB Braunschweig and developed a new fast flow source principle, which after further development is now used in commercial GD-MS equipment. His present research includes pulsed discharges to improve thin layer analysis and plasma imaging. From 2006 to 2012 he was chairman of the European Working Group for Glow Discharge Spectroscopy, and he is secretary of the corresponding German workgroup.

Jorge Pisonero is an Associate Professor of Physics (since 2012) at University of Oviedo (Spain), from which he obtained his PhD degree (November 2004) working on glow discharge spectroscopy. After his PhD, he was awarded a two-year Marie Curie Intra-European Fellowship for a postdoctoral stay at ETH (Switzerland) to work on laser ablation-based techniques. Afterwards, Jorge obtained the prestigious "Ramon and Cajal" research contract and went back to University of Oviedo, where in collaboration with Dr Nerea Bordel established the Laser and Plasma Spectroscopy Research Group (www.unioviedo.es/gelp). His current research interests are focused on fundamentals and applications of atmospheric and low pressure GD spectroscopies, LIBS and LA-ICP-MS. Moreover, Jorge is co-author of more than 60 scientific articles and several book chapters.

SI-05 Time-of-Flight and Distance-of-Flight Mass Spectrometry for Atomic Analyses, Sunday, January 12, 8 am, Steven J. Ray, State University of New York at Buffalo, Department of Chemistry, Buffalo, NY 14260, sjray2@buffalo.edu; Alexander Gundlach-Graham, graham@inorg.chem.ethz.ch, Department of Chemistry and Applied Biosciences, ETH Zurich, Switzerland

This short course will provide an introduction to the fundamental aspects of both time-of-flight mass spectrometry (TOFMS) and distance-of-flight mass spectrometry (DOFMS) as they are used in atomic spectrometry. Underlying principles of instrument design and construction, specific equipment and techniques used in the experiments (including solid-state detectors for MS), topics in data analysis, and the recent applications from the literature will be reviewed.

Keywords: Inductively coupled plasma mass spectrometry; time-of-flight mass spectrometry; distance-of-flight mass spectrometry

Steven Ray is an assistant professor at SUNY-Buffalo. He was an associate scientist in the Department of Chemistry at Indiana University, where he received his PhD. He has over 15 years experience in the design, construction, and use of time-of-flight mass spectrometers, with a particular emphasis on their development for elemental ionization sources. Dr. Ray has coauthored over 40 papers, four book chapters, holds four patents, and has presented numerous papers at international conferences on elemental TOFMS.

SI-06 ICP-MS I: Introduction, Saturday, January 11, 1 pm, John Olesik, Ohio State University, School of Earth Sciences, 125 S. Oval Mall, 026 Mendenhall Labs, Columbus, OH 43210-1002, olesik.2@osu.edu

This course is intended mainly for the newcomer to ICP-MS. ICP characteristics as an ion source, ion extraction, operating principles of ion optics, ion focusing, quadrupole and sector mass analysis, and detectors will be described. The general analytical capabilities, applications survey, and an introduction to matrix effects will be presented.

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Keywords: ICP-MS characteristics, instrumentation, interferences, applications

SI-07 ICP-MS II: Advanced Topics, Sunday, January 12, 1 pm, John Olesik, Ohio State University, School of Earth Sciences, 125 S. Oval Mall, 026 Mendenhall Labs, Columbus, OH 43210-1002, olesik.2@osu.edu

This course is intended for those who complete Part I and for the experienced ICP-MS user. Detailed consideration will be given to basic cases of matrix effects, removal of polyatomic ion interferences (solvent removal, collisional dissociation, high resolution, and cool plasma), alternate mass analyzers, solid sampling, analysis of limited solution volumes, and combining ICP-MS with chromatography for speciation and removal of interferences.

Keywords: ICP-MS operation and measurement effects, interference corrections, sampling, chromatography

SI-08 Theory and Practical Use of Reaction Cells and Collision Cells for ICP-MS, Monday, January 13, 7 pm, John Olesik, Ohio State University, School of Earth Sciences 125 S. Oval Mall, 026 Mendenhall Labs, Columbus, OH 43210-1002, olesik.2@osu.edu

The design and operation of reaction cells and collision cells used for isobaric interference removal in ICP-MS will be discussed. The course begins with an introduction to the principals and kinetics of ion-molecule reactions and the operation of the rf devices (quadrupoles, hexapoles, octapoles, etc.). The various efficiencies of the ion chemistry (primarily ion reactivity, reactivity, production of the ions within the cell) will be evaluated, concluding that where high efficiency of the primary chemistry is obtained, reaction of the analyte ion with impurities and the formation of new interferences within the cell becomes important. Various means of suppressing these effects, including kinetic energy discrimination and band pass operation of the cell will be contrasted and compared, and effects related to the order of the multipole device will be considered. Examples of the application of reaction cell and collisions cell methods in the semiconductor, environmental, clinical, geochemical, and isotopic analysis will be presented.

Keywords: Collision cell, reaction cell, spectral interference, chemical resolution, pressurized multipole, chemistry, ion dynamics, ion-molecule chemistry, in-cell produced interferences, multipole operating point, energy discrimination

SI-09 Interferences in ICP Spectroscopy, Sunday, January 12, 1 pm, José Luis Todolí, Department of Analytical Chemistry, Nutrition and Food Sciences, University of Alicante, PO Box 99, 03080 Alicante, Spain, jose.todoli@ua.es
Matrix effects make difficult the use of ICP techniques for some particular applications. The first step to overcome them is to understand the mechanisms and the main sources of interferences. The present course deals with the detection of the origin of the ICP-OES and ICP-MS interferences. The discussions will be based on selected applications (clinical, organic, food analysis...). Advice to improve the accuracy of the determinations will be given.

Keywords: Matrix effects, liquid sample introduction system, inorganic acids, organic solvents, easily ionized elements, ICP-AES, ICP-MS, clinical analysis, fuel analysis, food analysis

SI-10 Identification and Correction of Interferences in Practical ICP-OES, Saturday, January 11, 7 pm, Deborah Bradshaw, Atomic Spectroscopy Consulting, PO Box 536307, Orlando, FL 32853-6307, bradshawdk@cs.com

The identification and correction of interferences for ICP-OES can be critical to obtain accurate data in the analytical laboratory. The interferences and their corrective techniques that will be addressed include sample transport, sample matrix, and spectral. Procedures used to correct for transport and matrix interferences include the use of appropriate internal standards, matrix matching, optimizing plasma conditions, using buffer solutions, and the correct choice of sample introduction systems. Spectral interference correction approaches include optimizing the method parameters as well as choosing the appropriate correction technique such as interelement corrections and multiple linear regression techniques. Some of these may be limited to the specific instrumental hardware and software available to the analyst. The merits and disadvantages of the various correction approaches that are used will be examined, with practical examples of the use of these corrections to obtain accurate data.

Keywords: Transport interferences, matrix interferences, spectral interferences, interelement correction, multiple linear regressions, inductively coupled plasma atomic emission

SI-11 Identification and Correction of Interferences in Practical ICP-MS, Sunday, January 12, 7 pm, Deborah Bradshaw, Atomic Spectroscopy Consulting, PO Box 536307, Orlando, FL 32853-6307, bradshawdk@cs.com

The identification and correction of interferences for ICP-MS can be critical to obtain accurate data in the analytical laboratory. The interferences and their corrective techniques that will be addressed include sample transport, sample matrix, and spectral. Procedures used to correct for transport and matrix interferences include the use of appropriate internal standards, matrix matching, optimizing plasma conditions, and the correct choice of sample introduction systems. Spectral interference correction approaches include optimizing the method parameters as well as choosing the appropriate correction equations. The merits and disadvantages of the various correction approaches that are used will be examined, with practical examples of the use of these corrections to obtain accurate data.

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Keywords: Transport interferences, matrix interferences, spectral interferences, correction equations, inductively coupled plasma mass spectrometry

SI-12 Direct Analysis with Ambient Mass Spectrometry: Chemical Analysis of Things as They Are, Sunday, January 12, 8 am, Jacob Shelley and Brian T. Molnar, Rensselaer Polytechnic Institute, Department of Chemistry and Chemical Biology, 228 Cogwell Laboratory, 110 8th St., Troy, NY 12180, shellj@rpi.edu

The ultimate goal of analytical chemistry is to provide, what G.E.F. Lundell described as, “the chemical analysis of things as they are” such that a comprehensive assessment of sample constituents is directly obtained in a way that is nondestructive, while the sample is interrogated in its native environment. Recent efforts in mass spectrometry ionization source development have demonstrated these attributes to be possible. In such ambient mass spectrometry experiments, the source desorbs molecules from a surface, softly ionizes them, and transfers these ions into a mass spectrometer. This course will cover fundamental principles of desorption/ionization processes, as well as applications of these ionization sources. In this course a particular emphasis will be placed on plasma-based systems.

Keywords: Direct Analysis, molecular mass spectrometry, DART, glow discharge, ambient ionization

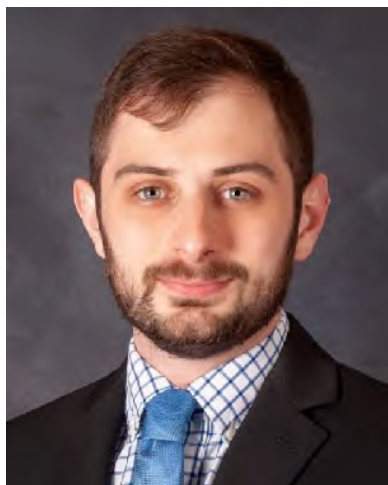
Jacob Shelley was born in Albuquerque, NM in 1984. He earned his B.S. in Chemistry from Northern Arizona University in Flagstaff, AZ in 2005. His research at NAU, while working under Prof. Diane Stearns, was focused on examining metal-DNA adducts with ICP-AES. He worked at Los Alamos National Laboratory for four summers on a wide range of projects including metallomics with X-ray fluorescence detection, developing nanoporous silica substrates for matrix-free MALDI, and method development for detecting various of radioactive materials. He completed his Ph.D. under Prof. Gary Hieftje in 2011 at Indiana University where his research focus was on the development, characterization, and application of novel plasma ionization sources for ambient, molecular mass spectrometry. Jake started his postdoctoral research in 2011 with Prof. R. Graham Cooks at Purdue University where he developed portable mass spectrometers capable of *in situ* analyses. In 2012 Jake was awarded an Alexander von Humboldt Post-Doctoral Fellowship to work with Dr. Carsten Engelhard at the University of Münster in Germany. In 2014 Jake became an Assistant Professor at Kent State University specializing in fundamental characterization of plasma-based ionization methods for mass spectrometry. In August 2016 Jake became the Alan Paul Schulz Career Development Chair at Rensselaer Polytechnic Institute in Troy, NY. In 2017 Shelley was presented the Bunsen-Kirchoff Award by the German Working Group for Analytical Spectroscopy in the German Chemical Society. Recently, Shelley was named to the Analytical Scientists Top 40 Under 40 Power List. His current research interests lie in the development of new hardware and software tools for mass spectrometry, which enable rapid and sensitive detection and identification of analytes in complex matrices. Thus far, he has authored 36 published journal articles, five United States patents/patent applications, a book chapter, and has given more than 40 invited presentations at national and international venues.



Brian T. Molnar was born and raised in Greenville, South Carolina. Brian began his studies in Chemistry at The Citadel: The Military College of South Carolina, where he studied photocatalytic decomposition of amino acids in Martian soil simulants and used inductively coupled plasma optical emission spectroscopy to study the concentration of toxic metals in fish from the Ashley River in Charleston, SC. He graduated with a B.S. in Chemistry in the spring of 2016. Brian joined the graduate program at Rensselaer Polytechnic Institute in the summer of 2016. Brian worked with Professor K.V. Lakshmi and collaborators to use density functional theory to model a newly synthesized compound and predict its absorption spectrum. In the spring of 2017, Brian joined the lab of Professor Jacob Shelley where, he began working on fundamental

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studies of the flowing atmospheric-pressure afterglow (FAPA) ionization source. Brian is presently continuing to study the fundamental chemistry associated with FAPA, but is also using advanced tools such as computational fluid dynamics and fluid flow visualization to improve the sensitivity and reproducibility of FAPA-MS analyses.



SI-13 Atmospheric-Pressure Glow Discharge and Liquid-Based Plasmas for Spectrochemical Analysis, Saturday, January 11, 1 pm, Steven J. Ray, and Andrew Schwartz, State University of New York at Buffalo, Department of Chemistry, Buffalo, NY 14260, sjray2@buffalo.edu

Atmospheric-pressure glow discharges have come to the attention of the spectrochemistry community due to both their versatility and simplicity. These inexpensive plasmas are useful for analysis of a wide variety of samples (gases, liquids, and solids) by both optical emission and mass spectrometry. This course will review topics in atmospheric-pressure glow discharges as used for spectrochemical analysis, and focus specifically on the use of liquid-electrode or liquid-sampling plasma systems. Recent advances and future outlook of these liquid-based glow discharges will be discussed. Performance compared to established methods (such as ICP-AES/MS) will be critically evaluated.

Keywords: Atmospheric pressure glow discharges, field-portable instrumentation, microdischarges, and novel instrumentation, spectrochemical analysis

SI-14 New Calibration Strategies in Spectrochemical Analysis, Sunday, January 12, 1 pm, George L. Donati, Wake Forest University, Department of Chemistry, Salem Hall, Box 7486, Winston-Salem, NC 27109, donatigl@wfu.edu
Calibration is a crucial component of quantitative spectrochemical analysis. In recent years, several alternative calibration methods have been proposed to improve precision, accuracy and sample throughput. Five of these new strategies will be discussed in this short course: standard dilution analysis (SDA), multi-energy calibration (MEC), interference standards (IFS), multi-isotope calibration (MICal), and multispecies calibration (MSC). The theoretical basis of each method, as well as their application in atomic absorption, atomic emission and mass spectrometry will be discussed. There will also be opportunity for hands-on data processing using MS Excel and ICP OES, ICP-MS, MIP OES and HR-CS FAAS experimental results. Please b-ring your computer with MS Excel installed.

Keywords: Accuracy; sample throughput; external standard calibration; standard additions; standard dilution analysis; multi-energy calibration; interference standard; multi-isotope calibration; multispecies calibration; non-traditional calibration methods

George L. Donati received his M.Sc. in Analytical Chemistry from the Federal University of São Carlos (UFSCar, Brazil, 2004), and his Ph.D. in Analytical Chemistry from Wake Forest University (WFU, 2010). During his postdoctoral fellowship at UFSCar, George collaborated with Prof. Joaquim Nóbrega to develop the first concepts of the interference standard method (IFS). George is an Associate Research Professor at the Department of Chemistry of Wake Forest University, in Winston-Salem, NC, where he developed the methods of multi-energy calibration (MEC), multi-isotope calibration (MICal) and multispecies calibration (MSC), and contributed to the development of Prof. Bradley Jones's standard dilution analysis method (SDA). His research interests include portable instrumentation and novel methods for spectrochemical analysis, as well as the use of atomic spectrometry and advanced statistical tools to diagnose and understand diseases. George is a member of the editorial board of the *Microchemical Journal*, and has published more than 70 peer-review papers and three book chapters on several topics associated with spectrochemical and trace element analysis.

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SI-15 Flow Injection Analysis for Increased Productivity with ICP Spectrometry, Diane Beauchemin, Sunday, January 12, 7 pm, Queen's University, Department of Chemistry, 90 Bader Lane, Kingston, ON K7L 3N6, Canada, diane.beauchemin@queensu.ca

Reproducibly injecting small sample volumes into a continuous flow of carrier allows more samples to be analyzed in a given amount of time. It also reduces solid deposition on cones and lenses in ICPMS, thereby decreasing downtime for instrument maintenance. Furthermore, continuous rinsing by the carrier effectively minimizes memory effects. Moreover, under suitable conditions, all these benefits are achieved while preserving sensitivity. For additional benefits, air-sandwiching the sample plug can be carried out, which improves sensitivity and detection limit two-fold while reducing peak width, thereby further increasing sample throughput. The optimization of such flow injection systems will be discussed.

Keywords: Flow injection analysis, monosegmented flow analysis, increased sample throughput, reduced memory effect, preserved or improved sensitivity and detection limit



Sample Introduction Approaches

SS-01 A Practical Guide to Nebulizers and the Part They Play in Modern Sample Introduction, Saturday, January 11, 1 pm, Gerhard Meyer, Promerus LLC, 9921 Brecksville Rd., Breckville, OH 44141, gary.meyer@promerus.com
This course will give participants an overview of the popular methods for introducing liquid samples used by today's instruments. A wide variety of nebulizers will be presented along with a discussion of how they work, which ones to use for particular matrices, and how to properly care for them. Along the way we will also feature ideas for best connecting pump tubing of a wide variety of sizes to these various devices. Once a firm understanding of nebulizers and their operation is established, the course will continue with a detailed discussion of sample matrices, properties of aerosols and segregation chambers that are important for good spectrochemical analysis, how matrices affect nebulizer performance

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and what can be learned about these matrices from the spectroscopic results. Since nebulization implies working with aerosols, participants will be provided a window into novel sample collection techniques that use nebulizers as part of the whole sample introduction scheme. Engaging discussions among the participants will be encouraged, so that everyone can share their experiences and come away with new and practical information with which to return to the lab.

Keywords: Nebulizers, spray chambers, desolvation, aerosol diagnostics, process monitoring, transport efficiency

Gerhard Meyer is Chief Analyst at Promerus LLC, a subsidiary of Sumitomo Bakelite North America located in Brecksville, Ohio, where he performs determinations of trace levels of impurities in high purity organic electronic materials using ICPOES and ICPMS, as well as works in the area of thermal analysis and tensile testing. He received his PhD at the University of Massachusetts – Amherst, and has worked at Dow Chemical Company, Battelle Memorial Institute, Thermo Jarrell Ash, Ametek/EDAX, and The Ohio State University. His outside research interests include the application of spectroscopic techniques to workplace air quality and hot fume emissions monitoring, and the design and manufacture of aerosol particle extraction instruments.

SS-02 Laser Ablation Mass Spectrometry I, Friday, January 10 1 pm, Bodo Hattendorf and Detlef Günther, Department of Chemistry and Applied Biosciences, ETH Zurich, Vladimir-Prelog-Weg 1 8093 Zurich, Switzerland, bodo@inorg.chem.ethz.ch, guenther@inorg.chem.ethz.ch

The course is designed to give participants an introduction to the analytical capabilities of laser ablation - inductively coupled plasma spectrometry and should be of particular benefit to spectroscopists interested in developing a laser ablation facility. LA-ICP-MS has become one of the most common solid sampling technique for major, minor and trace element analysis. The course will explain how LA-ICP-MS works. Details about basics in lasers and ICP-MS instrumentation and their combination will be explained. Examples for transient data acquisition, method development, and a large number of applications will be discussed to give a feel for the quantification capabilities of this analytical technique. Topics also will include terms and terminology, laser selection, ablation cell design and interfacing, ablation processes, transport phenomena, and measurement systems. Participants do not need previous knowledge about this technique.

Keywords: Lasers, ablation, aerosol transport systems, carrier gas, calibration, atomization and ionization, ICP-MS, interface, applications

SS-03 Laser Ablation Mass Spectrometry II, Friday, January 10, 7 pm, Detlef Günther and Bodo Hattendorf, Laboratory of Inorganic Chemistry, Department of Chemistry and Applied Biosciences, ETH Zurich, Vladimir-Prelog-Weg 1 8093 Zurich, Switzerland, guenther@inorg.chem.ethz.ch, bodo@inorg.chem.ethz.ch

The course will provide detailed knowledge about recent instrumentation and method developments in LA-ICP-MS. Various problems in laser sample interaction, aerosol transport, and atomization and ionization will be discussed. Elemental fractionation, its source, and various strategies to overcome this problem for different laser and ICP-MS systems will be extensively discussed. Furthermore, different quantification strategies and non-matrix matched calibration examples will be given. A few non-routine applications will also be discussed. Participants should have some knowledge or practical experience with LA-ICP-MS or should have taken the basic LA-ICP-MS course (SS-02).

Keywords: Laser-sample interaction, elemental fractionation, aerosol size and aerosol transport, atomization and excitation, ICP-MS, interface and ICP-optimization

Detlef Günther was born in Köthen, Germany in 1963. He obtained his Diploma degree in Chemistry in 1987 and a Ph.D. degree in Analytical Chemistry from the Martin-Luther-University Halle-Wittenberg under supervision of L. Moenke - Blankenburg in 1990. After carrying out postdoctoral work in the Institute of Plant Biochemistry Halle where he worked on the development of analytical methods to characterize heavy metal-binding proteins using HPLC-ICP-MS, he joined the group of H.P. Longerich at the Memorial University of Newfoundland, Canada. From 1995 until 1998 he was in the group of C.A. Heinrich at the Institute of Isotope Geology and Mineral Resources at ETH Zürich. In 1998 he was appointed Assistant Professor in the Laboratory of Inorganic Chemistry at the ETH Zürich. He was promoted to Associate Professor for Trace Element and Micro Analysis in 2003 and became Full Professor in 2008. From 2010 until 2012 he was Chair of the Department of Chemistry and Applied Biosciences at ETH Zurich and since 2015 he is Vice President for Research and Corporate Relations at ETH Zurich. He is recipient of the Ruzicka Award (2002), the European Award for Plasma Spectrochemistry (2003), the Fresenius Award (2007), and the Lester Strock Award (2007), and he received in 2013 the "Einstein Visiting Fellowship" to Humboldt University Berlin (Germany) and the "Thousand Talent Fellowship" (Wuhan University, China). In 2014 he became a member of the German National Academy of Science Leopoldina. His research program focuses on fundamental and applied studies in inductively coupled plasma-mass spectrometry (ICP-MS) and laser ablation-inductively coupled plasma-mass spectrometry (LA-ICP-MS), including studies on laser- sample interaction, aerosol transport, and plasma-related excitation processes. As well particle plasma interaction and particle vaporization for single nanoparticle analysis have been studied. Fundamental processes of UV-nns and UV-fs laser ablation used with Q-ICP-MS, SF-ICP-MS, TOF-ICP-MS, and MC-ICP-MS as well as alternative excitation sources, such as glow discharge

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are currently under investigation. The improvements in trace element and microanalysis and isotope ratio determinations have been demonstrated on a wide variety of applications (e.g., quantification of fluid inclusions, gemstones, metals, minerals, ceramic, and various nano materials).

SS-04 Latest Advances in Laser Ablation-Based Chemical Analysis and Emerging Applications: LIBS, LA-ICP-OES/MS, and Tandem LA – LIBS, Monday, January 13, 7 pm, Jhanis Gonzalez, Applied Spectra, Inc., 46661 Fremont Blvd, Fremont, CA 94538, jhanis@appliedspectra.com, jjgonzalez@lbl.gov; Rick Russo, Lawrence Berkeley National Laboratory, 1 Cyclotron Rd, Berkeley, CA 94720, rerusso@lbl.gov

Laser ablation has advanced over the last 50 years to become a successful technology for numerous chemical analysis applications. Breakthroughs in understanding the science of the ablation process and development of improved laser and detector components have led to reliable analytical measurement performance. The course will summarize key underlying mechanisms of the ablation process that are critical for accurate and precise measurements using LIBS and ICP-MS. This course will cover state of art system and performance, example applications and directions for future capabilities.

Keywords: Laser ablation, ICP-MS, LIBS, chemical analysis, elemental isotopic and molecular analysis, nano-analysis, imaging

Jhanis José González Chacon is director of Applications Lab Operations, Applied Spectra, Inc, Fremont, CA, and project scientist at Lawrence Berkeley National Lab, Berkeley, CA. He received a BS and PhD in chemistry from Central University of Venezuela, and he joined the Laser Spectroscopy and Applied Materials Group at Lawrence Berkeley National Laboratory, under the supervision of Dr. Richard E. Russo. He was a postdoctoral fellow from 2004 to 2007. His research is focused on fundamental mechanisms of laser-material interaction, including laser energy coupling to solid samples, laser induced plasma properties, particle formation and transport, and developing new applications for laser technologies, in particular laser induced breakdown spectroscopy (LIBS) and laser ablation inductively coupled plasma mass spectroscopy (LA-ICP-MS).

Richard E. Russo is founder and scientific director of the laser material interactions group at the Lawrence Berkeley National Laboratory (LBNL). His group has pioneered the development of laser ablation for chemical analysis, with an almost 30 year contribution to fundamental and applied research topics. Programs in this group are closely integrated to DOE basic science, industrial technologies and nonproliferation activities. His research has led to breakthroughs in laser ablation understanding and development. Dr. Russo has an international scientific reputation in chemistry and physics related to nanosecond and femtosecond laser-material-interactions (laser ablation), is co-inventor of the nanowire laser, and developer of a real-time standoff laser ultrasonic sensor (R&D100 2006). He also is co-inventor of a process for ion nano-texturing (ITEX) thin-films, lead-inventor of the ion-assisted pulsed laser deposition (IBAD) process, and a pioneer in elucidating fundamental laser heating and laser ablation processes for chemical analysis. The group achieved 450 nm spatial resolution and a detection limit of 220 ag using a single laser pulse for LIBS (laser induced breakdown spectroscopy) measurements. By pioneering near-field scanning optical microscopy (NSOM) with laser ablation, the group achieved 30-nm diameter sampling and analysis. Finally, the group demonstrated and patented the use of laser plasmas (LIBS) for real-time measurement of isotopes. Russo has over 220 scientific publications; 45 refereed proceedings; 250 (115 Invited) presentations, nine book chapters, and nine patents. Fourteen students have received their PhD degree under his direction at the University of California, Berkeley.

Dr. Russo is president and founder of Applied Spectra, Inc. (ASI). The company is the world leader in laser ablation based chemical analysis using LIBS and laser ablation with ICP-OES and ICP-MS. The ASI staff members are experts in utilizing laser ablation for solving the most challenging chemical analysis problems. Applied Spectra's LIBS and laser ablation instruments offer superior performance in commercial, military, and security markets. These LIBS and LA-ICP-MS systems provide significant cost benefits to traditional chemical analysis, delivering real time elemental and isotopic analysis with excellent spatial and depth resolution, and without sample digestion. The ASI bench top RT100 LIBS system is successfully deployed in energy, environmental, health, industrial and security markets. The company continues to drive laser ablation capabilities and instrumentation based on strong in-house research, and instrumentation and applications (methods) development.

SS-05 Application of a Microdroplet Generator in Plasma Spectrochemistry, Jutta Tentschert, Saturday, January 11, 8 am, German Federal Institute for Risk Assessment (BfR), Department of Chemical and Product Safety (BfR), 10589 Berlin, Germany, jutta.tentschert@bfr.bund.de; Daniel Rosenkranz, BAM Federal Institute for Materials Research and Testing, Unter den Eichen 87, 12205 Berlin, Germany, daniel.rosenkranz@bfr.bund.de

SS-06 Microplasma for Chemical Analysis. Sunday, January 12, 7 pm, Vassili Karanassios, University of Waterloo, Department of Chemistry and Waterloo Institute for Nanotechnology, Waterloo, ON N2L 3G1, Canada, vkaranassios@uwaterloo.ca

Microplasmas have been arbitrarily defined as those with one "critical" dimension (e.g., depth, height, radius) in the μm or

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sub-mm regime [1]. In this short course, microplasmas for optical emission and mass spectrometry described in the literature will be reviewed. Battery-operated microplasmas fabricated *on-chips* using a variety of technologies (ranging from clean room-based and micro-machining to 3D-printing) will be emphasized. Analytical performance characteristics will be discussed and selected applications will be highlighted.

[1] V. Karanassios, "Microfluidics and Nanofluidics: Science, fabrication technology (from cleanrooms to 3D printing) and their application to chemical analysis by battery operated microplasmas-on-chips." Invited, open-access book-chapter, Chapter 1, Pages 1-34, InTech Publishing, Aug. 22, 2018, DOI: 10.5772/intechopen.74426.

Keywords: Sample introduction; micro- and nano-samples; field sampling, applications

Vassili Karanassios is a Professor of Chemistry at the University of Waterloo (Ontario, Canada) and a co-founder of a degree-program in nano-technology engineering. Professor Karanassios received his Ph.D. from the University of Alberta (Edmonton, Canada) and was a Post Doctoral Fellow at McGill University (Montreal, Canada). In 2009 he held a Leverhulme award in the UK where he was a visiting Professor in Chemistry (Sheffield University), and an Overseas Fellow of Churchill college (Cambridge University, UK), and a visiting Professor of Engineering (Cambridge University, UK) in the Center for Advanced Photonics and Electronics (CAPE). Karanassios and his group were the first to operate microplasmas from a battery, and have published extensively in the areas of sample introduction for ICPs and on microplasmas.



SS-07 Laser-Induced Breakdown Spectroscopy (LIBS), Saturday, January 11, 7 pm, Vassilia Zorba, Laser Technologies Group, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, vzorba@lbl.gov

This course will cover the basic principles, mechanisms, and instrumentation of laser-induced breakdown spectroscopy (LIBS). Laser-induced breakdown spectroscopy (LIBS) has emerged as a unique analytical technique for the qualitative and quantitative analysis of a variety of solid materials. The minimal sample preparation requirements, high spatial resolution capabilities, rapid analysis time, simple instrumentation, and applicability to all media make LIBS especially appealing to industry. This course will introduce the fundamentals and instrumentation of LIBS and provide a brief review of current applications. The utility of LIBS for the analysis of solid materials will be covered, including its application to coating analysis, homogeneity determination, contaminant identification, and elemental quantitative analysis.

Keywords: LIBS, atomic spectroscopy, mechanisms, instrumentation, solid analysis

Plasma Spectrochemical Techniques

ST-01 On-the-Job and Soft Skills for Technology Developers (Things You Were Not Taught in School), Saturday, January 11, 8 am and 1 pm, Andrew T. Zander, Consultant, Gerson Lehrman Group, 1632 Hickory Ave, Torrance, CA 90503, atzander1027@gmail.com

In this full day course, topics that technologists need for success in their professional careers are covered. Among the topics to be covered that are neglected or never covered in formal education programs for chemists, physicists and engineers will be (not inclusive): Work Environment; Being Organized; Confidential Documents; Credentials; Project Management Basics; Budgets; Finances for Development; the Cost of RDT&E; Personnel Management Basics; Electronic Communications and Networking on the job; Innovation (and why it is problematic); Leadership in the technical domain. Adequate time for questions and discussion is incorporated into the course.

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The material in this course is geared toward finishing graduate students about to embark on corporate positions and new hires in industry. It is also beneficial for seasoned technology developers wishing to upgrade their soft skills or who have been recently promoted to leadership positions in technical departments.

Keywords: Professional training, personal development, soft skills, technology development, project management, leadership

Andy Zander is a successful technology developer and manager of engineering and scientific professionals. The majority of his product development experiences were in the analytical instrument domain, for a variety of industries ranging from semiconductor equipment; analytical, life sciences and biotechnology instrumentation, and drug discovery tools businesses. He has managerial and technical experience in Dept. of Defense RDT&E from a 30 year career with the U.S. Naval Reserve, 21 years of which were as a Scientific Liaison Officer for the Office of Naval Research.

Over the course of his 44-year career as an analytical chemist and RDT&E Director, Andy performed, managed, led or directed the development of instrumentation, subsystems and devices in a wide variety of technologies, including: X-ray technologies and components; atomic and molecular spectroscopy, spectrometry and spectrophotometry; Gas and Liquid chromatography; mass spectrometry; hyphenated instruments; field/ruggedized instruments; atomic force microscopy; and 3D Flash LIDAR

Andy has had published 29 peer-reviewed journal articles, 21 non-refereed publications (e.g., book chapters) and authored multiple manuals and training documents for project management. He has four patents. Andy is a technical consultant with the Gerson Lehrman Group.



ST-02 Isotopic Measurements Using ICP-MS, Monday, January 13, 7 pm, Frank Vanhaecke, Ghent University, Department of Analytical Chemistry, Campus Sterre, Krijgslaan 281 - S12, 9000 Ghent, Belgium, frank.vanhaecke@ugent.be, and Nancho Garcia Alonso, University of Oviedo, Oviedo, Spain, jiga@uniovi.es

In this short course, the measurement of both natural variation and induced changes in isotope ratios using ICP-MS will be discussed. We will discuss the use of enriched stable isotopes and isotope abundance measurements for total elemental analysis, speciation, traceability and metabolism studies. The theory of Isotope Dilution Mass Spectrometry applied to the different fields will be described in detail as IDMS is recognized by the Bureau International des Poids et Mesures (BIPM) as a potential primary measurement method, directly traceable to the International System of units. Trace element speciation is another field where enriched stable isotopes have been applied successfully as they can correct for degradation and interconversion reactions, which can occur during sample preparation or measurement. Another application field for enriched isotopes is in the traceability of manufactured goods and living organisms. We will describe a double-isotopic labeling technique, which can be applied for traceability purposes.

The sources of natural variation in the isotopic composition of the elements will be discussed. Specific attention will be devoted to elements with radiogenic nuclides (e.g., Sr, Pb) and to mass-dependent and mass-independent isotope fractionation. The importance of isotope ratio precision will be underlined and hints for optimization of the instrument settings and data acquisition parameters aiming at an optimum isotope ratio precision will be provided for single-collector and multi-collector ICP-MS. Correction for detector dead time (pulse counting detectors) and for instrumental mass discrimination, required to convert the raw measurement data into "true" isotope ratios, will be discussed. Examples of applications relying on the determination and quantification of natural isotope ratio variation will include provenance determination of raw materials used in the manufacturing of ancient artifacts, environmental applications, geo-/cosmochemical applications and the use of isotopic analysis for medical diagnosis.

Keywords: Isotope ratio, isotopic composition, isotope fractionation, radiogenic nuclide, MC-ICP-MS

J. Ignacio García Alonso obtained his PhD in analytical chemistry from the University of Oviedo, Spain in 1985 and subsequently became a postdoctoral fellow at the University of Plymouth, UK before returning to Oviedo in 1987. For five years he was a scientific officer of the European Commission, based in Karlsruhe, Germany, and in 1995 he returned to

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the University of Oviedo, where he is now Full Professor of Analytical Chemistry. He is head of the research group on Enriched Stable Isotopes. Prof. Garcia Alonso is founding member of the spin-off company ISC-Sciences (www.isc-science.com) devoted to the synthesis and commercialization of isotopically labeled compounds particularly for speciation and food analysis. He is co-author of the book *Isotope Dilution Mass Spectrometry* published by the Royal Society of Chemistry in the UK.

Frank Vanhaecke received a PhD from Ghent University (Belgium) in 1992. Currently, he is Senior Full Professor in Analytical Chemistry at Ghent University, where he leads the 'Atomic & Mass Spectrometry – A&MS' research group that is specialized in the determination, speciation and isotopic analysis of (trace) elements *via* ICP-mass spectrometry (ICP-MS). His group studies fundamentally oriented aspects of the technique and develops methods for solving challenging scientific problems in an interdisciplinary context. High-precision isotopic analysis using multi-collector ICP-MS is an important research line in his group. Methods for high-precision isotopic analysis are developed for applications in, among other, the fields of geo- and cosmochemistry, archaeometry, the environmental sciences, and medicine ("isotopic diagnosis"). Frank was co-editor of the book *Isotopic Analysis – Fundamentals and Applications using ICP-MS* published by Wiley-VCH.

ST-03 Isotope Dilution for Accurate, Precise and SI Traceable Measurements, Sunday, January 12, 8 am, Lu Yang, National Research Council Canada, 1200 Montreal Rd., Ottawa, ON, K1A 0R6, Canada, lu.yang@nrc-cnrc.gc.ca

This short course provides an overview of the fundamentals of isotope dilution technique and recent developments in this area. Single, double, triple and quadruple isotope dilution techniques will be discussed in detail. In addition, this short course provides metrological principles and rules in order to achieve accurate, precise and SI traceable measurements. Examples of the determination of trace metals and organometallic compounds in various sample matrices, such as drinking water, seawater, sediments and biological tissues using ICPMS will be provided. Excel file templates for the calculation of combined uncertainty of final result obtained by double and triple isotope dilution methods will be provided to the participants.

Keywords: Isotope dilution, accurate, precise, SI traceable measurements, trace metals, seawater, sediments and biological tissues

Lu Yang is a research officer at National Research Council of Canada (NRC, Ottawa, Canada), leading research in applications of inductively coupled plasma mass spectrometry (ICP-MS) and MC-ICP-MS. Her research focuses on the development of the most accurate, precise and SI traceable methodologies for the determination, speciation and isotopic analysis of trace elements using ICP-MS and MC-ICP-MS. She has published over 100 research papers. She is a member of the IUPAC Subcommittee on Stable Isotope Reference Material Assessment under the Inorganic Division, and the Commission on Isotopic Abundances and Atomic Weights. She is a NRC's representative at the Inorganic Analysis Working Group of CCQM (Consultative Committee for Amount of Substance) of the BIPM (International Bureau of Weights and Measures). She is an Editorial Board member of *JAAS* and *Spectroscopy*.



ST-04 Isotopic Analysis of Heavy Elements for Environmental, Forensic, Biomedical and Industrial Applications, Saturday, January 11, 7 pm, Olivier Donard, MARSS-IPREM, University of Pau, Pau, France, olivier.donard@univ-pau.fr

The development of ICP/MS with multicollection allows promoting the routine use of isotopic signatures as an addition of the current inorganic information that is the total metal content, and/or the speciation of the elements of interests. ICP MS sources are very useful and have allowed promoting the increasing use of isotopic information of elements in a wide range of applications. Initially promoted in the field of geochemistry, it is now gaining major applications in a whole array of applications dealing with our daily life: environment, life sciences, nuclear or clinical applications, and now in topics such as food authenticity or even in industrial uses. There is therefore a rapid need of raising the awareness of the potential use, increasing of simplification and rationalization of isotopic signatures to these new routine domains extending then the frontiers of atomic spectrometry. The course will include a. Overview of the fundamental of isotopic uses and information.

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b. Traditional and classical aspects of the full analytical chain from sampling, extraction and detection of isotopes of interested species. c. Main traditional analytical approaches for most commonly used isotopes: Sr, Pb, Hg, Cd, Cu,... d. Review, examination and critically assess major developments in sample collection, preservation, preparation, analyte detection and validation, and e. Identification of the areas of growing demand.

Keywords: ICP-MS, isotope analysis, source identification, forensic, biomedical, industrial applications

ST-05 Isotope Fractionation Correction Methods for Accurate Isotope Amount Ratio Measurements by MC-ICP-MS, Saturday, January 11, 8 am, Lu Yang, National Research Council Canada, 1200 Montreal Rd., Ottawa, ON, K1A 0R6, Canada, lu.yang@nrc-cnrc.gc.ca

This short course focuses on the latest developments related to isotopic fractionation/mass bias and its correction models for MC-ICP-MS. In addition to commonly believed mass-dependent fractionation (MDF) phenomenon, recognition and reporting of mass-independent fractionation (MIF) within MC-ICP-MS itself has proliferated in the last decade. MIF has a significant impact on the choice of these isotopic fractionation correction models, as the use of mass-dependent models to correct for instrumental bias for isotopes which display mass-independent fractionation would result in biased isotope amount ratios. Implication of MIF on several popular mass bias correction models, the core concepts and assumptions for each model, its pros and cons, and individual practical aspects for isotope amount ratio measurements will be discussed in detail. Graduate students, researchers and chemists from the subject areas of archaeology, provenance studies, medical science, nuclear and forensic sciences, geosciences, and environmental science will profit from this course

Keywords: Isotopic fractionation, mass bias, mass-dependent fractionation, mass-independent fractionation, standard-sample bracketing, double spike model, regression model, full gravimetric isotope mixture model

ST-06 Contamination Control for Elemental Analysis, Sunday, January 12, 1 pm, Brad McKelvey, Seastar Chemicals Inc., 10005 McDonald Park Rd., Sidney, BC V8L 5Y2, Canada, bmckelvey@seastarchemicals.com

Current instrumentation has the ability to determine many elements down to the ppt and ppq level. However, many analytical techniques for trace element determinations are limited by the blank. The focus of this course will be contamination control and strategies to determine and eliminate contamination sources. This course will discuss contamination sources from the environment, labware, reagents, sample handling and sample introduction systems. Participants will be encouraged to discuss their contamination problems and experiences.

Keywords: Contamination control, trace element analysis, blanks

Brad McKelvey is Senior Research Scientist at Seastar Chemicals Inc. Seastar Chemicals is a global supplier of high purity reagents for trace element analysis. Dr. McKelvey has over 20 years experience in ICP-MS analysis, sample preparation, and contamination control for ultra-trace elemental analysis.

ST-07 Launching or Modifying Your Laboratory for Trace Analyses, Saturday, January 11, 1 pm, Ela Bakowska, Elba Elemental Consulting, PO Box 1050, Corning, NY 14830, ela@bakowska.com, bakowska@corning.com

Reducing and eliminating sources of elemental contamination and by optimizing the laboratory layout achieve the improvements of trace or ultra-trace capabilities. The contamination of a sample may occur during collection, storage, preparation and analysis. Specific examples of appropriate reagents and lab supplies will be listed. Cost saving alternatives for lab design and operation will be presented. Sample preparations considerations for different applications (semiconductor, environmental, clinical) will be discussed. Sources of specific elemental contaminations and ways of eliminating or minimizing them will be discussed. Guidelines for procurement of a new ICP-MS will be shared with the participants. The course would benefit scientists and managers adapting their current laboratory (renovating or remodeling) or designing a new laboratory to optimize the performance of new or existing ICP-MS instrumentation.

Keywords: Laboratory design/upgrade, contamination sources, contamination prevention, supplies, pharmaceutical, sample preparation, automation

Ela Bakowska is Research Associate at Corning Research and Development Corporation and Technical Director at Elba Elemental Consulting and has more than 30 years of experience in ICP-MS. Ela holds an M.S. in Physical Chemistry from the Warsaw University (Poland) and Ph.D. in Analytical Chemistry from the University of Massachusetts, Amherst. During her career Ela established the first application ICP-MS lab at HP and expanded and modernized several other labs. For eight years she was an application chemist for HP/Agilent, and in this role she assisted multiple new users in modernizing and upgrading their labs. Since 2001 (being again a user), she purchased multiple ICP-MS systems from various vendors. Ela's experience includes development of methods for preparation and analysis of various types of glass, ceramics, raw materials, plastics, semiconductor, clinical, forensic, environmental, nuclear, and pharmaceutical samples. Ela is continuously upgrading and automating her seven labs, especially sample preparation areas dedicated to ultra-trace levels testing.



ST-08 IUPAC Commission on Isotopic Abundances and Atomic Weights (CIAAW): Tables of Isotopic Composition of the Elements and Standard Atomic Weights and Their Relevance for the Plasma Spectrochemist.

Johanna Irrgeher, Sunday, January 12, 8 am, Montanuniversität Leoben, Department of General, Analytical and Physical Chemistry, Chair of General and Analytical Chemistry, Isotope Research Group; Franz Josef-Strasse 18, 8700 Leoben, Austria, johanna.irrgeher@boku.ac.at, johanna.irrgeher@unileoben.ac.at

This short course gives an introduction to the Commission, its key tasks and functions as well as current projects relevant to the mass spectrometric community. Practical considerations for the plasma spectrochemist are provided concerning (1) the appropriate/inappropriate use of the CIAAW publications and the tabulated atomic-weight and isotope-abundance values; (2) the importance of correct and transparent extraction and application of these values and recommendations and in analytical chemistry; (3) isotope-abundance measurements and certified reference materials, and (4) the importance of measurement uncertainty along with a guide on how to calculate and extract uncertainties from tabulated values. Recommendations will be discussed interactively on examples taken from daily lab routine. This short course is relevant to all users of standard atomic-weight and isotopic-abundance values, spanning from undergraduate students to experienced plasma spectrochemists. Insights into how tabulated values and their uncertainties are generated within the Commission are explained along with guidelines on how to extract values and associated uncertainties for different analytical questions and calculations. Colleagues from academia and industries as well as instrument manufacturers are welcome.

Keywords: CIAAW, IUPAC, isotopic abundances, atomic weight, uncertainty, isotope ratio measurements

Johanna Irrgeher has held a position as head of the Isotope Research Group at the Montanuniversität Leoben since January 2019. She graduated from the University of Natural Resources and Life Sciences (BOKU), Vienna with honors in 2013. Amongst others, she was visiting researcher at the NRC Canada, the National Cheng Kung University Tainan, the University of Calgary, and the University of Alaska, Fairbanks. From 2015 to 2018, she was post-doctoral fellow at the Helmholtz Centre in Geesthacht, Germany. Johanna is a lecturer at BOKU and in 2018 she was appointed adjunct professor at the University of Calgary. Currently, she is chair of the Subcommittee on Isotopic Abundance Measurement of the IUPAC Commission on Isotopic Abundances and Atomic Weights (CIAAW). Her current research interests are dedicated to analytical mass spectrometry and the application of isotope tools in medical, environmental and material sciences including the implementation of fundamental metrological methods. Among other awards, she received the Agilent Rising Star Award at the EWPCS 2017.

ST-09 Microwave-Assisted Sample Preparation for Trace Elemental Analysis: Think Blank and Go Green, Sunday, January 12, 8 am, Joaquim A. Nóbrega, Federal University of São Carlos, Department of Chemistry, São Carlos, SP, Brazil, djan@terra.com.br

This short course presents both the theory and selected applications for sample preparation featuring microwave-assisted digestion for trace elemental analysis. Specific sample preparation approaches for AAS, ICP-MS and ICP OES including microwave power, reagent temperature, pressure, matrices, chemical compatibility, and practical standard methods will be discussed. Trace analysis will be discussed considering analytical blanks and contamination control. Effects caused by reagent and materials impurities, laboratory environment, and analytical procedures will be stressed. Procedures for purifying acids and cleaning vessels will be discussed. Benefits resulting from closed vessels digestion and special procedures, such as digestions using dilute nitric acid solutions with emphasis on green procedures using minimum amount of reagents and generating minimum amount of residues will be presented. Role of oxygen gas on chemical

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oxidative reactions also will be discussed. Applications for different types of samples, such as biological and botanical tissues, medicines and foods, will be highlighted. Special applications based on digestions in closed vessels will be discussed with emphasis on new United States Pharmacopeia 232 and 233 regulations.

Keywords: Microwave-assisted digestion, analytical blank, green procedures, dilute nitric acid, reagent purification, reagent recovery

Joaquim A. Nóbrega received his Ph.D. from the State University of Campinas (1992) and completed his postdoctoral training with Ramon Barnes (University of Massachusetts, Amherst, MA, 1996) and with Bradley Jones (Wake Forest University, Winston-Salem, NC, 2003). He is Professor in the Department of Chemistry at the Federal University of São Carlos (São Carlos, São Paulo State, Brazil) and Visiting Professor in the Faculty of Pharmacy at the University of Concepción (Concepción, Chile). His research interests are sample preparation for inorganic analysis, atomic absorption spectrometry, atomic emission spectrometry, and inductively coupled plasma mass spectrometry. He co-authored a chapter in 2011 on "Microwave-Assisted Sample Preparation for Spectrochemistry" published in the online *Encyclopedia of Analytical Chemistry*. He is a member of the Brazilian Society of Chemistry, Brazilian Society for the Advancement of Science, American Chemical Society, Society for Applied Spectroscopy, International Union of Pure and Applied Chemistry, and fellow member of the Royal Society of Chemistry.



ST-10 Plasma Diagnostics: Fundamentals, Measurements, and Applications, Sunday, January 13, 7 pm, Igor B. Gornushkin, BAM, Federal Institute for Materials Research and Testing, Berlin, Germany, igor.gornushkin@bam.de This course will provide an introduction to plasma diagnostic techniques. The major focus of the course will be on the discussions of the practical procedures as well as the underlying physical principles for the measurements of plasma fundamental characteristics (e.g., temperatures, thermodynamic properties, and electron number density). Particular emphasis will be placed on inductively coupled plasma–atomic emission spectrometry, but other analytical plasmas will also be used as examples when appropriate. Selected examples on how one can manipulate the operating conditions of the plasma source, based on the results of plasma diagnostic measurements, to improve its performance used for spectrochemical analysis will also be covered. Topics to be covered include thermal equilibrium, line profiles, temperatures, electron densities, excitation processes, microreactions, pump and probe diagnostics, tomography, temporal and spatial resolution. Basis of plasma computer modeling will be presented.

Keywords: Thermal equilibrium, plasma processes, electron number density, temperatures, emission line profiles, spatial information, plasma modeling

Igor B. Gornushkin is a physicist and analytical chemist with major expertise in fundamental and applied spectroscopy including LIBS, emission, absorption, fluorescence and Raman. He received his PhD from the University of Florida in 1998 and at present works at BAM Federal Institute of Material Research, Berlin (Germany). He develops spectroscopic methods for environmental, industrial, and laboratory applications, and he has strong background in physics, optics, and computer modeling.

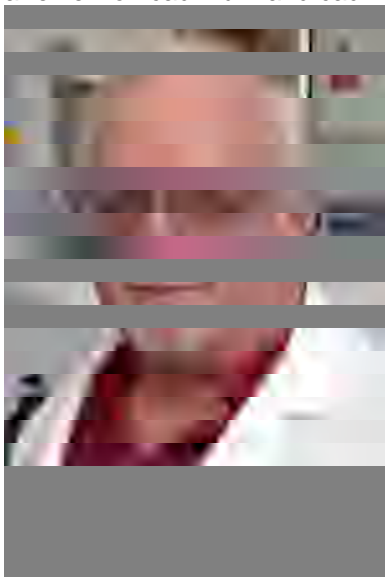
ST-11 Triple Quad (QXQ) ICP-MS, Sunday, January 12, 1 pm, R. Steven Pappas, and Nathalie Gonzalez-Jimenez, Centers for Disease Control & Prevention, 4770 Buford Hwy NE, MS F44, Atlanta, GA 30341-3717, rpappas@cdc.gov Development of the Agilent 8800/8900 QQQ and ThermoFisher iCAP TQ were major steps in next generation quadrupole instrumentation development, adding new capabilities, increased sensitivity, and new approaches for addressing analytical interferences. This course will describe choice of reactive gas to accomplish "mass shift" to avoid interferences,

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how to use internal standards in different modes, how to use instrument settings to overcome problems with high intensity analytes in the same method with low intensity analytes. The course will focus on the QQQ instrument, but most approaches are applicable to the TQ as well. Questions are welcomed. Analysts who are investigating the potential of triple quad ICP-MS instrumentation, how to take advantage of its capabilities, how to apply it to multielement, multimode methods, internal standard choices, practical applications will find this course useful.

Keywords: Triple Quad, QQQ-ICP-MS, interference, reactive gas, quadrupole, reaction cell

Steve Pappas earned his B.S. in Chemistry at Middle Tennessee State University in 1986. He completed his doctoral training in Biochemistry at Vanderbilt University. After holding faculty positions at Middle Tennessee State University and Georgia State University, he was employed at the Centers for Disease Control and Prevention (CDC) to develop methods for analysis of toxic metals in urine and blood for emergency response state health department laboratory training. In the second phase of his work at CDC, he became responsible for development of methods for analysis of tobacco and smoke for toxic metals. He subsequently became the Tobacco Inorganics Group Team Lead. He oversees method development, ISO 17025 accreditation, and analyses for toxic metals in tobacco and smoke. He is responsible for publishing and interpreting data in terms of public health risks. In addition to application manuscripts, he has written the Annex behind World Health Organization Technical Report Series 967 on toxic metals in tobacco and smoke with emphasis on inflammation and sensitization responses in animal and human studies, and a *Metalomics* review on the same topic, and a review on cadmium and cadmium/zinc ratios in tobacco-related disease.



Nathalie González Jiménez received her B.S. in Chemistry at Inter American University of Puerto Rico in San German in 2012. After completing her degree in chemistry, and is presently working toward her Masters while working in the Tobacco and Volatiles Branch of CDC in the Tobacco Inorganics group under Dr. Steve Pappas. Her assignments have included determination of cigarette and little cigar physical properties, development and utilization of methods for analysis of toxic metals in tobacco and tobacco smoke using microwave digestion, development of a low metals trap for e-cigarette aerosol, quadrupole ICP-MS, "Triple Quadrupole" ICP-MS, and combustion mercury analyzer, as well as analysis of tobacco smoke carbonyls and diacetyl.



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ST-12 Quadrupole, Triple Quad, and Sector Field ICP-MS, ETV-AAS, ICP-AES/ICP-OES Method Development Problem Solving, Saturday, January 11, 1 pm, R. Steven Pappas and Mark R. Fresquez, Centers for Disease Control and Prevention, 4770 Buford Hwy NE, MS F-44, Atlanta, GA 30341-3717, rpappas@cdc.gov

After preparation of liquid or digested samples, one takes advantage of instrument capabilities to accomplish analytical goals. Approaches to utilization of kinetic energy discrimination, reactive gases, and mass shift for quadrupole and "triple quad" ICP-MS, the use of resolution, mass windows, mass offset, and similar techniques for magnetic sector ICP-MS, and the use of desolvating introduction systems for increased sensitivity and decreased interferences will be discussed. Interferences and troubleshooting will be discussed for ICP-AES/OES. Optimization, troubleshooting, and matrix modification will be discussed for ETV-AAS. If communicated by email in advance, individual problems are welcomed. Analysts who confront problems in method development will benefit from approaches to taking advantage of strengths from different types of instrumentation, how to apply them in practical applications.

Keywords: Triple quad, magnetic sector, interference, reactive gas, quadrupole, reaction cell, desolvation

Mark Fresquez earned his B.S. in Chemistry at New Mexico State University in 1988, and subsequently his graduate training in Analytical Chemistry at the same institution. Mark began his career in commercial environmental trace metal analysis laboratories working with a wide variety of matrices and instrumentation including GFAA and ICP-OES for 13 years. Afterwards he was employed at the Centers for Disease Control and Prevention (CDC) working with arsenic speciation in urine utilizing HPLC-ICP-MS and mercury speciation in blood using GC-ICP-MS. Subsequently at CDC he was responsible for development of methods for analysis of tobacco and smoke for toxic metals. He has over 25 years of inorganic trace metals analysis experience with a wide range of instrumentation including ETV-AAS, ICP-OES/AES, ICP-MS, HPLC-ICP-MS, GC-ICP-MS, and ETV-ICP-MS.



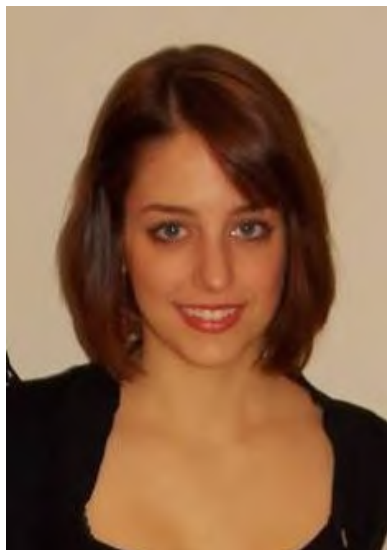
ST-13 Sample Preparation Problem Solving for Atomic Mass Spectrometry, Saturday, January 18, 8 am, R. Steven Pappas and Naudia Gray, Centers for Disease Control and Prevention, 4770 Buford Hwy NE, MS F44, Bldg 110, Atlanta, GA 30341-3717, rpappas@cdc.gov

Topics include preparation of liquid samples such as water, urine, and blood, biological solid sample digestion, very brief coverage of difficult inorganic oxide and metal sample dissolution, chemistry related to analytes of interest including chelation and avoiding memory effects. Approaches to optimization and the use of desolvating introduction systems for increased sensitivity and decreased interferences will be discussed. Limited discussion will touch on special needs such as considerations necessary for organic solvents and use of electrothermal vaporization.

Keywords: Sample preparation, memory effects, chelation, digestion, desolvation, environmental and biological samples, electrothermal vaporization

Naudia Martone Gray received her Bachelors and Masters degrees in Environmental Science at Duquesne University under Dr. Skip Kingston in 2012. Her graduate project involved the use of species specific isotope dilution for speciation of chromium with quadrupole ICP-MS. After completing her masters, she began to work in the Tobacco and Volatiles Branch of CDC in the Tobacco Inorganics group under Dr. Steve Pappas. Her projects have included determination of cigarette and little cigar physical properties, development and utilization of methods for analysis of toxic metals in tobacco and tobacco smoke using microwave digestion, development of a low metals trap for e-cigarette aerosol, quadrupole ICP-MS, triple quadrupole ICP-MS, and combustion mercury analyzer.

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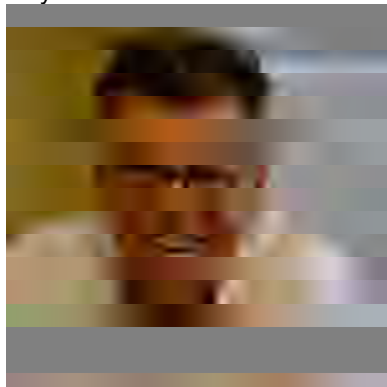


ST-14 Validation Assessment and ISO/IEC 17025: An Interactive Session, Sunday, January 12, 1 pm, Rob Ritsema, RR Quality Consultancy, Amersfoort, The Netherlands; robritsema@gmail.com; Petra Krystek, VU Amsterdam, The Netherlands, petra.krystek@vu.nl

This course will give an overview about the validation of analytical methods and procedures, which is an integral part of any good analytical practice. Method validation is the process used to confirm that the analytical procedure employed for a specific test is suitable for its intended use. Results from method validation can be used to judge the quality, reliability and consistency of analytical results. For making this information as practice relevant as possible, several examples like a procedure for the determination of selected elements in water by ICPMS will be discussed in detail. Special attention will be given to sampling and storage. Other examples from the inorganic analytical field of environmental, food and biological matrices will be covered too. Besides the methodological aspects and the obtained analytical results, the ten most relevant performance characteristics (limit of detection, recovery, repeatability, reproducibility, measuring range, trueness, lack of fit, expanded uncertainty of measurement, robustness and selectivity) are defined, calculated and discussed; also in relation if the analytical method should fulfill to section 5.4.5 of the accreditation standard ISO/IEC 17025. Crucial aspects of the new version of ISO/IEC 17025 will be discussed too. This course will be held as an interactive session.

Keywords: Quality assurance, validation assessment, performance characteristics, ICPMS

Rob Ritsema obtained his PhD in 1997 at the Université de Pau et des Pays de l'Adour, Pau, France. For 15 years he has worked at the accredited laboratory of the National Institute of Public Health and the Environment (RIVM) in the field of ICP-MS, focusing on environmental, food and body fluid analysis. For the past year he started his own company RR Quality Consultancy. Since 1998 he has been a freelance assessor the Dutch Accreditation Council (RvA) performing approximately 20 ISO 17025 technical assessments on a yearly base at laboratories mainly in the Netherlands. Recently he started at RvA as a freelance lead assessor. He is board member of the working group Atomic Spectrometry of the Royal Netherlands Chemical Society (KNCV).



ST-15 Uncertainty of Measurements: Practical Approaches to Determine Measurement Uncertainty Budgets

Thomas Prohaska, Sunday, January 12, 7 pm, Chair General and Analytical Chemistry, Montanuniversitaet Leoben, Franz Josef-Strasse 18, 8700 Leoben, Austria, Thomas.prohaska@unileoben.ac.at

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Metrology in chemistry is defined as the science of measurements. Even though we do take care about the best measurement results with respect of precision or the deviation from the 'true value', the validity of these results is determined by their uncertainties. Thus, a proper understanding of uncertainty budgets and the sources of error is crucial for providing validated measurement results. This short course provides the basic understanding for building an uncertainty budget and provides different approaches for doing so with a main focus on Monte Carlo calculations. Working on practical examples, the participants should be able to transfer the knowledge to their own measurement results.

Keywords: Uncertainty budget, metrology, errors, calculations

Thomas Prohaska is Chair for General and Analytical Chemistry at the Montanuniversität Leoben, Austria. He studied technical chemistry at the Vienna University of Technology and received his PhD with summa cum laude in 1995. In the same year he became scientific researcher at the University of Natural Resources and Life Sciences (BOKU), Vienna and was in charge to set up a laboratory for elemental trace analysis. From 1998 to 2000 he was researcher at the EC joint research center IRMM in Geel, Belgium. He returned to BOKU with a new focus on isotope ratio analysis in 2000. In 2004 he received the FWF-START award to setup a new research laboratory (VIRIS) for isotope research. He was associate professor at the BOKU from 2002-2018 before moving to Leoben. His current research focus is based on elemental and isotopic analysis using mass spectrometry, chemical imaging techniques and metrology with more than 150 peer-reviewed publications.



ST-16 Nanomaterials: Regulations, Standards, Measurement Advances and Remaining Challenges, Monday, January 13, 7 pm, Heidi Goenaga-Infante, LGC Limited, Queens Rd, Teddington, Middlesex TW11 OLY, UK, heidi.goenaga-infante@lgcgroup.com

This short course will cover regulatory aspects of the use of engineered nanomaterials by industry, linked to the EU definition of nanomaterial, the related analytical needs and challenges as well as the measurement strategies and standards driven by those challenges. It will be divided into three parts as follows: The first part of the course will cover key regulations, which have emerged from the increasing use of nanomaterials in several industrial applications (*e.g.*, novel food, food contact materials, cosmetics, *etc.*). It will also discuss the measurement capability needed to comply with those regulations and for future risk assessment.

The second part of the course will discuss existing analytical technology and advances in measurement capabilities for the characterization of nanomaterials and their input on key relevant ISO standards. Focus will be on inorganic nanomaterials and on multi-modal platforms combining hyphenated ICP-MS with spectroscopy and microscopy techniques. Examples of key analytical challenges and recommendations for overcoming such challenges will be given through (i) the quantification and characterization of metal oxide nanoparticles in food and cosmetics by asymmetrical field-flow-fractionation hyphenated to multiple detectors and (ii) the characterization of nanomaterials released from medical devices by single particle ICP-MS for toxicology testing. Finally, the short course will touch on measurement lessons learnt from international intercomparisons as well as highlight future measurement requirements and associated challenges. It will also provide the attendees with information on the existing reference materials for method development

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and validation and discuss remaining gaps for matrix/measurand combinations. The course presentation will be informal allowing for questions or remarks from the participants to be raised and discussed at any time.

Keywords: Regulations, engineered nanomaterials, reference nano-materials, measurement, characterization, AF4

ST-17 Metrology Concepts in Plasma Spectrochemistry, Zoltán Mester, Saturday, January 11, 7 pm, National Research Council of Canada (NRC), 1200 Montreal Rd, Building M-58, Ottawa, ON K1A 0R6, Canada, zoltan.mester@nrc-cnrc.gc.ca

An overview of the basics of chemical measurement science will be given. Concepts related to measurement traceability, comparability, and uncertainty will be discussed.

Keywords: Chemical measurements, traceability, uncertainty