

**XXI<sup>st</sup> Slovak - Czech Spectroscopic Conference**  
dedicated to the memory of Prof. Ing. Mikuláš Matherný, DrSc.

**October 16 - 20, 2016**  
**The Low Tatras - Liptovský Ján, Slovakia**



**BOOK OF ABSTRACTS**

peer reviewed

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and

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Dear colleagues.

It is a great pleasure for me to welcome you to the international XXI<sup>st</sup> Slovak-Czech spectroscopic conference organized by Slovak spectroscopic society (SSS), member of the Association of Slovak scientific and technological societies, and Ioannes Marcus Marci spectroscopic society (JMMSS). This year our conference will take place in Hotel Sorea Máj in Liptovský Ján, that is a gate to the Jánska valley, known and sought-after tourist and recreational locality in The Low Tatras National Park. The conference builds on cooperation between the Slovak and Czech spectroscopic society, which was restored in the form of national spectroscopic conferences in 2008 by XIX<sup>th</sup> Slovak-Czech spectroscopic conference in Častá-Papiernička and in the same time it continues in the tradition of Slovak spectroscopic conferences, which began as a workshop in Hrabušice in 1970. These scientific meetings are known for their tradition, high scientific level and wide professional public interest. The conference, with respect to its scope, provides a space for the presentation of the contemporary state and trends and problem solving at all stages of the analytical procedure relating to the application of spectroscopy in the analysis of various materials. It covers wide range of atomic and molecular spectroscopy, special spectroscopy techniques and their applications in different fields of analytical interests. Thanks to interest of distinguish scientists, researchers, students, workers from different universities, institutions and laboratories as well as commercial companies we were able to create high-quality professional program that is worth seeing.

The XXI<sup>st</sup> Slovak-Czech spectroscopic conference is dedicated to the memory of nestor of Slovak spectroscopy, Prof. Ing. M. Matherny, DrSc., professor emeritus, who passed away last year on 22 June. His outstanding job, life and friendship will remind us three commemorative lectures of his life-long friends and colleagues.

This year conference will be hosting about 114 participants from 6 European countries. The scientific program is divided into 11 scientific sessions, involving poster session. It consists of 3 commemorative lectures, 10 invited lectures, 29 oral presentations, 25 poster displays and exhibition of 14 companies representing leading manufacturers of laboratory instrumentation and distributors of laboratory equipment.

The XXI<sup>st</sup> Slovak-Czech spectroscopic conference offers occasion to honor outstanding personalities of Slovak and Czech spectroscopy. Four honorary memberships of SSS and three Nicolaus Konkoly-Thege medals will be awarded by Slovak Spectroscopic Society and Ioannes Marcus Marci medal will be awarded to one outstanding scientist. To support students, the best student lecture presentation, the best student poster presentation and the best three poster presentations of all posters, will be evaluated by international committees. Award ceremony will take place in the official part of conference dinner.

I would like to thank our general sponsors Pragolab, s.r.o. and ThermoFisher Scientific, Inc. as well as Messer Tatragas, Shimadzu-Slovakia, Centralchem, Labicom, Spectro APS, Chromspec-Slovakia, Analytika, Merck, Optik Instruments, Amedis, Renishaw, Lambda Life and Specion as the sponsors for their notable support and cooperation.

On behalf of organizing committee of the XXI<sup>st</sup> Slovak-Czech spectroscopic conference I wish let these four conference days have brought to you not only new inspirations and ideas in your work, but also new experience, friendships and memories. At the same time, take the opportunity to relax and recharge your energy in the beautiful nature of The Low Tatras.

Silvia Ružičková  
chairperson of the organizing committee



Mikuláš Matherny, professor emeritus of the Technical University of Košice, outstanding personality of the Slovak chemical community, internationally recognised scientist, a spectrochemist colleague and a good friend passed away last year on 22 June. Professor Matherny was born in Prešov on 3 July 1930, and graduated from the well-known Lutheran College high school. In 1952, he obtained his diploma at the Faculty of Chemical Engineering of the Slovak Technical University in Bratislava. He started his professional career at the Department of Mineralogy and Crystallography in the Faculty of Natural Sciences of the Comenius University.

In 1960, he moves to Košice for political reasons and joins the Department of Chemistry in the Faculty of Metallurgy at the Technical University; he soon takes over the leadership of the department and stays at its head until 1973. In parallel, he also assumes duties at the Faculty of Natural Sciences of the Pavol Jozef Šafárik University in Košice; he organises and leads the Department of Analytical Chemistry until 1973. He chose his colleagues purposefully and created a workplace that came to be known as “the Košice spectroscopic school” both at home and abroad. He encourages his students with the Faraday motto “work-finish-publish”, and this motto was also Professor Matherny’s lifelong objective. He established his international relations purposefully as well, mostly with colleagues from Hungary and both Germanys. In 2001, the Hungarian Spectrochemical Society awarded him the Tibor Török Commemorative Medallion for his achievements in the realisation of Hungarian-Slovak scientific cooperation.

He did an outstanding job in the different scientific societies operating within the framework of the Slovak and Czechoslovak Academies of Sciences. He founded the East-Slovak Commission of the Slovak Chemical Society in 1962 and stayed at its head until 1990. For these activities, the society awarded him its Gold Medallion (1990) and an honorary membership (1995). He actively took part in the Czechoslovak Spectroscopic Society’s work; from 1970 onwards, he regularly organised the seminars of atomic spectroscopy that ultimately became the Slovak Spectroscopic Conference in 1990. For this reason, he was awarded the Johannes Marcus Marci Commemorative Medallion as well as the Konkoly-Thege Commemorative Medallion of the Slovak Spectroscopic Society.

Professor Matherny’s scientific and teaching activities primarily prevailed in the fields of analytical chemistry, spectral analysis and chemometrics; he disclosed his results in approximately 250 scientific papers. In 1982, he took over the leadership of the department once again; he developed and introduced an environmental study program. Between 1986 and 1990, he also creates a common workplace (Laboratory of rare elements) with the Slovak Academy of Sciences as a coordinator of a public research program; his results thus achieved in the fields of physics and chemistry are rewarded by a Dionýz Ilkovič Golden Plaque. He was the academic supervisor of sixteen CSc (now PhD) students; two of his colleagues became doctors of chemical sciences, and three became university professors of analytical chemistry. Professor Matherny retired in 1998, but remained actively involved with the department’s scientific endeavours as professor emeritus. On the occasion of the Golden Jubilee of the Technical University of Košice, he was awarded the university’s Gold Medallion.

His colleagues home and abroad, his students and his friends lovingly preserve the memory of Professor Mikuláš Matherny, who – by his life-work – gave an example of the creative realisation of cross border cooperation.

**Professor Mikuláš Matherny and his Košice Spectroscopy School:  
History and Scientific Milestones**

Karol Flórián

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Professor Mikuláš Matherny (full professor since 1982) moved from Bratislava to Košice in 1960. Having some experience in spectroscopy, at the early times of his stay at TU he established a working group, later well known as “Košice spectroscopy school”. In spite of the fact that Košice was the centre of magnesite industry at that time, the main interest of analytical chemists was oriented towards natural materials mainly in the form of powdered samples. As spectrography was at that time one of the leading instrumental analytical methods, logically this method was preferred. The first published papers were devoted to basic problems of spectrography: the influence of quality of spectral electrodes on excitation process was checked, as well as the possibilities of spectrographic analysis of magnesite and later of CaO-matrices. Besides these typical analyses of powdered samples (today’s solid sampling), appropriate interest was paid also to the solution methods of the analysis. The basic problem of both solution and powder spectroscopy was the phenomenon designated as matrix-effect. This was described and clearly defined by prof. Matherny and a complex procedure for checking of this effect in spectrography was evaluated. In spite of the fact that quantitative spectrochemical analysis was based since Gerlach’s proposal on the use of spectral line pairs (analytical-X vs. reference-R line), the examination of their correlation has become of high importance. The method of scatter diagrams proposed by Holdt, Strasheim and Keddy was applied by prof. Matherny and his school in various spectrographic methods. Including two further parameters to the mentioned correlation-regression analysis of spectral line pairs, the complex method for checking the homology of spectral line pairs was established, using an own computer program for this evaluation (used at that time also by other spectrographic groups not only in Slovakia, but also in Hungary). Later, besides modernized instrumentation, the evaluation process has also been changed – the systematic use of statistical methods as well as of own computer programs in evaluation are typical. Summarizing papers about the use of computers in spectrographic evaluation as well as about determination of limiting criteria in spectrography were published by prof. Matherny and his co-workers. The weak points of quantitative spectrography at that time were both the measurement of densities on the photographic spectral plates and their transformation process. The determination of transformation constants ( $\gamma$  and  $\kappa$ ) of used  $\ell$ -transformation as well as the transformation of densities using tables was very difficult and laborious. Therefore computer programs were developed and their reliability was tested. Another alternative method (for powdered samples of environmental origin), the double arc method was applied in Slovak-German cooperation as a result of Professor Matherny’s stay in the Research Centre in Jülich / Germany as visiting professor (research group headed by prof. Hubertus Nickel). In environmental applications, the gravitation dust sediments were analysed and evaluated using chemometrical procedures in cooperation with the F. Schiller University in Jena, but the methodology and possible chemometrical investigations in environmental analysis in general were also described. This research had a continuation in comparison of solid sampling spectrochemical methods by means of multivariate statistics and information theory which was realized in German-Slovak-Hungarian cooperation using the evaluation procedure based on the information characteristics, elaborated by prof. Matherny. The fruitful scientific career of prof. Matherny ended in June 2015. This was also the time when the research in the scientific field of chemistry as well as the PhD study programmes in analytical chemistry were stopped at the Faculty of Metallurgy. As a result of these facts it seems that the Košice spectroscopic school established by prof. Matherny reached its end.

**Slovak Spectroscopic Society (SSS)** – *member of the Association of Slovak Scientific and Technological Societies* is a voluntary organization of scientific, scientific-pedagogical and professional workers in the field of spectroscopy. The main aim of the society is to participate in the further development and enhancing of the level of spectroscopy in the Slovak Republic, in the conceptual work as well as in the dissemination and implementation of the scientific results.

**The honorary members of SSS:**

- doc. RNDr. Bohumil Dočekal, CSc.
- prof. RNDr. Viktor Kanický, DrSc.
- RNDr. Ján Medveď, CSc.
- doc. RNDr. Mária Žemberyová, CSc.



**Ioannes Marcus Marci Spectroscopic Society (IMMSS)** is a non-profit organization of scientific, educational and professional technical workers in spectroscopy, eventually legal entities engaged in scientific or application activities in this field, all associated in joint activities with the aims of promoting and fostering advancement in the field of spectroscopy. **Ioannes Marcus Marci** was a Bohemian doctor and scientist, rector of the University of Prague, and official physician to the Holy Roman Emperors.

**The Laureate of IMM Medal:**

- doc. RNDr. Jana Kubová, PhD.



**Nicolaus Konkoly-Thege (NKT)** was mainly interested in the new methods of celestial photography and astrophysics – especially spectroscopy. In 1898 he presented his observatory to the Hungarian government, together with the funds necessary to ensure its continuation. **The Nicolaus Konkoly-Thege Medal** is an award given for exceptional contributions to the development of the spectroscopy.

**The Laureates of NKT Medal:**

- prof. RNDr. Jiří Dědina, CSc. DSc.
- prof. Dr. Viliam Krivan
- prof. Ing. Jozef Sitek, DrSc.



## Scientific Program of the XXI<sup>st</sup> Slovak - Czech Spectroscopic Conference, October 16 - 20, 2016, Low Tatras - Liptovský Ján, Slovakia

Conference venue: *Hotel Sorea Máj\*\*\*\**, Liptovský Ján

### Sunday, 16 October 2016

14:00 – 20:00 Registration

### Monday, 17 October 2016

08:00 – 18:00 Registration

09:30 – 09:45 Welcome address

#### *Commemorative Lectures*

09:45 – 10:15 (CL1) **Karol Flórián:** Professor Mikuláš Matherny and his Košice Spectroscopy School: History and Scientific Milestones

10:15 – 10:30 (CL2) **Hubertus Nickel:** In Memory of Prof. Dr. Mikuláš Matherny

10:30 – 10:45 (CL3) **Eduard Plško:** Memory of Prof. Dr. Matherny.

#### *Invited Lectures*

*Chairperson: Hubertus Nickel*

10:45 – 11:15 (IL1) **Bohumil Dočekal,** Zbyněk Večeřa, Pavel Mikuška, Pavel Šurýn, Michaela Dufka, Pavel Coufalík: Analysis of Mice Organs and Blood from Inhalation Experiments with Selected Metal Oxides Nanoparticles

11:15 – 11:45 (IL2) **Gyula Záray:** Determination of Pharmaceutical Residues in Waste, Surface and Drinking Water by GC-MS/MS

#### *Session – Spectroscopy and Spectrometry*

*Chairperson: Viera Vojteková*

13:30 – 14:00 (IL3) **Jiří Dědina,** Jan Kratzer, Marek Talába, Adam Obrusník, Pavel Dvořák: Recent Advances in Hydride Generation for Atomic Absorption Spectrometry: Atomizer Optimization by Two-Photon Absorption Laser-Induced Fluorescence



- 14:00 – 14:20 (OL1) **Stanislava Matějková**, Luisa Šerá, Martin Loula, Jan Mengl: Inductively Coupled Plasma Optical Emission Spectroscopy with Electrothermal Vaporisation: An Effective Tool for Direct Multielemental Analysis of Biological Samples
- 14:20 – 14:40 (OL2) **Ingrid Hagarová**: Separation and Preconcentration of Ultratrace Elements by Using New Modes of Cloud Point Extraction: Utilizable in Connection with Spectrometric Methods
- 14:40 – 14:50 (FL1) **ANALYTIKA s.r.o.**  
Daniela Weisserová, **Vladimír Patera**: Laboratory Reference Materials Supplied by Analytika s.r.o.

*Session – Atomic Spectrometry*

*Chairperson: Karol Flórián*

- 15:10 – 15:40 (IL4) **Ernest Beinrohr**, Ľubomír Machyňák, František Čacho: Determination of Trace Concentrations of Chlorine and Fluorine by Continuum Source High Resolution Graphite Furnace Atomic Absorption Spectrometry
- 15:40 – 16:00 (OL3) **Jan Kratzer**, Petr Novák, Pavla Zurynková, Ondřej Duben, Michal Albrecht, Milan Svoboda, Jiří Dědina: Dielectric Barrier Discharge Plasma Atomizers of Volatile Compounds in Atomic Absorption Spectrometry: Applications, Mechanisms and Future Perspectives
- 16:00 – 16:20 (OL4) **Manfred Sager**: Sample Preparation for Determination of High Iodine Levels by ICP-OES
- 16:20 – 16:40 (OL5) **György Heltai**, Karol Flórián, Remeteiová Dagmar, Márk Horváth, Éva Széles, Gábor Halász, Ilona Fekete: Application and Development Sequential Extraction Procedures for Fractionation of Heavy Metal Content of Soils, Sediments, and Gravitation Dusts
- 16:40 – 16:50 (FL2) **PRAGOLAB s.r.o.**  
**Róbert Cibula**: Using of Extra Techniques in Connection with ICP/MS
- 17:00 Slovak Spectroscopic Society General Assembly

**Tuesday, 18 October 2016**

***Session – Other Spectroscopic methods, instrumentation, and methodology***

*Chairperson: Marcel Miglierini*

- 09:00 – 09:30 (IL5) **Adriana Lančok:** Temperature Degradation of Vivianite as Related to Historic Paintings
- 09:30 – 09:50 (OL6) **Lukáš Pašteka, Marcel Miglierini:** Study of Stainless Steel LC200N by Mössbauer Spectrometry
- 09:50 – 10:10 (OL7) **Ivana Bonková, Marcel Miglierini, Marek Bujdoš:** Mössbauer Spectrometry Applied to Biological Samples
- 10:10 – 10:20 (FL3) **Messer Tatragas s.r.o.**  
**Michael Hanish:** Calibration Gases – Reference Materials acc. To ISO Guide 34 and ISO/IEC 17025

***Session – Other Spectroscopic methods, instrumentation, and methodology***

*Chairperson: Adriana Lančok*

- 10:40 – 11:00 (OL8) **Marcel Miglierini:** Hyperfine Interactions of Disordered Alloys Probed by Nuclear Resonances
- 11:00 – 11:20 (OL9) **Milan Štefánik, Martin Cesnek, Marcel Miglierini:** Neutron Activation Analysis of Steel Samples at the VR-1 Training Reactor and NG-2 Cyclotron-Based Neutron Generator
- 11:20 – 11:50 (IL6) **Jozef Sitek, Dominika Holková, Július Dekan:** Radiation Influence on Nanocrystalline Alloys

***Session – Molecular Spectroscopy***

*Chairperson: Přemysl Lubal*

- 13:30 – 14:00 (IL7) **Pavel Matějka, Martin Král, Alžběta Kokaislová, Marcela Dendisová, Marie Švecová, Adéla Jenišťová, Jiří Janoušek:** From Surface-Enhanced Vibrational Spectroscopy to Vibrational Nanoscopy
- 14:00 – 14:20 (OL10) **Adriana Šturcová, Nikolay Kotov, Alexander Zhigunov, Vladimír Raus, Jiří Dybal:** The Effect of Water on Structural Transitions of 1-Butyl-3-Methylimidazolium Chloride as Investigated by Vibrational Spectroscopy and WAXS
- 14:20 – 14:40 (OL11) **Markéta Pazderková, Petr Maloň, Václav Profant, Vladimír Baumruk, Lucie Bednářová:** Chiroptical Properties of the Antimicrobial Peptide *Lasiocepsin* and of its Analogs

14:40 – 15:00 (OL12) **Veronika Sutrová**, Ivana Šloufová, Martin Kalbáč, Ewa Pavlova, Martina Nevoralová, Blanka Vlčková: Enhanced Raman Spectra of Ag-Ethanedithiolate and Graphene from Graphene/Ag-NPs-Ethanedithiol Hybrids: Interplay between Surface- and Graphene-Enhanced Raman Scattering

15:00 – 15:10 (FL4) **Merck s.r.o.**  
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*Session – Molecular Spectroscopy; Spectroscopy and Spectrometry*

*Chairperson: Pavel Matějka*

15:30 – 15:50 (OL13) Alžběta Jebavá, Lenka Řezáčová, **Přemysl Lubal**, Karel Novotný: Synthesis and Analytical Applications of CdTe-QD's Nanoparticles

15:50 – 16:10 (OL14) **Branislav Hruška**, Tadeáš Gavenda, Darina Tokarčíková, Andrea Černá, Mária Chromčíková, Marek Liška: Interpretation of Raman Spectra Depth Profile of Weathered Glass Surface by Advanced Statistical Methods

16:10 – 16:30 (OL15) **Lucia Kořenková**, Martin Urík: Application of FTIR Spectroscopy in Soil Water Repellency Assessment

16:30 – 16:40 (FL5) **SHIMADZU SLOVAKIA, o.z.**  
**Johan Leinders**, Uwe Oppermann, Jan Knoop: ICPMS-2030: Peace of Mind for Users and Lab Managers

19:00 – 21:00 Poster session

**Wednesday, 19 October 2016**

*Session – Spectroscopy and Spectrometry; Mass spectrometry*

*Chairperson: Bohumil Dočekal*

08:30 – 09:00 (IL8) **Viktor Kanický**, Karel Novotný, Markéta Holá, Michaela Vašinová Galiová, Tomáš Vaculovič, Aleš Hrdlička: Recent Developments in Laser Assisted Plasma Spectrometry

09:00 – 09:20 (OL16) **Henrieta Šoltýsová**, Jarmila Nováková, Augustín Majchrák: Determination of Some Elements in Samples of Emissions by ICP-MS

- 09:20 – 09:40 (OL17) **Viera Vojteková**, Daniel Kupka, Daniela Sabolová: Multi-element Analysis in Complicated Sample Matrices Utilizing Single-Set Experimental Conditions of ORC-ICP-QMS
- 09:40 – 10:00 (OL18) **Pavel Pořízka**, Tomáš Zikmund, Markéta Tesařová, David Procházka, Jan Novotný, Jozef Kaiser: Utilization of Computed Tomography and Laser Spectroscopy for 3D High Resolution Mapping
- 10:00 – 10:10 (FL6) **AMEDIS s.r.o.**  
**Fabrizio Jakubec**: PQ MS Technological Progress

*Session – Atomic Spectrometry; Spectroscopy and Spectrometry*  
*Chairperson: Viktor Kanický*

- 10:30 – 11:00 (IL9) **Ewa Bulska**: On the Use of Non-Routine Analytical Approaches for Understanding Chemical Speciation in Environmental Samples
- 10:00 – 11:20 (OL19) **Michal Hlodák**, Martin Urík, Peter Matúš: Evaluation of Mercury Immobilisation and Transformation Processes in the Soil – Plant – Microscopic Filamentous Fungi System Using CV AAS Method
- 11:20 – 11:40 (OL20) **Michaela Hložková**, Michaela Vašinová Galiová, Renáta Čopjaková, Jindřich Kynický, Viktor Kanický: Application of Laser Ablation Sampling for the Multielemental Analysis of Dinosaur Skeletal Remains: a Diagenetic Study
- 11:40 – 11:50 (FL7) **CHROMSPEC-SLOVAKIA s.r.o.**

**Thursday, 20 October 2016**

*Session – Spectroscopy and Spectrometry*  
*Chairperson: Gyula Záray*

- 08:30 – 08:50 (OL21) **Hana Dočekalová**: Prediction of Bioavailability of Metals in Aquatic Systems: Comparison between Diffusive Gradient in Thin Films Technique and Living Organism
- 08:50 – 09:10 (OL22) **Eva Duborská**, Jana Kubová: Analytical Methods for Iodine Determination in Environmental Samples

- 09:10 – 09:30 (OL23) **Martin Urík**, Marek Bujdoš, Katarína Boriová, Marcel Miglierini: Application of Spectroscopic Methods for Evaluation of Toxic Metals and Metalloids Mobility in Defined Multicomponent Systems During Static Cultivation of Common Fungal Strains
- 09:30 – 09:50 (OL24) **Martin Šebesta**, Martin Urík, Marek Kolenčík, Peter Matúš, Gabriela Kratošová, Ivo Vávra, Andrej Vojtko, Eva Majková: Characterizing ZnO Nanoparticles and their Interaction with Humic Acids
- 09:50 – 10:20 (IL10) **Viliam Krivan**: Analysis of High Purity Advanced Materials: the Present-Day Importance of Wet-Chemical and Direct Solid Sampling Spectrometric Methods

***Session – Spectroscopy and Spectrometry; Other Spectroscopic methods, instrumentation, and methodology***

*Chairperson: Daniela Mackových*

- 10:40 – 11:00 (OL25) **Michal Rečlo**, Erkan Yilmaz, Mustafa Soylak, Vasil Andruch, Yaroslav Bazel: Switchable Hydrophilicity Solvent Based Microextraction of Nickel Prior to Determination by Flame Atomic Absorption Spectrometry
- 11:00 – 11:20 (OL26) Marek Bujdoš, Hana Vojtková, **Marek Kolenčík**, Martin Urík: The Leaching of Zn, Pb, and Cu from Polymetallic Ore Using Heterotrophic Bacteria such as *Pseudomonas*, *Rhodococcus* and *Cupriavidus* Compare to Fungal Strain *Aspregillus Niger*
- 11:20 – 11:40 (OL27) **Filip Polák**: Fungal Accumulation of Selected Metals from Mining Waste
- 11:40 – 12:00 (OL28) **Martin Pavlačka**, Karel Ventura, Kateřina Kortánková, Jiří Bláha, Michal Zástěra, Roman Mázl, Petra Bajerová: Analysis of Stimulants Using Differential Mobility Spectrometry
- 12:00 – 12:20 (OL29) **Jozef Bednarčík**: Experimental Possibilities at the High-Resolution Powder Diffraction Beamline P02.1
- 12:20 – 12:30 Closing ceremony

## POSTER SESSION

*Members of evaluation committee: E. Beinrohr, A. Lančok, H. Nickel, G. Záray*

- PP1 **Andrea Černá**, Branislav Hruška, Darina Tokarčíková, Mária Chromčíková, Marek Liška: AFM and Raman Study of Heavy Weathered Surface of Barium Crystal Glass.
- PP2 **Marianna Dorková**, Dagmar Remeteiová, Silvia Ružičková, Vladislava Mičková: Utilization of MW-Assisted Decomposition and HR-CS AAS for Evaluation of Heavy Metals Pollution in Sedimentary Ecosystems
- PP3 **Miroslav Fišera**, Jiří Mlček, Pavel Budinský, Helena Velichová, Lenka Fišerová: Determination of Selenium Species by ICP-MS Method in Biological Samples.
- PP4 **Ingrid Hagarová**: Simplex Method for Optimization of Cloud Point Extraction: Utilizable for Determination of Ultratrace Elements by Using Spectrometric Methods.
- PP5 Silvia Ružičková, Mariana Dorková, Dagmar Remeteiová, Vladislava Mičková, **Gabriela Holéczyová**: Determination of Heavy Metals in the Soil by High-Resolution Continuum Source Flame Atomic Absorption Spectrometry (HR-CS FAAS)
- PP6 **Petr Chrást**, Michaela Vašinová Galiová, Viktor Kanický: Inductively Coupled Plasma Mass Spectrometry in the Analysis of Geological Materials.
- PP7 **Adéla Jenišťová**, Jaroslava Šmolíková, Martin Flegel, Pavel Matějka: Vibrational Spectroscopic Study of Interactions between Skin and Peptides Based on the Argireline Structure.
- PP8 **Antonín Kaňa**, Jiřina Száková, Oto Mestek: Effect of Dietary Selenium Intake on Inter-Element Interactions in Rat Livers.
- PP9 **Lubomír Machyňák**, Martin Němeček, František Čacho, Ernest Beinrohr: High-Resolution Continuum Source Electrothermal Absorption Spectrometry of SrF and InCl Molecules.
- PP10 **Irena Matulková**, Ivana Šloufová, Jana Vejpravová, Tim Verhagen, Ivan Němec, Blanka Vlčková, Veronika Sutrová, Miroslav Šlouf, Martin Kalbáč: Raman Spectroscopy Study of Thermal Effects in Graphene on Au Nanoislands.
- PP11 **Vladislava Mičková**, Silvia Ružičková, Marianna Dorková, Dagmar Remeteiová: Temperature Influence on Electrothermal Vaporization Process of Heavy Metals in Different Matrices by Use of ETV-ICP-OES Method.
- PP12 **Martin Němeček**, Lubomír Machyňák, Ernest Beinrohr, František Čacho: Application of High-Resolution Continuum Source Molecular Absorption for the Determination of Nitrate.



- PP13 **Eliška Nováková**, Václav Červený, Petr Rychlovský: Determination of Se in Dietary Supplements by Photochemical Volatile Species Generation Atomic Absorption Spectrometry.
- PP14 **Markéta Prusková**, Ivana Šloufová, Jiří Vohlídal, Blanka Vlčková, Miroslav Šlouf: SERS Study of Self-Assembled 2D Nanocomposites of Ag and Au Nanoparticles with Terpyridine and its Derivatives.
- PP15 **Dagmar Remeteiová**, Marianna Dorková, Silvia Ružičková, Vladislava Mičková: Evaluation of Heavy Metals Impact from Various Types of Sediments to their Ecosystem by Fractionation Extractions and High-Resolution Continuum Source Flame Atomic Absorption Spectrometry.
- PP16 **Tina Resslerová**, Jakub Hraníček: Determination of Tellurium in Flavoured Mineral Waters by Electrochemical HG-AFS.
- PP17 **Silvia Ružičková**, Dagmar Remeteiová, Mariana Dorková, Vladislava Mičková: Optimization of Microwave-Assisted Decomposition for Heavy Metals Determination in Lichens.
- PP18 **Daniela Sabolová**, Viera Vojteková, Daniel Kupka: Inductively Coupled Plasma Mass Spectrometry in Trace Analysis of Sulphur.
- PP19 **Milan Svoboda**, Jan Kratzer, Věra Šindelářová, Marek Straka, Jakub Hraníček, Antje Michels, Joachim Franzke, Jiří Dědina: Novel Designs of Dielectric Barrier Discharge Atomizers of Volatile Compounds for AAS and AFS.
- PP20 Charles S. Huber, Mária G. R. Vale, Morgana B. Dessuy, **Milan Svoboda**, Jiří Dědina: Arsenic Speciation in Baby Food by HG-CT-AAS.
- PP21 **Lucie Šimoníková**, Lubomír Prokeš, Vlastimil Kubáň, Viktor Kanický: Elemental Analysis of Wine by Inductively Coupled Plasma Optical Emission Spectroscopy.
- PP22 Barbora Svatošová, **Michaela Vašinová Galiová**, Jitka Míková, Lubomír Prokeš, Hélène Tabouret, Christophe Pécheyran, Viktor Kanický: Analysis of Antarctic Otoliths by Laser Ablation Inductively Coupled Plasma Mass Spectrometry.
- PP23 **Éva Cseperke Vizsolyi**, Imre Varga, Győző G. Láng, József Varga, Gyula Záray: Case Study of Groundwater Remediation.
- PP24 **Viera Vojteková**, Anna Ballóková, Daniela Sabolová, Daniel Kupka: Optimization of Analytical Method for Determination of the Trace Phosphorus Contents by Using ORC-ICP-QMS.
- PP25 **Jiřina Vontorová**, Václav Dobiáš, Petr Mohyla: Utilization of GDOES for the Study of Friction Layers Formed on the Surface of Brake Discs During the Friction Process.

## **ABSTRACTS OF INVITED LECTURES**

## Analysis of Mice Organs and Blood from Inhalation Experiments with Selected Metal Oxides Nanoparticles

Bohumil Dočekal, Zbyněk Večeřa, Pavel Mikuška, Pavel Šurýn, Michaela Dufka,  
Pavel Coufalík

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The increasing amount of heavy metals used in manufacturing equivalently increases hazards of environmental pollution and occupational exposure by industrial products, especially in metallurgical processes or in application of engineered nanoparticles. One of the main routes of exposure is via inhalation. Inhaled nanoparticles are transported and deposited in the various parts of the respiratory tract. Very small sized particles are able to penetrate deep inside the alveolar regions. Their subsequent transport is influenced by phagocytosis, endocytosis and transcytosis across epithelial cells, which may result in their release into blood and lymph circulation.

This contribution focusses on the study of fate of inhaled nanoparticles of Cd, Mn, Pb, Ti and Zn oxides in the organism of small “white” mice (female, ICR strain), on translocation of metals from primary to secondary target organs by blood. Some critical steps of trace and ultra-trace determination in analysis of individual organs (lung, liver, kidney, spleen, heart and brain) and blood fractions (blood cells, protein and low molecular fractions) are shown. Methods of taking samples, sample preparation and decomposition by various procedures (microwave assisted high pressure mineralization, dry ashing in nitrous oxide/ozone atmosphere - APION) are presented. Some spectral interference effects in determination of selected metals by electrothermal atomic absorption spectrometry and inductively coupled plasma mass spectrometry are discussed. Basic characteristics of nanoparticles used and consequences of their inhalation to organ tissues and cellular structures are also given on transmission electron microscopy and histology pictures.

*Acknowledgements: This work was supported by the Czech Science Foundation (grants No. P503/11/2315 and P503/12/G147).*

**Determination of Pharmaceutical Residues in Waste, Surface and Drinking Water  
by GC-MS/MS**

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Municipal wastewater contains residues of different pharmaceutical and personal care products. Considering the fact that the wastewater treatment technologies applied worldwide are based first of all on mechanical and biological treatment, the biodegradation of different artificial molecules is a key question. Unfortunately, there are pharmaceutical products that pass through the sewage treatment plants without any degradation. Since the treated wastewater is introduced into rivers or even into lakes, their long-term effects on the ecological system or their appearance in the drinking water reservoirs should be taken into consideration. This issue is especially critical if the drinking water production is based on bank filtration technology. Due to the climate change, the reuse of treated wastewater has an increasing importance; therefore, the water technologies require advanced analytical techniques in order to follow the fate of the pharmaceutical products or even that of their metabolites.

At first our research program was focused on the determination of anti-inflammatory drugs (Diclofenac, Ibuprofen, Ketoprofen, Naproxen) in wastewater, treated wastewater, surface water, (Danube river water) as well as drinking water. In the next step a multiresidue analysis procedure was developed which permits the identification and quantification of sixty-three water-soluble pollutants. Subsequent to their solid-phase extraction (SPE) enrichment, analyses of species have been carried out from one solution, by a single injection, as their trimethylsilyl-oxime ether/ester derivatives, by gas chromatography-mass spectrometry, within 31 min. Based on our optimized extraction, derivatization and mass fragmentation studies separation have been performed in the total ion current mode, identification and quantification of compounds have been carried out on the basis of their selective fragment ions: including various pharmaceuticals, benzoic acid, its substituted species, different aromatic carboxylic acids, cholic acids, unsaturated and saturated fatty acids, aliphatic dicarboxylic acids, as well as synthetic pollutants of various origins (2,4-di-tert-butylphenol, different phthalates). Responses, obtained with derivatized standards proved to be linear in the range of 4-80 µg/L levels. Limit of quantification values varied between 0.92 ng/L (4-hydroxyphenylacetic acid) and 600 ng/L (dehydrocholic acid) concentrations. One of the most important question was the determination of origin of blank values. It was shown that contaminants, mainly 2,4-di-ter-butylphenol, different phthalates and fatty acids, are sourced both from the reagents and mainly from the SPE procedure, independent on the cartridge applied. Reproducibilities, characterized with the relative standard deviations (RSDs) of measurements, varied between 0.71 % and 10 %, with an average of 4.38 % RSD. This analytical technique made it possible to follow the changes of residue concentrations during the development of post-treatment procedures applying oxidation or adsorption technologies.

**Recent Advances in Hydride Generation for Atomic Absorption Spectrometry:  
Atomizer Optimization by Two-Photon Absorption Laser-Induced Fluorescence**

Jiří Dědina<sup>1</sup>, Jan Kratzer<sup>1</sup>, Marek Talába<sup>2</sup>, Adam Obrusník<sup>2</sup>, Pavel Dvořák<sup>2</sup>

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Our research is focused on analytical applications of hydride generation for atomic absorption and atomic fluorescence detectors. To fully utilize the potential of hydride generation the atomization step has to be optimized. Currently, the optimization is typically performed on the purely trial and error basis. The reason is that hydride atomization in the most often employed atomizers, quartz tubes and flames, proceeds via analyte interaction with hydrogen radicals which are extremely difficult to detect even though they are present in these atomizers at concentration several orders of magnitude above the equilibrium. There were attempts to prove hydrogen radical presence in quartz tube atomizers but no conclusive results were found because of the extreme complexity of employed techniques.

A new approach to hydrogen radical detection, based on a direct observation of free hydrogen radicals by two-photon absorption laser-induced fluorescence, in hydride atomizers will be reported. This approach makes possible to visualize the distribution of hydrogen radicals in atomizers. Consequently it offers a potential to disclose how the distribution of hydrogen radicals depends on atomizer design and on actual experimental parameters. It should be highlighted that two-photon absorption laser-induced fluorescence allows a straightforward optimization of the atomization step of analytical methods for trace element and speciation analysis based on hydride generation and on their atomization in atomic absorption and atomic fluorescence detectors. Outlooks of this exciting approach to atomizer optimization and to further investigation of mechanism of hydride atomization will be outlined.

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## Determination of Trace Concentrations of Chlorine and Fluorine by Continuum Source High Resolution Graphite Furnace Atomic Absorption Spectrometry

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Trace concentrations of chlorine and fluorine in aquatic samples were determined by graphite furnace continuum source high resolution atomic absorption spectrometry (GF-CS-HR-AAS) by making use of formation of diatomic InCl and SrF species. The influence of Indium and Strontium concentration, chemical modifiers, ashing and atomisation temperatures was investigated.

The detection limit and precision of the method are below 1 µg/l and 5 %, respectively for chlorine and 0.03 mg/l and 3.6 % for fluorine, respectively. The method was used for analysis of various water samples including surface water, underground water and waste water.

Keywords: chlorine, fluorine, CS-HR AAS

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## Temperature Degradation of Vivianite as Related to Historic Paintings

Adriana Lančok

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Vivianite has been used as a pigment for several centuries (documented usage in Europe ranges from 1050 to 1780) in various types of artworks: from polychromy on wood and stone to wall paintings, as well as paintings executed on wooden panels and canvases. The resulting colour of the paint with vivianite was usually blue (commonly in mixture with lead white, sometimes also with other blue pigments like azurite, smalt or ultramarine), more rarely green (e.g., in complex mixtures of pigments including yellow lake and yellow earth).

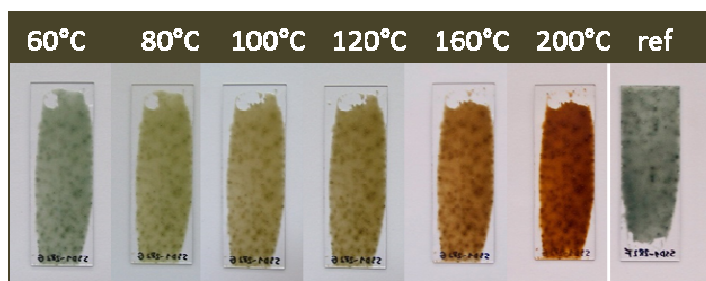


Fig. 1 - Temperature-related degradation of synthetic vivianite

Temperature-related degradation of pure synthetic as well as partly oxidised natural vivianite has been studied by high-temperature X-ray diffraction (HT-XRD) covering the whole extent of the temperature related stability of its structure. While temperatures around 70 °C are already damaging to vivianite, exposition to 160 °C results in complete amorphisation of both the vivianite and its oxidation products. As indicated by Mössbauer spectroscopy, temperature-induced oxidation of vivianite starts at 90 °C. To study the occurring structural as well as accompanying colour changes in more detail, model vivianite paint layer samples with different historic binders were prepared and subjected to increased temperatures. Exposition to 80 °C caused pronounced colour changes of all the samples: ground natural blue vivianite became grey – a colour change which has been described in actual works of art. Regarding the binders, the oil seemed to facilitate the transfer of heat to vivianite's grains. To simulate conditions of conservation treatment under which the painting is exposed to increased temperatures, oil-on-canvas mock-ups with vivianite were prepared and relined in a traditional way using iron. The treatment affected preferentially larger grains of vivianite; the micro-samples documented their change to grey, and their Raman spectra showed the change from vivianite to metavivianite.

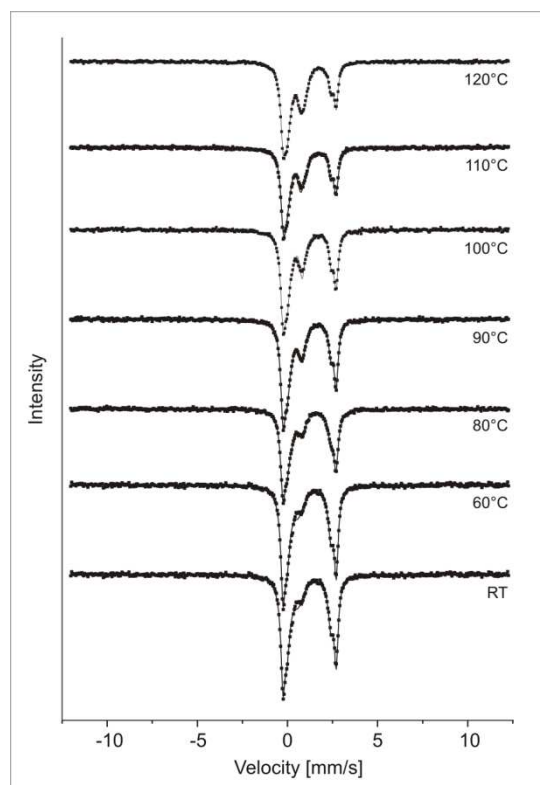


Fig. 2 – Temperature dependences of Mössbauer spectra of vivianite

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**Radiation Influence on Nanocrystalline Alloys**

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Influence of different types of radiation at nanocrystalline alloys were studied by Mössbauer spectroscopy. Electron-beam irradiation up to 4 MGy, neutron irradiation up to  $10^{17}$  neutrons/cm<sup>2</sup> and irradiation with Cu ions beam were applied. All types of irradiation had an influence on the magnetic microstructure and structural composition. The effect was manifested as a change in direction of the net magnetic moment, intensity of internal magnetic field and volumetric fraction. All these parameters could be determined from the measured Mössbauer spectra. The most sensitive parameter was the direction of the net magnetic moment with respect to the sample surface. The results indicated that the changes of the microscopic parameters induced by irradiation depend also on the content of the constituent elements and phase composition. The limit dose of radiation were set to values, at which the alloys do not show significant changes yet. Below these limits, the alloys can be considered to be radiation resistant. Results of nanocrystalline samples were compared with their amorphous precursors.

### From Surface-Enhanced Vibrational Spectroscopy to Vibrational Nanoscopy

Pavel Matějka<sup>1</sup>, Martin Král<sup>1</sup>, Alžběta Kokaislová<sup>1</sup>, Marcela Dendisová<sup>1</sup>, Marie Švecová<sup>2</sup>, Adéla Jenišťová<sup>1</sup>, Jiří Janoušek<sup>2</sup>

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Surface-enhanced vibrational spectroscopy (SEVS) is represented by two complementary techniques based on either surface-enhanced Raman scattering (SERS) or surface-enhanced infrared absorption (SEIRA) effect. SEVS techniques are valuable tools for physico-chemical studies of the metal-adsorbate interface and for analytical applications focused on detection of low/trace amounts of various substances. Nevertheless, their disadvantage is inadequate lateral resolution which is equal to the lateral resolution of corresponding “normal” Raman and infrared (micro-)spectroscopy limited by light diffraction. The irradiated surface area in usual SEVS micro-spectroscopic experiment contains relatively huge quantities of adsorbed molecules. However, for exact description of adsorption processes and intermolecular interactions, it is necessary to obtain spectra of single molecules and/or assemblies of several molecules, and thus the information obtained by classic SEVS methods is insufficient.

Techniques that offer the best lateral resolution are those integrating SEVS spectroscopic techniques with scanning probe microscopy (SPM), especially atomic force microscopy (AFM). The most important ones are tip-enhanced Raman spectroscopy (TERS) and scanning near-field infrared microscopy (SNIM). TERS combines SPM with Raman spectroscopy and enables both outstanding detection sensitivity down to single-molecule level and high spatial resolution down to sub-nanometers. Thus, TERS provides chemical information and morphological description about the nano-scaled surface simultaneously. The tips used in TERS are silver/gold or silver/gold-coated materials. The apex is usually only a few atoms wide, which makes it the dominant enhancing source of Raman signals. The electromagnetic field, arising in the close proximity of the tip apex on which the laser beam is focused, gives rise to the signal of molecules or even one molecule in this (near) field. The reliability of TERS results relies essentially on the stability and reproducibility of the TERS tips. In the case of SNIM, the source of irradiation is a tunable IR laser, adjusted to a specific wavenumber for an imaging/mapping experiment. The laser beam is focused to a space under the tip and coupled with tip oscillations. SNIM measurement reveals the chemical nano-scaled imaging information on the sample based on “distribution” of absorption and radiation phase shifts at the selected wavenumber for the molecules which absorb the radiation at this wavenumber and are located in the gap between the tip and supporting surface/substrate.

One-year experiences related to the TERS and SNIM studies performed on various model samples focused on either nanomaterial development or chemico-structural analysis of biologically relevant samples will be overviewed and discussed in this contribution.

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**Recent Developments in Laser Assisted Plasma Spectrometry**

Viktor Kanický, Karel Novotný, Markéta Holá, Michaela Vašinová Galiová, Tomáš Vaculovič, Aleš Hrdlička

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Laser assisted plasma spectrometry (LA-ICP-MS, LIBS) represents still vast area of fundamental and applied research and nowadays yields many useful advanced applications in elemental analysis of solid materials of various origin and matrix. For quantification, characteristics of laser-produced aerosol are of utmost importance and therefore, it is studied by means of various devices for particle size distribution measurement and microscopy techniques. As concerns nature of analysed materials, research and development is focused on spatially resolved analysis of soft and hard biological tissues, such as thin sections of tumours, animal tissues and plants, and biomineral-based parts. Analytical methods for monitoring the penetration of candidate anti-cancer drugs into cancer cells and to study mechanism of action of tissues and/or cultivated cells by LA-ICP-MS are developed. Local microanalysis of selected spots as well as elemental mapping of areas of interest in geological samples is performed by means of LA-ICP-MS. Archaeological samples, such as glass artefacts, are investigated. Besides LA-ICP-MS, laboratory-made LIBS facility in single- and double-pulse implementation is used in the analysis of some of above materials, for which contents of elements of interest are above detection limits of LIBS.

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## On the Use of Non-Routine Analytical Approaches for Understanding Chemical Speciation in Environmental Samples

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Increased attention is focus on the investigation of chemical speciation in various kind of environmental samples. The mechanisms of bio-transformation and translocation of selected species in e.g. soil, sediments, animal and plants tissues were evaluated on the basis of the analytical results towards obtaining complementary information of the biological and chemical characterization of the investigated objects.

Total content of elements of interest was determined by inductively coupled plasma mass spectrometry (ICP MS). High-performance liquid chromatography (HPLC), coupled to ICP MS, was used for the evaluation of chemical speciation for the compounds being identified by the know standards. In the case of unknown species the Orbitrap was validated and apply for the structural analysis of the extracted compounds. Moreover the isotopic profiles and isotopic ratio was monitored with the use of high-resolution ICP-MS. In this case species specific isotopic dilution MS procedure was used towards definite measurements for the certification of the chemical standard. Additionally, several imaging techniques were used for the investigation of the spatial distribution of the element of interest over the tissues and solids samples. The imagines from confocal and light microscopy were compared with the distribution maps obtained by LA ICPMS.

To conclude, in this presentation the advantageous of multi-technique approach towards obtain complementary information about selected environmental samples will be highlighted and exemplified.

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**Analysis of High Purity Advanced Materials: the Present-Day Importance  
of Wet-Chemical and Direct Solid Sampling Spectrometric Methods**

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Most modern technologies are based on the use of high and ultrahigh purity materials meeting specified purity requirements between 5N and 9N. For the challenging purity specifications at such extremely low concentrations, high performance analytical methods are needed providing required accuracies and LODs down to 10 pg/g level. Meanwhile, a number of spectrometric techniques based on various physical principles have become available for routine trace and ultra trace analysis of materials. The most of them can be used in connection with both the liquid sampling involving sample decomposition and often also analyte/matrix separation, and the direct solid sampling.

The applicability of atomic, mass and X-ray spectrometric methods based on liquid sampling of sample digests is, mainly due to the contamination risk, seriously limited, and is decreasing with increasing material purity grade. Nevertheless, working under cleanest conditions and meticulous optimization of the analytical procedure, in favourable cases for which examples will be given, LODs at the sub-ng/g level can be achieved under routine conditions. However, for the analysis of the majority of ultrapure materials, the application of wet-chemical spectrometric methods is seriously limited or not possible at all. Therefore, direct solid sampling graphite furnace atomic absorption spectrometry (SoS-GF AAS), solid sampling electrothermal vaporization inductively coupled plasma optical emission or mass spectrometry (SoS-ETV-OES/MS) and direct current high resolution glow discharge mass spectrometry (GDMS) have gained great importance.

During the last two decades, considerable progress has been achieved in the development of direct SoS-GF AAS and SoS-ETV-ICP methods for ultratrace analysis of advanced materials. In the determination of almost all analytes in a broad range of materials by these methods, good accuracies have been obtained by using calibration curves measured with aqueous standard solutions for quantification. Owing to nearly complete freedom of blank and application of sample masses up to several 10 mg per analysis cycle, for most analytes, LODs at the lower 10 pg/g range can be achieved. All these methods require the development of a matrix-specific procedure for each material. In some cases, a complete analyte release can be achieved only by using an adequate modification.

Of all currently available techniques for ultra trace analysis of conductive materials, GDMS is the most powerful and the most universal one. It provides the highest simultaneity, matrix universality, exceptionally large dynamic range, and LODs at lower ng/g and sub-ng/g levels. For analysis of h.p. non-conductive materials, several sample preparation techniques have been developed being capable of rendering final samples that are conductive. However, the sample preparation leads to significant reduction of the performance, especially to higher LODs.

The feasibilities, potentials and limitations of the routine methods will be discussed and their performance demonstrated by using selected examples.

## **ABSTRACTS OF ORAL LECTURES**

## Inductively Coupled Plasma Optical Emission Spectroscopy with Electrothermal Vaporisation: An Effective Tool for Direct Multielemental Analysis of Biological Samples

Stanislava Matějková<sup>1</sup>, Luisa Šerá<sup>1,2</sup>, Martin Loula<sup>2</sup>, Jan Mengr<sup>3</sup>

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Solid sampling electrothermal vaporization (ETV) inductively coupled plasma optical emission spectroscopy (ICP-OES) is an analytical method providing simple and rapid multi-elemental analysis of major, minor and trace elements without the need for pre-treatment (such as mineralization) of solid or liquid samples. Therefore, by comparison with more common ICP-OES combined with a solution nebulization, the risk of contamination of analysed samples is reduced. Furthermore, the detection limits and the sample quantity needed for analysis by means of ETV-ICP-OES decrease as a result of the almost complete transport of the sample aerosol into the ICP torch. The connection of ETV unit to simultaneous ICP-OES instrument capable of rapid transient signal processing allows us the fast direct analysis of numerous samples. The technique enabled the combined, matrix-matched or matrix-free calibration with home-made or certified solid and aqueous standards. Hence, ETV-ICP-OES is a powerful analytical method for environmental, forensic, biomedical and/or clinical applications where only very small amounts of material (a few milligrams or less) are available for sampling. In our IOCB analytical service laboratory, the methodologies were developed for the following studies:

1/ Only boron or together boron and cobalt contents were directly estimated in fresh frozen mice tissues (serum, brain and liver) for tracking the carboran-based candidate-drugs time dependent concentration and for their pharmacokinetic evaluation.

2/ The amounts of heavy metals and other elements in the collected insect samples from both polluted postindustrial and healthy areas were determined. Based on the use of also atypical, less sensitive lines, the simultaneous analysis of macro- and trace-elements is possible. 44 separated analytical lines for totally 18 elements (Ag, Al, As, Ba, Ca, Cd, Co, Cr, Cu, Fe, Hg, Mn, Ni, Pb, Se, Sr, V a Zn) were simultaneously monitored, calibrated and used for measurement of about 1-mg dried and grounded insect sample aliquots.

3/ A method for determination of biologically important major (Ca, K, Mg, P, S) and minor elements (Ba, Co, Cu, Fe, Mn, Na, Se, Sr, Zn) in plants from selenised and untreated fields was developed.

4/ The method was used for metal impurities determination in derived graphene material and for controlled purification of defined amounts of this special substance.

The LODs' in all developed applications ranged from 0.001 mg/kg for trace metals (e.g. Co) to 304 mg/kg for K in dry plant material (measured concentration values in % range). The typical RSD values were less than 10 % depending on material homogeneity (usually under 5 %) and the recovery obtained by certified material analysis was in the range 82 – 115 %.



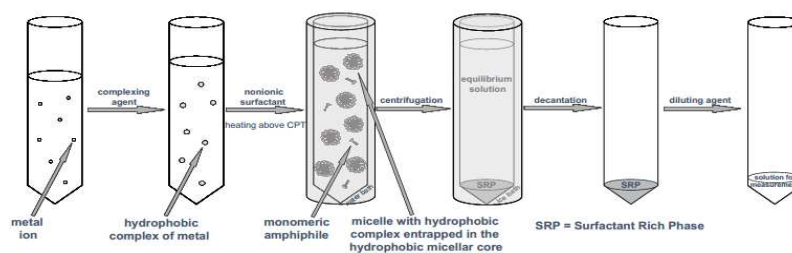
## Separation and Preconcentration of Ultratrace Elements by Using New Modes of Cloud Point Extraction: Utilizable in Connection with Spectrometric Methods

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In recent years, cloud point extraction (CPE) has become widely utilized for separation/preconcentration of (ultra)trace elements. CPE uses the property of nonionic and zwitterionic surfactants in aqueous solutions to create micelles and to become turbid when heated to particular temperature, so-called cloud point temperature. Above this temperature, the micellar solution separates into two phases: a surfactant-rich phase of a small volume, and a diluted aqueous phase. Conventional CPE needs to be heated in water bath to realize cloud point phenomenon (see Fig.1). This CPE procedure has many steps, which makes it quite time- and labor-consuming. Recently, researchers constantly looking for ways to improve conventional CPE in order to shorten procedure time and reduce steps needed or to improve selectivity. On the other hand, longer procedures such as the conventional CPE have been proposed to overcome troubles with organic solvents (which are used for the dissolution of the surfactant-rich phase). In this contribution, theoretical principles and practical designs of conventional CPE will be explained together with new approaches to the CPE procedures such as displacement CPE, rapidly synergistic CPE, dual CPE, ultrasound-assisted CPE, microwave-assisted CPE, and flow-based CPE [1]. Examples from the literature to illustrate the use of these extractions for separation/preconcentration of (ultra)trace elements before their spectrometric determination will be also presented.



**Fig. 1.** Schematic representation of a conventional cloud point extraction.

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## Dielectric Barrier Discharge Plasma Atomizers of Volatile Compounds in Atomic Absorption Spectrometry: Applications, Mechanisms and Future Perspectives

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Plasma devices based on dielectric barrier discharges (DBD) can be used in many applications in analytical spectrometry including atomizers of volatile compounds in atomic absorption (AAS) and fluorescence (AFS) spectrometry. The fundamental drawback of all the present DBD works dealing with DBD atomizers of volatile compounds is that they include only optimization of the basic DBD parameters followed by analytical figures of merit quantified for the DBD atomizers only. Neither comparison to any reference atomizer employing the same detector is presented, nor are results of interference studies reported. No effort is made to quantify atomization efficiency in DBD and atomization processes in the DBD plasma are not understood. As a consequence, it is difficult to judge the applicability of the methods reported with such a limited amount of information.

Atomization of five hydride forming elements has been investigated in detail using the same hydride generator, DBD atomizer and AAS detector making thus the results fully comparable. Moreover, the performance of the novel DBD atomizer was compared to that of a routine externally heated quartz tube atomizer (QTA). The effects of DBD power, discharge gas nature and its flow rate as well as modification of inner surface on analyte response in AAS were investigated for Bi, Sb, Se, As and Pb. Analytical figures of merit have been subsequently studied in the DBD atomizer for all individual elements followed by comparison of the results with those reached in QTA. Argon was found as the best discharge gas. A significant increase in sensitivity was observed for Bi and Pb in a DBD atomizer with its inner surface treated by a silanization agent (dimethyldichlosilane - DMDCS). Optimum atomization conditions for individual elements will be presented and detection limits reached in DBD and QTA atomizers under optimum atomization conditions will be compared. The results reached demonstrate that the detection limits between DBD and QTA atomizers are comparable (As, Se, Sb), whereas worse LOD (by a factor of 2-5) is reached for Pb and Bi in DBD, respectively. The interference studies indicate the resistance of the DBD towards interferences of other hydride forming elements is comparable or slightly better than in QTA. As a consequence, DBD atomizers seem to be promising alternative to QTA.

Mechanism of hydride atomization in the DBD was explored by a number of spectrometric techniques. The role of hydrogen radicals during atomization in a DBD plasma will be discussed and atomization efficiency of individual analyte hydrides will be assessed. Possibility of *in situ* preconcentration of hydrides in DBD will be presented.

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**Sample Preparation for Determination of High Iodine Levels by ICP-OES**

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Ambient levels of iodine in Europe range within 0.02 – 0.1 mg/kg dry mass, but items of suspiciously high iodine content (e.g. some algae) have to be controlled by food control for reasons of toxicity. The ICP-MS, which is the usual equipment for ambient iodine levels, has a strong memory in case of high iodine levels, thus a preliminary screening by ICP-OES seems useful. The emission line at 178 nm is not really sensitive (DL about 0.1 µg/ml), and is largely overlapped by a neighbouring P-line. Because in biological materials, always much more P than I has to be expected, a separation seems mandatory. After digestion with  $\text{KClO}_3\text{-HNO}_3\text{-H}_2\text{O}$ , all iodine is present as non-volatile iodate in acid solution. The test solution was put to a centrifugation tube, Al-sulfate or Fe-chloride added, and phosphate co-precipitated with Al- or Fe-hydroxide by addition of ammonia. In alkaline solution, iodate is not adsorbed at the precipitates, which can be removed by centrifugation. The solution can be transferred to another test tube to be measured by ICP-OES, which shows significant reduction of the P-peak, ready for correction calculations. Conditions of precipitation, and tests with real samples, will be given.

## Application and Development Sequential Extraction Procedures for Fractionation of Heavy Metal Content of Soils, Sediments, and Gravitation Dusts

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Risk assessment of potentially toxic element (PTE) contamination in environmental systems can be estimated by fractionation with sequential extraction procedures based on modeling the environmental mobilization pathways [1]. In Europe mostly the BCR (Community Bureau of Reference) procedure is applied which was issued in 1993 and modified in 2001. This is only the fractionation procedure to which certified reference material (BCR 601 and 701) was issued for fractionation of six PTE (Cd, Cr, Cu, Ni, Pb, Zn) in aquatic sediments [2]. For fractionation of PTE content of soils and sediment CRM is not available. The BCR batch leaching methodology is very labour and time consuming and does not keep the PTE-species intact and due to the many operations and application of several extractant reagents there is a significant risk of laboratory-contamination and matrix effects during the extractions and spectrochemical element detection. In the lecture a summary will be given of a forty years research cooperation between TU Kosice and Szent István University in the field of improvement of PTE analysis in solid environmental samples (gravitation dust, soils, aquatic sediment, biofilms). Started from solid sample spectrochemical methods the sequential extraction methodologies were developed. The important results of these developments: (1) acceleration of BCR methodology by sonication; (2) elaboration of continuous flow extraction methodology and (3) the optimization of ICP-OES multielemental calibration for different extraction matrices will be discussed.

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## Study of Stainless Steel LC200N by Mössbauer Spectrometry

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Mössbauer spectrometry (MS) is particularly suited technique for characterization of steel materials and for determination of iron compounds in these materials. MS can determine arrangement of iron lattice (fcc – face-centered cubic, bcc – body-centered cubic) as well as iron oxidation state. Element characterization was performed by neutron activation analysis (NAA) and X-ray fluorescence (XRF).

In this work, we focus on characterization of LC200N stainless steel by back-scattering Mössbauer spectrometry. This geometry was used due to high thickness of samples (0.5 mm). We investigated the effect of thermal treatments and surface treatment. Our disc-shaped samples were cut off from three original rods with different thermal history: non-hardened, hardened and hardened with subsequent rapid quenching. Each sample was polished from one side to see the different properties of polished and “as cut” sides. By parameters of the Mössbauer spectra taken from both sides of the investigated samples we were able to identify variations in the microstructure imposed by different thermal and surface treatments.

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## Mössbauer Spectrometry Applied to Biological Samples

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Mössbauer spectrometry is a very sensitive technique used for study of iron electronic and magnetic structures in various materials. The Mössbauer parameters such as isomer shift ( $IS$ ), quadrupole splitting ( $QS$ ), magnetic hyperfine field ( $B_{hf}$ ), linewidth ( $\Gamma$ ) provide valuable information about the state and local environment of the  $^{57}\text{Fe}$  resonant nuclei. Application of Mössbauer spectrometry to the study of iron containing biological molecules was very useful in understanding the structure-function relationship [1–4].

In this contribution, properties of iron in various samples of biological tissues were analyzed from the point of view of their magnetic properties and structural positions. In doing so,  $^{57}\text{Fe}$  Mössbauer spectrometry in transmission mode was applied. Absorption Mössbauer spectra have been measured directly on lyophilized tissues of human brain, human and horse spleen. Mössbauer measurements were performed at room temperature (~300 K) and at the temperature of 4.2 K using liquid helium bath cryostat. Each spectrum obtained at room temperature exhibits doublet-like features which indicate a presence of very small non-magnetic particles. Low-temperature Mössbauer spectra are superpositions of sextets and one doublet. Spectral parameters of the sextet-like components are similar to those for hematite, ferrihydrite or possibly magnetite.

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## Hyperfine Interactions of Disordered Alloys Probed by Nuclear Resonances

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Metallic glasses (MGs) are typical representatives of disordered alloys. They exhibit amorphous structure that is lacking any long-rang order. Because of this and taking also into consideration their unique soft magnetic properties that are governed by appropriate chemical composition MGs are suitable candidates for magnetic shielding, transformer cores, sensors, etc. Because the beneficial soft magnetic properties of MGs are closely related to their structural arrangement it is inevitable to understand fully the ways how and under what conditions the originally amorphous material undergoes structural transformation which could eventually lead to their partial crystallization. It is noteworthy that formation of crystallites might severely deteriorate the desired magnetic parameters. That is why this process is studied to fine details by employing thermal treatment upon the MGs.

It is possible to follow the formation of crystalline phases by several analytical techniques comprising X-ray diffraction, differential scanning calorimetry, transmission electron microscopy or via magnetic measurements. Only few of them (e.g., DSC or magnetic measurements) however, provide a direct *in situ* investigation in real time. And even if such experiments are performed we do not have unambiguous information on the type of the newly formed crystalline phases.

The above mentioned drawback is overcome by the use of synchrotron radiation featuring extremely high brilliance. Because of a high photon flux the time needed for data acquisition is short enough to ensure sufficient statistics. Consequently, structural transformation from amorphous into crystalline structure can be followed in real time during continuous increase of the measuring temperature. In this presentation, evolution of crystallization in selected MGs will be demonstrated using a method of nuclear forward scattering (NFS) of synchrotron radiation [1-3]. This method scans the local surroundings of resonant <sup>57</sup>Fe nuclei in time domain. Along with description of structural arrangement also information on magnetic states of the investigated material is available. The presented results will be complemented by findings from <sup>57</sup>Fe Mössbauer spectrometry which uses the same principles as NFS but works in energy domain.

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**Neutron Activation Analysis of Steel Samples  
at the VR-1 Training Reactor and NG-2 Cyclotron-Based Neutron Generator**

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Neutron activation analysis (NAA) is a radioanalytical method that makes it possible to study chemical compositions of unknown samples after irradiation in a neutron field [1]. Together with the nuclear gamma-ray spectroscopy technique [2], it is widely used at the research nuclear reactors and accelerator-driven fast neutron sources. The neutron activation method is often utilized as a primary technique for neutron field spectrometry and neutron beam monitoring at nuclear facilities. At the VR-1 training reactor of the Czech Technical University in Prague [3], the NAA with gamma-ray spectrometry is also successfully employed to study historical coins, meteorites, and dietary supplements.

Within this work, the qualitative method of NAA was used for investigation of the composition of steels. Several kinds of steels were irradiated in the vertical channel of the VR-1 training reactor with a thermal neutron flux up to  $10^9$  n/cm<sup>2</sup>s. For comparison, the selected samples were also irradiated in a neutron field from the accelerator-driven fast neutron source NG-2 (thick beryllium target) of the Nuclear Physics Institute of the CAS [4] with a neutron flux of  $10^{11}$  n/cm<sup>2</sup>s (the integral neutron fluence of  $10^{16}$  n/cm<sup>2</sup> at the sample position). After irradiation at the reactor and neutron generator, the induced radioactivity of the steel samples was repeatedly measured by calibrated semiconductor HPGe detectors. The observed gamma-lines were identified on the basis of their energies, intensities, and half-life periods. In total, up to 25 reactions products were observed in gamma-ray spectra.

The irradiation experiments performed at the VR-1 training reactor and using the NG-2 fast neutron generator will be described, and the obtained results will be discussed in details.

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## The Effect of Water on Structural Transitions of 1-Butyl-3-Methylimidazolium Chloride as Investigated by Vibrational Spectroscopy and WAXS

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Ionic liquids are a promising alternative to the currently used cellulose solvents – they are more environmentally friendly but still costly. In ionic liquids, water is often present as an impurity; when more water is added, it can act as a co-solvent or as an anti-solvent during the dissolution process. The work, that will be presented, attempts to relate molecular-level events (such as change in ionic liquid conformation and in cation–anion and ion–water interactions) to the changes in macroscopic behavior of 1-butyl-3-methylimidazolium chloride (bmimCl) upon addition of water.

We have kept neat bmimCl and bmimCl/water mixtures at the temperature of  $-25\text{ }^{\circ}\text{C}$  for prolonged periods of time and then investigated the process of bmimCl crystallization by Raman and infrared spectroscopy and WAXS. Neat bmimCl crystallized in a monoclinic lattice denoted as M0. In samples with water concentrations 0.4 and 2.9 wt %, a metastable monoclinic form, denoted as M, was detected. The metastable form later converted into the monoclinic form M0 (0.4 wt % of water) or into an orthorhombic form O (2.9 wt % of water). The liquid–solid and the solid–solid transitions in the two mixtures were accompanied by a phase separation into a water-rich phase and a phase enriched in bmimCl. The hydrodynamic phenomena during the phase separation created local stresses on the newly formed crystallites of bmimCl, which led to formation of the metastable crystal form M. Raman spectroscopy showed that the conformation of the butyl group in the bmim cation was gauche–anti for the crystal form M0 and anti–anti for the orthorhombic form O. The differences in the conformation and crystal forms adopted in mixtures with different content of water were ascribed to the effect of capillary forces and H-bonding on the liquid–solid and solid–solid transitions. Infrared spectroscopy in combination with quantum chemical calculations confirmed changes in the strength of hydrogen bonds between chloride anion, bmim cation, and water.

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**Chiroptical Properties of the Antimicrobial Peptide *Lasiocepsin* and of its Analogs**

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We report chiroptical properties of the novel antimicrobial peptide (AMP) lasiocepsin (LAS, 27As) containing two disulfide bridges [1] and of its three analogs designed to study the influence of heterodetic disulfide-closed rings. The set of peptides included the natural LAS (H-Gly-Leu-Pro-Arg-Lys-Ile-Leu-Cys-Ala-Ile-Ala-Lys-Lys-Lys-Gly-Lys-Cys-Lys-Gly-Pro-Leu-Lys-Leu-Val-Cys-Lys-Cys-OH), two analogs with just one disulfide bridge and the remaining two cysteines replaced by alanine residues (Las[Cys17-Cys27, Ala8,25] – LAS 2; Las[Cys8-Cys25, Ala17,27] – LAS 3), and a linear analog having all four cysteines replaced by alanines (Las[Ala8,17,25,27] – LAS 4A). LAS 2 retains reduced activities against common pathogens while LAS 3 and LAS 4A are inactive [1]. The effect of changing the disulfide bridge pattern on secondary structure is investigated by electronic circular dichroism (ECD) and vibrational optical activity (VOA) including Raman optical activity (ROA) and vibrational circular dichroism (VCD). A combination of these techniques helps us to clarify the role of disulfide bridges in stabilization of LAS's conformation. ECD indicates similar conformation of the disulfide bridge for analogs containing one disulfide (LAS 2, LAS 3), while ROA enables us to determine sense of disulfide torsion, even in the more complicated case of natural LAS containing two disulfide groups. The experimental mainly ROA results were compared to theoretical spectral dependences which were based on known NMR structure of natural lasiocepsin [2].

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## Enhanced Raman Spectra of Ag-Ethanethiolate and Graphene from Graphene/Ag-NPs-Ethanethiol Hybrids: Interplay between Surface- and Graphene-Enhanced Raman Scattering

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SERS spectroscopy of molecules on plasmonic metal nanostructured surfaces is currently a well established spectroanalytical tool [1]. By contrast, the ability of single layer graphene (SLG) to enhance Raman spectra of some aromatic molecules (denoted as GERS) has been only recently explored and reviewed [2]. Furthermore, the ability of SLG to enhance SERS of an aromatic molecule by factors of 3 – 9 has been reported as well [3]. In this contribution, we report enhanced Raman spectra of Ag-ethanethiolate species and SLG obtained from the glass/SLG/AgNPs-ethanethiolate film hybrid systems at 445, 532, 633 and 780 nm excitations, and their comparison to those of the appropriate reference systems. The 2-dimensional (2D) AgNPs-ethanethiol films were prepared according to [4]. Raman spectra obtained from glass/AgNPs-ethanethiol film hybrids provide evidence for Ag-ethanethiolate surface species formation and indicate its pronounced SERS enhancement. Excitation wavelength dependence of Raman spectra of Ag-ethanethiolate species and of SLG obtained from the glass/SLG/AgNPs-ethanethiol samples in the straightforward geometry (i.e. with the AgNPs-ethanethiolate film on the top) has revealed that at 633 and 532 nm excitations, the 2D mode of SLG experiences SERS enhancement by factors 6 and 4, respectively. Interestingly, the Raman modes of the Ag-ethanethiolate species experience an additional, SLG induced enhancement of their SERS by an average factor of 4 at both these wavelengths, although the species does not fulfill the conditions for GERS [2]. By contrast, the inverse geometry (ie. SLG on top) measurements of the same sample revealed vanishing of the additional enhancement of SERS of Ag-ethanethiolate, together with the increase of the SERS enhancement of 2D mode of SLG to the factor of 18 at 633 nm excitation. The reason of this rather complex interplay between SERS and the graphene-induced enhancement can be tentatively attributed to the amplified photoresponse of SLG [5] (namely the reflectance) induced by the optical near field formed by the resonance excitation of surface plasmons in the 2D Ag NP assembly. This explanation is supported by the reference experiment in which an average additional enhancement of Ag-ethanethiolate SERS by a factor of 40 has been achieved by deposition of the AgNPs-ethanethiol film on a strongly reflecting Al mirror.

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## Synthesis and Analytical Applications of CdTe-QD's Nanoparticles

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The recent nanotechnological methods enable the assembly and characterization of well-defined objects in nanometer scale. The quantum-dot (QD) colloid particles of diameter 1-10 nm are usually low-soluble CdTe compounds and their solubility is increased by surface covering of thiol containing compounds (*e.g.* mercaptopropionic acid) and also by increase of solution pH which leads to dissociation of functional carboxylate and/or protonated amine groups. Their exceptional physico-chemical and optical properties as well as higher photostability compared to organic fluorophores can be used for development of new analytical methods for the detection and determination of ions and molecules important in biology and medicine. QD-based nanoparticles exhibit broad excitation and narrow emission band where their position depends on their kind, morphology and size and thus the maximum of emission band can be tuned by synthetic process.

This contribution deals with synthesis and characterization of various QD-CdTe nanoparticles covered by thiol containing compounds (*e.g.* mercaptopropionic acid, dimercaptosuccinic acid, glutathione, cysteine, 2-mercapto-ethanesulfonic acid *etc.*). The physico-chemical processes of nanoparticles in presence of Cu(II) and Pb(II) ions were studied and some of them were employed for their analytical determination by means of laser-induced luminescence spectroscopy. The analytical procedure was optimized for experimental conditions (*e.g.* pH, concentration of nanoparticles and analyte) and then it was utilized for determination of both metal ions in water samples. The proposed simple and fast method can be employed for environmental analysis.

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## Interpretation of Raman Spectra Depth Profile of Weathered Glass Surface by Advanced Statistical Methods

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The stratified structure of glass weathered surface was studied by Raman spectra depth profiling [1]. The series of Raman spectra of weathered barium crystal glass surface were recorded with different focusing depth level ranging from surface level to 5-7  $\mu\text{m}$ . After the baseline subtraction and thermal correction the number of independent spectral components was determined by the Principal Component Analysis (PCA). Then the spectra of pure components (so called loadings) and their relative abundances (so called scores) were determined as a function of focusing depth by the multivariate curve resolution method (MCR) [2-4]. The proposed treatment allows the study of corrosion/weathering products with very small dimensions (small lateral dimensions and small thickness) not allowing recording of pure individual Raman spectra.

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## Application of FTIR Spectroscopy in Soil Water Repellency Assessment

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Soil is a very complex medium consisting of several constituents that affect the spectral reflectance of soil. Based on the chemical and physical composition, different soils have specific absorption of reflection at different wavelengths [1]. Soil is a highly complex and variable material, consisting of a solid phase comprised of inorganic rock particles and organic materials, a soil solution containing dissolved solutes and a gas phase [2]. It can range from a mineral soil with almost no organic matter present to an entirely organic soil or peat. Soil constituents affect the spectral reflectance of soil; based on the chemical and physical composition, different soils have specific absorption of reflection at different wavelengths [1]. Even some soil properties, such as moisture content, soil organic matter content, particle size and surface conditions, have been found to affect the spectral reflectance of soils, but general behaviors are usually not possible to conclude [3]. The previously mentioned properties belong to those soil water repellency is closely related to. Fourier transform infrared (FT-IR) spectroscopy is a method with a lot of advantages. It allows characterization of very small samples of material, requires relatively simple sample preparation, it is non-destructive, rapid, low cost, and can be performed in laboratory as well as in field conditions. It provides detailed qualitative and quantitative chemical information about both the organic and inorganic components in a sample. This is highly advantageous for soil because it means that from a single IR spectrum, aspects of the mineralogy and the nature of the soil organic matter present can be determined [4]. Besides being widely used for soil quality assessment (i.a. for evaluation of hydrophobic/hydrophilic organic components in soil), FT-IR is also involved in soil environmental monitoring and in forensic examination of soil evidence.

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**Determination of Some Elements in Samples of Emissions by ICP-MS**

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Mass spectrometry is an advanced analytical methodology for determination of the concentration of elements in samples with various matrices and low detection limits. Typical applications for this instrument: determination of trace element in water, food, pharmaceutical and biological materials, determination of species toxic elements and isotopes identification.

This work describes preparation and validation of the method for determination of As, Be, Cd, Co, Cr, Cu, Mn, Ni, Pb, Sb, Se, Sn, Te, Tl, V and Zn in samples of emissions from stationary sources of air pollution [1, 2]. The sample is withdrawn isokinetically from the source. Particulate emissions are collected in the probe on a heated filter. Gaseous emissions are then collected in an aqueous-acidic solution of hydrogen peroxide [3]. The recovered samples are digested with acids and diluted before analyses. The absorption solutions are directly analyzed by inductively coupled argon plasma – mass spectrometer Agilent 7900 ICP-MS. The sample which contains more than 100 µg /l of the analyte is diluted to that level, or below, for the final analysis [2, 3]. Instrument uses octopole reaction system (ORS) which eliminates almost all molecular interferences. He collision mode is the standard operating mode for the ORS. Collision effects are the major factor for interferences removal [1]. Method validation was performed using commercially available reference materials. Accuracy, precision and limit of detection analyzed elements are satisfied the requirements of Decree no. 410/2012 Coll. as amended Ministry of Environment of the Slovak Republic, which implements certain provisions of the Clean Air Act.

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## Multi-Element Analysis in Complicated Sample Matrices Utilizing Single-Set Experimental Conditions of ORC-ICP-QMS

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Collision-reaction cells are accepted as the preferred means for removing of spectral interferences in quadrupole ICP-MS [1, 2]. However, only the octopole cell of the 3<sup>rd</sup> generation (ORC) allows its use by single-set experimental conditions for many selected analytes across diverse range of sample matrices.

In this work is presented optimization of ORC experimental conditions, for different concentrations of tested isotopes, in real and model sample matrices, using the inert collision cell gas (He), and operating in the mode of kinetic energy discrimination. Influence of He flow-rate on the background-equivalent concentration (BEC) of isotopes in the mass range from 7 to 208u has been studied.

Multi-element analysis of creek-, seepage- and acid mine waters from Slovakia was realized, research-interesting elements were determined (Li, Na, Mg, Al, K, Ca, Cr, Mn, Fe, Co, Ni, Cu, Zn, As, Se, Sr, Mo, Cd, Sb, Ba, Pb) and basic validation characteristics were estimated. The optimal operating conditions of ORC, with chosen He flow-rate of 4.3 mL min<sup>-1</sup>, ensured the reduction of majority polyatomic ions, caused no reactive loss of analyte signal, and meant also improvement of BEC and the next validation and calibration parameters.

Accuracy was evaluated by recoveries of the SRM analyses (98-103 %) and by comparison with the reference method analysis, atomic absorption spectrometry (98-104 %). Precision, evaluated by repeatability was ranged from 0.03 to 10 %.

The used external analytical calibrations were linear, and chosen working ranges were 0-5 mg L<sup>-1</sup> for Li, Na, Mg, K, Ca, and 0-100 µg L<sup>-1</sup> for the others studied elements. Limits of detection (3σ-criterion) have varied from 0.24 ng L<sup>-1</sup> (for cadmium) to 0.062 µg L<sup>-1</sup> (for selenium), in the calibration range 0-100 µg L<sup>-1</sup>.

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## Utilization of Computed Tomography and Laser Spectroscopy for 3D High Resolution Mapping

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The simultaneous utilization of analytical techniques, Laser-Induced Breakdown Spectroscopy (LIBS) and X-Ray Computed micro-Tomography ( $\mu$ CT), proved to be powerful in visualizing the sample structure together with chemical mapping. The relative simplicity of the LIBS and  $\mu$ CT techniques makes their synergy very attractive for a large variety of applications. Their capability to provide 3D high resolution mapping was verified for the use in i) clinical research and ii) geology.

Firstly we demonstrated the 3D visualization capabilities in the analysis of soft tissues. Special emphasis was given to provide the distribution of Gd nanoparticles administered in murine organs. Thus, this combination enables a novel analytical approach how to quickly visualize and recognize different elements in soft tissues and can in turn induce a significant breakthrough in clinical research. In the second application, the simultaneous application of LIBS and  $\mu$ CT was tested for 3D visualization of Pt distribution in selected mineral. In both applications, the resulting  $\mu$ CT scans and LIBS chemical maps were successfully combined to prepare 3D chemical map of the sample together with its structure.

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## Evaluation of Mercury Immobilisation and Transformation Processes in the Soil – Plant – Microscopic Filamentous Fungi System Using CV AAS Method

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The aim of this work is geochemical evaluation of transfer and phytotoxicity of mercury bioavailable species from contaminated soil in selected plant species, study of mercury phytoavailability in these soils using chemical and biological separation techniques and study of mercury biotransformation by chosen microscopic filamentous fungi species. Study of mercury biogeochemistry in soil – plant system contaminated with water-soluble mercury under laboratory conditions (up to 130 mg.kg<sup>-1</sup> Hg) showed, that despite high mercury sorption capacity of this soil ( $S_{\max} = 13.2 \text{ mg.g}^{-1} \text{ Hg}$ ), the absence of the mercury ageing process in the soil resulted in extreme mercury translocation and accumulation in barley shoots (*Hordeum vulgare* L.) (up to 195 mg.kg<sup>-1</sup> Hg). Mercury phytotoxicity effects in barley biomass were also observed. On the other hand, laboratory and field cultivation of barley in the aged soils and analysis of selected wild and culture plants from mercury-contaminated area (up to 30.9 mg.kg<sup>-1</sup>) showed low mercury bioavailability in such environment (barley shoot mercury accumulation only up to 0.07 mg.kg<sup>-1</sup> Hg), where mercury exists predominantly in stable form. Study of selected chemical and biological separation techniques suitability for soil mercury phytoavailable fraction content evaluation in aged mercury-contaminated soils indicated us extractions with microbial metabolites of microscopic filamentous fungi, especially *Alternaria alternata* and *Cladosporium* sp., synthetic rainwater and diffusive gradient in thin films technique appropriate for this purpose. Laboratory cultivation of various microscopic filamentous fungi isolates from both aged mercury-contaminated and non-contaminated soils on culture medium contaminated with water-soluble mercury showed us the dominant role of biovolatilization processes in mercury resistance strategy of microfungi. *Aspergillus niger* and some of *Cladosporium cladosporioides* isolates volatilized almost 80 % of total mercury in culture medium also at highest initial mercury concentration (32.7 mg.l<sup>-1</sup>). High rate of biovolatilization in mercury resistance strategy of microfungi isolates, especially those of *A. niger* and *C. cladosporioides*, indicates the potential of these fungi utilization in remediation techniques.

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## Application of Laser Ablation Sampling for the Multielemental Analysis of Dinosaur Skeletal Remains: a Diagenetic Study

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Laser ablation-inductively coupled plasma-mass spectrometry (LA-ICP-MS) has become a powerful technique of trace element microanalysis, as it offers high sensitivity, low limits of detection, multielemental capability, high spatial resolution and minimal sample preparation. These features represent invaluable merits for determining elemental distributions and contents of selected elements in fossil skeletal remains. Fossil skeletal tissues, including teeth and bone, provide information about, for instance, diet, migration/mobility, physiology, taphonomy, diagenesis, paleo-environmental reconstructions and paleo-redox conditions. Mineral phase of skeletal tissues is hydroxyapatite, however, it could be modified *via* substitutions by cations and/or anions during diagenesis. These *post-mortem* changes depend on many factors (properties of skeletal tissue and surrounding natural conditions).

In dinosaur skeletal remains originating from Mongolia, high total levels of REE (up to units of % m/m) as well as presence of various mineral phases were observed. Positive and/or negative Ce anomaly was found out depending on analyzed phase. Elemental association was revealed in particular mineral phases. The obtained information about elemental contents, distributions and associations in analyzed fossils can be used to determine the level of diagenesis. As a comparative method, Electron Micro Probe Analysis (EMPA) was applied to verify LA-ICP-MS results.

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## Prediction of Bioavailability of Metals in Aquatic Systems: Comparison between Diffusive Gradient in Thin Films Technique and Living Organism

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The metal bioavailability and bioaccessibility in environment are critical to the risk assessment process. There is, therefore, great interest in finding efficient environmental monitoring methods for their determination. Analytical testing of chemical pollutants based on various separation and leaching procedures provides a simple classification of water, soil and sediment metal fractions, but these are based on arbitrary responses to chemical reagents and do not provide information on the potential impact of pollution on resident organisms. Therefore, there is a need for a simple procedure which reliably estimates metals accessibility and predicts the uptake of toxic metals by plants and animals. There is, thus, an ever increasing interest in using biomonitoring methods such as analysis of organisms that are bioaccumulators. However, it is not generally assumed that different organisms transport metals by the same mechanisms and the transport is affected by external environmental conditions. A lack of understanding of the basic physiological, biochemical, and molecular mechanisms prevents the correct evaluation of their influence on metal transport to living organisms. Therefore, new approaches are still being sought to obtain a better characterization of bioaccessible forms of metals and their transport to the living specimen. An *in situ* technique known as Diffusive gradient in thin films technique (DGT) capable of quantitatively measuring labile metal species in aqueous systems has been developed [1-3]. This technique working on principle of Fick's 1<sup>st</sup> law of diffusion is based on a simple tight-fitting piston designed assembly that accumulates metal ions on a selective binding cation-exchange resin, immobilized in thin layer of hydrogel, after passage through a well-defined diffusion layer.

The lecture presents some of our results focused on the relationship between concentrations of metals measured by DGT and their elevated levels in aquatic moss (*Frontinalis antipyretica*), terrestrial plants (*Raphanus sativus*, *Taraxacum officinale*) and fishes (*Cyprinus carpio* L.). Our results demonstrate that DGT predicts metal uptake by living organisms and can be used as physical surrogates for plant and fish metals uptake. And so DGT offers the possibility of simple test procedure for metal bioavailability assessment.

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## Analytical Methods for Iodine Determination in Environmental Samples

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Iodine is an essential micronutrient for most living being including humans. In spite of various efforts through various iodine deficiency disorders elimination programs such as salt iodization, iodine deficiency disorders still persist [1]. Sub-clinical deficiencies of iodine often have endemic character and are characteristic to a certain area where iodine is deficient or inaccessible in the geochemical environment, especially in soil or drinking water or food [2, 3]. Therefore iodine distribution in content in soils, plants and other environmental matrixes is a long term interest of environmental chemistry, environmental and medical geochemistry.

Extraction and fractionation of naturally occurring iodine from these matrixes followed by spectroscopic determination is the most used method for iodine determination. Nowadays, iodine determination by inductively coupled mass spectrometry (ICP-MS) is the most common and reliable method of total iodine content determination in environmental samples and foodstuff, although other methods such as liquid or gas chromatography which besides iodine quantification enable to distinguish individual iodine species.

The aim of this work is to summarize the most widely used analytical and sample preparation methods for iodine determination in environmental matrixes focused on soil and plant tissues.

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## Application of Spectroscopic Methods for Evaluation of Toxic Metals and Metalloids Mobility in Defined Multicomponent Systems During Static Cultivation of Common Fungal Strains

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Manganese and ferric oxides significantly participate in redox and sorption reactions over a wide pH range in soils and sediments. Therefore, they are recognized as an important natural geochemical barrier due to their ability to scavenge various elements and compounds, including antimony (Sb). Therefore we evaluated fungal manganese and ferric oxides biodeterioration and its effect on Sb mobility, bioavailability, accumulation and volatilization by common soil fungus *Aspergillus niger* using atomic absorption spectroscopy, as well as X-Ray diffraction analysis and Mössbauer spectroscopy. XRD identified manganese oxides as hausmannite and amorphous characteristics of ferric oxides. After cultivation, hausmannite was bio-transformed into manganese oxalate (lindbergite), while amorphous characteristics of ferric oxides were not changed. Presence of ferric and manganese oxides significantly reduced adverse antimony effects on fungal growth. This finding is explained by excellent sorption properties of applied mineral phases restricting antimony bioavailability. At initial growth stages almost 85 % and 94 % of total Sb was immobilized in manganese and ferric phase, respectively. Biologically induced hausmannite dissolution and transformation into lindbergite leached almost 99 % of immobilized antimony in fungal presence, while ferric oxides were relatively unaffected by the fungus, with adsorbed antimony more resilient to microbial leaching. Bioleached antimony was available for fungal bioaccumulation and biovolatilization. The volatilization efficiency of uptaken antimony ranged from 56 % to 64 %, except for ferric phase treatment where significant decrease in bioavailable antimony resulted in 34 % volatilization efficiency. Our findings suggest the fungal role in manganese and ferric oxides transformation and antimony mobility, and we clarify these interactions at presence of the ubiquitous fungal *A. niger* strain.

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## Characterizing ZnO Nanoparticles and their Interaction with Humic Acids

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Use of engineered nanoparticles is growing in both commercial products and technological applications. Their precise characteristic is needed in the technically advanced applications but also for evaluation of their potential hazard when released to the environment. In this study, sol-gel synthesized nanoparticles of zinc oxide (nZnO) were analyzed to find their size and other properties. Size and crystalline structure was determined by powder X-ray diffraction (XRD). The size measurements were also taken by inductively coupled plasma-mass spectrometry (ICP-MS) and by scanning and transmission electron microscopy (SEM and TEM). During SEM procedure the nZnO were also analyzed by energy-dispersive X-ray spectroscopy (EDS). The nZnO nanoparticles deposited on a resin were inspected by atomic force microscopy (AFM). UV-vis spectrophotometry was applied to observe the sorption of humic acids (HA) onto nZnO and the change of sedimentation of bare and HA-coated nZnO (Fig. 1). These different spectroscopic and spectrometric methods provide us with the needed information to characterize the properties of nanoparticles relevant for their further study.

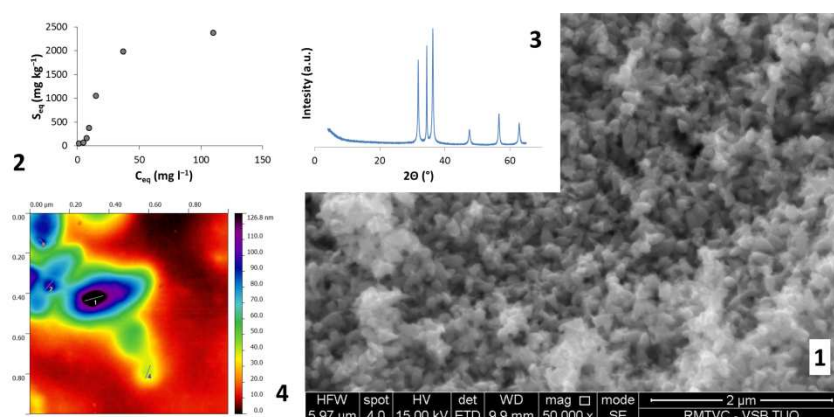


Fig. 1 SEM image of nZnO (1); adsorption graph with HA (2); XRD diffractogram showing zincite nanocrystal structure (3); AFM image of nZnO aggregate (4)

*Acknowledgement: The study was supported by Comenius University in Bratislava under grant UK/139/2016.*

### Switchable Hydrophilicity Solvent Based Microextraction of Nickel Prior to Determination by Flame Atomic Absorption Spectrometry

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A combination of switchable solvent and microextraction is presented for extraction of nickel prior to determination by flame atomic absorption spectrometry. Switchable solvents, also called as green solvents, introduced by Jessop et al. [1], are capable of reversible change of their physical properties. Nickel, so widely used in different branches of industry, present some risk for health of people. Just contaminated food and cigarette are widely way of exposure of people to nickel.

Reverse change of hydrophilicity of extractant, 1-ethylpiperidine, involves effective extraction without additional solvents. CO<sub>2</sub> was used for preparing of stable amine-water extraction mixture. The mixture was added in sample solution, while homogenous solution was observed. NaOH was used as stimulus for separation of amine from sample-amine solution; nickel was collected in amine phase. After phase separation, nickel was determined by FAAS. A linear analytical response was obtained in the range 30 – 500 µg L<sup>-1</sup> of nickel with the limit of detection 8.7 µg L<sup>-1</sup> of nickel. Accuracy of the method was tested by analyzing of two certified reference materials. Method was successfully applied on determination of nickel in food and cigarette samples.

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*Acknowledgements: This work has been supported by Erciyes University, Kayseri, Turkey, and by the Scientific Grant Agency of the Ministry of Education, Science, Research and Sport of the Slovak Republic and the Slovak Academy of Sciences under the VEGA contract (Grant No. 1/0253/16, 2016 – 2019).*



**The Leaching of Zn, Pb, and Cu from Polymetallic Ore Using Heterotrophic Bacteria such as *Pseudomonas*, *Rhodococcus* and *Cupriavidus* Compare to Fungal Strain *Aspergillus niger***

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The aim of this paper was evaluated effect of leaching ability of Cu, Zn and Pb from polymetallic ore gained from Hodruša-Hámre (Slovak republic) using heterotrophic bacteria strains *Pseudomonas*, *Rhodococcus* and *Cupriavidus* compare to filamentous fungi *Aspergillus niger*. Alternative biohydrometallurgical method (using different kind of microorganisms) takes more advantage by the confrontation with the traditional the chemical, pyrometallurgical, hydrometallurgical technology due to economic and environmental point of view [1,2]. There is some evidence that heterotrophic bacteria genus *Pseudomonas* leached Zn, Pb and Cu more effectively than *Rhodococcus*, *Cupriavidus* and comparison with fungal strain *Aspergillus niger* strains. For quantification bioleaching processes of lead, copper and zinc was used atomic absorption spectroscopy (AAS) also with morphological and chemical characterisation of parent material (polymetallic ore) which was carried out scanning electron microscope (SEM) and for mineral (crystallographic) identification was apply X-ray analysis. Our research confirmed more appropriate biohydrometallurgical methods using heterotrophic bacteria genus including *Pseudomonas*, *Rhodococcus* and *Cupriavidus* compare to fungal strain *Aspergillus niger*.

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*Acknowledgement: This work was supported by Scientific Grant Agency of the Ministry of Education, Science, Research and Sport of the Slovak Republic and the Slovak Academy of Sciences under the contract VEGA 1/0274/13, and by the Slovak Spectroscopic Society, member of the Association of Slovak Scientific and Technological Societies with the following logo*



## Fungal Accumulation of Selected Metals from Mining Waste

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The main objective of our research was investigation of *Aspergillus niger*'s efficiency in metal leaching of Au, Pb, Cu and Zn from mine tailings collected from Hodruša-Hámre gold mine. Mining waste used in this study represented fraction below 0.1 mm size diameter, and contained 6.11 mg Au.kg<sup>-1</sup>, 403 mg Pb.kg<sup>-1</sup>, 126 mg Cu.kg<sup>-1</sup> and 6723 mg Zn.kg<sup>-1</sup>. Four different wild *A. niger* strains were used; three isolated from soils collected in Šobov, Pezinok and Slovinky with elevated concentrations of heavy metals, and one strain isolated from habitat without environmental impact in Gabčíkovo. Accumulation took place under stationary conditions at 25 °C during 14- and 28-day cultivation in Sabouraud broth medium supplemented with 0.5 or 1 g of mine waste. After cultivation, the grown mycelia were isolated, dried and analyzed for total concentration of selected metals after acidic digestion. For metal determination atomic emission spectroscopy with inductively coupled plasma (AES-ICP) was used. Works of Huang [1], Kapoor [2] and Wang [3] confirmed that pH is an important factor for efficient metal extraction from waste materials. However, at lower pH values the H<sup>+</sup> ions also occupy sites on fungal biomass where metal ions can be bound preferentially. Therefore, the fungal accumulation rate decreases with decreasing value of pH. Thus, Šobov strain showed in most cases the poorest results because it kept low levels of pH, mostly below 3. On the other hand, strains from Gabčíkovo, Pezinok and Slovinky were able to keep close to neutral or slightly alkaline pH. This led to higher metal accumulation efficiency by these strains, and possibly also includes biologically induced precipitation of studied metal ions. While Gabčíkovo strain accumulated up to 127 mg.g<sup>-1</sup> of Pb, the Pezinok strain was the most efficient accumulator of Cu, Zn and Au with determined biomass concentrations of 18.2, 385 and 0.2 mg.g<sup>-1</sup>, respectively.

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*Acknowledgement: This work was supported by Scientific Grant Agency of the Ministry of Education, Science, Research and Sport of the Slovak Republic and the Slovak Academy of Sciences under the contract project VEGA 1/0482/15.*

## Analysis of Stimulants Using Differential Mobility Spectrometry

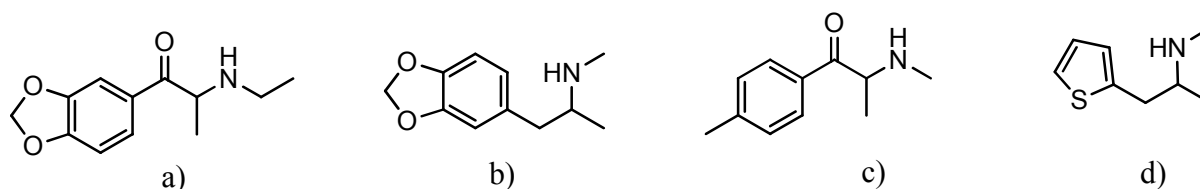
Martin Pavlačka<sup>1</sup>, Karel Ventura<sup>1</sup>, Kateřina Kortánková<sup>2</sup>, Jiří Bláha<sup>2</sup>, Michal Zástěra<sup>2</sup>,  
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Derivatives and analogues of phenethylamines and cathinones belong to the main group of abused stimulants. This work also gives special attention to methiopropamine-structural analogue of methamphetamine (thiophen ring replacing benzene ring) which appears as a drug of abuse since 2011. Stimulant effect of methiopropamine is similar to methamphetamine [1]. Ecstasy (MDMA) is a typical representative of phenethylamines frequently named as a classical recreational drug. Synthetic cathinones are structurally related to cathinone, a compound that is naturally observed in the Khat plant [2]. Ethylone and mephedrone are representatives of synthetic cathinones. The reasons for increasing interest in range of cathinone derivatives have been attributed to the low cost and stimulant effect similar to amphetamines [3].

This work deals with analysis of ethylone, MDMA, mephedrone and methiopropamine (Figure 1) using differential mobility spectrometry. Dispersion plots of measured compounds as well as time plots with differential mobility spectra were analysed.



**Figure 1** Chemical structure of ethylone a), MDMA b), mephedrone c) and methiopropamine d).

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**Experimental Possibilities at the High-Resolution Powder Diffraction Beamline P02.1**

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High Resolution Powder Diffraction (HRPD) Beamline P02.1 is part of the “Hard X-ray Diffraction Beamline P02” at PETRA III (DESY Hamburg, Germany). P02.1 is operated at a fixed energy of 60 keV. Its design is optimized for high resolution powder diffraction as well as the analysis of highly disordered materials and real-time (time resolved) investigation of chemical and physical transformations in a variety of materials.

X-ray diffraction (XRD) using high-energy photons has proven to be well suited for describing the structure of highly disordered systems such as metallic glasses (MG). Time-resolved in situ XRD experiments may nowadays be performed at high-brilliance synchrotron radiation sources for a variety of conditions which help to elucidate the structure–property relations. It has been recently demonstrated that the high energy X-ray diffraction represents very powerful tool to track tiny structural changes in the structure of metallic glasses when exposed to thermal or mechanical load. The first part of this contribution presents mapping of strain fields of indented Zr-based BMG using high-energy micro-diffraction technique. Results presented in the second part show how high-intense photon beams coupled with fast X-ray detectors can be used in studying of the fast crystallization kinetics. At the end an overview of the experimental possibilities at the P02.1 beamline will be presented.

## **ABSTRACTS OF FIRM LECTURES**

**CERTIFIED REFERENCE MATERIALS CertiPUR® Merck**

Zuzana Antalová

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In order to obtain accurate analytical results, it is essential to calibrate all of the instruments used for analysis before commencing. However, such calibration work is only meaningful if reliable reference materials are employed. With Merck CertiPUR® reference materials you can have always confidence in your analytical results. All CertiPUR® reference materials and standards come with a comprehensive Certificate of Analysis (CoA), where all batch specific parameters and important inspection-relevant data are documented: used analytical method, uncertainty data, traceability including batch number, date of release, minimum shelf life and the responsible laboratory head.

With the worldwide globalization, analytical results have to become more comparable and transparent. Quality management especially for reference material is gaining in importance with respect to the accuracy and precision of analytical measurements. Using high sophisticated reference materials leads to avoid repeat analysis and save qualitatively costs.

Our ICP standards are analyzed using ICP/OES and ICP/MS methods. The true value is certified by an accredited calibration laboratory according to ISO/IEC 17025. For this analysis, a method has been developed for 68 element standards. The advantage is obvious: a high degree of precision; this is reflected in the uncertainty data, which can vary, depending on the chemical nature of the element concerned. Our ICP single-element standards are produced according to ISO Guide 34. Our AAS standards are normally determined titrimetrically. Depending on the element involved, the ICP/OES method is also used [1].

ICP standards are directly traceable to an international standard from NIST. Traceability to the primary standard is documented in the CoA with indication of the batch used. Standards used in AAS are also traceable to SRM from NIST. Analysis of content is generally carried out titrimetrically and is traceable to the original volumetric standard.

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**ICPMS-2030: Peace of Mind for Users and Lab Managers**

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In March 2016 Shimadzu launched the ICPMS-2030 Inductively Coupled Plasma Mass Spectrometer; the company's first global ICPMS platform. The ICPMS-2030 is designed for high stability, excellent sensitivity and low interference. The instrument offers peace of mind on all levels: The software is user friendly, offers assistant functions to those with less experience and is backed by a central software platform for compliancy. The running costs set a new benchmark with low argon consumption and quality demand, easy to maintain hardware and Shimadzu's highly appraised level of service and support.

The new ICPMS-2030 is primarily designed to respond to the ICH-Q3D guidelines for elemental impurities in pharmaceutical products. The ICH-Q3D specifies allowable limits of daily intake of 24 elements of toxicological concern, and requires high sensitive and high precision measurement of such elements. The ICPMS-2030 satisfies these requirements with ppt level high sensitivity while offering FDA 21 CFR Part 11 compliance, automated analytical method development function. US pharmacopoeia indicates limits of elemental impurities (USP232) and detection technique by ICP-MS (USP233), which will be in effect in January 2018.

Also in the food market many applications can be found for the ICPMS-2030. Focal point in this market will certainly be the simultaneous evaluation of nutritional elements present in high concentrations (Na, K, Ca, Mg...), in combination with the evaluation of trace elements and toxic elements in very low concentrations (Pb, Cd, As, Hg, Th, Se...). Looking at the food market in Europe there is a clear dominance by beverage producers; Breweries, dairy producers, drinking water producers, distilleries and wine makers make up a significant part of the market.

## **ABSTRACTS OF POSTER PRESENTATIONS**



**AFM and Raman Study of Heavy Weathered Surface of Barium Crystal Glass**

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Glass samples of barium crystal glass produced by RONA, a.s. Lednické Rovne glass works were weathered at controlled conditions (60 °C, 90 % relative humidity) for 2 months. The morphology of weathered glass surface was studied by AFM using a tapping mode [1, 2]. The micro Raman spectroscopy (inVia Reflex Raman – Renishaw) was used for study of corrosion products observed by the optical microscopy [3]. Raman spectra were recorded in the range of (200-1500) cm<sup>-1</sup> by RENISHAW inVia Reflex Raman spectrometer with the Leica DM2500 microscope. A 532 nm laser with 28.5 mW power was used as the excitation source for a spot of about 1 mm diameter.

Only the largest pieces of weathering products enabled recording of Raman spectra with sufficient quality. The obtained Raman spectra were compared with the spectral database (S.T. Japan spectral databases). Obtained results contribute to the explanation of weathering mechanism and will be utilized for protecting the barium crystal glass products against weathering.

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## Utilization of MW-Assisted Decomposition and HR-CS AAS for Evaluation of Heavy Metals Pollution in Sedimentary Ecosystems

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The aim of the carried out experiments was to point out the use of MW-assisted decomposition in the evaluation of heavy metals (Cu, Ni, Pb and Zn) ecosystem contamination. These decompositions are from the „green chemistry“ point of view classified as the most effective, as they minimalize not only the amount of decomposition agents, but also the time of the decomposition [1, 2]. The total content determination of the chosen heavy metals in the solutions after individual decompositions was performed by high resolution-continuum source flame atomic absorption spectrometry (HR-CS FAAS) using contraAA 700 spectrometer.

Studied samples of anthropogenic sediments come from sludge beds Ajka (Hungary) and Lintich (Slovakia). Samples of natural sediments come from Hornád river (Slovakia) in the area of neighbourhoods Ťahanovce, Nad Jazerom (Košice) and Ida river. Samples of biofilms come from Hornád and Ida rivers. Previous experiments formed the basis for the assessment of the most effective decomposition for sediments at 200 °C, decomposition time 15 minutes, sample amount 0.3 g and decomposition mixture HCl:HNO<sub>3</sub>:HF in the ratio of 6:2:2. The most effective mixture of agents for the biofilm decomposition was the combination of HNO<sub>3</sub>:H<sub>2</sub>O<sub>2</sub> in the ratio of 7:1 at 200 °C, decomposition time 15 minutes and sample amount 0.5 g.

Comparing the measured total contents of given heavy metals in the sediments, it is clear, that they have different physical and chemical characteristics, which causes their different sorption properties. For better explanation of this issue, the comparison of the total contents of metals in the sediments and biofilms from the one sampling site is also given. This contribution also presents the application of different decomposition mixtures of agents on sediment Ajka, which unlike other sediments has alkaline character.

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*Acknowledgements: This work was supported by Scientific Grant Agency of the Ministry of Education, Science, Research and Sport of the Slovak Republic and the Slovak Academy of Sciences under the contracts VEGA (projects Nos. 1/0126/14 and 1/0130/14), and by Slovak Spectroscopic Society, member of the Association of Slovak Scientific and Technological Societies with following logo*



**Determination of Selenium Species by ICP-MS Method in Biological Samples**

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The opinion on selenium influence on human organism has varied in the course of the past century. At first, selenium was considered to be badly toxic up to cancerogenic. As time went by, it was discovered to have an essential role in human organism. In human organism selenium is a part of many enzyme systems, e.g. glutathione peroxidase, and as a part of antioxidant defense system it has an expressive preventive effect against cardiovascular and oncogenic diseases. An interesting fact is a relatively narrow range between concentrations with favorable and toxic effects on the human organism. The toxicity of selenium doesn't only depend on its amount but also on its chemical form or species (oxidation state, organic or inorganic form, eventually the occurrence of single isotopes) and that is why the compounds speciation becomes unavoidable.

Many laboratories deal with speciation analysis of various elements, one of which is selenium. Various studies are used in various analytical methods (typically in an online ordering e.g. IEC-ICP-AES and HPLC-(UV)-HG-AFS and off-line HPLC-ETA-AAS) for the determination of different forms of selenium. However, as the most suitable, in terms of achieving very low detection limits, appears combination HPLC/IC-MS. In this work are shown the possibilities of this application, recently reported methods for the analysis of various forms of selenium compounds in biological materials [1, 2].

Analytical chemists have increasingly realized that determining total contents of the elements cannot provide the required information about mobility, bioavailability, and finally the impact of elements on ecological systems or biological organisms. Only knowledge about the chemical species of the elements can lead to understanding of chemical and biochemical reactions involving these species, thus providing information about toxicity or essentiality. This is why speciation analysis has become an essential tool for risk assessment of elements in the environment, leading to more effective diagnosis and therapy, to understanding the toxicity and the moving of trace elements and to better nutrition and health.

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## Simplex Method for Optimization of Cloud Point Extraction: Utilizable for Determination of Ultratrace Elements by Using Spectrometric Methods

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Cloud point extraction (CPE) is based on the property of nonionic and zwitterionic surfactants in aqueous solutions to create micelles and become turbid when heated to particular temperature referred to as cloud point temperature. Above this temperature, the micellar solution separates into a surfactant-rich phase (SRP) of a small volume, and a diluted aqueous phase. In element analysis, a chelating agent is usually added to create the hydrophobic chelate which can remain in the hydrophobic core of the micelles in the SRP, thus being extracted and preconcentrated. The separation of the small volume of the SRP is greatly promoted by placing the extraction tube, after centrifugation, in ice bath to increase the viscosity of the phase. Finally, after removing of residual aqueous phase, the highly viscous SRP is diluted by methanolic or ethanolic solution of mineral acid (mainly HNO<sub>3</sub>). Such diluted sample is used for measurement.

Proposal of a reliable CPE procedure takes some time. It is traditionally performed by monitoring the influence of one variable at a time on a given experimental response. In this type of optimization, so-called univariate optimization, when the level of a factor is changed, the levels of other factors of interest are kept at constant values. In case of CPE, where many variables can influence the magnitude of the studied response, numerous experiments are needed. Recently, in effort to reduce number of experiments, multivariate optimization is more frequently applied. It results in lower costs of reagents and time consumption. A large number of chemometric tools, such as two-level fractional designs, mixture designs, Doehler and Box-Behnken designs, etc. can be used for this purpose. The simplex method suggests the optimization of various studied factors without the need to use more specific mathematical-statistical expertise as required in response surface methodology [1]. The main goal of this contribution is to show the use of simplex optimization in developing a reliable CPE procedure for separation/preconcentration of ultratrace elements before their spectrometric determination.

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**Determination of Heavy Metals in the Soil by High-Resolution Continuum Source Flame Atomic Absorption Spectrometry (HR-CS FAAS)**

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Actual extreme climate conditions in combination with industrially developed societies represent degradation factors which significantly affect the quality of the environment and its individual components. In the case of soil it is mostly about its contamination with heavy metals, acidification, erosion and desertification. Population growth, industrial plants, use of natural resources (natural gas, oil), transport, and today's consumer society annually produces millions of tons of waste that is recycled, incinerated, but substantial portion is amassed in the controlled and uncontrolled landfills. In terms of protection of human health, land resources and environmental quality, uncontrolled landfills represent a significant risk of soil contamination. This work is focus on the assessment of the possible contamination of agricultural land near by the uncontrolled landfill in the city Tornaľa (southern Slovakia). Prerequisite for reliable analytical results is the proper implementation of all steps of chemical analysis in accordance with applicable standards, therefore, adequate attention has been paid on the sampling planning, correct soil sampling and subsequent sample processing before itself analysis. Samples were taken from a fixed point (landfill body), at a distance of 10 m and 20 m from a fixed point, and in the landfill body from the depth 80 cm to 90 cm (assessment of the mobility elements). Due to seasonal comparison, autumn and spring sampling was carried out. For the purposes of spectral analysis, samples were decomposed using microwave energy (Ethos One, Milestone, Italy) and decomposition mixture reagents (8 ml 65 % HNO<sub>3</sub>, 5 ml 37 % HCl and 1 ml 40 % HF) to ensure the total decomposition. Evidence of presence of elements was carried out by ICP-OES method using axially plasma torch (Iris AP, Thermo Jarrell Ash, Germany). Determination of total contents of determined elements was performed by HR CS FAAS method (contrAA 700, Analytik Jena, Germany). Obtained results showed, that contents of some heavy metals in the soil in this area exceed the statutory limits (Cu 60 mg/kg, Pb 70 mg/kg, Zn 150 mg/kg of dry mass) as follows: Cu 306.27 mg/kg; Pb: 423.44 mg/kg; Zn: 193.50 mg/kg of dry mass. Values of total elements content in dependence on the distance from the landfill body showed the highest mobility of Cr and Ni in the environment, particularly in the spring season. The results show that the soil in the vicinity of the uncontrolled landfill is not suitable for agricultural purposes. For its re-use would be appropriate to focus attention on her recultivation, for example through the phytoremediation technology.

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**Inductively Coupled Plasma Mass Spectrometry in the Analysis of Geological Materials**

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Inductively coupled plasma mass spectrometry (ICP-MS) with laser ablation sampling (LA-ICP-MS) is widespread instrumental method, which has found its place in geology for microanalysis of geological samples, such as monitoring of elemental distribution or single grain microanalysis. It is complementary method to electron microprobe analysis (EMPA) with advantages being low limits of detection (hundreds of  $\mu\text{g kg}^{-1}$ ) and  $\mu\text{m}$  scale spatial resolution. However, the lack of suitable reference materials in an issue hampering the matrix matching in LA-ICP-MS.

Laser ablation sampling results in stoichiometric disagreement between sample aerosol and sample composition, called fractionation. It occurs at different rates, depending on the disagreement between sample and reference material matrix. The parameters of laser ablation affecting the degree of elemental fractionation are pulse duration, laser wavelength, fluence and frequency, for instance. Additionally, carrier gas type and physicochemical properties of the sample are the additional aspects of fractionation.

This exploratory study investigates the means and limitations of two commercially available laser ablation devices in terms of fractionation degree, when various matrices, such as synthetic glass standards (SRM NIST), basalt glass (BCR-2G), Max Planck Institute – Dingwell reference materials (MPI-DING) and columbite are sampled. The fractionation was investigated to estimate the contribution of wavelength, fluence and frequency, as well as ablation modes to overall degree of fractionation.

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## Vibrational Spectroscopic Study of Interactions between Skin and Peptides Based on the Argireline Structure

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For the treatment or leveling off the wrinkles toxic protein botulinum toxin (Btx) with acute toxicity about 10 – 13 ng/kg is used [1]. From N-terminal part of the protein SNAP-25 was derived peptide Argireline which is in contrast to Btx practically nontoxic. Argireline is acetylated hexapeptide with the Ac-EEMQRR-amide sequence [2, 3] which prevents the formation of skin lines and wrinkles in a similar way as Btx. Argireline is distributed on the market by the company Lipotec Argireline® and it appears in many cosmetic products against wrinkles [3].

In this study the structure of Argireline peptide was modified by increasing its hydrophobicity. In the terms of peptides synthesis, methionine residues were substituted by norleucine and acetyl groups in N-terminal part of Argireline were replaced by a suitable terpenoid. The both cooperative changes affect jointly the properties of obtained Argireline analogues.

Samples of pig skin provided by the Department of Organic Technology UCT Prague were used to study skin interaction with four synthesized Argireline analogues. Skin samples were treated by solutions of individual peptides with mass concentration of 50 mg/ml. As reference data, skin samples treated by the same volume of pure water (without peptide) were used. Mutual interactions between selected peptide and skin layers were studied by Raman and infrared spectroscopy, especially by Attenuated Total Reflection (ATR) technique, and by confocal Raman microscopy for depth profiling measurements.

Obtained data were evaluated by multivariate statistical methods namely Linear Discriminant Analysis (LDA), Partial Least Squares (PLS), Principal Component Analysis (PCA) and Soft Independent Modelling of Class Analogy (SIMCA). The measured spectra show that peptides can penetrate through the upper parts of the skin. We also detected changes in the intensity ratios and spectral shifts of some peptide bands, concluding that peptides interact with the skin constituents. Kinetic monitoring of skin spectral changes enables reliable prediction of time based on the spectral data. Hence, it is possible to elucidate changes in the skin caused by the peptides by vibrational spectroscopic techniques.

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**Effect of Dietary Selenium Intake on Inter-Element Interactions in Rat Livers**

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Selenium belongs to the most important essential elements for animals and various beneficial effects were reported [1]. The effect of Se-enriched defatted rape seeds [2] added to the diet on the response of essential micro- and macronutrients (I, Se, Cu, Ca, Fe, K, Mg, Mn, P, S, and Zn) in rat livers was investigated in model conditions. The experimental diets for the individual experimental groups were prepared as follows: i) the control diet with 14 % of the soybean meal; ii) 30 % of the soybean meal in the diet was replaced with defatted rape seeds; iii) 60 % of the soybean meal in the diet was replaced with defatted rape seeds; and iv) 100 % of the soybean meal in the diet was replaced with defatted rape seeds.

Whereas Se contents in liver of the rats remained unchanged, the decreasing Cd contents in the rat liver with increasing Se content in the diet confirming antagonism of these elements was observed. Concerning most of the essential elements, the application of the selenized defatted rape seeds did not result in any serious imbalance of these elements utilization. In the opposite, Se addition led to significant changes in the total iodine content, but no obvious dependence on the portion of selenized defatted rape seeds was observed. The abundance of inorganic iodine did not significantly differ between groups.

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### High-Resolution Continuum Source Electrothermal Absorption Spectrometry of SrF and InCl Molecules

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Non-metals normally cannot be determined by AAS, because their most sensitive resonance lines are in the vacuum ultraviolet region of the electromagnetic spectrum. Molecular absorption spectrometry (MAS) is a technique originally developed in the 1970s which allows the determination of the halogens by low resolution, line source atomic absorption spectrometry (AAS) instrumentation. These techniques are based on formation of a diatomic molecule whose absorbance is monitored. According to the low resolution, application of MAS for practical analysis is limited by the unavailability of excitation wavelengths, poor spectral resolution, and the presence of spectral interferences. The situation changed dramatically with the introduction of high-resolution continuum source atomic absorption spectrometry (HR-CS AAS). This kind of spectrometer is capable of resolving completely or almost completely the rotational fine structure of electron excitation spectra of diatomic molecules. Due to the use of a continuum radiation source, any of the rotational lines can be selected at high resolution and used for the indirect determination of the halogens via thermally stable, gaseous diatomic molecules.

The aim of this study was to develop a new procedure for the determination of F and Cl by HR-CS MAS using molecular absorption line of SrF and InCl formed in graphite furnace. The effects of graphite furnace program, chemical modifiers and amount of modifier on the sensitivity and accuracy were investigated. Under optimized conditions, experimental parameters (sensitivity, linearity, accuracy, limit of detection) were determined. Furthermore, matrix effects were investigated to characterize spectral and non-spectral interferences. Optimized method was used for analysis of various water samples including surface water, underground water and wastewater.

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**Raman Spectroscopic Study of Thermal Effects in Graphene on Au Nanoislands**

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Graphene as a hexagonal single layer arrangement of carbon atoms is very promising material for variety of applications where charge transfer plays a significant role. The charge doping and strain effects between the substrate and the graphene layer with the temperature evolution were studied very rarely [1-5]. Previously, the graphene was placed on the top of the Si/SiO<sub>2</sub> substrate and the irreversible changes were observed in the band positions, linewidths and relative intensities of 2D and G Raman bands. The authors [1] concluded that the doping of the sample played the major role in comparison with strains effects.

In our study, we focused on the temperature dependence of strain and doping in monolayer graphene placed on a glass slide decorated with Au nanoislands, which were prepared by sputter coating. The temperature behaviour was investigated by surface-enhanced Raman spectroscopy (SERS) in the temperature range 303 – 573 K. The analysis of the SERS spectra of the graphene monolayer measured with 780 nm excitation revealed that (i) the SERS enhancement increases by a factor of 10<sup>0</sup> after the thermal treatment, and (ii) the position of the 2D Raman mode was redshifted with the increasing temperature by *c.a.* 35 cm<sup>-1</sup>, which is higher in comparison to the literature [1].

To enable deeper interpretation of the observed effects, the changes of the morphology of the annealed sputtered Au island films were studied by scanning electron microscopy and UV/Vis spectroscopy. Recrystallisation of the film was confirmed. In contrast to the previous observations [1], we conclude that the strain is the dominant factor originating the Raman band shift as corroborated by the G – 2D correlation analysis. Finally, we addressed the interaction of the graphene and the Au nanoislands, which is evidenced by fine structure of the G mode [6]. The G-band splitting increased after the first annealing cycle, which suggests enhancement of the graphene – Au interaction due to better adhesion of the graphene layer.

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## Temperature Influence on Electrothermal Vaporization Process of Heavy Metals in Different Matrices by Use of ETV-ICP-OES Method

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Direct analysis of solid samples offers quick, accurate and reliable results along with an easy manipulation of the sample and minimum analyte loss. Small amount of samples and thus appropriate homogeneity of analysed material are needed. The aim of work is to discover optimal conditions for vaporization of heavy metals (Cd, Cr, Ni, Pb) from solid samples in order to determine them by use of method connecting optical emission spectrometry (OES) with inductively coupled plasma (ICP) as an excitation source and furnace with electrothermal heating (ETV) as a vaporization device, ETV-ICP-OES.

To achieve required figures of merit of the method it is necessary to apply suitable program of electrothermal vaporization to guarantee complete evaporation of determined elements. For easy handling of method several different types of reference materials were chosen for this study that would be replaceable in analytical calibration in practice. Different sample types used to elements vaporization study were model samples prepared according to the real environmental samples, soil sample, sediment sample and two different certified reference materials of sediment origin.

The vaporization process was taken in the ETV device enabling to program a thermal course of electrothermic vaporization according to the type of sample. Three different temperature programs of electrothermal vaporization were applied varying in duration and temperature values for drying, ashing and evaporating step in order to find the most suitable one to achieve complete vaporization of determined elements in the shortest time. The vaporization process of chosen metals was evaluated by achieved signal intensity, by standardized vaporization curves expressing the course of vaporization and finally by accuracy of measurement expressed by relative standard deviation (RSD) values.

Results showed that measured signal intensity of all determined elements was the highest by use of one of applied ETV programs. Furthermore, Cd, Cr and Ni had identical vaporization behaviour in all types of samples. Exception is Pb with significant differences of vaporization course for all samples. RSD values are lying under 5.00 % for Cd and Cr in all six samples. Nickel exceeds this in soil sample with 7.86 % and lead in sediment with 6.60 %, respectively 25.95 %.

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## Application of High-Resolution Continuum Source Molecular Absorption for the Determination of Nitrate

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Nitrogen species such as nitrite play an important role in environmental and human health. In aquatic ecosystems nitrites are produced by microorganisms as nitrogen sources and at higher concentrations can be toxic or cause eutrophication. Nitrites are very important indicators of water pollution [1, 2, 3]. In the human body, nitrite can react with secondary or tertiary amines forming nitrosamines, which are recognized as carcinogenic agents [2, 3]. The presence of nitrites in blood at high concentrations can react with iron(II) causing formation of methemoglobin which is not able to carry oxygen.

The determination of nitrite has been the study object of numerous researches and various analytical methods can be used for their quantification. These include gas chromatography–mass spectrometry [4], electrochemical methods [5, 6] and molecular absorption spectrometry [7, 8, 9].

The molecular absorption of NO was measured with an Analytik Jena AG Model ContrAA 700 high-resolution continuum source spectrometer (Jena, Germany) equipped with a xenon lamp operating in hot-spot mode as a continuum radiation source.

In this work NO line at 215.360 nm was used [7], and new method for the determination of nitrites was developed and optimized. Determination parameters, such as pyrolysis and vaporization temperature were obtained and analytical method was validated. Developed and optimized method was applied for analysis of real samples.

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**Determination of Se in Dietary Supplements by Photochemical Volatile Species  
Generation Atomic Absorption Spectrometry**

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The technique of volatile species generation has recently seen renewed interest due to the development of new generation approaches. The main advantage of this technique is the separation of the analyte from the sample matrix and the subsequent possibility to decrease spectral interference and improve the limits of detection in comparison with the direct analysis of liquid samples by atomic spectrometric methods.

Regular intake of selenium is recommended for its cancer protective effects and for improving the state of human skin, hair and nails [1] making it a common component of dietary supplements. However, regular intake of high doses of Se may lead to garlic breath, poor dental health, disorders of the nervous system and skin and hepatic toxicity caused by accumulation in liver. It may also increase the risk of type II diabetes [2]. Development of methods to control the content of Se in dietary supplements may soon become necessary.

This contribution proposes determination of Se in multivitamin dietary supplements containing either Na<sub>2</sub>SeO<sub>3</sub> or Na<sub>2</sub>SeO<sub>4</sub>. The method is based on the photochemical generation of volatile compound of selenium from the medium of acetic acid with the aid of the TiO<sub>2</sub> photochemical catalyst and AAS determination. The pre-reduction of Se is eliminated, because it takes place during the generation process. Similar figures of merit were observed for Se (IV) and Se (VI), however the species require different extraction conditions.

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## SERS Study of Self-Assembled 2D Nanocomposites of Ag and Au Nanoparticles with Terpyridine and its Derivatives

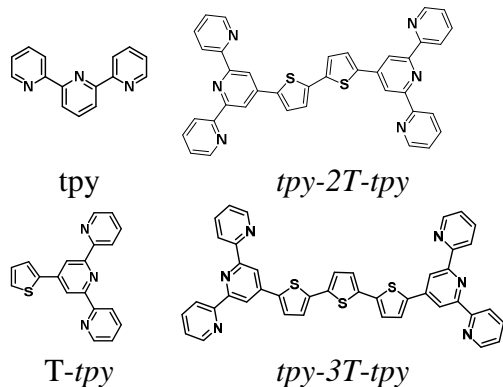
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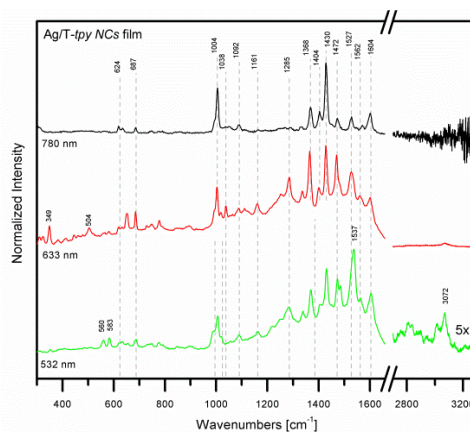
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2,2':6',2''-terpyridine (tpy) complexes and tpy-based oligomers [1] are currently the subject of interest due to their applications as building blocks of light-emitting devices and dye-sensitized solar cells as well as the building blocks of metallocsupramolecular polymers [2] and dynamers [3]. Assembling of plasmonic (predominantly Ag and Au) nanoparticles (NPs) through selected molecules into 2D and 3D systems allows the observation of adsorbed molecules by surface-enhanced Raman scattering (SERS) spectroscopy [4].

In this contribution, we have focused on the spectroscopical characterization of the two-dimensional (2D) self-assembled nanocomposite (NC) of Ag and/or Au nanoparticles (NPs) with tpy and tpy-based oligomers. The SERS study of the prepared NCs proved the existence of two forms of the surface complexes – with and without the MLCT (metal-to-ligand charge transfer) transition in Ag and/or Au/tpy and Ag and/or Au/T-tpy NCs. The existence of surface complexes with MLCT transition was not proved for the systems derived from bis(tpy) NCs.



**Figure 1:** Structures of used adsorbates.



**Figure 2:** SERS excitation profile of Ag/T-tpy NC.

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**Evaluation of Heavy Metals Impact from Various Types of Sediments to their Ecosystem by Fractionation Extractions and High-Resolution Continuum Source Flame Atomic Absorption Spectrometry**

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The behaviour (bioavailability, mobility, toxicity) of heavy metals in the solid environmental samples depends mainly on their chemical forms or type of the binding in samples, upon which phases the elements occur in the samples, and which chemical and physical processes these phases are subjected [1]. Single-step extractions by various extraction reagents (no-buffered solutions of inorganic salts, organic complexing reagents, weak organic or strong inorganic acids...) were originally proposed for fractionation of heavy metals in soils [2] but their application on sediments it is possible to obtain information about environmental behavior of metals in this samples [3].

This contribution presents results of fractionation analysis of various types of natural sediments from different river/lake ecosystems and anthropogenic sediments from sludge beds with different character of the suspended material. The single-step fractionation extraction by several reagents with different extraction ability ( $1 \text{ mol dm}^{-3} \text{ MgCl}_2$ ,  $0.43 \text{ mol dm}^{-3} \text{ CH}_3\text{COOH}$ ,  $0.05 \text{ mol dm}^{-3} \text{ EDTA}$ ,  $2 \text{ mol dm}^{-3} \text{ HNO}_3$ ) and the determination of Cu, Ni, Pb and Zn content in extracts by the FAAS method were realized. The obtain results were evaluation from two point of view: environmental (Cu, Ni, Pb and Zn impact from sediments to environment) and analytical (effect of individual extraction reagents on the signal of the atomic absorption). For the FAAS analysis, the high-resolution continuum source flame atomic absorption spectrometer (HR-CS FAAS, equipment: contrAA 700, Analytik jena, germany) was used and structured background spectral absorption by matrix molecules/atoms, which may affect the individual signals determined by Aspect CS software were valuated.

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**Determination of Tellurium in Flavoured Mineral Waters by Electrochemical HG-AFS**

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Tellurium is one of the heavier trace elements and its high amounts in environment are not welcome. It belongs to the group of elements which readily form volatile hydrides. This makes a hydride generation coupled with atomic spectrometry the first choice method for its analysis. Hydride generation is a sample introduction technique commonly used in atomic spectrometry. Its main advantages are an easy separation of the analyte from a matrix, possibility to use milder atomization temperatures and reduction of atomization interferences leading to an increase of the determination sensitivity. Conventionally the hydride generation is performed chemically, but the main disadvantage of this conventional method is the necessity to use tetrahydridoboritanes. These are very reactive and unstable and need to be prepared daily or stored frozen; in addition to their high cost. One of alternatives to the chemical approach is the electrochemical generation, using electrical current as the reductant and a solution of a strong mineral acid as a source of hydrogen.

The presented study focuses on the investigation of the electrochemical tellurium hydride generation and its atomization in microflame AFS. A laboratorymade electrolytic cell was designed for the purpose and the generation setup was optimized and subsequently the analytical figures of merit were determined; the obtained limit of detection is 4 ng ml<sup>-1</sup> (4 ppb). In addition an interference study was carried out. The studied interferents were chosen from various groups of metals: i) other hydride forming elements, ii) transition metals, iii) alkali metals and iv) alkali earth metals. The great performance of the method, especially for the last two mentioned interferent groups, suggests that it allows water samples to be analyzed without any pre-treatment. This also brought up the question of interference of organic compounds. Mineral water with artificial flavorings was chosen as model sample contaminated with organic interferents. Unsweetened mineral water and several randomly chosen flavors were acidified, spiked with tellurium standard solution and analyzed. Even though more complex water matrices presented some problems, the analytical process was practically not influenced by the majority of flavors and sugar; with exception of raspberry flavored water, which interfered strongly. The developed electrochemical hydride generation method coupled with AFS thus proved to be a complex method capable of direct determination of tellurium in real samples.

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## Optimization of Microwave-Assisted Decomposition for Heavy Metals Determination in Lichens

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At present, environmental pollution represents the global problem which did not avoid either Slovak Republic. Increased pollution can be found in the vicinity of certain industrial and urban centers. The main sources of pollution is natural and anthropogenic activity. The main sources of environmental pollution derived from anthropogenic activities include industrial facilities, mining and ore processing. These sources produce emissions that can be released into the atmosphere and as a result of sedimentation (rainfalls or dust) are getting into the water and soil. For monitoring of environmental contamination as well as for control of the environmental components condition, in addition to the known matrices (air, soil and water), bio-indicators of plant or animal origin are also used. For bio-indicator it is generally considered an organism that occurs in a specific place and according to him it is possible to identify certain specific characteristics of the environment. These organisms may contain much higher concentrations of some contaminants than usually are detected in the environmental components. In recent decades, one of the most important and frequently studied plant bio-indicators are lichens. The work is aimed to find suitable conditions of biological material decomposition lichens using decomposition mixture of reagents, microwave radiation and following spectral analysis in order to determine the effectiveness of the decomposition. Two most widespread species of lichens in Slovakia (*Xanthoria parietina* and *Hypogymnia physodes*) were collected, processed and decomposed. Microwave decomposition system Ethos One (Milestone, Italy) for acid pressure decomposition was applied for sample decomposition. Three procedures for total sample decomposition (weight of sample 0.5 g) were used: 1. 7 cm<sup>3</sup> 65 % HNO<sub>3</sub>, 1 cm<sup>3</sup> H<sub>2</sub>O<sub>2</sub>, 2. 2 cm<sup>3</sup> 65 % HNO<sub>3</sub>, 6 cm<sup>3</sup> HCl, 2 cm<sup>3</sup> HF, 3. 2 cm<sup>3</sup> 65 % HNO<sub>3</sub>, 2 cm<sup>3</sup> H<sub>2</sub>O<sub>2</sub>, 6 cm<sup>3</sup> HCl. Using ICP-OES method (spectrometer Iris AP, Thermo Jarrell Ash, Germany), following heavy metals were identified: Ag, Fe, Co, Cr, Cu, Mn, Ni, Pb, Sb, and Zn. Finding of proper decomposition procedure for given type of biological sample means verification of decomposition effectivity on the base of determination of total element content. For this purpose, highly sensitive HR CS FAAS method (spectrometer contrAA 700, Analytik Jena, Germany) was used and Fe, Cu, Mn, Ni, Pb, and Zn elements were determined. Obtained results showed, that the most suitable decomposition procedure is that, using mixture of reagents HNO<sub>3</sub>, H<sub>2</sub>O<sub>2</sub> and HCl.

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**Inductively Coupled Plasma Mass Spectrometry in Trace Analysis of Sulphur**

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In this work is presented development of analytical method for sulfur determination in the complex water matrices, using ICP-QMS with octopole collision-reaction cell (ORC) for analysis of trace sulfur contents.

Sulfur analysis utilizing quadrupole-based inductively coupled plasma mass spectrometry (ICP-QMS), remain challenging in complicated sample matrices, according to the spectral interferences, and to the high first ionization potential, resulting in poor sensitivity compared to elements with ionization potentials in range of 6-8 eV [1]. The most intense interferences for isotopes <sup>32</sup>S and <sup>34</sup>S, are coming from polyatomic ions based on nitrogen, oxygen and hydrogen (e.g. O<sub>2</sub>, NO, NOH and NOH<sub>2</sub>).

Octopole collision-reaction cell (ORC) is one of the technical novelty for elimination spectral interferences in ICP-QMS that is utilizable for element determinations of complex and variable sample matrices on trace and ultra-trace concentration levels [1, 2].

The optimization of experimental conditions for ORC in collision operating mode using helium as the inert collision gas was carried out, and basic calibration and validation parameters were estimated. The helium flow-rate was optimized, and its impact at the background equivalent concentration (BEC) of interfering and in the collision cell arising ions were monitored. For this purpose, there were chosen and monitored the interfering species in mass range from 34 to 74u that are interesting for sulfur analysis.

Optimized ORC conditions meant improvement of BEC and next calibration and validation parameters. The accuracy was evaluated as recovery (Rec) of the model prepared laboratory reference material (Rec = 95-100 %), and the precision as repeatability of the real water samples (RSDs - in the range - 0.05-2.63 %).

During the analytical development, external calibrations were used and working range for sulfur determination was estimated (the linear range was in the concentration interval of 0-1000 µg L<sup>-1</sup>). The quadratic calibration function was more suitable in range of 0-5000 µg L<sup>-1</sup>. The limit of detection (3σ-criterion) was 96 ng L<sup>-1</sup> for linear and 321 ng L<sup>-1</sup> for non-linear working range.

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## Novel Designs of Dielectric Barrier Discharge Atomizers of Volatile Compounds for AAS and AFS

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Miniature dielectric barrier discharge (DBD) plasma atomizers of volatile compounds can replace the commonly used quartz tube atomizers in AAS or diffusion flames in AFS. A DBD atomizer design with planar configuration of compact metal strip electrodes is used in AAS. All the main system components, i.e. radiation source-atomizer-detector, lie on a straight line in AAS (180° geometry). Analyte absorption is measured through the whole volume of a planar DBD. Thus, it is well suited for routine applications. However, current design does not allow plasma diagnostics (discharge longitudinal homogeneity, etc.) since the electrodes are not transparent. Such measurements might significantly contribute to the understanding of the atomization mechanisms and further improvement of the DBD atomizers. Novel planar DBD atomizers with (semi)-transparent electrodes will be presented to overcome the above mentioned limitations. They include planar DBD with (i) one or both electrodes made of metal grid or (ii) electrodes made of indium tin oxide (ITO). ITO is an electrical conductive material being optical transparent at the same time. Atomization conditions for arsane as model analyte will be optimized in these novel designs and their performance subsequently compared to that of common DBD with compact electrodes. Emission spectra will be recorded and effect of experimental parameters on plasma emission profiles investigated.

Contrary to AAS, a 90° geometry is dictated by AFS principle. A cylindrical (tubular) design of DBD atomizer is suited for AFS employing concentric arrangement of the electrodes. The signal in AFS is usually recorded above the top of the DBD atomizer since metal non-transparent electrodes are used in common designs. However, this region accessible for signal detection lies completely outside the plasma area, where the analyte atomization takes place. As a consequence, a decay of free analyte atoms resulting in impaired sensitivity occurs in that region even when employing a protecting gas flow using a shielding unit. This limitation of the DBD atomizers with AFS is solved by newly proposed design, in which fluorescence could be detected directly from the plasma region. The discharge is ignited between two thin electrodes and it is shielded from the ambient atmosphere by an inert gas flow. The atomization performance of the novel DBD atomizer construction will be compared to that of cylindrical DBD as well as to quartz tube and diffusion flame atomizers using AAS detection. Subsequently, its applicability to AFS will be discussed.

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**Arsenic Speciation in Baby Food by HG-CT-AAS**

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The determination of trace and ultratrace element concentrations in commercially available baby foods is necessary to control the dairy intake of essential and toxic elements. Among the toxic elements, the arsenic takes a prominent place. Infants, toddlers and preschooler children, consume relatively more food than an adult, when comparing the ratio of the mass ingested by weight. Because of that, it is important to determine the arsenic content in baby food. The identity of arsenic species (inorganic and organic) controls their toxicity in food in general as well as in baby food. There are two inorganic arsenic forms, arsenite (iAs(III)) and arsenate (iAs(V)) and more than fifty organic arsenic compounds, among them the most abundant are methylarsonate (MAs), dimethylarsinate (DMAs) and trimethylarsine oxide (TMAOs). While the methods for analysis of iAs(III) and iAs(V) are well-known, the analysis of methylated species are not usual. An automated system for hydride generation-cryotrapping-atomic absorption spectrometry with multiatomizer (HG-CT-AAS), which was recently developed for arsenic speciation analysis in biological samples [1], is being applied for baby food slurry samples. In general, the use of hydride generation-atomic absorption spectrometry require a sample pretreatment. A total sample dissolution is usually accomplished with the use of acids and microwave sample digestion in closed vessels. Regarding the arsenic speciation, the use of strong oxidizing reagents such H<sub>2</sub>SO<sub>4</sub>, HNO<sub>3</sub>, HClO<sub>4</sub>, HBr and aqua regia, besides being a time-consuming process, is not recommended to avoid the arsenic species conversion. In order to maintain the original speciation, the sample preparation using mild reagents is being evaluated. Up to now, two sample preparation approaches were tested, the first one using HCl 1 mol L<sup>-1</sup> and the second one using tetramethylammonium hydroxide 0.96 mol L<sup>-1</sup> (TMAH), both heated at 85-90 °C for 15 min and after that placed in ultrasound bath for 15 min. The optimum conditions for sample preparation and arsines generation will be demonstrated.

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## Elemental Analysis of Wine by Inductively Coupled Plasma Optical Emission Spectroscopy

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Wine is significant commercial commodity of which quality reflects the plant geographic origin, grape variety and processing, for instance. Thus unsurprisingly the quality and provenance inspection play important role for verification of authenticity. The history of wine analysis with respect to the geographic origin establishing dates back to eighties of last century and it is based on determination of elemental content. Nowadays, the development of various analytical techniques leads to extension of element to be analysed in terms of LOD and accuracy improvement. Moreover, currently used equipment is quite robust and enables to analyze wine without mineralization. Taking into account analysis of elements at the trace and ultratrace level, low degree of sample dilution is required.

The contribution is focused on elemental analysis of Moravian organic wine by optical emission spectroscopy. The influence of the sample dilution during direct nebulisation of wine and quantification approach is discussed. The results were also subjected to advanced statistical analysis in order to find the link between elements and between selected ratios as well as Moravian organic wine were compared to wine from Spain, Italy and Hungary.

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### Analysis of Antarctic Otoliths by Laser Ablation Inductively Coupled Plasma Mass Spectrometry

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Otolith, so-called earstone, consisting of calcium carbonate is located in inner ear of the teleost fish. It is responsible for ability of hearing and keeping the balance. From the chemical point of view, it can serve as indicator of biological and environmental events due to changes in trace elemental content in the matrix. Moreover, otolith grows continually from the nucleus and thus is characterized by the specific structure with incremental layers corresponding to particular lifetime. Using suitable analytical approach for direct investigation of solid samples, the fish life can be described.

This study is focused on analysis of Antarctic otoliths origination from five different species caught in James Ross Island. Using laser ablation sampling connected to inductively coupled plasma mass spectrometry, content of selected elements and their distributions as well as strontium isotope ratio were determined.

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### Case Study of Groundwater Remediation

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It is an important question nowadays, how to purify the polluted groundwaters. There are more treatment options, e. g. biodegradation, filtration, adsorption and oxidation. Our research group developed an electrochemical way for continuous production of ferrate (FeVI) solution which can be mixed directly to the polluted groundwater. This strong oxidation agent makes possible the degradation of different organic molecules. In the groundwater 44 organic compounds were identified and quantified by headspace gas-chromatograph mass spectrometer system. The main compound was isopropyl-alcohol, about 50 % of the total organic pollutants. The halogenated hydrocarbons and aromatic hydrocarbons formed the other 50 %. The chemical oxygen demand (COD) and the total organic carbon content (TOC) amounted to about 4000 and 1000 mg/L, respectively.

The ferrate treatment was carried out in 3 steps applying 5 or 30 min treatment time in each treatment step and ferrate dosage of 50, 300 and 500 mg/L. It means fresh ferrate solution was added three times to the groundwater to be treated in the concentrations mentioned above. The pH value was adjusted to 7 in all cases. Between the 2<sup>nd</sup> and 3<sup>rd</sup> ferrate treatment a sedimentation step was applied in order to remove the Fe-oxyhydroxide.

Using this technological procedure and ferrate concentration of 500 mg/L about 70 % of isopropyl-alcohol content was removed and simultaneously the COD and TOC values also decreased by 70 %.

Comparing the 5 min and 30 min treatments, it can be stated, that 5 min treatment time is sufficient in all treatment step to achieve the maximal removal efficiency. It is an interesting observation that the removal efficiency values for toluene and xilenes (o-, m-, p-xilene) at similar initial concentration (40mg/L) are different and the toluene is a less degradable compound than the xilenes. An other important result that the three different xilenes can be removed with the same efficiency. It means, the positions of the functional groups on the benzene nucleus have not influence on the effectiveness of oxidation. On basis of these results and observations, it can be established that the ferrate treatment is an effective technology to reduce the COD below to a prescribed limit value and then the treated groundwater can be introduced into the wastewater pipes as a sewage.

## Optimization of Analytical Method for Determination of the Trace Phosphorus Contents by Using ORC-ICP-QMS

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Analysis of trace phosphorus contents in complex water and organic solutions presents a number of challenges to ICP-QMS [1,2], many of which have been overcome to varying degrees by using technological advances including a Peltier-cooled spray chamber, fast variable-frequency impedance matching solid state RF generator and octopole-based collision-reaction cells (ORC).

However, even with these advances, phosphorus remains challenging according to relatively high 1<sup>st</sup> ionization potential. Phosphorus is also subject of the intense interferences from polyatomic ions based on carbon, nitrogen and oxygen, which are difficult to completely remove using conventional ICP-QMS. Examples include COH, NOH, N<sub>2</sub>H, NO and CO on <sup>31</sup>P.

In this work the optimization of experimental conditions of collision-reaction cell is presented. In accordance with the optimization measurements for 10-200 µg L<sup>-1</sup> (1<sup>st</sup> calibration range), and for 75-750 µg L<sup>-1</sup> (2<sup>nd</sup> calibration range), the optimal helium flow-rate of 3 mL min<sup>-1</sup> was evaluated for the both calibration ranges. Optimized experimental conditions of ORC-ICP-QMS have resulted in improvement of background equivalent concentration (BEC) and next calibration and validation parameters. Precision was evaluated as repeatability, and the RSDs of repeated analyses of the real water samples were ranged from 0.4 to 5.8 %. Accuracy was evaluated by recovery (Rec) of the model prepared reference sample, and it was ranged from 97 to 100 %. Limit of detections (3σ-criterion) were 4 ng L<sup>-1</sup> for the 1<sup>st</sup> calibration range, and 6 ng L<sup>-1</sup>, for the 2<sup>nd</sup> calibration range. The used external analytical calibrations were linear for the both chosen working ranges.

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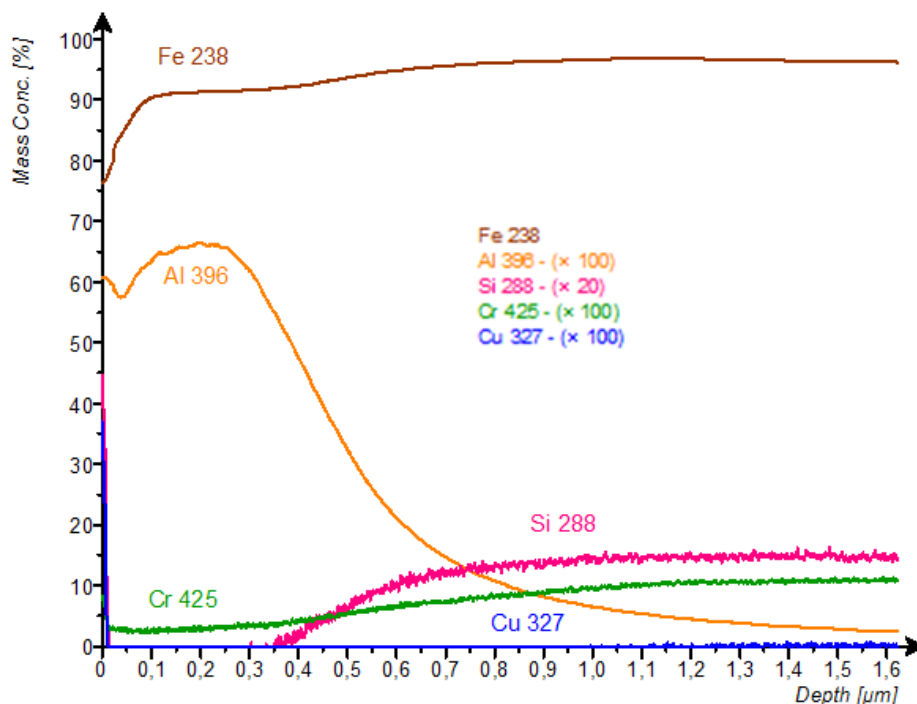
## Utilization of GDOES for the Study of Friction Layers Formed on the Surface of Brake Discs During the Friction Process

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The paper deals with the chemical characterization of friction layer, generated on surface of friction materials during the friction test by using the glow discharge optical emission spectrometry (GDOES) (Fig. 1). Friction layer is formed during the friction process and its character is dependent on several factors and one of the most important is the composition of brake pads and brake disc. When the brake pressure is released at the end on the brake event the specific friction layer remains on the surface of both counter partners (brake pads and brake disc). Using the GDOES profile analysis the thicknesses of friction layers were estimated and these results were compared with results obtained by scanning electron microscopy coupled with X-ray microanalysis (SEM-EDX).



**Fig. 1** GDOES analysis of friction layers on the surface of brake discs after the friction test

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