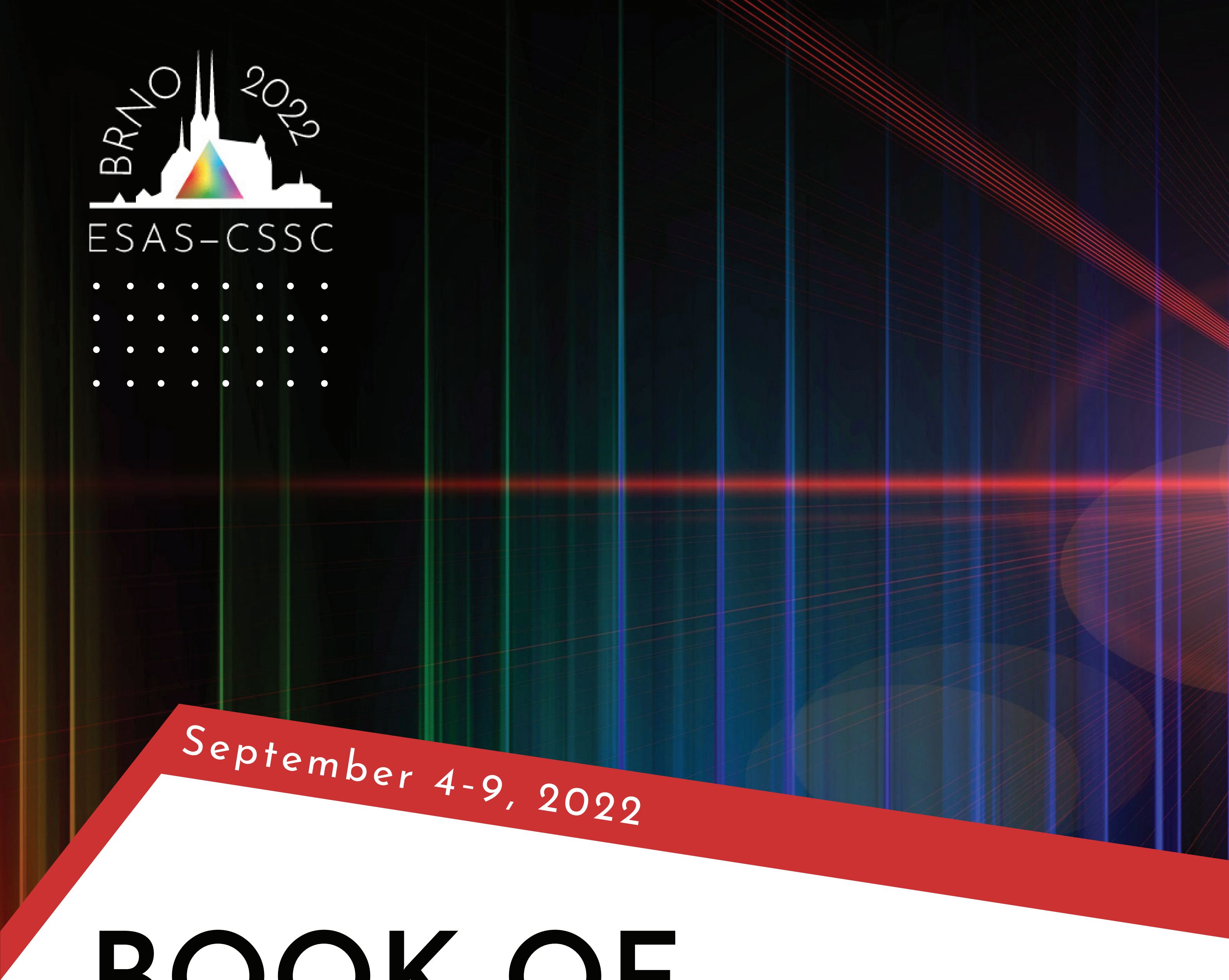

BRNO 2022

ESAS-CSSC

September 4-9, 2022

BOOK OF ABSTRACTS

2022

European Symposium on Analytical Spectrometry

Czech-Slovak Spectroscopic Conference

MUNI SCI

Ioannes Marcus Marci Spectroscopic Society

UNIVERSITY OF CHEMISTRY AND TECHNOLOGY PRAGUE

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WELCOME WORDS

Dear Colleagues,

It is with pleasure that we warmly welcome you on behalf of all the organizers of the joint scientific event combining the European Symposium on Analytical Spectrometry (ESAS) 2022 and the 17th Czech-Slovak Spectroscopic Conference (CSSC).

After a two-year break caused by the pandemic, this is the first international meeting of spectroscopists in the ESAS series, and at the same time, ESAS is taking place for the first time in a broader spectral range than that corresponding to atomic spectrometry. The replacement of the term "atomic spectrometry" with "analytical spectrometry" in the title of the symposium fully corresponds to current trends when the study of an analytical problem is carried out using numerous analytical techniques and multispectrally. The scientific meeting thus brings together the international scientific community of spectroscopists investigating analytical issues in the full breadth of current trends and mediates a much more versatile exchange of information, experience, and results. This year's ESAS & CSSC is, after joint meetings in 2012 in Tatranská Lomnica, Slovakia, and in 2014 in Prague, Czechia, the third joint scientific event of the ESAS series, which takes place in the territory of Czechia and Slovakia and follows on from the very successful meetings of ESAS 2010 in Wroclaw, ESAS 2016 in Eger and ESAS 2018 in Berlin. This year's meeting takes place in the Moravian capital of Brno, allowing participants to experience the extraordinarily pleasant and hospitable atmosphere of Moravia.

On behalf of the organizers, we would like to thank cordially the interest of participants from many, not only European, countries, from academic institutions and various technology companies, who created together a very professional program worth seeing. During the conference, on the proposal of the Jan Marek Marci Spectroscopic Society, the medal named after the patron of this society, the crucial Bohemian renaissance polyhistorian and humanist Jan Marek Marci from Kronland, will be awarded to three outstanding world scientists. Laureates are Érico Marlon de Moraes Flores, Detlef Günther and Yukihiro Ozaki. Warm congratulations to the honorees.

In addition to the scientific contribution, the conference should also be a pleasant and inspiring meeting of colleagues and friends. Therefore, we have prepared social events in interesting places, including Welcome party at the conference venue (the Atrium of Faculty of Social Studies of Masaryk University, close to the city centre), Evening with the stars and planets at the Brno Observatory and Planetarium, Brno excursions and Conference dinner in the beerhouse with typical Czech food and beer right in the city centre. We should like to take this opportunity to thank everyone who participated in the realization of the conference, especially the sponsors for their financial support, as well as the Faculty of Science, Masaryk University, Brno, and University of Chemistry and Technology Prague for the organisational support.

We believe that we create a pleasant and inspirational atmosphere and the right conditions for you to work, discuss, get inspiration, and meet interesting people. We wish you a valuable and enjoyable week spent with memorable experiences and the establishment of new fruitful contacts.

With our best regards,

Markéta Holá

Chair of the organizing committee

Viktor Kanický and Pavel Matějka

Chairmen of the ESAS & CSSC

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WELCOME PARTY	
17:00 – 20:00	ATRIUM FACULTY OF SOCIAL STUDIES

MONDAY, SEPTEMBER 5TH

OPENING CEREMONY (Hall P31)		
8:00 - 8:30	KANICKÝ, MATĚJKA	
SURFACE-ENHANCED RAMAN SPECTROSCOPY (Hall P31) CHAIR: MATĚJKA		
8:30 – 9:15	PL 1: Y. OZAKI	Chiral-label-free SERS and TERS strategies for chiral discrimination
9:15 – 9:35	OL 1: B. VLČKOVÁ	SERS and SERRS spectroscopy as a tool for probing and monitoring plasmon catalysed decarboxylation of Ru(II)-dicarboxybipyridine complexes
9:35 – 9:55	OL 2: M. PROCHÁZKA	New approaches in plasma-assisted nanostructured platforms for surface-enhanced Raman scattering (SERS) spectroscopy
9:55 – 10:15	OL 3: J. PÁSZTOR	Molecular spectroscopy NICOLET 1992-2022
10:15 – 10:35	OL 4: S. BERUS	The integration of a handheld Raman device and a SERS-based sensor for spectral recognition of vaginal fluids alterations
10:35 – 11:05	COFFEE BREAK (ATRIUM FACULTY OF SOCIAL STUDIES)	

Explanatory notes:

ESAS-CSSC BRNO 2022

●	Social events
●	Poster session
●	Plenary lecture
●	Invited lecture
●	Student lecture
●	Lunch/coffee

MONDAY, SEPTEMBER 5TH

PARALLEL SESSION

RAMAN SPECTROSCOPY & IR SPECTROSCOPY 1 (Hall P31) CHAIR: JOHNSON		
11:05 – 11:35	IL 1: E. KOČIŠOVÁ	Drop coating deposition Raman (DCDR) spectroscopy for sensitive detection of biologically important molecules
11:35 – 12:05	IL 2: A. BARTH	Structure and interactions of amyloid-β peptide aggregates unraveled by novel infrared spectroscopy approaches
12:05 – 12:25	OL 5: P. MOJZEŠ	Raman microscopy survey of intracellular purine inclusions: New paradigm of biocrystallization in eukaryotes
12:25 – 12:45	OL 6: V. PROFANT	Raman optical activity as a promising tool for mononucleotide g-quadruplexes studies
12:45 – 13:05	OL 7: M. LIBÁNSKÝ	Fluorescence-free material identification with new XTR technology from Metrohm
13:05 – 14:45		LUNCH (MU RECTORATE)

MONDAY, SEPTEMBER 5TH

PARALLEL SESSION

ICP-MS/OES (Hall P51) CHAIR: MATOUŠEK		
11:05 – 11:35	IL 3: M. CORTE-RODRIGUEZ	In-vivo and in-vitro studies on metal release (ions and nanoparticles) from dental implants using single-cell and single-particle ICP-MS
11:35 – 11:55	OL 8: F. GELMAN	Analysis of PTFE micro-particles by ICP-QMS operated in a single-particle mode
11:55 – 12:15	OL 9: M. GODULA	iCAP TQe ICP-MS: For samples where single quadrupole performance isn't enough
12:15 – 12:35	OL 10: J. DOBEŠ	Isotopic tools for uranium ores dating: application of uranium-lead and lead-lead dating systems
12:35 – 12:55	OL 11: J. VYHNANOVSKÝ	Photochemical vapor generation of rhodium and rhenium – on the way towards real sample analyses
13:05 – 14:45		LUNCH (MU RECTORATE)

MONDAY, SEPTEMBER 5TH

PARALLEL SESSION

RAMAN SPECTROSCOPY & IR SPECTROSCOPY 2 (Hall P31)
CHAIR: BARTH

14:45 – 15:15	IL 4: R. BETTENCOURT DA SILVA	Identification of microplastics by micro-FTIR: Validation and uncertainty evaluation
15:15 – 15:35	OL 12: M. HÁKOVÁ	Microplastics analysis by agilent 8700 LDIR
15:35 – 15:55	OL 13: K. BOTUROVÁ	Spectroscopic characterization of humic acids in chernozems
15:55 – 16:15	OL 14: J. ŠTUBŇA	Identification of gemstones in watch by Raman spectroscopy
16:15 – 18:15	POSTER SESSION (AULA OF FACULTY OF SOCIAL STUDIES)	
18:30 – 22:00	BRNO OBSERVATORY (SEE DETAILS IN SOCIAL PROGRAMME)	

MONDAY, SEPTEMBER 5TH

PARALLEL SESSION

SPECIATION ANALYSIS 1 (Hall P51)
CHAIR: FELDMANN

14:45 – 15:15	IL 5: G. SCHLEMMER	Instrumental Analysis in 30 minutes: bridging the techniques
15:15 – 15:35	OL 15: T. MATOUŠEK	Simultaneous ultratrace speciation analysis of arsenic and germanium in natural water
15:35 – 15:55	OL 16: K. CHIBA	Speciation analysis of Gd-based contrast agents in river water using HPLC-ICP-MS
15:55 – 16:15	OL 17: P. NOMNGONGO	Miniaturised liquid phase extraction of butyl and phenyltins in sediment samples using deep eutectic solvent: Optimisation and HPLC-ICP-MS analysis
16:15 – 18:15	POSTER SESSION (AULA OF FACULTY OF SOCIAL STUDIES)	
18:30 – 22:00	BRNO OBSERVATORY (SEE DETAILS IN SOCIAL PROGRAMME)	

TUESDAY, SEPTEMBER 6TH

AAS 1 (Hall P31) CHAIR: DĚDINA		
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9:20 – 9:50	IL 6: E. BEINROHR	High resolution continuum source AAS for determination of nonmetals
9:50 – 10:10	OL 18: V. CYPRICHOVÁ	Study of distribution of zinc in ZnO nanoparticles in soil colloids (extracted from samples collected at various agricultural and forest sites in Slovakia) by sequential centrifugation and flame AAS
10:10 – 10:40	IL 7: M. ARRUDA	What metals/speciome can tell us about bioanalytics applied to health and plant science
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TUESDAY, SEPTEMBER 6TH

PARALLEL SESSION

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11:40 – 12:10	IL 9: J. DĚDINA	Employing laser induced fluorescence and selected ion flow tube mass spectrometry to understand what happens in hydride atomizers
12:10 – 12:30	OL 19: F. SIMON	An improved method for the determination of PFAS using HR-CS-GFMAS via GaF detection
12:30 – 12:50	OL 20: Z. KOWALEWSKA	Spectral aspects in determination of fluorine via GaF, CaF and SrF molecules using high-resolution continuum source molecular absorption spectrometry
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TUESDAY, SEPTEMBER 6TH

PARALLEL SESSION

RAMAN SPECTROSCOPY & IR SPECTROSCOPY 3 (Hall P51) CHAIR: KOČIŠOVÁ		
11:10 – 11:40	IL 10: I. NĚMEC	Promising molecular-based materials for nonlinear optics – spectroscopic, diffraction and optical study
11:40 – 12:10	IL 11: M. JOHNSON	Nanoscale infrared spectroscopy studies of cellulose
12:10 – 12:30	OL 21: P. MATĚJKA	Nanoscopic techniques related to molecular vibrations
12:30 – 12:50	OL 22: J. HORÁK	Chemistry at the nanoscale – AFM meets IR spectroscopy
12:50 – 14:30		LUNCH (MU RECTORATE)

TUESDAY, SEPTEMBER 6TH

PARALLEL SESSION

SPECIATION ANALYSIS 2 (Hall P31) CHAIR: DONARD		
14:30 – 15:00	IL 12: J. FELDMANN	Elemental speciation from metals, metalloids to non-metals in environmental science: successes and problems
15:00 – 15:20	OL 23: A. RAAB	Arsenic and rice (*Oryza sativa L.*)
15:20 – 15:40	OL 24: A. ORLOWSKA	Comparison of mobile phases for cation exchange HPLC-ICP OES
15:40 – 16:00	OL 25: A. KAŇA	Selenium transformation by food-grade microorganisms
16:00 – 16:20	OL 26: J. PROCH	Determination of metals and metalloids species using self-designed hyphenated systems based on detection by optical emission spectrometry
16:20 – 16:40	OL 27: V. MUELLER	Mass balance analyses of PFAS in soil, snowmelt and ski waxes
16:45 – 18:45	POSTER SESSION (AULA OF FACULTY OF SOCIAL STUDIES)	

TUESDAY, SEPTEMBER 6TH

PARALLEL SESSION

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15:00 – 15:30	IL 14: V. SVOBODA	Ultrafast time-resolved probes of chirality during photochemical reactions
15:30 – 15:50	OL 28: D. MATOUŠEK	FTIR-FPA and FTIR-QCL microscopy: Breakthrough techniques in infrared imaging
15:50 – 16:10	OL 29: P. LUBAL	The optical chemosensor array for analysis of halides or small biological molecules
16:45 – 18:45	POSTER SESSION (AULA OF FACULTY OF SOCIAL STUDIES)	

WEDNESDAY, SEPTEMBER 7TH

PARALLEL SESSION

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9:00 – 9:20	OL 30: A. KOHOUTOVÁ	Stopping efficiency simulation of cryogenic gas stopping cell
9:20 – 9:40	OL 31: E. BULSKA	Fluoroproteomics uncovers the effects of fluorinated drugs
9:40 – 10:00	OL 32: M. VIDO	Structural characterization of hydrophobic hyaluronan derivatives by comprehensive 2D-LC-MS
10:00 – 10:20	OL 33: J. KUČERA	The first AMS laboratory in the Czech Republic installed at the Nuclear Physics Institute of the CAS, Řež
10:40 – 11:10	COFFEE BREAK (ATRIUM OF FACULTY OF SOCIAL STUDIES)	

WEDNESDAY, SEPTEMBER 7TH

PARALLEL SESSION

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9:00 – 9:20	OL 34: I. MACHADO	Microwave plasma atomic emission spectrometry for metallomics of bioactive rhenium compounds
9:20 – 9:40	OL 35: B. CIEŚLIK	Heavy metals fractions analysis in sewage sludge ash obtained on laboratory scale and from industrial origin
9:40 – 10:00	OL 36: A. RAGYÁK	Time travel with honeys - The MP-AES analysis coupled with AMS age determination of Hungarian acacia samples
10:00 – 10:20	OL 37: A. MOLLO	Advances in mercury determination by CV – MIP OES with nitrogen plasma, in drinking and surface water
10:20 – 10:40	OL 38: Z. SAJTOS	Time travel with honeys - The MP-AES analysis coupled with AMS age determination of Hungarian rape, sunflower and multifloral samples
10:40 – 11:10	COFFEE BREAK (ATRIUM OF FACULTY OF SOCIAL STUDIES)	

WEDNESDAY, SEPTEMBER 7TH

PARALLEL SESSION

SPECIAL SPECTROSCOPY 1 (Hall P31) CHAIR: KANTNEROVÁ		
11:10 – 11:40	IL 17: P. NEUGEBAUER	High frequency rapid scan electron spin resonance spectroscopy
11:40 – 12:00	OL 39: A. OPÍCHAL	Data analysis from catcher foil experiment for cross-sections measurement of ^{40}Ar + ^{144}Sm reaction
12:00 – 12:20	OL 40: M. JIRUŠ	Mechanical and gamma-absorption properties of selected heat resistant materials used in development of sealed reaction chambers
12:20 – 12:40	OL 41: P. LIŠKA	Correlative high-resolution optical and chemical imaging of $CsPbBr_3$ nanocrystals
12:40 – 14:30		LUNCH (MU RECTORATE)
15:00		EXCURSION (SEE DETAILS IN SOCIAL PROGRAMME)

WEDNESDAY, SEPTEMBER 7TH

PARALLEL SESSION

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11:40 – 12:10	IL 19: Z. WEISS	Excitation in a glow discharge and an inductively coupled plasma: similarities and differences
12:10 – 12:30	OL 42: J. KRATZER	Next generation of dielectric barrier discharge atomizers for ultratrace element analysis
12:40 – 14:30		LUNCH (MU RECTORATE)
15:00		EXCURSION (SEE DETAILS IN SOCIAL PROGRAMME)

THURSDAY, SEPTEMBER 8TH

LA-ICP-MS (Hall P31) CHAIR: KANICKÝ		
8:00 – 8:50	PL 3: D. GÜNTHER	Recent developments in laser ablation and inductively coupled plasma mass spectrometry
8:50 – 9:10	OL 43: B. WAGNER	Comparative analysis of inks from the Chopin's manuscript Impromptu in a flat major, Op. 29: a proof of concept for a non-invasive image-based investigations of written cultural heritage
9:10 – 9:30	OL 44: M. KUCHYNKA	Bioimaging of elements and proteins by LA-ICP-MS in medicine and pharmaceutical research
9:30 – 9:50	OL 45: K. SOBEK	Imaging of chemical and structural processes in minerals
9:50 – 10:15	COFFEE BREAK (ATRIUM OF FACULTY OF SOCIAL STUDIES)	

THURSDAY, SEPTEMBER 8TH

PARALLEL SESSION

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10:45 – 11:15	IL 21: D. SCHAUMLOFFEL	Nanoscale Secondary Ion Mass Spectrometry for elemental bioimaging in cells and tissue
11:15 – 11:35	OL 46: L. KRONLACHNER	Depth-resolved elemental and molecular analysis of polymeric composites using chemometric evaluation
11:35 – 11:55	OL 47: P. NEČAS	Application of spectroscopic methods in research of geochemical processes in the Upper Silesian coal basin
11:55 – 12:15	OL 48: M. BURŠÍKOVÁ	Evaluation of the element content in geologial units and its importance in the environment evaluation – spectroscopy study
12:15 – 14:00		LUNCH (MU RECTORATE)

THURSDAY, SEPTEMBER 8TH

PARALLEL SESSION

MÖSSBAUER SPECTROSCOPY 1 (Hall P51) CHAIR: MIGLIERINI		
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10:45 – 11:05	OL 49: V. HEGER	Polymorphism and crystal structure of iron(II) oxalate
11:05 – 11:25	OL 50: P. NOVÁK	Lamb-Mössbauer factor determination of powders by resonance Mössbauer spectroscopy
11:25 – 11:45	OL 51: J. KOPP	Thermally induced solid-state reaction of $Fe_2(SO_4)_3$ with NaCl or KCl : a route to β-Fe_2O_3 synthesis
11:45 – 12:05	OL 52: S. VYHNÁLEKOVÁ	Speciation analysis of iron in the biological matrix of filamentous fungi using Mössbauer spectrometry
12:15 – 14:00		LUNCH (MU RECTORATE)

THURSDAY, SEPTEMBER 8TH

PARALLEL SESSION

MÖSSBAUER SPECTROSCOPY 2 (Hall P31) CHAIR: KOPÁNI		
14:00 – 14:30	IL 23: M. MATULOVÁ	Application of spectroscopic techniques for speciation analysis of Iodine, Selenium and iron used in studies of processes in the near- and far-field regions of spent nuclear fuel disposal system
14:30 – 14:50	OL 53: S. LISNÍKOVÁ	Nickel-iron and zinc-iron bimetal oxalates: preparation, characterization and thermal decompositon to spinel ferrites
14:50 – 15:10	OL 54: M. MIGLIERINI	Mössbauer spectrometry of metallic alloys
15:10 – 15:30	OL 55: D. GREY	Mössbauer spectroscopy study of tin-containing metallic glasses
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THURSDAY, SEPTEMBER 8TH

PARALLEL SESSION

ICP-MS/OES 2 (Hall P51) CHAIR: HOLÁ		
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14:20 – 14:40	OL 57: L. NYABA	Seasonal variation of drinking water quality and human health risk assessment: a case study in rural village of the eastern cape
14:40 – 15:00	OL 58: J. KARASIŃSKI	High precison measurements of lead isotope ratio without matrix separation
15:00 – 15:20	OL 59: T. MUNONDE	Magnetic Fe_3O_4@Mg/Al-layered double hydroxide adsorbent for preconcentration of trace metals in water matrices
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THURSDAY, SEPTEMBER 8TH

PARALLEL SESSION

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16:30 – 17:00	IL 25: M. KOPÁNI	Application of analytical techniques in the study of biological systems
17:00 – 17:20	OL 60: M. URÍK	Speciation of iron in microbial biomass and natural ochric precipitates as affected by fungal activity
19:00	CONFERENCE DINNER (POUPĚ BREWERY)	

THURSDAY, SEPTEMBER 8TH

PARALLEL SESSION

SPECIAL SPECTROSCOPY 2 (Hall P51) CHAIR: NEUGEBAUER		
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17:00 – 17:20	OL 61: A. VOJS STAŇOVÁ	Finding of needle in a haystack -- nontargeted mass spectrometry analysis of environmental samples
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9:30 – 10:00	IL 29: J. LASERNA	Understanding the correlation of LIBS and acoustic measurements of rock and soil found in the traverse of Perseverance rover across the Jezero crater, Mars
10:00 – 10:20	OL 62: K. NOVOTNÝ	Laser induced breakdown spectroscopy imaging of uranium ores
10:20 – 10:40	OL 63: Y. DEGUCHI	LIBS applications of online monitoring and 2D/3D mappings for advanced control of industrial processes
10:40 – 11:10	COFFEE BREAK (ATRIUM OF FACULTY OF SOCIAL STUDIES)	

FRIDAY, SEPTEMBER 9TH

LASER INDUCED BREAKDOWN SPECTROMETRY (Hall P31) CHAIR: LASERNA		
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11:40 – 12:10	IL 31: J. KAISER	Enhancing the sensitivity of laser-induced breakdown spectroscopy for the detection of nanoparticle-labeled cancerous tissues
12:10 – 12:30	OL 64: P. KOLEČKÁŘ	Polychromator ORCA (Optimized Rowland Circle Alignment)
12:30 – 12:50	OL 65: D. HAHN	Aerosol analysis with laser-induced breakdown spectroscopy: Sampling approaches and recent applications
12:50 – 13:10	ESAS-CSSC 2022 CLOSING CEREMONY	
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MONDAY, SEPTEMBER 5TH

MONDAY'S POSTER SESSION – AULA OF FACULTY OF SOCIAL STUDIES

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MP 2	RAGYÁK	The Effect of farnesol and tyrosol treatment for the intracellular metal content of candida auris
MP 3	KRÁLOVIČ	The process of photopolymerization of acrylated soybean oil based epoxides investigated by positron annihilation lifetime spectroscopy
MP 4	WEIß	Quantitative determination of supramolecular complex stabilities using collison-induced dissociation and Fourier transform ion cyclotron resonance mass spectrometry
MP 5	KUIŽOVÁ	Drop coating deposition raman spectroscopy of liposomes on nanostructured fluorocarbon film
MP 6	ROGOLL	Determination of the impact of LA-ICP-MS parameters during soft material analysis
MP 7	ŠTÁDLEROVÁ	Comparison of radiation sources for atomic fluorescence spectrometry
MP 8	WIGGERSHAUS	Method development for the analysis of highly saline samples using TXRF
MP 9	FARKAS	Mobilization of potentially toxic elements from mine drainage ochres by Aspergillus species
MP 10	ACHLEITNER	Realisation of a LIBS method to determine the degree of imidization of polyimides
MP 11	ISHIKAWA	The evaluation of solid state of rice flour by IR and NIR spectroscopy
MP 12	ADAMCOVÁ	Novel cell for transcorneal permeation studies using vibrational spectroscopy techniques
MP 13	FRIEBEL	Application of emission spectroscopic solid sampling methods on biomass samples for co-combustion
MP 14	NOVÁKOVÁ	Efficiency of chemical vapor generation of zinc
MP 15	KOKO	Multielemental speciation analysis of Cd^{2+}, Pb^{2+} and $(CH_3)_3Pb^+$ in herb roots by advanced hyphenated technique HPLC/ICP-DRC-MS
MP 16	DUBORSKÁ	Soil Iodine fractionation by sequential extraction followed by ICP-MS determination
MP 17	ŠVÁBENSKÁ	Spectroscopic methods in the analysis of wear particles
MP 18	KOUTENTAKI	3D Raman mapping as an investigation tool for particle coating thickness
MP 19	KAŇKOVÁ	Overview of XRF versus ICP applications in elemental analysis of glass materials

MONDAY, SEPTEMBER 5TH

MONDAY'S POSTER SESSION – AULA OF FACULTY OF SOCIAL STUDIES

MP 20	HAGAROVÁ	Two extraction procedures coupled to ETAAS quantification employed for speciation of inorganic antimony
MP 21	KOPAL	Another perspective at the origin of alien bands in the surface-enhanced Raman spectra of 4-aminobenzenethiol
MP 22	KREMPL	Laser ablation synthesis of tellurium clusters
MP 23	WILLNER	A novel standard addition approach for matrix-matched calibration with LA-ICP-MS via spray deposition
MP 24	HRANÍČEK	Chemiluminescent determination of vitamin B12 using automatic sequential injection analysis
MP 25	NOVÁKOVÁ	Determination of rare earth elements in geological samples by ICP-MS
MP 26	ŠVANCAROVÁ LAŠTINCOVÁ	Suitable methods of heavy metals determination in wines by ETA-AAS
MP 27	ŠVEHLA	Examples of the use of selected spectrometric techniques in the practice of the Customs Tech Lab. in the Czech Republic.
MP 28	HEGROVÁ	Evaluation of toxicity and bioaccumulation of metals from transport and their effect on the mineral composition of green alga Desmodesmus Subspicatus using ICPMS/MS
MP 29	VYTISKOVÁ	Detection of biomolecules labeled with photon-upconversion nanoparticles by laser-induced breakdown spectroscopy
MP 30	URÍK	Evaluation of heterotrophic leaching of arsenic in multicomponent humic acid/amorphous ferric oxohydroxide/bentonite system using atomic spectrometry
MP 31	CIFRANIČOVÁ	Positron annihilation spectroscopy as a tool for examining microstructural properties
MP 32	POLÁŠKOVÁ	Polypropylene treated by atmospheric plasma jets: correlating plasma chemistry with surface modifications
MP 33	ZAORALOVÁ	Application of X-ray diffraction and scanning electron microscopy to clay minerals
MP 34	HEIMLER	Tabletop CμXRF spectrometer for nondestructive depth-resolved element analysis
MP 35	BILAVČÍKOVÁ	Tracing new potential chemoterapeutics using ICP-MS and LA-ICP-MS
MP 36	DOBŠÍKOVÁ	Synthetic cannabinoids: structure determination and characterization by molecular spectroscopy
MP 37	BUŇOVÁ	Simulated stability of selected elements in TRIS buffer solution
MP 38	KUBINYIOVÁ	Enhancement of luminescence signal of tetracyclines antibiotics by deuterated water

MONDAY, SEPTEMBER 5TH

MONDAY’S POSTER SESSION – AULA OF FACULTY OF SOCIAL STUDIES

MP 39	COELHO	Plasma-mediated vapor generation by dielectric barrier discharge: Direct analysis of mercury by AAS
MP 40	SAGAPOVÁ	Ultrasensitive determination of cadmium by atomic spectrometry
MP 41	BEDNÁŘOVÁ	Structural investigation of a/g-hybrid peptide oligomers
MP 42	ŠIMONÍKOVÁ	Multielemental analysis of tantalum ores by ICP-OES
MP 43	ČECHOVÁ	LIBS analysis of Cannabis sativa after long-term exposition in cadmium-contaminated soil
MP 44	DENDISOVÁ	Microscopic and nanoscopic study of polymer membranes
MP 45	MESKO	Multitechnique determination of halogens and sulfur in human hair

TUESDAY, SEPTEMBER 6TH

TUESDAY'S POSTER SESSION – AULA OF FACULTY OF SOCIAL STUDIES

TP 1	BOSÁKOVÁ	Instrumental configuration effect on the libs acoustic signal response
TP 2	VEJVODOVÁ	Biorecognition tools
TP 3	LOULA	Graphene analysis by ICP-OES: The importance of sample preparation
TP 4	SIHLAHLA	Vortex assisted liquid-liquid microextraction for extraction of Selenium in food samples using alcohol based-DES prior to ICP-OES: One step closer to achieving green analytical chemistry
TP 5	BOKOV	Rearrangement of intracellular crystalline guanine as an adaptation for various illumination levels
TP 6	PODSEDNIK	Analysis of non-metals in technologically relevant materials using laser-induced breakdown spectroscopy (LIBS)
TP 7	ASARE	The distribution of potentially toxic and risk elements in the organs of Rumex alpinus
TP 8	BAHELKOVÁ	Where cadmium accumulates after inhalation of cadmium-based nanoparticles
TP 9	SVOBODA	In-situ trapping of volatile species in DBD atomizers: new approach to preconcentration of cadmium and selenium
TP 10	FIŠERA	Selected spectrometric methods for determination of iodine in biological samples
TP 11	MAŠLÁŇ	Mössbauer study of thermal behavior of CL20ES and CL50WS steel powders used in selective laser melting
TP 12	TSUBOI	Raman spectroscopic study of minerals in granitic rocks
TP 13	JURGA	The luminescence of NIR-excited up-converting nanoparticles in the blood solution
TP 14	TARASENKA	Spectroscopic analysis of laser ablation plasma in liquid during nanoparticles synthesis
TP 15	KRČMÁŘ	Charge ordering and hyperfine interactions in magnetite at liquid helium temperature
TP 16	ZVĚŘINA	Zn and Fe in vegetables: simultaneous determination using HR-CS GF-AAS
TP 17	HANNIG	Alkaloid fagaronine and its interaction with non-canonical DNA structures
TP 18	KOHOUT	Simulations of Ion funnel of multi-reflection time-of-flight mass spectrometer
TP 19	BHAT	A brief study of plasma plume parameters from laser ablation of mica under argon ambient

TUESDAY, SEPTEMBER 6TH

TUESDAY'S POSTER SESSION – AULA OF FACULTY OF SOCIAL STUDIES

TP 20	HAĆ	Mercury in various tobacco products
TP 21	MATÚŠ	Application of spectroscopic methods for analysis of humic acids' interactions with aluminium(III)
TP 22	WOŹNY	Temperature dependent luminescence of $FeS_2@YF_3:Yb^{3+}/Er^{3+}$ nanocomposites
TP 23	BURA	Isotopic labeling of microalgae: Raman study
TP 24	NEPAL	Scope and challenges of IR spectroscopy: Theoretical aspects
TP 25	SŮRA	Synthesis of gold nanoparticles using tetrahydroxy-1,4-benzoquinone oxocarbon as a capping agent
TP 26	MICHALICOVÁ	Arsenic species in the air of Brno city park
TP 27	MUSIL	Atomization of tellurium hydride in a dielectric barrier discharge and its in-situ trapping for atomic absorption spectrometry.
TP 28	KOŽNAROVÁ	Analysis of chemotherapeutics in extracellular vesicles
TP 29	ADAMEC	Risk elements in soils in selected areas of northwestern Bohemia
TP 30	KOŠKOVÁ	Alnus glutinosa short rotation coppice for HCH contaminated area - Chemical and microbiological evaluation
TP 31	RIGASOVÁ	Recognition of proteins using metal-based nanoparticles
TP 32	MATOUŠEK	Speciation analysis of tellurium in water samples by Selective HG-ICP-MS/MS with $TiCl_3$ as pre-reducing agent
TP 33	KANTOROVÁ	Analysis of high-molecular selenium species in lactic acid bacteria
TP 34	KRAJANOVÁ	Raman Spectroscopy of metal oxalates
TP 35	ŠIRŮČKOVÁ	The spectroscopic study of kinetic properties of Pb(II) complexes with phosphonic acid derivative ligands
TP 36	DUVIVIER	Evaluation of current benchtop energy dispersive XRF instrumentation in comparison to wavelength dispersive XRF
TP 37	BAZEL	Design of new microextraction procedure for ammonium determination
TP 38	LANDRY	Is digital scanner suitable as cheaper alternative of a spectrophotometer?

TUESDAY, SEPTEMBER 6TH

TUESDAY'S POSTER SESSION – AULA OF FACULTY OF SOCIAL STUDIES

TP 39	SAJTÓS	The elemental analysis of the mummies of Vác, Hungary
TP 40	GAJARSKÁ	Feature engineering to improve classification in LIBS
TP 41	ACHLEITNER	Determination of K and N within functionalized polystyrene beads for glycan purification
TP 42	KOPAL	Contribution of the chemical mechanism to the overall enhancement in the surface-enhanced Raman spectra of methylene blue
TP 43	ŠVECOVÁ	Nanoscopic Investigation of wood cell walls
TP 44	IVANOVA	Mössbauer study of the stainless steel surface after annealing in the temperature range 700 - 1000 °C
TP 45	HRDLIČKA	Laser-induced breakdown spectroscopy in analysis of algae contamination on the filter

ORAL
ABSTRACTS

PL1

A CHIRAL-LABEL-FREE SERS AND TERS STRATEGIES FOR CHIRAL DISCRIMINATION

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Efficient and generic enantioselective discrimination of various chiral molecules is achieved by SERS through charge–transfer (CT) contributions.[1] The intensities of the SERS peaks of a chiral selector are strongly dependent on the chirality of its surroundings including the chirality of a hot spot itself. This highly distinct spectral discrepancy may be due to the tendency of chiral isomers to form intermolecular hydrogen-bonding complexes with the chiral selector in different molecular orientations, resulting in different CT states and SERS intensities of the adsorbates in the system. The selectivity originated from the enantioselectivity of the intermolecular hydrogen bonding interactions. The difference in the protonation of the Ag–MPY complex through hydrogen bonding led to the formation of different CT states of the Ag–MPY complex, which are involved in the CT process, and further manifested in a tremendous difference in the SERS spectra. These results provide important improvements in the field of label-free enantioselective discrimination without the employment of any chiral agents.[1]

Discrimination between enantiomers is also achieved by TERS using a silver tip that is chemically modified by an achiral para-mercaptopyridine (*p*MPY) probe molecule.[2] Differences in the relative intensities of the *p*MPY spectra were monitored for three pairs of enantiomers containing hydroxy (-OH) and/or amino ($-NH_2$) groups. The N: or N^+-H functionality of the *p*MPY-modified tip participates in hydrogen-bond interactions with a particular molecular orientation of each chiral isomer. The asymmetric arrangement of silver atoms at the apex of the tip induces an asymmetric electric field, which causes the tip to become a chiral center. Differences in the CT states of the metal-achiral probe system in conjunction with the asymmetric electric field produce different enhancements in the Raman signals of the two enantiomers. TERS with tailored chemical modification is firstly proposed to distinguish the enantiomers. CT transition of *p*MPY-Ag complex can encourage the slight difference in the electronic structure of two complexes of enantiomers through the preferable hydrogen bonding interaction.[2] Of note is that the TERS tip itself has some chirality.

References

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OL1

SERS AND SERRS SPECTROSCOPY AS A TOOL FOR PROBING AND MONITORING PLASMON CATALYSED DECARBOXYLATION OF RU(II)-DICARBOXYBIPYRIDINE COMPLEXES

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Plasmon catalysis represents a challenging possibility of conversion of light energy into chemical bond energy. In this contribution, we report the strategy of revealing plasmon-catalysed decarboxylation reactions of Ru (II) bis(2,2‘-bipyridine)(4,4‘-dicarboxybipyridine) /Ru(bpy)$_2$(dcbpy)/ and of Ru(II) tris(4,4‘-dicarboxybipyridine) /Ru(dcbpy)$_3$/ complexes in hydrosol systems with Ag nanoparticles (NPs) conditioned by the presence of Ag(0) adsorption sites on Ag NP surfaces. In the first step, SERRS (at 445 nm excitation) and SERS (at 532 nm excitation) spectral marker bands of Ru-bpy and Ru-dcbpy units in Ru(bpy)$_2$(dcbpy) complex have been established and re-confirmed by comparison with SERRS and SERS spectra of Ru(bpy)$_3$ and Ru(dcbpy)$_3$. Consequently, both Ru(bpy)$_2$(dcbpy) and Ru(dcbpy)$_3$ were found to undergo decarboxylation reaction in systems with Ag NPs modified by chlorides and in systems with reduction-driven Ag NP growth, yielding Ru(bpy)$_3$ as the final product. The characteristic common to both types of systems is the presence of Ag(0) adsorption sites on Ag NPs surfaces. Furthermore, by a series of targeted experiments, the decarboxylation reaction has been identified as a light-induced surface reaction. SERS spectral detection of the reaction progress at 532 nm excitation eliminated surface photochemistry and indicated plasmon catalysis. Another series of targeted experiments enabled us to establish the mechanism of the decarboxylation reaction as plasmon catalysis by charge carriers, i.e., hot electrons and hot holes, and propose the following reaction scheme:

$$(bpy)_2\text{-Ru(II)-bpy-}(COO^-)_2 + 2\text{hot } h^+ + 2H^+ + 2\text{hot } e^- \rightarrow Ru(II)(bpy)_3 + 2CO_2$$

Finally, we conclude that the crucial role of Ag(0) adsorption sites in the decarboxylation reactions undergone by the complexes and catalyzed by the charge carriers is the creation of an appropriate interface for the interfacial transfer of hot e$^-$ to H$^+$ ions. In particular, we reason that provided that only oxidized Ag$^+$ adsorption sites were present on Ag NPs surfaces, hot e$^-$ would be used primarily for reduction of these adsorption sites.

OL2

NEW APPROACHES IN PLASMA-ASSISTED NANOSTRUCTURED PLATFORMS FOR SURFACE-ENHANCED RAMAN SCATTERING (SERS) SPECTROSCOPY

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In this contribution we report some new approaches in the preparation of nanostructured platforms for SERS by means of plasma-based techniques such as:
1. Gradient nanostructured Ag surfaces, i.e. nano-islands with gradually changing optical properties (LSPR) in one direction, prepared by magnetron sputtering [1].
2. Nanostructured bi-metallic Ag/Au films prepared by magnetron sputtering. We found that by Ag-coating of Au nanostructures it is possible to tune in a certain range independently the position and the intensity of LSPR peak [2].
3. Physically produced Ag/C:H:N:O core-satellite nanoparticles upon deposition on a planar substrate forming mesoporous nanoparticle films with SERS-active Ag nanoparticles evenly distributed on the surface of supporting C:H:N:O cores [3].
4. Magnetron sputtered Ag nanoislands on Au surface. We used them to investigate the permeability of zwitterionic carboxybetaine-based polymer brushes with respect to small molecules. The method is based on rafting the polymer brush to a custom-made SERS substrate. By checking SERS spectra of the reporter molecule penetrating through the brush we are able to gain information about the polymer brush permeability.

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OL3

MOLECULAR SPECTROSCOPY NICOLET 1992-2022

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Brief historical overview and interesting steps at world leading manufacturer of Nicolet brand molecular spectroscopy instruments.
30 years of our FT-IR and Raman spectroscopy method development at the EMEA region and worldwide.
Recent development and news from Nicolet CZ portfolio: FT-IR, SNOM and IR-SNOM nanomicroscopy, FT-NIR, NIR, Raman, FT-Raman, FT-FAR, UV-VIS, UV-VIS-NIR, THz. NMR, PL and LIBS spectroscopy, incl. microscopes, process analysers, portable and handheld spectrometers...

OL4

THE INTEGRATION OF A HANDHELD RAMAN DEVICE AND A SERS-BASED SENSOR FOR SPECTRAL RECOGNITION OF VAGINAL FLUIDS ALTERATIONS

Sylwia Magdalena BERUS[1], Beata MŁYNARCZYK-BONIKOWSKA[2], Monika ADAMCZYK-POPŁAWSKA[3], Tomasz SZYMBORSKI[1], Agnieszka KAMIŃSKA[1]

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Vaginal infections (vaginitis) are among the most common and problematic disorders that affect almost 70% of women during their whole lifetime at least once – the most prevalent are bacterial vaginosis (BV) and vulvovaginal candidiasis (VVC). Vaginitis is associated with the feeling of discomfort and can cause many severe diseases and complications *e.g.* premature rupture of membranes. The accurate diagnosis and implementation of appropriate medicines is an inherent element in successful treatment and provides protection against recurrence of infection - this makes the differential diagnosis of vaginal infections of the utmost importance. Surface-Enhanced Raman Spectroscopy (SERS) is based on the inelastic scattering of incident light by molecules adsorbed onto a roughened metal substrate (SERS substrate). SERS has been proved as a beneficial method due to its ultra-sensitivity and non-destructive nature that reveals specific fingerprint-like information down to the molecular level. This technique was utilized to study many biological systems such as: human tissues, cells, body fluids [1].

In this study for the first time, we used SERS and chemometric method - Partial Least Squares Regression (PLSR) to track the spectral response of vaginal fluids caused by different types of infections. We proved that the biochemical alterations that result from infections can be translated into a specific spectral image that is unique for each infection and hence their differentiation is possible at high level of explained information by PLSR. The integration of SERS-based sensors with a small, portable Raman spectrometer leads to the development of a handheld point-of-care device.

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IL1

DROP COATING DEPOSITION RAMAN (DCDR) SPECTROSCOPY FOR SENSITIVE DETECTION OF BIOLOGICALLY IMPORTANT MOLECULES

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The drop coating deposition Raman (DCDR) scattering technique is a relatively new unique detection method based on drying of a small drop (2-5 µl) of molecular solution or suspension of interest deposited on a special hydrophobic surface. The drying process of the drop very efficiently accumulates the molecules in the forming pattern from which the Raman spectrum of very good quality can be measured. The hydrophobic surface enables to dry the droplet in a manner of either "coffee-ring effect" or a small pattern without a clear peripheral ring. In the former case, the dispersed material is carried by the flow of a liquid in the evaporating droplet to its edge, where it forms a ring. The latter case was proposed as a universal "solvent removal" method applicable to samples in aqueous solutions deposited on highly hydrophobic surfaces. Both approaches lead to the possibility of measuring the Raman signal not only from small volumes but also from low initial concentrations by using a confocal Raman microspectrometer. The lecture will focus on the introduction and possible application of the DCDR technique, emphasizing the detection of biologically important molecules. The importance of the DCDR hydrophobic substrates and the possibilities of commercially available ones will be discussed. An attempt to improve the method led to the development of a novel type of surfaces with metallic nanoparticles. Their preparation is based on nanostructuring of magnetron sputtered hydrophobic C:F films by a base layer of metallic nanoparticles that were fabricated employing a gas aggregation source of the original construction. It will be demonstrated that the surface roughness of resulting coatings has a strong influence on surface wettability and properties/shapes of formed dried patterns. DCDR spectra of a set of molecules, including lipids, porphyrins, food contaminants (melamine), pesticides (thiram, bentazon), dipicolinic acid as anthrax marker, will be presented [1-3].

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IL2

STRUCTURE AND INTERACTIONS OF AMYLOID-BETA PEPTIDE AGGREGATES UNRAVELED BY NOVEL INFRARED SPECTROSCOPY APPROACHES

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The most common neurodegenerative disease is Alzheimer's disease, in which the amyloid-ß (Aß) peptide aggregates to amyloid fibers that accumulate in plaques in the human brain. Key aspects of the disease are still unclear and our work sheds light on two of them: (i) the structure of Aβ oligomers in aqueous solution and (ii) interactions of Aβ with other peptides. Here, we exploit the particular advantages of isotope-edited infrared (IR) spectroscopy using both uniform and site-specific ^{13}C-labeling.
Our results confirm a hairpin structure of individual peptides in the oligomers. They indicate a building block of two adjacent strands for the shorter Aβ variant Aβ40 and of two or more adjacent strands for the longer variant Aβ42 [1]. For more detailed structural models, we use ^{13}C–labeling of specific amide groups in the backbone to identify intra– and intermolecular contacts similar to solid state nuclear magnetic resonance. First results indicate that the β-sheets of oligomers are composed of different residues in oligomers of different sizes (Vosough & Barth, manuscript in preparation).
To study Aβ's interaction with other peptides, we use uniform ^{13}C–labeling of one of the interaction partners. We found that Aβ40 and Aβ42 form mixed β-sheets in oligomers [2]. With IR nanospectroscopy, we were able to identify both interaction partners in nanoscale images of the IR absorption. Our results indicate that an anti-amyloid peptide dissolves or coats Aβ fibers.

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OL5

RAMAN MICROSCOPY SURVEY OF INTRACELLULAR PURINE INCLUSIONS: NEW PARADIGM OF BIOCRYSTALLIZATION IN EUKARYOTES

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Despite the widespread occurrence of crystalline inclusions in unicellular eukaryotes, scant attention has been paid to their composition, functions, and evolutionary origins. Using Raman microscopy, we revisited the broad diversity of eukaryotes examining more than 200 species in all major supergroups [1, 2]. We found that 80% of cellular crystalline inclusions contain purines, such as anhydrous guanine (62 %), guanine monohydrate (2%), uric acid (12%), and xanthine (4%), which shifts the paradigm assuming the presence of calcite, and oxalates. Purine crystals emerge in microorganisms in all habitats, *e.g.*, in freshwater algae, endosymbionts of reef-building corals, deadly parasites, anaerobes in termite guts, or slime mold amoebas. Hence, purine biocrystallization seems to be a general and ancestral eukaryotic process likely present in the last eukaryotic common ancestor. Purine crystalline inclusions were already shown to serve as high-capacity and rapid-turnover reserves of nitrogen in photosynthetic protists [3], however, even in unicellular eukaryotes they can have other functions, *e.g.*, serving as optically active elements in light manipulation and sensing.

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OL6

RAMAN OPTICAL ACTIVITY AS A PROMISING TOOL FOR MONONUCLEOTIDE G-QUADRUPLEXES STUDIES

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The tendency of guanosine-5´-monophosphate (5´-GMP) to self-associate at higher concentrations into regular higher-order arrangements, – G-quartets and further to G-quadruplexes (G4s) – is known for 60 years[1], therefore it has been thoroughly studied and has significant possible applications both in pharmaceutics and nanotechnology. These associates hold together through a combination of several contributions: Hoogsteen base pairing, base stacking, hydrophobic interaction, cation coordination, and H-bond network among phosphates and ribose hydroxyls of different 5´-GMP. The latter effect has a major impact on the stability of the associate (as we show further) but has not been sufficiently described yet.

We studied 5´-GMP associates using Raman spectroscopy and its chirally sensitive variant Raman optical activity (ROA)[2] which benefits from the inherent nucleotide chirality. Data were analyzed by the multivariate factor analysis. Usage of Raman spectroscopy enabled simple aqueous solution measurements (unlike X-ray diffraction) and studies of highly concentrated samples (unlike absorption-based techniques). At the same time, we can easily change the external conditions (e.g., temperature, pH, and ions) which affects the higher-order structure, stability, and dynamics of these assemblies.

We obtained well-resolved Raman and ROA spectra of 5´-GMP associates over the full range of fundamental molecular vibrations (~50 – 4500 cm^{-1}) and found ROA to be much more sensitive to the formation of G4s than Raman scattering. In ROA, agglomeration is reflected by sharpening and double intensity increase of vibrational features in the fingerprint region and striking over the magnitude signal increase in the terahertz region (50 – 200 cm^{-1}) reflecting the higher-order arrangement of the observed systems in the presence of different stabilizing cations (Na, K, Li, etc.). Moreover, we observed a major loss in G4s stability (melting temperature dropped by ~30°C) when ribose was changed for 2´-deoxyribose in 5´-GMP, pointing to the crucial role of H-bond networking.

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OL7

FLUORESCENCE-FREE MATERIAL IDENTIFICATION WITH NEW XTR TECHNOLOGY FROM METROHM

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In Raman spectroscopy, accurate and sensitive identification of chemicals and materials can be compromised by fluorescence from laser excitation of the target substance itself and/or interferents in the sample matrix. Fluorescence emission in Raman spectra reduces the signal-to-noise ratio and can obscure signature peaks assigned to the unique Raman-active vibrational modes of molecules.

Recent advances have had some success in mitigating the impact of fluorescence on data quality; however, compact commercially available Raman devices that provide a universal solution for suppressing fluorescence are lacking. MIRA **XTR** DS 785nm system fills this void with a state-of-the-art handheld Raman system that revolutionizes material identification in complex environments due to outstanding XTR technology.

XTR® technology (which stands for «Raman eXTRaction») is Metrohm Raman's patent-pending proprietary method to differentiate the signals stemming from fluorescence and Raman scattering and bin them into two distinct spectra. MIRA XTR DS produces a fluorescence spectrum with its corresponding intensity and shape, and it generates a pure Raman spectrum of just the Raman scattered light. The XTR technology is useful at places where use of smaller and safer 785 nm system is advantageous.

The field of application ranges from the identification of hazardous substances *in-situ* through the food industry to the conventional chemical industry. The identification of Arabic gum powder and microcrystalline cellulose, detection of counterfeit honey, on-site detection of hexavalent chromium in protective paint primers or fentanyl analysis in hazmat work are applications which show capability of this new technology.

The goal of this research was to develop and introduce new Metrohm XTR technology for reduction of negative impact of fluorescence during Raman spectroscopy analysis.

IL3

IN-VIVO AND IN-VITRO STUDIES ON METAL RELEASE (IONS AND NANOPARTICLES) FROM DENTAL IMPLANTS USING SINGLE-CELL AND SINGLE-PARTICLE ICP-MS.

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Dental implants made of titanium alloys with aluminium and vanadium are broadly used as replacement of lost teeth. Despite being considered inert, these titanium alloys are known to undergo degradation in the human body environment, mainly due to tribocorrosion. As a consequence, the release of titanium ions from orthopaedic implants is well documented and can cause severe consequences in the long term. However, the release of metals in the form of nanoparticles is not so well known, although they may be involved in the induction of the implant failure [1]. Additionally, some surgical procedures used for the treatment of periimplantitis, produce a great amount of ions and metal debris in the form of macro- and microparticles, and may include a high amount of nanoparticles.

This presentation will show the application of single-particle and single-cell-ICP-MS strategies aimed to the detection and characterization of metal ions and nanoparticles released by dental implants. An *in vitro* model, including bacteria and osteocyte cell cultures, will be used to address the formation of nanoparticles by dental implants. Additionally, an *in vivo* animal model that simulates the consequences of implantoplasty will be used to study both the production and fate of titanium, aluminium and vanadium ions and the translocation of titanium-based nanoparticles to other organs from the implant site.

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OL8

ANALYSIS OF PTFE MICRO-PARTICLES BY ICP-QMS OPERATED IN A SINGLE-PARTICLE MODE

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During the last decades, environmental contamination with plastics has become a major cause of concern. Plastic waste released into the environment is a virtually non-degradable persistent pollutant, which can be found in soil, sediments, and water. The chemical composition of the polymer influences its environmental behavior and toxicity level. One of the significant classes of microplastics is fluoropolymers, which are widely used in various consumer products. Currently, thousands of tons of fluoropolymers are produced every year and their production is steadily increasing. Fluoropolymers are extremely persistent under environmental conditions. However, even possessing exceptional stability, fluoropolymers are disintegrated into microplastics by various mechanical processes, accelerating their further dispersion and increasing their bioavailability. Despite the noticeable advantage in the detection of microplastic particles based on $13C^+$ analysis by single-particle (SP)-ICP-MS [1], this technique cannot be used for distinguishing between the types of microplastics. In the present study, we propose to apply fluorine SP-ICP-MS analysis for the detection of fluorinated microparticles. Our analytical method is based on the earlier proposed approach for fluorine detection by ICP-MS through the formation of $[BaF]^+$ ions (m/z 157) [2]. NexION 2000 s ICP-qMS has been used for the method development. To reduce the level of interfering ions at m/z 157, reaction cell mode with O_2 was applied. Under the optimized operating conditions, a calibration curve for dissolved fluoride ($y= 6616x + 21318$; $R^2= 0.999$) was obtained in a continuous mode. The instrumental conditions optimized for the determination of dissolved fluoride were applied for PTFE analysis by ICP-qMS operated in a single-particle mode. Using the short dwell time (50 µs) for the analysis reduces considerably a background signal at m/z 157. In the analyzed sample containing PTFE microparticles, signal spikes produced by individual PTFE particles were detected by monitoring the $[BaF]^+$ signal.

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OL9

ICAP TQE ICP-MS: FOR SAMPLES WHERE SINGLE QUADRUPOLE PERFORMANCE ISN'T ENOUGH

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The issue of spectral interferences in quadrupole ICP-MS and the negative effects these have on trace element data accuracy and detection limits has been known since the early days of the technology. During the 1990’s, the advent of collision cell technology enabled significant reduction of a range of the most well-known interferences, such as ArO (on Fe), ArCl (on As) and ArAr (on Se) to be achieved, but challenges, such as doubly-charged ion and isobaric (same isotope mass) overlap interference, remained. The development of triple quadrupole ICP-MS in the last few years has provided a solution to these challenges by enabling much more selective interference control. With triple quadrupole instruments, this selectivity is achieved through a combination of mass pre-filtering prior to the collision cell of the instrument and use of reactive gases, such as oxygen, hydrogen and ammonia in the cell, to remove interferences via chemical reactions. In part 1 of this this 2-part webinar series, the theory and practice of triple quadrupole ICP-MS in comparison to single quadrupole ICP-MS will first be presented. The focus of the presentation will then move on to the performance of a new, workhorse instrument that utilises only He and O2 collision / reaction cell gases to remove the most commonly encountered interferences, the Thermo Scientific™ iCAP™ TQe triple quadrupole ICP-MS.

OL10

ISOTOPIC TOOLS FOR URANIUM ORES DATING: APPLICATION OF URANIUM-LEAD AND LEAD-LEAD DATING SYSTEMS

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Isotopic tools used in geoanalysis are highly discussed topic nowadays. Many approaches for age determination of rocks and minerals are being developed relying on various isotope systems. Deposit Rožná appears to be a remarkable example including uranium minerals, e.g. uraninite, in which uranium has been stable and bound for more than 250 million years. Uraninite dating using U-Pb / Pb-Pb systems is possible, but with challenges remaining. [1-3]

Precise and accurate technique for isotope ratios measurements has been introduced already – Multi-Collector Inductively Coupled Plasma Mass Spectrometry (MC-ICP-MS). Other techniques, e.g. ICP-(Q)MS or ICP-(SF)MS, provide only acceptable results. [3, 4]

Three approaches have been used. (I) Solution nebulization with specific sample preparation to eliminate matrix effects; (II) Laser Ablation MC-ICP-MS hyphenation [3], combined with standard solution nebulization; (III) Electron Probe Microanalysis (EPMA) to check the mineral phases analysed.

Matrix effects elimination, instrumentation maintenance, tuning parameters and correction models need to be considered. All these parameters affect the ability to get the precise and accurate isotope ratios and ages, respectively. Our data which will be presented will be used to discuss the advantages and disadvantages of different analytical approaches.

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OL11

PHOTOCHEMICAL VAPOR GENERATION OF RHODIUM AND RHENIUM - ON THE WAY TOWARDS REAL SAMPLE ANALYSES

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Photochemical vapor generation (PVG) is an emerging alternative sample introduction technique for analytical atomic spectrometry and its use has been described for some 30 elements so far [1]. Feasibility of PVG was previously demonstrated for both rhodium [2,3] and rhenium [4]. However, the analytical performance was found inadequate for real samples analysis, which indicates a rather low overall PVG efficiencies.

In this work, the volatile rhodium and rhenium compounds (believed to be metal carbonyls, but the true identity of these compounds is yet to be confirmed) were generated in a flow-injection system using a thin-film flow-through photoreactor and directed by a carrier argon to ICP-MS for detection. The individual parameters affecting PVG of both elements, i.e., the type and concentration of photochemical agent, pH, irradiation time, carrier argon flow rate, the type and concentration of sensitizers or other parameters, were optimized to reach as high overall PVG efficiency and as low limits of detection as possible. The severeness of interferences arising from inorganic acids and their salts and also other elements will be discussed with respect to real sample analyses in various environmental samples. Lastly, the analytical figures of merit (repeatability and limit of detection) and overall PVG efficiency at optimized conditions will be presented and the mechanism of PVG including the effect of transition metal sensitizers will be proposed.

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IL4

IDENTIFICATION OF MICROPLASTICS BY MICRO-FTIR: VALIDATION AND UNCERTAINTY EVALUATION

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The determination of the contamination with microplastics of environmental samples involves the characterisation and counting of particles in portions of the analysed sample. Microplastics are characterised by the type of polymer, shape, size, and colour of the particles, being this information useful for identifying the contamination source. When relevant contamination sources are identified, environmental protection policies should be reviewed.

The most popular technique for microplastic identification is the comparison of micro-ATR-FTIR spectrum with reference spectra of polymers. The agreement between particle and reference spectra can be quantified by spectra correlation being available several algorithms to quantify this match. However, spectra identification is affected by the microplastic's ageing and/or biofilm contamination. These effects reduce the agreement between spectra of the particle and reference polymer, making the definition of minimum Match for automatic particle identification difficult. This work describes a methodology for defining the minimum Match value for polymer identifications with a True Positive Rate, *TP*, of 95%, ensuring that the minimum Match produces less than 5% of false-positive results. The bootstrap method is used to model the distribution of Match values of the agreement between aged particles and reference plastic. Models of the distributions are subsequently used to quantify False Positive Rate, *FP*, and the uncertainty of polymer identification as a Likelihood ratio (*TP*/*FP*) [1,2].

A flowchart with different algorithms for spectra matches quantification and minimum match values if proposed for the automatic identification of microparticles in sediment samples with adequate uncertainty (qualitative analysis uncertainty) [2].

The valid identification of particles supports the quantification of the contamination, which can also be expressed with uncertainty (measurement uncertainty) [3].

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OL12

MICROPLASTICS ANALYSIS BY AGILENT 8700 LDIR

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The popularity of microplastics has grown significantly over the last few years. There are many studies focused on the research of microplastics. The most commonly used analytical techniques within microplastic research are Raman and infrared spectroscopy, as well as gas chromatography. If more insightful and complex information is required, the spectroscopic technique is recommended. The biggest disadvantage of these methods is time consumption. Additionally, spectroscopic techniques also need very experienced operators. Agilent have introduced a unique technique which is incorporated into the Agilent 8700 LDIR instrument. The quantum cascade laser (QCL) is used in the Agilent 8700 LDIR, and this adds much needed speed into microplastic analysis. The second most important aspect of this instrument is the possibility of automatization. Almost anyone can use that instrument with just basic training, and the end result is that you receive your results very quickly. Dedicated software generates all the important sample information. You receive information about sample size, chemical identity, number of particles and also the microplastic distribution.

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OL13

SPECTROSCOPIC CHARACTERIZATION OF HUMIC ACIDS IN CHERNOZEMS

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Hydrophobicity of soil humic acids (HA) was studied using diffuse reflectance infrared Fourier transform spectroscopy (DRIFT). Hydrophobicity is an important parameter for the evaluation of humic acids stability against microbial degradation. Hydrophobicity and humification degree also affect other soil chemicals properties such as aggregate stability, water retention, and leaching of organic and inorganic pollutants. For this reason, three soil humic acids were isolated from the transect along the hill and the effect of management practices on soil quality/ health was studied. Three different soil types were classified in the transect – *Calcic Chernozem – control site, Calcaric Regosol – erosion site, and Calcic Chernozem Colluvic – accumulation site.* Results showed that the humification degree was the highest in HA isolated from *Calcic Chernozem Colluvic (accumulated site)* and lower in HA isolated from *Calcic Chernozem (control site), and Calcaric Regosol (erosion site).* Hydrophobicity index showed the same sequence (the highest value was in HA isolated from *Calcic Chernozem Colluvic).* We concluded that *Calcic Chernozem – control site* is strongly affected by intensive management practice and erosion processes. DRIFT spectroscopy is a rapid and reliable technique, which helps us to assess soil aberration and soil degradation.

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OL14

IDENTIFICATION OF GEMSTONES IN WATCH BY RAMAN SPECTROSCOPY

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Identification of gemstones by Raman spectroscopy is commonly used [1, 2]. It is used where general gemmological identification procedures cannot be used [3]. Gemstones are part of jewellery such as rings, earrings, pendants, bracelets and necklaces [4]. Man has been measuring time for a very long time. The hours gradually decreased until they decreased. Nowadays, watches are worn on the wrist and have become a fashion accessory and a piece of jewellery. In this paper, we focused on gemstones, which are used in the watch industry and have primarily a decorative function. The most frequently used of stones are diamond, glass and cubic zirconia [1]. The cover glass on the watch is acrylic, glass or corundum. Identifying the stones that are on the dial is very difficult. In this case, Raman spectroscopy is useful because it can identify the material behind the glass [4]. In the paper, we mainly identified diamonds on the dial, which often reach very small dimensions, about 1 mm. We analysed 10 pieces of models come from manufacturers of wristwatches, which can be commonly bought in watch shops. They represent a representative sample of gemstones, which are most often used in wristwatches.

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IL5

INSTRUMENTAL ANALYSIS IN 30 MINUTES: BRIDGING THE TECHNIQUES

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Multitudinous analytical instruments are commercially available as tools for analytical chemists in the laboratories and research institutes. They are invented, developed, and built to answer numerous questions in virtually all fields of modern life, where data-based decisions must be made. The instruments and the physicochemical base behind their function are multitudinous as well. However, a few basic tasks in the measurement process are necessary for the measurement. They relate to important terms or definitions such as e.g., „resolution, sensitivity, noise, background, specificity, interference "which apply for most of these techniques. Looking from the viewpoint of these fundamental Figures of Merit (FOM), similarities between instruments will be obvious. Examples will be given in the first part of the contribution.

Once a method is developed in principle, the feasible hardware must be selected and combined by engineers, physicists, and chemists to optimize requirement (FOM), technical outlay, and cost. This process, executed in the research and development departments of instrument manufacturers will define whether a concept will become a successful product. Exceedingly complex physical ideas or solutions may lead to an effective and efficient instrumental feature. This will be explained- as an example- by the methods to achieve resolution in mass spectrometry.

Both, the users of equipment as well as the executive suite of the instrument manufacturers will finally decide whether a method, perfect with respect to FOM and analytical capability, will be able to survive in the market. A few examples of success and failure will illustrate the market aspect in the third part of this contribution.

OL15

SIMULTANEOUS ULTRATRACE SPECIATION ANALYSIS OF ARSENIC AND GERMANIUM IN NATURAL WATER

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Arsenic is a toxic element, quite well studied and with established analytical procedures. Much less is known about germanium, an element essential for modern technologies and quite rare in the nature. Methylated species of both elements are present in natural waters, but only As has also redox speciation.

Both elements can form volatile hydrides at similar conditions, and (methyl substituted) hydrides of both elements can be collected and separated in a cryotrap (HG-CT). Ge is very poorly atomized in simple atomizers for AAS, but As speciation in natural water can be achieved by HG-CT with quartz multiatomizer or novel atomizers based on dielectric barrier discharge (DBD) with simple AAS detection atomizer, as will be presented on example of water reference materials. However, the detailed speciation including quantification of minor As species present in low tens of ng L^{-1} requires more sensitive detection. Ge levels in natural waters are typically in ng L^{-1}, i.e. even 3 orders of magnitude lower than As levels.

A method for simultaneous ultratrace speciation analysis of arsenic and germanium based on selective HG-CT from TRIS buffer medium, with L-cysteine as reaction modifier and detection by ICP-MS/MS in O_2 mode will be presented. A practical application, simultaneous analyses of As and Ge in depth profiles of Lake Geneva will be shown, with total As concentration of approximately 1 µg L^{-1} and total Ge concentration about 1.4 ng L^{-1}. Species of these two elements showed very different behavior over the productivity period in spring 2021: iAs^{V}, a dominant As species in winter, was reduced to iAs^{III} in the surface layers and the methylated As species appeared as a product of biota metabolism. iGe was incorporated in diatoms and depleted from water at the surface, but enriched near the bottom from dissolving frustules of dead diatoms, in a pattern identical to silicon. Conservative concentrations of methylated Ge species (0.1 ng L^{-1} MGe and ~0.03 ng L^{-1} MGe) were found by a Ge specific method [1].

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OL16

SPECIATION ANALYSIS OF GD-BASED CONTRAST AGENTS IN RIVER WATER USING HPLC-ICP-MS

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Magnetic resonance imaging (MRI) is now one of the requisite imaging methods for medical diagnostics. Gadolinium (Gd) is used as the contrast agent for MRI to enhance the contrast of an image because of its strong paramagnetic property. Gadolinium-based contrast agents are administrated to patients in chelated form, because Gd^{3+} is well known for its toxicity. In recent decades, several studies reported that the apparent positive anomalies of Gd in the REE pattern are shown in rivers running through metropolitan areas [1-3]. It shows that a part of the Gd-based contrast agents is emitted to river water without being processed during the sewage treatments, even though the long-term risks of Gd-based contrast agents for living organisms are not well elucidated so far.

Recently, our group has developed a new HPLC-ICP-MS technique using the hydrophilic interaction chromatography (HILIC) column with the water-based eluent for the separation of Gd-based contrast agents [4]. In this study, the presented technique was applied to the speciation analysis to identify Gd-based contrast agents in river water in Japan. River water samples were collected from the Muko River (Hyogo, Japan) in June 2018 and November 2020 near Sanda City, which is a suburban city with a population of 200,000. The concentrations of Gd in the samples collected in 2018 and 2020 were 97 ng L^{-1} and 51 ng L^{-1}, and the magnitudes of the anomalies were calculated 39 and 17, respectively. The anomalies are much smaller than those reported in metropolitan areas, however it is very important to show that the anthropogenic Gd emission to the river is not only a matter in metropolitans but also a matter in small cities. Gd-species in the river water samples were also investigated using the HILIC-ICP-MS technique with the water-based eluent. As a result, 3 kinds of the cyclic type of Gd-based contrast agents, which are approve in Japan, were found in samples of 2018 and 2020. The concentration of these Gd-species makes up 70% of the anthropogenic Gd. It clearly shows that the Gd anomalies are caused by MRI reagents emitted from the WWTP without being treated.

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OL17

MINIATURISED LIQUID PHASE EXTRACTION OF BUTYL AND PHENYLTINS IN SEDIMENT SAMPLES USING DEEP EUTECTIC SOLVENT: OPTIMISATION AND HPLC-ICP-MS ANALYSIS

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Organotins are persistent organic pollutants that were used to be of high importance as biocides in polymers and antifouling agents in ship paints. However, due to their toxic effects, bioaccumulation and endocrine disrupting properties, their extensive application has been banned. However, due to their persistence nature, traces of organotins are still present in the environment especially in sediments. In the present study, A rapid and environmentally friendly analytical method was developed for simultaneous extraction of tributyltin (TBT), diphenyltin (DPhT), dibutyltin (DBT), monophenyltin (MPhT), monobutyltin (MBT) and triphenyltin (TPhT) s from sediments. The extraction efficiencies of hydrophobic deep eutectic solvents were investigated. and the extracted organotins were quantified using high-performance liquid chromatography–inductively coupled plasma-mass spectrometry (HPLC-ICP-MS). The experimental parameters affecting the extraction process were optimized using response surface methodology. Under optimized conditions, the limits of detection and limits of quantification ranged from 0.2 -1.1 ng g-1 and 2.3-6.0 ng g-1 respectively. The accuracy expressed in the form of percentage recoveries ranged between 89.2 % and 105 %. The developed extraction method was applied for the extraction of organotins in to freshwater and seawater sediments. The results obtained demonstrated that TBT and TPhT were present in seawater sediments.

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PL2

ADVANCES AND TRENDS IN SAMPLE PREPARATION FOR ANALYTICAL SPECTROMETRY

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Currently, although there are many digestion systems developed for a high number of matrices, most of them still use concentrated reagents (acids in case of further metals determination) to assure an efficient digestion and make solutions more suitable to be analyzed. The recent trends in analytical chemistry require methods with lower consumption of reagents and lower generation of laboratory residues. However, high concentrated reagents are usually necessary to obtain suitable digests for further determination of elements by spectrometric or chromatographic techniques. Moreover, the digestion efficiency of these systems presents some limitations for many matrices. In this sense, even using methods based on microwave-assisted closed vessels some drawbacks can occur for some matrices (as crude oil, high carbon content samples, etc) and incompleteness of digestion is frequently reported. In addition, it is important that digests are suitable for the determination techniques avoiding excessive dilution or higher blank levels. On this aspect, the main trends for sample preparation will be presented in this lecture for further metals and also non-metals determination. The use of diluted solutions using oxygen pressurized systems, combustion systems and pyrohydrolysis will be covered and the main aspects of sample preparation for the determination of metals and halogens will be discussed. Recent applications will be presented showing the advantages of methods using diluted reagents (combustion, UV digestion) for determination using ICP-MS and ICP-OES and ion chromatography.

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IL6

HIGH RESOLUTION CONTINUUM SOURCE AAS FOR DETERMINATION OF NONMETALS

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Trace concentrations of nonmetals such as nitrogen, sulphur, fluorine, chlorine, bromine and a metal (aluminium) 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 species.
The influence of molecule forming elements concentration, chemical modifiers, ashing and atomisation temperatures was investigated. The elaborated procedures were applied for analyses of real water samples.

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OL18

STUDY OF DISTRIBUTION OF ZINC IN ZNO NANOPARTICLES IN SOIL COLLOIDS (EXTRACTED FROM SAMPLES COLLECTED AT VARIOUS AGRICULTURAL AND FOREST SITES IN SLOVAKIA) BY SEQUENTIAL CENTRIFUGATION AND FLAME AAS

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The zinc oxide nanoparticles (ZnO NPs) have been shown, if applied foliarly, to improve the growth, yield, and physiological parameters of some agricultural plants [1]. However, widespread use of nanoparticles as fertilizers or ever-growing demand for ZnO NPs-containing consumer goods can significantly increase the risk of their transfer to (waste) water streams or sediments. Therefore, the ZnO NPs' fate and behavior in environmental matrices (e.g., soils and sediments) need to be closely monitored [2]. The fate and transport of nano-objects (e.g., natural, or engineered nanoparticles) in soil or any other chemically heterogeneous porous medium is primarily regulated by aggregation, (de)sorption, straining and exclusion [3]. In our experiment, the behavior of soluble and bulk ZnO NP in water-extracted colloids has been investigated by adding 20 mg/L of ZnO NP. The soil colloids were collected from various soil types (e.g., calcic chernozem), mixed with ZnO NP and size-fractioned (1000 – 450 nm, 450 – 100 nm, below 100 nm) by the differential centrifugation with centrifugal forces calculated for synthetic ZnO-nanoparticles according to Stokes' law. The concentration data in each fraction, which have been correlated with physicochemical properties of soils (such as pH, SOC...) and extracted colloids, show some effect of a manganese component on zinc partitioning. This indicates the heteroaggregation of ZnO-nanoparticles (or their reactive products) with manganese-bearing minerals.

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IL7

WHAT METALS/SPECIOME CAN TELL US ABOUT BIOANALYTICS APPLIED TO HEALTH AND PLANT SCIENCE

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Paraphrasing Philippus Aureolus Theophrastus Bombastus von Hohenheim, better known as Paracelsus, *Dosis sola facit venenum* (Only the dose makes the poison), which, in fact, means that all substances are poisons; there is no one that is not poison. The right dose differentiates a poison from a medicine. The same is true when considering metals, and metalloids in the human health. A large variety of metals ions are required to humans for keeping the body in good health so that they are divided into essentials, non-essentials, and toxic [1]. The lack or excess of these elements can produce an imbalance in the homeostasis of themselves or others, unleashing a myriad of undesirable processes inside the human body, which can lead to a variety of diseases from A to Z (from Alzheimer to Zellweger syndrome, among others), or in the cultivation of plants. Then, we are intending to provide a comprehensive overview of how trace elements, and the speciome [2] are involved in some of these diseases and how they can be used to better understand the process involved in such diseases, as well as to a culture of soybean (transgenic or not), which growth in the presence of nanoparticles. For this task, the ICP-MS and its platforms are a powerful tool for attaining this demand, and some of them are discussed.

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IL8

PLASMA INDUCED CHEMICAL VAPOR GENERATION: A NEW GREEN AND EFFICIENT SAMPLE INTRODUCTION METHOD FOR ATOMIC SPECTROSCOPY

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Chemical vapor generation method is widely employed in elemental analysis because of its high sample introduction efficiency and capability of matrix separation. However, conventional CVG methods are typically achieved by the use of reducing reagents（e.g. Na/KBH_4）, which is not stable and expensive. In addition, these methods are susceptible to the interferences from transition metal ions. To solve these issues, plasma induced vapor generation (PIVG) method has been developed simply by the plasma induced reactions without the use of additional oxidation/reduction reagents. It provides a promising new vapor generation technique coupled with atomic and mass spectrometry, notable for its enhanced sensitivity and selectivity [1, 2,3], and now it has been successfully applied to the vapor generation of As, Sb, Bi, Se, Te, Hg, Tl, In, Pb, Cd, Zn, Ag, Os, and I.

PIVG offers several advantages including avoiding the use of unstable chemical reduction/oxidation reagents, high vapor generation efficiency, fast reaction speed, simple device structure, and easy construction. In this presentation, we will firstly provide an overview of the developments and applications of plasma induced-CVG, including liquid electrode discharge PIVG and dielectric barrier discharge PIVG. Then, the influence of different discharge devices, operating parameters, and the interference of coexisting ions on the vapor generation method will be summarized. Furthermore, the possible mechanism and future development trend of PIVG are also discussed.

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IL9

EMPLOYING LASER INDUCED FLUORESCENCE AND SELECTED ION FLOW TUBE MASS SPECTROMETRY TO UNDERSTAND WHAT HAPPENS IN HYDRIDE ATOMIZERS

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Hydride generation (HG) combined with atomic fluorescence (AF) or atomic absorption (AA) spectrometry for determination of hydride forming elements is a viable alternative to the conventional approaches based on the liquid phase sampling inductively coupled plasma mass spectrometry. The most popular hydride atomizers for AF and AA spectrometry, respectively, are miniature flames and externally heated quartz tube atomizers (QTA).

For the most successful application of the whole procedure of element determination based on HG, it is essential to understand what really happens in hydride atomizers. The underlying theory – the radical theory of hydride atomization – is based on a formation of high concentration of free hydrogen atoms serving to atomize hydrides. Consequently, the knowledge of H atom distribution in miniature flames and in QTA is vital for the further development of analytical methods based on HG coupled to AF or AA. The aim of this presentation is to demonstrate how two different spectrometry methods, two-photon absorption laser-induced fluorescence and selected ion flow tube mass spectrometry, combined with a numerical model of the flame chemistry, gas dynamics and heat transfer can bring important information on H atom distribution and on the mechanism of H atom formation in hydride atomizers.

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OL19

AN IMPROVED METHOD FOR THE DETERMINATION OF PFAS USING HR-CS-GFMAS VIA GAF DETECTION

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Per- and polyfluorinated alkyl substances (PFASs) are a group of over 4730 individual compounds [1]. Several PFASs are extremely persistent, bioaccumulative and toxic [2]. The analysis of PFASs is challenging because of their various chemical and physical properties as well as the high number of compounds. Target-based approaches (e.g., LC-MS/MS) are limited to the availability of analytical grade standards and are not suitable for the analysis of new/unknown PFASs and transformation products. Therefore, PFAS sum parameter methods become increasingly important to indicate realistic PFAS pollution levels. PFAS sum parameters display the proportion of organically bound fluorine that can either be extracted (EOF) or adsorbed to activated carbon (AOF). For the instrumental analysis of such sum parameters, a fluorine selective detector is needed. High resolution-continuum source-graphite furnace molecular absorption spectrometry (HR-CS-GFMAS) is a sensitive and highly selective tool for fluorine determination. The method is based on the *in situ* formation of diatomic gallium-mono fluoride (GaF) in a graphite furnace at a temperature of 1550°C. The molecular absorption of GaF can be detected at its most sensitive wavelength at 211.248 nm providing limits of quantification of c(F) 2.7 µg/L [3]. Here, we present an improved method for the determination of PFASs using HR-CS-GFMAS via GaF detection. The optimized method includes a Ga pretreatment as described by Gawor et al. [4] resulting in overall lower detection limits. Furthermore, during optimization the influence of species-specific responses during HR-CS-GFMAS analysis was reduced resulting in a more accurate determination of PFAS sum parameters. To test the applicability of the improved method, we analyzed soil samples from a former fire-fighting training area combining the improved method for detection with our previously optimized extraction method for EOF determination in soils [5].

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OL20

SPECTRAL ASPECTS IN DETERMINATION OF FLUORINE *via* GaF, CaF AND SrF MOLECULES USING HIGH-RESOLUTION CONTINUUM SOURCE MOLECULAR ABSORPTION SPECTROMETRY

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Fluorine is an element of extreme properties (e.g. the highest electronegativity), which excludes or makes difficult its determination using many analytical techniques. One of the solutions is indirect analysis. Gallium, calcium and strontium monofluorides (MF) belong to the molecules most often used in high-resolution continuum source molecular absorption spectrometry (HR-CS MAS).

The following spectral aspects are considered in the method development step and can decide on the method figure of merit:

- selection of the spectral range of the highest absorption by the target molecule (based on the literature devoted to HR-CS MAS or coming from other indirect techniques, verified experimentally),
- a character of the spectrum of the target molecule (the number, position, height and shape of rotational lines) [1],
- occurrence of signals of other fluorine species in the spectral range,
- occurrence of signals of other complementary metal (M) species in the spectral range (e.g. Ga atomic lines, molecular spectra of CaOH or SrOH),
- the character of baseline,
- interferences due to absorption by molecules typically existing in the measurement space (e.g. OH molecules in flame),
- interferences due to possible components of samples (e.g. spectra of SiO or GaCl molecules, Pb, Ni, Fe atomic lines),
- availability of interferent species for generating good quality correction spectra (necessary in least-square background correction).

The presentation intents to show that many of the aspects listed above can be simultaneously important, which can lead to quite unexpected conclusions.

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IL10

PROMISING MOLECULAR-BASED MATERIALS FOR NONLINEAR OPTICS – SPECTROSCOPIC, DIFFRACTION AND OPTICAL STUDY

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Hybrid materials based on polarizable organic molecules as carriers of non-linear optical (NLO) properties are still very attractive field of material science. The selected molecules provide great potential for the crystal engineering of novel molecular crystals with advantageous physical and chemical properties. The obtained materials benefit from the existence of hydrogen bonds as a controlling interaction in the molecular self-assembly leading to the crystal formation. The energy of formed hydrogen bonds counteracts the natural tendencies of the organic molecules to form centrosymmetric pairs. The resulting NLO properties – based on $\chi^{(2)}$ and $\chi^{(3)}$ processes – could provide several technical applications ranging from harmonic generations to stimulated light scattering.

This contribution deals with the characterization of selected hydrogen-bonded molecular materials based on salts and co-crystals of guanidine, biguanide and pyrimidine derivatives, which were prepared in our research group, by the combination of experimental (i.e. vibrational spectroscopy, XRD and calorimetry) and theoretical (solid state quantum-chemical calculations) methods. Particular attention will be focused on vibrational spectroscopic study of phase stability and the explanation of the observed phase transformations. Moreover, linear and nonlinear optical properties of the materials obtained will be discussed.

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IL11

NANOSCALE INFRARED SPECTROSCOPY STUDIES OF CELLULOSE

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Cellulose is a sustainable and biodegradable material that has been used for thousands of years in numerous applications and is moreover the most abundant polymer in nature. In wood, cellulose is the main constituent, but cellulose can also be produced by animals such as tunicate. By extracting the smallest (~3-20 nm in diameter) and mainly crystalline structures of cellulose fibers, so called "nanocellulose" is obtained.[1] Important properties of this material are a high mechanical strength and a low weight, and examples of applications are to strengthen paper, in composite materials, and as a barrier for oxygen. Two types of nanocellulose are cellulose nanofibrils (CNFs) and cellulose nanocrystals (CNCs), being different in length and how they are produced. When characterizing the properties of a macroscopic sample of nanocellulose, a signal corresponding to both an amorphous and a crystalline character of cellulose is obtained, but it has been debated exactly where in the nanocellulose particles the amorphous and crystalline domains are located. In this study we have applied nanoscale infrared spectroscopy [2] to investigate where these amorphous and crystalline domains are located in individual nanocellulose particles with a lateral resolution of 20 nm. The studies have been performed on tunicate CNFs, cotton CNCs, and wood CNFs.

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OL21

NANOSCOPIC TECHNIQUES RELATED TO MOLECULAR VIBRATIONS

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In recent decades, a massive expansion of nanotechnology and nanomaterials is evident, changing industry, research areas and the daily life of people. Various classes of analytical techniques have been developed to cover the requirements of nanotechnology and the characterization of nanomaterials.

Molecular vibrations are directly related to the molecular structure. The techniques of vibrational spectroscopy, including those based on either infrared absorption/reflection or Raman scattering, are well-known analytical techniques. Their microscopic/microspectroscopic counterparts developed in the second half of the 20th century are limited in spatial resolution by light diffraction. Recently this limit has been overcome by the combination of near-field optics with scanning probe microscopy (SPM). Imaging techniques described by abbreviations like AFM-IR (atomic force microscopy – infrared (imaging)) and SNIM (scanning near-field infrared microscopy) are powerful analytical techniques for nanoscience and nanotechnology [1]. Nano-FTIR and TERS (tip-enhanced Raman scattering) combined the spatial and spectral information essential for both the design/development of new nanomaterials/nanosystems and a detailed description of biological systems. Nevertheless, individual experimental techniques require some specific sample preparation/treatment procedures.

The advantages and drawbacks of preparation procedures, individual imaging techniques, and spectroscopic data acquisition and processing will be demonstrated in several examples of studies [2-4] performed in our laboratory at UCT Prague.

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OL22

CHEMISTRY AT THE NANOSCALE – AFM MEETS IR SPECTROSCOPY

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Nanoscale Infrared spectroscopy [1] has been successfully demonstrated in an expanding range of applications in recent years due to significant increases in capability. One method of nanoscale infrared spectroscopy, atomic force microscope based infrared spectroscopy (AFM-IR) uses the tip of an AFM as a nanoscale detector of the expansion caused by absorption of IR radiation. AFM-IR can be used to obtain IR absorption spectra and chemical imaging with resolution as fine as the AFM tip radius, >100X smaller than spatial resolution limits of conventional infrared spectroscopy. The photothermal AFM-IR technique has demonstrated improvements in sensitivity, down to the scale of single monolayers, and speed with spectral acquisition times dropping by an order of magnitude. This presentation will describe the underlying technology and complementary techniques for nano-mechanical/nano-electrical and nano-thermal analysis. Additionally, we will also highlight numerous applications of nanoscale spectroscopy and chemical imaging in physics, materials and life sciences. Applications include nanoscale chemical analysis of polymers, composites, semiconductors, biological cells, proteins, tissue, and other areas.

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IL12

ELEMENTAL SPECIATION FROM METALS, METALLOIDS TO NON-METALS IN ENVIRONMENTAL SCIENCE: SUCCESSES AND PROBLEMS

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Processes in environmental science for toxic and essential elements cannot easily be described by analyzing the total elemental concentration in samples but must rather be described by their molecular form – their speciation. Here in this keynote lecture the general concept of speciation will be explained and illustrated by recent case studies conducted in the TESLA lab. The case study covers the environmental perturbation effects on biota from natural processes to the impact of industrial processes in the marine and terrestrial environments.

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Rice as one of the main staple foods in the world has attracted the attention of the research community since many years. One of the reasons is the ability of rice to accumulate different arsenic species in grain at relative high concentrations. In general, these arsenic species are dimethylarsinic acid (DMA) and inorganic arsenic with small amounts of monomethylarsonic acid being present as well. The organic arsenic species are not synthesised by the plant but taken up from the environment. This applies as well to other organic arsenic species sometimes found in rice like Roxasone or its bacterial breakdown products. Rice, like all so far studied terrestrial plants, tends to accumulate organic arsenic species preferably in leaves and seeds. It therefore can contain unusual arsenic compounds when the environmental conditions lead to their production. One such compound was recently identified as dimethylarsonyldimethylarsinic acid. This compound is a derivative of DMA whereby the arsenic atoms are joint via a methylene group and not via an oxygen bridge as in some synthetic compounds. SO far only one natural polynuclear arsenic compound Arsenicin A was known to occur in a marine sponge. In this presentation we will show how we this unusual compound was found and identified.

OL24

COMPARISON OF MOBILE PHASES FOR CATION EXCHANGE HPLC-ICP OES

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In environmental field of literature, there is a lot of information about speciation analysis of arsenic, mercury, selenium, antimony or chromium, as evidenced by the number of review articles [1]. For other elements, e.g. iron, cobalt, zinc, manganese, there is much less information about extraction and speciation procedures. Moreover, the detection technique which is used very often is the absorption of electromagnetic radiation in the near ultraviolet (UV) and visible range (Vis). The sensitivity of the high performance liquid chromatography inductively coupled plasma mass spectrometry technique (HPLC-ICP MS) and the ability to measure the signal for many elements at the same time make it an invaluable detector [2]. Those advantages and scarcity of methods encourage to create new procedures for speciation analysis with ICP MS as a detector. Therefore, as a first step, different mobile phases presented in literature and their modifications were tested on inductively coupled plasma optical emission spectrometer (ICP OES), which will be shown at my presentation. The tests have been done on standards and real samples with different matrix. The aim of this part of the research was to obtain the lowest possible concentrations of the eluent components while maintaining the separation of element forms, using the separation of iron forms Fe(II) and Fe(III) as a determinant.

Next step of this research will be application of the selected mobile phases to the HPLC-ICP (iCRC)MS technique in order to select the best eluent. The final step will be to optimize the chromatographic and spectrometric parameters. Afterwards the extraction methods will be investigated.

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OL25

SELENIUM TRANSFORMATION BY FOOD-GRADE MICROORGANISMS

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Inorganic selenium compounds are generally toxic in the cellular environment, therefore, the association of selenium with proteins throughout selenium metabolism is essential for cell survival. Microorganisms belonging to all three domains of life (bacteria, archaea, and eukarya) synthesize selenocysteine as the main form of organic selenium in the cells, which is incorporated into selenoproteins involved in several functions including redox signalling and antioxidant defence. This ability of microorganisms can be utilized in the preparation of functional dairy fermented foods enriched with selenium.

In our study we analysed how dairy microorganisms including lactic acid bacteria, bifidobacteria, and yeasts incorporate and transform selenite after being exposed to selenium enriched growth media. The highest ability to accumulate selenium (up to 201 mg/g, dry weight) was found in *Streptococcus thermophilus*, but most of the samples have an average Se content below 20 mg/g (dry weight). As expected, the main organic species was selenocystine, with the exception of strains of bifidobacteria where only 4–6% organically bound selenium was found in this species. A surprisingly high percentage of organically bound selenium (8–52 %) was found in the form of an atypical species (probably selenomethionine oxide). However, the most abundant species was selenium in the form of nanoparticles (SeNPs). SeNPs make up 57 % of the total selenium content. The only exceptions are yeast strains in which most of selenium is bound to organic species. The mean size of the SeNPs was the largest among the cocci strains and reached >200 nm. In the case of yeasts, bifidobacteria, and lactobacilli, smaller particles with a mean size of 80–140 nm were observed.

Furthermore, the cytotoxic effect of selenized strains on the viability of Caco-2/HT29 cells was evaluated. Cell viability was reduced by 40–75% using strains cultivated in 30, 50, and 100 mg/L Na_2SeO_3. In comparison, the same reduction in viability caused 5 mg/L inorganic selenium in the form of Na_2SeO_3.

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OL26

DETERMINATION OF METALS AND METALLOIDS SPECIES USING SELF-DESIGNED HYPHENATED SYSTEMS BASED ON DETECTION BY OPTICAL EMISSION SPECTROMETRY

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Although hydride generation (HG) is widely used as an effective analyte introduction technique in optical emission spectrometry (OES), relatively few hyphenated systems using this technique have been developed for last 10 years [1].

The presented research fills this gap by the usage of Multi-mode Sample Introduction System (MSIS) as an interface between anion-exchange (AE) or/and cation-exchange (CE) high performance liquid chromatography (HPLC), and optical emission spectrometry, both inductively coupled plasma (ICP OES) or microwave induced plasma (MIP OES).

Three hyphenated systems were designed, according to the three work modes of the MSIS chamber: (1) hydride generation (HG) to determine analytes forming volatile hydrates (e.g. three arsenic species) [2], (2) conventional nebulization (Neb) to determine forms of metals (e.g. two iron species) [3], and (3) Dual-mode, i.e. the combination of HG and Neb modes for the simultaneous determination of metal and metalloid forms occurring as cations and anions in the environment [4]. The applicability of the systems was presented on real samples, e.g. soils, sediments, food, plants or archaeological ceramics.

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OL27

MASS BALANCE ANALYSES OF PFAS IN SOIL, SNOWMELT AND SKI WAXES

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Per and polyfluoroalkyl substances (PFAS) are common additives in ski waxes for their water repellent characteristic [1,2]. Abrasion of ski wax leaves PFAS on the snow surface [3], however, little is known about the distribution and concentration of PFAS in snow and soil due to skiing. In this study we analysed using targeted HPLC-MS/MS analysis different ski waxes, snowmelts from skiing areas and soil from remote alpine location to understand more about PFAS distribution in the environment. We found that PFAS was present in all analysed media. The sum of all target PFAS ranges between <LOQ and 0.14 ng g^{-1} in snowmelt, 0.62 ng g^{-1} and 5.35 ng g^{-1} in soil and <LOQ and 874 ± 240 ng g^{-1} in ski wax samples. Mass balance of organic fluorine was conducted using combustion ion chromatography (CIC). Extractable organic fluorine concentrations ranged up to 2.12 ± 0.2 mg g^{-1} (wax samples). We also showed that the sum of all target PFAS accounts for only a few % in extractable organic fluorine content. This indicates that ski waxes can be a source for PFAS contamination in snow and soil and that non-target analysis is needed to get a better overview on PFAS distribution.

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IL13

INORGANIC NANOLUMINOPHORES CONTAINING LN IONS AND THEIR MULTIFUNCTIONALIZED SYSTEMS FOCUSED ON SENSOR AND ANALYTICAL APPLICATIONS

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This lecture presents selected nanomaterials based on inorganic matrices (e.g.: fluorides, vanadates, borates, phosphates, silicates, etc.) doped with luminescent lanthanide (Ln) ions, characterized by efficient emission properties. As application materials, they should show: phase purity, high crystallinity and homogeneity, small particle size and narrow particle size distribution, and should not be agglomerated. Examples of effective nanoluminophores (NL) and up-converting (UCNL) doped with Ln^{3+} (or Ln^{2+}) ions and their surface functionalized by coting with organic compounds hybrid systems for sensor and analytical applications are discussed in detail. We show that the luminescence of selected Ln^{3+} or Ln$^{/2+}$-doped NLs can be successfully used in (nano)-manometry as optical pressure sensors, capable of measuring pressure and multifunctional optical sensors for (nano)-manometry & (nano)-thermometry, high-pressure and temperature upconversion luminescence of Ln^{3+} doped NLs [1,2]. We also present luminescent-magnetic NPs of the core/shell type, doped with Ln^{3+} ions, which have been used as modifiers for cellulose fibers. Such multifunctional NLs are excellent materials for textile and documents protection against counterfeiting [3].

NPs functionalized with organic compounds have also proved to be very useful for analytical purposes. We have developed new, highly selective fluorescence methods based on energy transfer from the analyte ion to the Tb^{3+} ion (benzoic acid–capped CaF$_2$:Tb^{3+} NPs [4], or Eu^{3+} ion (adenosine capped CaF$_2$:Eu^{3+} nanocrystals [5] and DPA capped-LaF$_3$:Eu^{3+} NPs) for the determination of metal species (e.g. WO$_4^{2-}$, MnO$_4^{-}$, Cu^{2+}) in real water samples.

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IL14

ULTRAFAST TIME-RESOLVED PROBES OF CHIRALITY DURING PHOTOCHEMICAL REACTIONS

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Chirality is an important concept in chemistry and other natural sciences. Recently, molecular chirality in isolated gas-phase molecules has become accessible using photoionization of a chiral molecule and subsequent angle-resolved photoelectron detection, revealing the phenomenon of photoelectron circular dichroism (PECD).[1] PECD experiments have already evolved from synchrotron-based static measurements [2] to table-top laser sources with femtosecond temporal resolution.[3]

In this talk, we will focus on the first time-resolved PECD (TRPECD) experiments with circularly polarized harmonics. These experiments include several novel aspects: First, we have introduced a simple approach to generate circularly polarized vacuum ultraviolet (VUV) radiation based on low-order harmonic generation.[4] Second, we have performed a complete polarization measurement of the generated VUV harmonics.[4] Third, we have combined this light source with angle-resolved photoelectron detection to measure for the first time TRPECD during photoinduced chemical reactions, thereby introducing a general experimental approach for chiral femtochemistry.[5]

Selected chiral molecules are ionized in a (1 + 1')-pump-probe scheme involving linearly polarized 266 nm and circularly polarized 133 nm pulses with sub-100 fs temporal resolution. One of the structurally simplest chiral molecules, CHBrFI, will be discussed in terms of its molecular dynamics and time-dependent chirality associated with the photo-induced C–I bond breaking. The experimental results are supported by high-level *ab initio* electron-molecule scattering calculations. The broad applicability of the time-resolved PECD measurement scheme is demonstrated on another chiral molecule, 2-iodobutane. Whereas CHBrFI displays a non-vanishing PECD at long pump-probe delays, the PECD decays to zero after the photo-dissociation of 2-iodobutane, reflecting the effective chirality of the product radicals on long timescales.

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OL28

FTIR-FPA AND FTIR-QCL MICROSCOPY: BREAKTHROUGH TECHNIQUES IN INFRARED IMAGING

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Recent years brought significant development in the field of infrared microscopy. This proven and well-established technique always had several limitations regarding spatial resolution and measurement speed.

The technology of the focal-plane-array detector brings in the possibility of fast measurement of up to 128 x 128 pixels at once, which leads to the collection of up to 16.348 spectra with spatial resolution up to 1.25 µm at once. Even though this technology has existed for several years, current computing technology can collect and manipulate large datasets with millions of spectra inside and fully exploit the enormous potential of the FPA system. Therefore the collection of comprehensive spectral maps with unique spatial resolution and fast evaluation is finally possible.

The new technology of quantum cascade laser (QCL) expands the limits even more. With quantum cascade lasers as a highly intensive source of infrared light, the microscopes can use much more powerful detection systems (e.g., bolometer cameras), which leads to unmatched imaging speed (of 90.000 measurements per second) or even so-called LIVE chemical imaging – observation of chemical changes in the space in the real-time. This technology opens brand new possibilities in the field of tissue imaging, microorganism, or material research.

OL29

THE OPTICAL CHEMOSENSOR ARRAY FOR ANALYSIS OF HALIDES OR SMALL BIOLOGICAL MOLECULES

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Chemosensor arrays are assemblies of multiple chemosensors where it is supposed that a single chemosensor should exhibit the highest selectivity to give the highest response (analytical signal) for a single analyte [1, 2]. On the contrary, the methodology using arrays consisting of less selective chemosensor elements is more general because each element responds to more analytes present in the sample [1, 2]. Thus, this overall analytical signal can be decomposed into individual signals originating from the analytes using advanced chemometrics methods. The choice of the single chemosensor elements for an optical array followed by their sizing is a difficult task. It could be resolved by various approaches which depend on the knowledge of the target analyte(s) in a complex sample as well as their application for a qualitative or quantitative analysis (or for both qualitative/quantitative analysis in some cases) therefore it is necessary to know basic physico-chemical and metrological parameters of a single chemosensor. In this oral contribution, the examples of development of optical chemosensor array suitable for qualitative analysis of small organic molecules containing thiol group (*e.g.*, cysteine, glutathione) or phosphate (*e.g.,* AMP/ATP) as well as multicomponent quantitative analysis of halides [3] will be presented.

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IL15

IRMS ON THE TIDES OF THE PAST

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Isotope ratio mass spectrometry (IRMS) deals with changes in stable isotope ratios; most often, values of δ^{13}C (based on the ratio of ^{13}C/^{12}C) and δ^{18}O (reflecting the ratio of ^{18}O/^{16}O) are evaluated. During the exchanges of carbon and oxygen among the atmosphere, hydrosphere, and biosphere, these isotopic ratios undergo tiny changes, which are referred to as isotopic fractionation, and are also influenced by the current climatic conditions (temperature, precipitation). The actual isotopic ratios are archived in annual tree rings. IRMS could be applied for rediscovering of these values, which are subsequently used for the reconstruction of the paleoclimate in the relevant period.

In this study the values of δ^{13}C and δ^{18}O in the late-wood of oak tree rings (*Quercus* spp.) from 21 living oaks and from 126 core and disc samples originating from construction timbers, subfossil remains and archaeological excavations of the same genus, dated between 75 BCE and 2018 CE were used for the reconstruction of the paleoclimate in the period mentioned above. All samples were collected in the area of today's Czech Republic and part of southern Bavaria. The alpha-cellulose was extracted from individual tree rings and analyzed on a VarioPYROcube elemental analyzer connected with Isoprime 100 IRMS. In total, 13,496 δ^{18}O and 13,584 δ^{13}C values from annually resolved and absolutely dated samples were obtained. Based on the proven correlation of the combined inverse δ^{13}C and δ^{18}O values with Palmer's drought severity index [1] in June, July, and August during the variability of the period 1901-2018, the hydroclimate in the last 2110 years was reconstructed with high resolution [2].

The results obtained show a constant drying trend during the period under study, together with pluvials around 200, 720 and 1100 and droughts around 40, 590, 950, 1510 and now in the 21st century. However, the current summer droughts are unprecedented and, with a high probability, are caused by anthropogenic warming.

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OL30

STOPPING EFFICIENCY SIMULATION OF CRYOGENIC GAS STOPPING CELL

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The mass is a fundamental property of an atom comprising all information on its constituents and their interactions. Thus, it carries information on the internal structure of the nucleus, reveal the quantum mechanical shell structure within complex nuclei and determine the energy available for nuclear transformations in radioactive decay processes. Mass measurements allow us to benchmark nuclear models and thus contribute to investigations of the nature of the strong interaction itself. With the aim of high-precision mass measurement (HPMM) of heavy and super heavy elements, a new experimental setup is being built in FLNR, Dubna. The setup consists of the following parts: target unit; gas-filled separator of complete fusion reaction products; cryogenic gas stopping cell (CGSC); a radio-frequency system for transporting and cooling a low-energy beam; and a multi-reflection time of flight mass spectrometer (MR-TOF MS). CGSC is responsible for the final slowing down and thermalizing the energy-bunched fragments produced and selected in the Gas Filled Separator. The thermalization is achieved in a volume filled with ultra-pure helium gas at cryogenic temperatures. After the thermalization, the fragments are extracted and transported with a radio frequency quadrupole (RFQ) to the MR-TOF MS. The stopping and thermalization of the incoming fusion-evaporation residuals (EVRs) is a key step in HPMM of the heaviest elements. Due to the typically low incoming ion rates and low particle integrals CGSC has to be as efficient as possible. The HPMM requires at least a few ions for a measurement any loss should be avoided. The kinetic energy of the incident EVR, the entrance window foil type and thickness as well as the buffer-gas type and density of the CGSC condition the stopping efficiency. Only the ions that are stopped within the active gas volume of the CGSC can be extracted. The stopping efficiencies for EVRs cannot be tested on-line and one have to rely on simulations. To use the CGSC on ion beam the optimal entrance window foil thickness for every reaction is necessary evaluate. The Geant4 and SRIM software packages was used in these simulations with different entrance window materials and beam and target combinations.

OL31

FLUOROPROTEOMICS UNCOVERS THE EFFECTS OF FLUORINATED DRUGS

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The intentional replacement of hydrogen atoms or hydroxyl groups by fluorine in pharmaceuticals increase their bioavailability and biostability. However, there is not much knowledge on the interaction of fluorine released from fluorine-containing molecules with proteins. Thus, we aimed to evaluate the possible fluorination of proteins after administration of the fluorinated drug cinacalcet, which belongs to type II calcimimetics and is metabolised mainly in the liver. We applied the MS-based proteomics approach was used to identify proteins in Wistar rat's brain and liver tissues. The label-free proteomic approach was used, were chromatographic separation was followed by measurements performed by high-resolution mass spectrometry. In order to identify peptide/protein the Mascot algorithm was used. We succeed to identified few fluorinated proteins both in liver and in brain tissues.

Interestingly, among the treatment subgroup, ten up-regulated and three down-regulated proteins were detected in the liver and one upregulated protein in the brain compared to the control group. These proteins were involved in the enzyme regulator activity (36%), binding (31%) and catalytic activity (19%). Accordingly, the results obtained in the pilot study indicate that chronic cinacalcet therapy could impair phase II of enzymatic detoxication and may cause disturbances in blood homeostasis, lipid metabolism, and inflammatory mediators or contribute to the acceleration of cognitive dysfunction; therefore, appropriate patient monitoring should be considered.

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OL32

STRUCTURAL CHARACTERIZATION OF HYDROPHOBIC HYALURONAN DERIVATIVES BY COMPREHENSIVE 2D-LC-MS

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Hyaluronan (HA) is a polymeric biomolecule affiliated to glycosaminoglycans. It is promising macromolecule for many cosmetic and biomedical applications thanks to its biocompatibility and non-toxicity. Derivatives of HA with hydrophobic functional groups are often synthetized to prolong the resistance to natural degradation or to fabricate amphiphilic molecules with desired properties that can bind active compounds.[1] For complete characterization of novel derivatives not only essential parameters are needed, such as a degree of substitution (DS), molar mass distribution and polydispersity, but also distribution of substituents along the molecule chain[2] is indispensable for proper assessment of structure-property relationship of these polymers, due to the fact that HA derivatives with the same DS can differ in their properties.

A method, that utilizes comprehensive two-dimensional LC-MS for separation of oligosaccharides derived from HA derivatives, was developed. Oligosaccharides can be obtained by enzymatic degradation of polymeric derivatives with hyaluronidases, e.g. from Streptococcus Pneumoniae (SpHyl) and because of digestion they differ in their length (a number of HA monosaccharides) and in a number of bound substituents. Therefore, the combination of SEC in the first dimension and RP-LC in the second dimension was used to successfully separate complicated mixtures of oligosaccharides by size and polarity at the same time. Also, the active solvent modulation was used while connecting two modes of separation which can suppress a "breakthrough" effect[3] and further help with optimizing the separation. The method was optimized for characterization of HA oligosaccharides with two to twenty monosaccharide units that are either unmodified or modified with one to six lauroyl substituents, but it can be easily adjusted for analysis of HA oligosaccharides originating from different hydrophobic derivatives of HA, for instance oleyl or caproyl derivatives. In a part of the work, a detailed investigation of enzymatic degradation of 330 kDa derivatives of HA by SpHyl was provided, thus showing possibilities of this hyaluronidase.

Finally, the developed method provided more insight into understanding very important structure-property relationship. Group of samples that showed good correlation of swelling with their DS was analyzed and compared with other samples that showed high deviation from a dependence of swelling ratio on DS. Results enabled us to find structurally irregular patterns in distribution of substituents for these deviant samples and thus explain the differences in their properties in comparison with other samples.

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OL33

THE FIRST CZECH AMS LABORATORY AT THE NUCLEAR PHYSICS INSTITUTE, ŘEŽ

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We describe the first accelerator mass spectrometry (AMS) laboratory in the Czech Republic established by a consortium of the above given institutions. The laboratory has been built on the premises of the Nuclear Physics Institute and put into operation in February 2022. It is equipped with a 300 kV Multi-Isotope Low-Energy AMS system (MILEA) developed in a collaboration of Ionplus AG and ETH Zurich, Switzerland. Despite of a low terminal voltage, MILEA is capable of determination ^{10}Be, ^{14}C, ^{26}Al, ^{41}Ca, ^{129}I, isotopes of U, especially ^{236}U, Pu and other actinoids due to scientific progress in the development of new types of ion sources, accelerators and detectors. Since MILEA will be used for a considerable part of its operational time for 14C measurement and radiocarbon dating, the AMS system has also been equipped with a gas interface system, which allows for direct measurement of gaseous $^{14}CO_2$ instead of the determination ^{14}C in graphitized samples, with a preparative gas chromatograph for monitoring of targeted compounds and for compound-specific radiocarbon dating analysis, and with isotope-ratio mass spectrometer for determination of the relative abundance of stable isotopes (δ^{2}H, δ^{13}C, δ^{15}N, δ^{18}O, and δ^{34}S). Thus, MILEA and its accessories appear optimal for a Czech national project “Ultra-trace isotope research in social and environmental studies using accelerator mass spectrometry”, acronym RAMSES. A report on MILEA performance has already been given elsewhere [1,2], therefore we present here only the most important features of this AMS system together with the first results achieved till May 2022, including both radionuclide measurements and sample preparation procedures.

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IL16

OPTICAL EMISSION SPECTROMETRY COUPLED WITH MICROWAVE INDUCED PLASMA IN ANALYTICAL- AND NANO-CHEMISTRY

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In the last twenty years, optical emission spectrometry coupled with microwave induced plasma (MIP-OES) has become a promising tool in the analytical laboratory for determining different metal species with a high excitation capability and low spectral background. For example, MIP-OES coupled with headspace solid phase microextraction (HS SPME) and thermal desorption (TD) could be applied for determining semi-volatile compounds of analytes after their microwave-assisted extraction. Moreover, MIP-OES could be easily combined with photochemical vapor generation (PCVG), HS SPME and TD for the unified separation and preconcentration of analytes such as mercury compounds. Interestingly, the generation efficiency of Hg vapor in batch-mode PCVG-HS SPME system based on photochemical reduction was improved by thermal reduction effect [1]. Thus, this method is a viable alternative to continuous PCVG for the determination of trace-level mercury in real-life samples [1, 2] and could be used in nanomaterial science for characterization of nanoparticle-analyte interaction including kinetics of adsorption of analyte on nanoparticle surface.

One of the most promising approach based on MIP-OES is a newly developed system operating in a single particle mode (SP). SP-MIP-OES is a real-time fast detection mode that allows capture of the light radiation events occurring when individual nanoparticles are vaporized, atomized and excited in the plasma. This technique has been developed for characterizing powder nanomaterials, providing information about their size, dispersity and agglomeration [3]. The use of multi-element specific detection by MIP-OES give the possibility to provide multi-dimensional information about size-dependent chemical composition of nanoparticles. Thus, SP-MIP-OES technique enables identifying organic compounds present on the NPs surface and examining the molecular interaction between nanoparticles and other analytes. The nanoparticle-analyte conjugates are characterized by observation of synchronous signals from different particle components.

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MICROWAVE PLASMA ATOMIC EMISSION SPECTROMETRY FOR METALLOMICS OF BIOACTIVE RHENIUM COMPOUNDS

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Chagas disease constitutes an overwhelming health issue in Latin America, being its etiological agent the homoflagellated protozoan parasite *Trypanosoma cruzi* [1]. In this regard, five newly synthetized *fac*-Re(I) tricarbonyl compounds were explored as prospective antitrypanosomal agents. The biological activity of the whole series was preliminarily evaluated against the epimastigote form of *Trypanosoma cruzi*, showing good activity with IC_{50} values in the low micromolar range. The most active compound *fac*-$[Re(I)(CO)_3(tmp)(CTZ)](PF_6)$, with CTZ = clotrimazole and tmp = 3,4,7,8-tetramethyl-1,10-phenanthroline, showed good selectivity towards the parasites and thus was selected to carry out further metallomic studies. For this task, a newly bioanalytical method based on microwave plasma atomic emission (MP-AES) was developed and validated. This technique employs the concept of 'running on air' with a nitrogen plasma that operates at around 5000 K, which results in cost savings and the removal of expensive and flammable gases from the laboratory, and thus it can be considered as a good strategy for the determination of highly refractory elements such as rhenium [1]. The accuracy of the method was ensured by testing a certified reference material. Results of rhenium elemental analysis by MP-AES agreed with the proposed formula of the studied compounds, contributing to the overall validation of the method, which was then applied to evaluate the percentage of rhenium uptaken by the parasites and the association of the compound with parasite biomacromolecules. Metallomics results showed low total rhenium percentage uptaken by parasites (~1.2%) and preferential accumulation in the soluble proteins fraction (~82.8%). Thus, the method based on MP-AES turned out to be an economical and green alternative for metallomics studies involving potential rhenium metallodrugs.

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OL35

HEAVY METALS FRACTIONS ANALYSIS IN SEWAGE SLUDGE ASH OBTAINED ON LABORATORY SCALE AND FROM INDUSTRIAL ORIGIN.

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Scientists around the world are developing new methods for managing sewage sludge ash (SSA). The mentioned species are generated during industrial combustion processes with the use of fluidized bed furnaces. However, in many published research, tested SSAs are produced on a laboratory scale in muffled furnaces. In the research presented, heavy metal speciation analysis, using modified BCR sequential extraction techniques. Simultaneous analysis of SSA samples, produced on a laboratory scale, and SSA produced during industrial trials was performed. The content of the mentioned fractions of Cu, Cd, Pb, and Ni was determined with the use of the MP-AES. It has turned out that an effective determination of the total Hg content must be done using the more sensitive CV-AAS. The analysis showed significant differences in the share of particular heavy metal fractions between laboratory and industrially produced SSAs. Moreover, it was observed that the SSA obtained in the laboratory is characterized by a Hg content several dozen times lower than industrial-scale SSA. The analysis showed that the SSA samples obtained in the laboratory do not constitute representative research material. Moreover, MP-AES was considered as a useful analytical tool which could be a cheaper substitute for mostly used ICP-OES.

OL36

TIME TRAVEL WITH HONEYS - THE MP-AES ANALYSIS COUPLED WITH AMS AGE DETERMINATION OF HUNGARIAN ACACIA SAMPLES

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Honeys are excellent indicators of the environment, several studies show that the elemental content of honey entirely depends on the botanical and geographical origin, but the information is incomplete regarding time-dependent composition changes. Twenty-six acacia and four honey samples with unknown botanical origin were collected between 1958-2018 and analysed for elemental composition by microwave plasma optical emission spectrometry (MP-AES). The elemental analysis was coupled with independent dating method by accelerator mass spectrometry (AMS) to determine the real age of the honey samples and test the possibility of radiocarbon based dating of bee products, which has not been applied before. The 5-(hydroxymethyl)furfural (HMF) concentration of the old samples was followed by spectrophotometry for which the White method was modified. According to the analytical measurements and statistical analysis, we can conclude that the elemental composition shows change with time in the acacia honey during the last five decades. We have proven that honey preserves information of previous times and thus can be applied as an environmental indicator in reconstruction studies by analysing the non-degradable mineral content. Our results further show that acacia honey is a suitable material for radiocarbon dating, proved by the results compared to the atmospheric radiocarbon bomb-peak. The presented new approach for investigations of honey by radiocarbon-based age determination coupled with elemental analysis can be used in biological, dietary, archaeological or other multidisciplinary studies as well. Some samples show slightly depleted radiocarbon content, based on these results, honey could be used for atmospheric monitoring. The HMF content of the honeys showed a good correlation with age and samples older than 5 years old reached and exceeded the threshold value.

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OL37

ADVANCES IN MERCURY DETERMINATION BY CV – MIP OES WITH NITROGEN PLASMA, IN DRINKING AND SURFACE WATER

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The World Health Organization (WHO) included mercury as one of the 10 chemicals of major public concern. Its presence in water bodies can engage living organisms disturbing the ecosystems, impacting negatively in the drinking water quality and thus in the human health. The monitoring of mercury at low level concentration is thereby of great relevance. The Maximum Contaminant Level (MCL) in drinking water allowed by the United States Environmental Protection Agency is 0.002 mg L^{-1} and the guidance value for the total mercury given by WHO is 0.001 mg L^{-1}. For preventing aquatic life damage, concentrations of 0.002 mg L^{-1} should not be exceed in natural bodies of water. A cold vapour, microwave induced plasma atomic emission spectrometry (CV – MIP AES) methodology was developed for mercury determination in drinking and surface water. Mercury vapour was chemically generated with 2 % $NaBH_4$ (w/v) in 0.5 % (w/v) NaOH in a Multimode Sample Introduction System (MSIS); the reactor serves at a time as the gas liquid separator and the mercury atoms were sweep towards the nitrogen plasma for its determination by emission spectrometry at 253.652 nm. The chemical parameters evaluated for the optimum generation conditions were nitric acid concentration on the samples and reductant ($NaBH_4$) concentration. Instrumental parameters considered were the torch viewing position, the nitrogen flow-rate in the gas liquid separator, sample and reductant flow-rate and the conditioning time for the gas liquid separator prior to recording the measurements. The method was characterized in terms of linear range, limit of detection, precision of repeatability and trueness. The linear range assayed was from 1.2 to 10.0 μg L^{-1} (Intensity = 132.6 C (μg L^{-1}) + 27.9, R^2= 0.998). The limit of detection calculated as 3xσ (σ being the standard deviation in concentration units of the result of 10 replicate measurement of the blank reagent) found was 0.36 μg L^{-1}. Precision of repeatability calculated as the relative standard deviation of the concentration was 13,0 % (n=6) and 19,0 % (n=6) for drinking and surface water samples respectively. Trueness was assessed by spiking drinking and surface water samples and calculated as the relative spike mean recovery (110.5 % and 89.0 % respectively, n = 3). CV – MIP OES with nitrogen plasma was successfully applied for mercury screening in water samples showing a promising performance for mercury determination at low concentration levels, highlighting the capability of the technique as an economical alternative.

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TIME TRAVEL WITH HONEYS - THE MP-AES ANALYSIS COUPLED WITH AMS AGE DETERMINATION OF HUNGARIAN RAPE, SUNFLOWER AND MULTIFLORAL SAMPLES

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Our former study highlights that acacia honey can be successfully applied for long-term environmental assessment as old samples keep inorganic compounds preserved as well as they serve as a proper material for radiocarbon dating. Good agreement was observed between the radiocarbon activity of the acaica honeys and the atmospheric bomb-peak that was used for calibration. In present study the time-dependent elemental composition and AMS dating results of 36 rape, sunflower and multifloral honey samples are presented, collected between 1985 and 2018 in geographically close locations. Elemental concentration data were gained by MP-AES method. Based on the elemental analysis we concluded that bee products regardless the type provide useful environmental information of the previous decades, such as the decreasing trend of airborne Pb emission can be traced. However, radiocarbon results agree less with the atmospheric bomb peak. Random offsets were observed in the specific radiocarbon activity of the honey samples. FTIR-ATR analysis was used to gain a deeper knowledge regarding the organic material composition of the honey samples. Results indicate that neither the inorganic composition nor the organic constituents show corresponding pattern to the AMS deviation. Even the 5-(Hydroxymethyl)furfural content following the expected age trend in acacia honeys has no such pattern in present sample series. This work indicates that rape and sunflower honey samples are not as reliable materials for radiocarbon dating as acacia honeys. Thus, the complex application of honey samples for environmental reconstruction requires the species-separated investigation of bee products to reveal their adaptability for assessment approaches.

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IL17

HIGH-FREQUENCY EPR: CURRENT STATE AND PERSPECTIVES

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From its discovery, electron paramagnetic resonance (EPR) is a constantly developing technique following technological advances in generating and detecting microwaves, creating strong magnetic fields, and fast digitalization, among others. In the talk, I will discuss developments in the field of high-frequency EPR (HFEPR) with a special focus on experiments in the frequency domain compared to the traditional field domain EPR. I will report on the recent development of a high-frequency rapid scan electron spin resonance (FRASCAN) spectrometer at the Brno University of Technology. The basic principle of frequency rapid scan will be explained and compared to conventional methods. I will present significant progress in the experimental determination of Zeeman diagrams (frequency vs. field EPR maps) and discuss the advantages of HFEPR for investigating high-spin systems, particularly single-molecular magnets (SMMs). Besides, we dedicate a section to discuss the advances in the studies of the cyclotron resonance in thin-films and modern solid-state materials like graphene (graphite). Furthermore, the importance of HFEPR for dynamic nuclear polarisation (DNP) is discussed. At last, I will demonstrate the possibility of accessing very short relaxation times (ns) by implementing rapid frequency scans, emphasizing the power of frequency domain EPR. This technique allowed to perform, for the first time, multi-frequency relaxation studies in a single spectrometer at frequencies above 100 GHz.

FRaScan Spectrometer.

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OL39

DATA ANALYSIS FROM CATCHER FOIL EXPERIMENT FOR CROSS-SECTIONS MEASUREMENT OF 40AR + 144SM REACTION

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Cross-sections from the complete fusion reaction of 40Ar + 144Sm were measured by the catcher foil method [1]. Products from the complete fusion reaction were implanted into aluminum foils and radionuclides were identified by alpha spectrometry. Improved setup allowed measurement of the absolute cross sections of α-radioactive nuclei with half-lives ≥ 0.1 s. Advanced method of data analysis was proposed in the work taking into account TRIM [2], [3] and Geant4 [4] Monte-Carlo simulations for alpha spectra, PACE4 [5] fusion-evaporation code for residual nuclei energy distribution, Couple channel method calculation [6] for theoretical cross-sections and SRIM [3] evaluation of produced isotopes stopping ranges. Using this method, the 1pxn, 2pxn and 1αxn complete-fusion excitation functions are presented.

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MECHANICAL AND GAMMA-ABSORPTION PROPERTIES OF SELECTED HEAT RESISTANT MATERIALS USED IN DEVELOPMENT OF SEALED REACTION CHAMBERS FOR IN SITU MÖSSBAUER SPECTROSCOPY

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The concept of viewports has been used in industry and research for a long time, more so in applications that require direct observation of an ongoing process inside a sealed environment. Viewports that are transparent in UV-VIS spectrum are widely available, but for the application in gamma ray energies, the viewports cannot be used, and specialised types are very uncommon. In this work several proposed heat resistant materials were studied for the development of slit windows in viewports, specifically for reaction chambers in Mössbauer spectroscopy. The material separating the sample section from the source and detector sections is required to have low absorption coefficient (less than 1.0 cm^{-1} for energies of 14.4 keV). Therefore, their gamma-absorption properties were studied by multi-channel analysis measurements using a common Mössbauer source of gamma radiation (^{57}Co). Standard Mössbauer measurements were performed to determine any MS active contaminants presence that might influence the final spectra. Mechanical properties of the clamped window materials were determined by measuring mechanical hysteresis by laser displacement measurement. Windows were periodically deformed by applying a side load – chamber relative pressure in the range of - 0.9 to + 9.0 bars. Effects of prolong and repeated exposure to these conditions were discussed in detail. Based on the observations, reusability and application potential of materials are determined. The influence of modified measurement geometry on transmission Mössbauer spectrometer was established.

OL41

CORRELATIVE HIGH-RESOLUTION OPTICAL AND CHEMICAL IMAGING OF CSPBBR$_3$ NANOCRYSTALS

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Lead halide perovskite (LHP) $CsPbBr_3$ is a highly promising semiconducting nanomaterial exhibiting bright and narrow size-tunable photoluminescence (PL) with high quantum yield. In this paper, we present a correlative imaging leading to structural, optical, and chemical characterization of single $CsPbBr_3$ nanocrystals (NCs) with high lateral resolution.

This approach utilizes focused ion beam (FIB) which is used to mark the analyzed region by rectangular micro-markings. These markings are used for precise alignment of analyzed area on the sample for several imaging and characterization techniques and correlation of their results on the level of individual NCs. The techniques include scanning electron microscopy (SEM) and atomic force microscopy (AFM) for morphological characterization resulting in correlative imaging and reliable 3D reconstruction of the $CsPbBr_3$ NCs, PL imaging of PL integral intensity and PL peak wavelength and chemical characterization with time-of-flight secondary ions mass spectrometry (TOF-SIMS).

The $CsPbBr_3$ NCs exhibit bright anti-Stokes PL that is correlated to the morphology of the crystals. The dependence of the $CsPbBr_3$ NCs' PL peak wavelength on their size is described by effective mass approach (EMA), which is compared to the experimentally obtained data. This model is based on the idea of $CsPbBr_3$ NCs being arbitrary potential well in which is the exciton confined. The prediction for PL emission of $CsPbBr_3$ NCs is then made based upon their shape and size.

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IL18

GD- AND LA-ICP-(TOFMS): TWO POWERFUL SPECTROSCOPY TECHNIQUES FOR FAST HIGH SPATIALLY RESOLVED ANALYSIS

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Plasma-based atomic spectroscopy techniques, such as Glow Discharge Mass Spectrometry (GD-MS), or Laser Ablation Inductively Coupled Plasma Mass Spectrometry (LA-ICP-MS), provide excellent analytical capabilities for the direct elemental characterization of innovative materials, geological samples or biological tissues. These plasma-based techniques provide high sensitivity and high spatial resolution (depth resolution and/or lateral resolution). Moreover, they complement other well-established analytical techniques, including Auger electron spectroscopy (AES) and secondary ion mass spectrometry (SIMS), providing higher sample throughput analysis. [1]

Glow discharges have gained increasing importance as atomization, excitation and ionization plasma-based sources for depth profiling analysis. Although GDs are operated at rough pressure conditions (1-1000 Pa) they exhibit low matrix effects and good limits of detection (in the range of µg/g-ng/g). GD-based techniques can be applied to a high variety of materials; in particular, using radiofrequency (RF) power, both conducting and insulating materials can be analyzed. Coupling pulsed-RF-GD to TOFMS for fast depth profiling analysis of nanolayers is here described.

Complementarily, techniques based on Laser Ablation such as LA-ICP-MS have been widely used, rapidly evolving into well-established, mature powerful tools for direct, high sensitivity and high lateral resolution analysis in numerous fields such as geology, biology, metallurgy, or environmental sciences [2]. Significant research and advances continue to thrive for achieving the fastest, most accurate and efficient analysis, as those focused on improvements such as low dispersion setups and cell geometries for the finest control of aerosol trajectories [3]. In this context, the combination of a femtosecond laser ablation unit with fast response and novel ICP-TOFMS technology provides one of the top-most interesting analytical methods for high spatial resolution determination -imaging- in samples of different matrices and nature. In the present work, the potential of this novel ICP-TOFMS is investigated for fast elemental imaging applications and for single spot multielemental analysis. Additionally, the option of configuring the attenuation of the ion signals at different levels in multi-segmented methods allows for the analysis of very highly abundant isotopes next to other low abundant/trace ones boosting the dynamic range of LA-ICP-MS at the low micrometric scale.

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IL19

EXCITATION IN A GLOW DISCHARGE AND AN INDUCTIVELY COUPLED PLASMA: SIMILARITIES AND DIFFERENCES

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Recent studies based on high-resolution emission spectroscopy [1,2] brought a better insight than before into excitation mechanisms of analyte atoms and ions in a Grimm-type glow discharge and an inductively coupled plasma. High-resolution spectra spanning from vacuum UV to the visible region and consisting of many hundreds of lines ('complete' spectra) were analyzed, providing distributions of relative populations of excited levels of selected analyte atoms and ions (experimental Boltzmann plots) as well as the corresponding transition rate diagrams. These two formalisms are much more suitable than raw spectral data, i.e., mere linelists with calibrated intensities, to comparing the actual empirically established discharge characteristics with predictions based on idealized plasma models or computer modelling. The similarities and differences between glow discharge sources and the ICP, as resulting from such a comparison, will be discussed, and some conclusions concerning the fundamentals of both types of analytical discharges will be presented.

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OL42

NEXT GENERATION OF DIELECTRIC BARRIER DISCHARGE ATOMIZERS FOR ULTRATRACE ELEMENT ANALYSIS

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Dielectric barrier discharges (DBDs) are non-equilibrium plasmas formed between two electrodes separated by one or two dielectric barriers, powered by high alternating voltage. DBDs can be employed for atomization of hydrides produced during preceding hydride generation step to be subsequently detected by atomic spectrometry. Our aim was to find optimum atomization conditions of eight hydride forming elements (As, Sb, Bi, Ge, Sn, Pb, Se and Te) in the DBDs with detection by atomic absorption spectrometry (AAS), compare their performance to the most common hydride atomizers and understand the mechanisms.

Several novel designs of (i) DBD atomizers and (ii) their power supply sources were investigated. The influence of electrode design and alternating current power supply source construction was studied. Three apparatus arrangements were investigated including DBD atomizers with their electrodes either glued (GE) or sputtered (SE) while the DBD high voltage power supply source was either with sinusoidal (SIN) or square wave (SW) modulation. The possible combinations were thus: GE-SIN, SE-SIN and SE-SW. Moreover, 7 types of dryers were tested to reduce the load of water vapor into the DBD. Nafion tubes or solid NaOH dryers were found as the best. Subsequently, analytical characteristics found in DBDs were compared to those reached in a conventional externally heated quartz tube atomizer (QTA) or its advanced design – quartz multiatomizer (MMQTA). Sensitivity reached in DBDs for As, Se, Sb and Te was independent of DBD configuration and comparable to that of (MM)QTA. The best DBD configuration for Pb and Sn determination is SE-SW providing sensitivity improvement by a factor of two and three, respectively, compared to GE-SIN arrangement. However, even under these conditions the sensitivity is still 3-times (Pb) and 7-times (Sn) lower, compared to (MM)QTA. Atomization of GeH_4 in DBD was optimized for the first time ever. Sensitivity reached in DBD is ca 5-times higher than in MMQTA.

Deeper insights into mechanisms of hydride atomization, its efficiency and the fate of free atoms in the DBDs, obtained by advanced spectrometric methods, such as high resolution optical emission spectrometry, laser induced fluorescence or selected ion flow tube mass spectrometry, will be outlined.

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PL3

RECENT DEVELOPMENTS IN LASER ABLATION AND INDUCTIVELY COUPLED PLASMA MASS SPECTROMETRY

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The major challenges of our times request sustainability in everything we are planning in the future. Environmental protection, discovery of new resources, characterization of new and lightweight materials, material replacement and reduction in the construction industry, food protection and safety and life science and medicine are important topics, among others, where analytical chemistry plays major role.

The availability of the entire portfolio of analytical techniques is of utmost improtance while constant refinement and development is required in order to provide high compatibility and flexibility for applications in aforementioned research fields.

The group for Trace Element and Micro Analysis at ETH Zurich studied a variety of instruments, processes and methods related to element analysis and isotope ratio determinations. Instruments were developed which become more and more applied. For example, a significantly improved prototype inductively coupled plasma time of flight (ICP-TOFMS) led to the renaissance of TOF-MS instruments and they are now commercially available (TOFWERK AG, Thun Switzerland). These instruments contribute to knowledge generation in many fields of research, e.g. in life science, medicine, geology and chemistry. Here we report a new sample introduction system for laser ablation generated aerosols introduced into an ICP-TOFMS, which has recently been developed and tested in our group. The aerosol washout and the improvements in terms of image acquisition time will be discussed[1].

For many decades argon has been the plasma gas of choice for ICP-MS, even though alternative gases have been proposed and tested. To exploit the possibility of argon substitution, a recently introduced nitrogen plasma source (Radom, Milwaukee, USA)[2] has been studied in combination with laser ablation. We also report results on direct solid analysis by LA-ICP-MS using nitrogen as plasma gas.[3]

Finally, the analyses of single cells gained significant attention using a cy-TOF-MS. Therefore, the geometry of the ICP-MS has been modified to improve throughput of single cells and nanomaterials.[4] The system and the current performance will be presented.

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OL43

COMPARATIVE ANALYSIS OF INKS FROM THE CHOPIN'S MANUSCRIPT IMPROMPTU IN A FLAT MAJOR, OP. 29: A PROOF OF CONCEPT FOR A NON-INVASIVE IMAGE-BASED INVESTIGATIONS OF WRITTEN CULTURAL HERITAGE

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The possibility of in-direct retrieving a chemical homogeneity of inks forming historical manuscripts was assessed on the example of non-destructive, multi-elemental analysis of notes and music notation from *Impromptu in A flat major, Op. 29* composed by Fryderyk Chopin. The research involved in situ acquisition of X-ray fluorescence (XRF) spectra in the museum, followed by the use of paper indicators soaked in 4,7-diphenyl-1,10-phenanthroline. The use of the indicators enabled the immediate visual detection of Fe(II) in the inked areas of the manuscript and initial assessment of the overall state of the manuscript.

Further investigations of the used indicators based on imaging of their heterogeneity by laser ablation inductively coupled plasma mass spectrometry (LA-ICP-MS). Mapping of Fe distribution allowed for selection of areas written with different inks and comparison of their elemental fingerprint with variable Al, Co, Cu versus Fe ratio. Although the manuscript had undergone conservation and chemical treatments twice in the past, it was still possible to establish differences in the elemental composition of the inks assigned to the composer, the editor and the third one used for drawing of stave lines.

In the case of this valuable object, the possibility of cross-referencing inks with other manuscripts was lost. On the basis of the results obtained, it seems that the conservation-related modifications limit the possibility of inter-object comparison, allowing only for a relative analysis of selected areas for this one item. Nevertheless, the conclusion about the possibility of transferring elemental information beyond examined manuscripts into paper indicators soaked in 4,7-diphenyl-1,10-phenanthroline and the use of sensitive MS detection for indirect discriminatory analysis remained valid.

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OL44

BIOIMAGING OF ELEMENTS AND PROTEINS BY LA-ICP-MS IN MEDICINE AND PHARMACEUTICAL RESEARCH

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In the last decades, increased interest in imaging of elements/metals/proteins distribution, mainly in pharmaceutical, biomedicine research, or life science with direct application of research to specific problem/disease [1-3]. The main emphasis of this contribution is to demonstrate the unique method of laser ablation with inductively coupled plasma and mass spectrometry (LA-ICP-MS) not only as a method of element analysis, but also as a technique for the simultaneous specific determination of the protein of interest, which opens up the possibility of achieving the so-called multiplex analysis.

Proteins are imaged using a combination of immunohistochemical methods – binding of nanoparticles labeled antibodies to a specific protein. The main advantages of using LA-ICP-MS are not only the acquisition of complex (metallo)proteomic information about the tissue of a given disease (in this case, cancer or stroke), but also low detection limits compared to other conventionally used protein imaging techniques, or multiplex analysis of a single sample.

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OL45

IMAGING OF CHEMICAL AND STRUCTURAL PROCESSES IN MINERALS

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In order to understand certain chemical processes and how they correlate with inner structural changes in minerals, several analytical methods could be used. Studying such features in minerals and materials (mostly with industrial applications) is of great importance for understanding the processes taking place at the atomic or molecular level. The development of hyperspectral imaging on a LA-ICP-MS, electron microprobe and Raman spectroscopy brought interesting results in the field of crystallography and material research with great potential to improve both qualitative and quantitative interpretation of results. Combined data can provide a very comprehensive tool for the investigation of structural/phase transitions and chemistry changes in the samples [1].

If we detect changes in the chemical composition (mostly zonal development or the occurrence of different mineral phases) via electron microprobe, it is also possible to assume the existence of structural changes visible in the Raman spectra in form of a band shifts or bandwidth variations. Observed on example of studied carbonate system emerging from the selected drains of coal heaps in the Czech part of the Upper Silesian Basin, each of the carbonate minerals present (monohydrocalcite, aragonite, calcite) has a unique Raman spectrum [2] based on which the Raman imaging could be processed. Even presence of luminescence might serve as some form of impurity indicator [3]. Presence and distribution of such impurities may be confirmed by LA-ICP-MS imaging (especially sub-ppm elements previously not detected on EPMA).

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OL46

NEW OPPORTUNITIES IN ATOMIC SPECTROCHEMISTRY WITH HYPHENATED TECHNIQUES USING HR ICP/MS AND MC ICP/MS WHEN HYPHENATED WITH GC OR LASER ABLATION

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To better understand the fate and impact of trace elements in the environment and in industrial processes, we need to propose the concept of speciation to determine the chemical species responsible for the effects studied. Further, it is also important to have often a discrete information on the surface of the sample. In both cases, this requires transient signals generation. We will present the results of hyphenated techniques using either ICP/MS, HR ICP/MS, or MC ICP/MS as detectors and mainly hyphenated to gas chromatography. The development of novel femto-second laser ablation systems also generated transient signal that can be used for nano particles detection for example. In all instances, we need to have advances transient signal processing in order to improve the quality of information that we want to have at very sensitivities also. Both GC and laser ablation systems will generate fast transient signals that are sometime not adapted to the scanning speed of the detectors. We will also present the different analytical strategies developed for both laser and GC transient signals hyphenated to various plasma-based instrumentation. These results will show that we can use these novel hyphenated analytical detections to open up new fundamental biogeochemical questions in the environment, but also generate most interesting information in food traceability, nuclear sciences or in archaeometry.

IL21

NANOSCALE SECONDARY ION MASS SPECTROMETRY FOR ELEMENTAL BIOIMAGING IN CELLS AND TISSUE

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Chemical bioimaging provides an important contribution to the investigation of biochemical functions, biosorption and bioaccumulation processes at cellular and subcellular level. Scientific progress in this field is directly related to new instrumental and methodological analytical developments and the combination of analytical techniques. Nanoscale secondary ion mass spectrometry (NanoSIMS) relies on the sputtering of ions under high vacuum from a solid surface by focused positive or negative primary ion beams and the subsequent analysis of the produced secondary ions by a mass spectrometer. NanoSIMS allows chemical imaging of a sample surface with lateral resolution down to 50 nm pixel size combined with high sensitivity and thus it is perfectly suited to localize the distribution of chemical elements with high spatial resolution at cellular level. A novel radio frequency plasma oxygen primary ion source provides high sensitivity and high spatial resolution for trace metal detection. Correlative imaging can be realized with transmission electron microscopy, synchrotron-based µXRF as well as µ-X-ray tomography and Laser Ablation ICPMS.

This lecture highlights the application of NanoSIMS and related techniques for intracellular element and nanoparticle analysis. Challenges and limitations including sample preparation will be discussed. Sophisticated sample preparation techniques are necessary basing on by chemical fixation or cryofixation, followed by resin embedding and ultramicrotomy. Recent examples from our laboratory for (trace) metal and nanoparticle localization in biological cells and tissue will be presented and strategies for correlative imaging with other element imaging techniques will be discussed.

OL46

DEPTH-RESOLVED ELEMENTAL AND MOLECULAR ANALYSIS OF POLYMERIC COMPOSITES USING CHEMOMETRIC EVALUATION

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Polymeric composites consist of organic polymer materials with various organic and inorganic additives such as pigments, antioxidants and flame retardants that customize the compounds for individual purposes. Due to their versatile adaptability, they have a wide range of applications and find use as paints, varnishes, coatings, packaging materials, and many more. Often, more than one polymer, either in mixtures or in structured or layered systems, is required to achieve the desired property of the material. [1] For processing and recycling of these materials, as well as for forensic analytics, reliable analysis methods are required. Information such as type of polymer, prevailing additives and potential contaminants is necessary to characterize the materials' organic and inorganic composition. Conventional analytical techniques used for polymer analysis, such as Pyrolysis gas chromatography-mass spectrometry (Py-GC-MS), Matrix Assisted Laser Desorption/Ionization-MS (MALDI-MS), and Fourier transform infrared spectroscopy (FTIR), provide only molecular and no elemental information. Moreover, they cannot efficiently deliver depth-resolved information, hampering their applicability to investigate structured materials. Structured samples like polymer multilayers are especially challenging to analyze since depth-resolved measurements are crucial to determine the individual layers of a sample. Solely Laser induced breakdown spectroscopy (LIBS) enables elemental analysis as well as depth profiling but shows limited selectivity for organic materials. [2]

This work presents a novel multi-modal approach for direct composite material analysis enabling depth profiling. The method is based on the laser ablation of a solid multilayer sample and simultaneous online measurement of the ablation products by Electron ionization mass spectrometry (EI-MS) and Inductively coupled plasma optical emission spectrometry (ICP-OES). Successive ablation allowed the measurement of depth profiles where EI-MS determined the molecular structure of the fragments and ICP-OES detected the corresponding elemental composition. The data evaluation, allowing a reliable differentiation and characterization of the individual layers, was achieved using principal components analysis (PCA) and hierarchical cluster analysis (HCA) of the combined EI-MS and ICP-OES results. The applicability of the developed procedure is demonstrated by the depth-resolved analysis of the molecular structure and elemental composition of layered nail polish samples.

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OL47

APPLICATION OF SPECTROSCOPIC METHODS IN RESEARCH OF GEOCHEMICAL PROCESSES IN THE UPPER SILESIAN COAL BASIN

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The aim of the study was to describe mineralogical phases related to discharge of saline mine waters and draining waters of coal heaps. Special mineralogical phases crystallize from these highly mineralized waters when entering the river system [1]. By using several analytical methods in studying of mineral incrustations we are able to better understand the processes and to create a more precise geochemical model of processes [2]. For this study, four samples from mine drainage and five samples from coal dumps drainage were collected. The content of the elements was measured by portable X-ray fluorescence spectrometer (pED-XRF) and for the phase composition XRD method was used. Mineralogical nature of incrustations was determined by scanning electron microscope with energy dispersive X-ray spectrometer (SEM/ED-XRF). Subsequently, representative samples with atypical mineral composition were selected for a more detailed phase analysis by micro-Raman spectroscopy which discovered local changes in the degree of luminescence. Based on previous observations, selected elements (K, Ca, V, Cr, Mn, Fe, Zn, As, Sr, Ba, Pb, Th and U) were used to create chemical distribution maps in the incrustations via laser ablation (LA-ICP-MS) and major as well as trace cations and anions were measured in sampled waters by ICP-MS. The hydrochemical type of waters was evaluated by using the Geochemist's Workbench 12 Professional Edition with using Gtplot. All monitored water resources reach neutral to basic pH values (6.7-10.2). In the evaluated mine waters and dump drainages, the hydrochemical types of water (SO_4 – Cl^-) with a variable content of bicarbonates and cations (Na, K, Mg, Ca) were distinguished, which noticeably contribute to the formation of incrustations at the drain or bottom of streams. Phase analysis showed us three main dominant minerals (calcite, aragonite and monohydrocalcite) which bind different elements into their structure. Based on results from laser ablation and analyses from another spectroscopic methods, we can determine correlating systems between the mobility of individual elements in water and their entrance into the incrustations.

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OL48

EVALUATION OF THE ELEMENT CONTENT IN GEOLOGIAL UNITS AND ITS IMPORTANCE IN THE ENVIRONMENT EVALUATION – SPECTROSCOPY STUDY

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The aim of the study was to identify elements in primary background rocks and determine the conditions under which they can be released into the environment.

The study area is situated in the Upper Silesian Coal Basin that is one of the largest bituminous coal basins in Europe. At present, mining is declining, and the landscape is being revitalized. The excavated rocks present on the surface are gradually weathering and potentially hazardous elements are entering the environment in increased quantities.

For this study, ten borehole core samples and five bottom sediments from lakes were collected. The content of elements was determined by X-ray fluorescence spectrometer (XRF) and subsequently some samples were measured by ICP-OES. One sample with higher amount of Hg was measured by automatic mercury analyzer (AMA) to detect the total mercury content (Hg-T) and Thermal Desorption technique was used to identify mercury species. Rare-earth elements were analyzed by ICP-MS on ten samples and the strontium content was measured in four samples. There were eight water samples collected from five lakes and major anions and cations were measured in it. The hydrochemical type of waters was evaluated using the Geochemist's Workbench. Water analysis shows that there are three hydrochemical types of water. There is a chloride hydrochemical type of water in two localities (Liberďok, Kozinec). Next, there is one locality (Heřmanický rybník) with a sulphate-chloride hydrochemical type of water and two localities (Skučák, Rybník Pod Farou) with a carbonate hydrochemical type of water. However, there is also a larger ammount of sulphates in Rybník Pod Farou. The following toxic elements were monitored: lead, copper, zinc, arsenic, mercury and chromium. Increased amounts were measured for zinc and copper. The strontium content was also measured. In case of core samples, the strontium content was higher. In case of lake sediments, the highest content of mercury, copper and zinc was measured in Heřmanický rybník and the lowest content of toxic elements was detected in Liberďok and Skučák.

Finally, the results of the methods were compared and the explanatory power of the method for given elements was evaluated.

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IL22

MÖSSBAUER SPECTROSCOPY IN GAMMA-OPTICS, GAMMA-OPTICS IN MÖSSBAUER SPECTROSCOPY

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Recently an extension of quantum optics into the x-ray and gamma domain has frequently been discussed. This offers working with quantum information on the wavelength bellow one nanometer, easy performance of single photon experiments and new techniques in the metrology fields. One of the promising approaches to a coherent control of gamma radiation (using radioactive sources and also synchrotrons) is based on the Mössbauer effect. However, not only can the Mössbauer spectroscopy be helpful to handle the gamma photon field but also, conversely, manipulating with gamma photons can advance the Mössbauer spectroscopy. It aims, for example, to the enhancement of the signal to noise ratio and advancements in ghost imaging. In this contribution an application of the Mössbauer effect for manipulation with gamma photons is overviewed and discussed, mainly in connection with electrically and acoustically induced transparency. Simultaneously, new perspectives for Mössbauer spectroscopy will be outlined.

OL49

POLYMORPHISM AND CRYSTAL STRUCTURE OF IRON(II) OXALATE

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Anhydrous oxalates of transition metals MC_2O_4 (M = Mn, Fe, Co, Ni, Cu) are interesting materials for many researchers because of theirs use in various scientific and technological processes. For example, iron (II) oxalate has been reported as a useful precursor for ferrite preparation [1] or as novel material for lithium-ion batteries [2]. Iron (II) oxalate usually crystalizes in a hydrated form, either in α- or β- modification. In this work, we explore the transformations of both α-$FeC_2O_4{\cdot}2H_2O$ and β-$FeC_2O_4{\cdot}2H_2O$ crystal structures during the hydrous to anhydrous state transition. The separation of crystal-bound H_2O molecules is induced by a low-temperature calcination in the nitrogen atmosphere. The prepared samples, both prior and after calcination, were examined by X-ray powder diffraction, Mössbauer spectroscopy and scanning electron microscopy.

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OL50

LAMB-MÖSSBAUER FACTOR DETERMINATION OF POWDERS BY RESONANT MÖSSBAUER SPECTROSCOPY

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Lamb-Mössbauer factor is a crucial material parameter which reflects the lattice dynamics. The knowledge of its precise value is also essential for proper quantitative analysis of the Mössbauer experiments. We report on a method for the Lamb-Mössbauer factor determination on powder samples. The method is based on the resonant Mössbauer spectroscopy [1]. The principle of this method and the sample preparation is described in detail together with different experimental aspects of its application to powders. The method is demonstrated on the investigation of powder iron oxalate. The thickness dependence of iron oxalate nuclear absorption was measured by resonant Mössbauer spectrometer and analyzed by fitting the spectra using the full transmission integral based approach.

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OL51

THERMALLY INDUCED SOLID-STATE REACTION OF FE$_2$(SO$_4$)$_3$ WITH NACL OR KCL : A ROUTE TO Β-FE$_2$O$_3$ SYNTHESIS

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A detailed in-situ investigation of a thermal solid-state reactions of $Fe_2(SO_4)_3$ + NaCl and $Fe_2(SO_4)_3$ + KCl mixtures (molar ratio 1:3) is presented. Previously, the former mixture was reported as a precursor for the formation of a rare β-Fe_2O_3 polymorph[1–3]. However, the synthesis of β-Fe_2O_3 is sensitive to reaction conditions and the contamination with α-Fe_2O_3 is possible[3]. In this study the effect of the alkali salt selection on the thermal transformation processes is shown. The results of Mössbauer spectroscopy and in-situ X-ray powder diffraction show that potassium is more willing to form bimetal sulphates, i.e. the key intermediates to β-Fe_2O_3, than sodium. As a result, the formation of β-Fe_2O_3 is less sensitive to the heating profile, proposing the thermal decomposition of $Fe_2(SO_4)_3$ + KCl mixture as a more controllable route for β-Fe_2O_3 preparation.

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OL52

SPECIATION ANALYSIS OF IRON IN THE BIOLOGICAL MATRIX OF FILAMENTOUS FUNGI USING MÖSSBAUER SPECTROMETRY

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Microscopic filamentous fungi are ubiquitous organisms whose typical habitat is soil. In this environment, fungi interact with the soil mineral surfaces, effectively regulating the bioavailability and mobility of mineral nutrients [1], including iron [2]. They also contribute to precipitation of biogenic iron-bearing mineral phases [3], whose analysis is usually performed by Mössbauer spectroscopy. This technique is especially advantageous for analyzes of iron speciation in synthetic or natural materials [4]. Since it has been successfully applied for analysis of transformants of ochric materials [5] in the presence of filamentous fungi [6], we have also applied Mössbauer spectroscopy to study a microbially induced transformation of magnetic nanoparticles which has been triggered by the presence of *Aspergillus* strains. However, our preliminary results indicate that even though the iron is extractable by fungi (up to 20%), magnetic nanoparticles are relative stable and resists the microbially induced transformation into new biogenic minerals.

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IL23

APPLICATION OF SPECTROSCOPIC TECHNIQUES FOR SPECIATION ANALYSIS OF IODINE, SELENIUM AND IRON USED IN STUDIES OF PROCESSES IN THE NEAR- AND FAR-FIELD REGIONS OF SPENT NUCLEAR FUEL DISPOSAL SYSTEM

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Selenium and iodine have long-lived radioactive isotopes formed by the nuclear fission of uranium. However, since it is easily adsorbed onto the ferric and manganese minerals, their mobility in the natural environment or removal from contaminated waters is generally not an issue [1-4]. However, both exhibit peculiar redox properties, especially in the presence of ferrous ions. ^{79}Se and ^{129}I can be accessible in case of radionuclides leaching from the radioactive waste disposals, where the anoxic conditions prevail and, thus, the ferrous ions and minerals predominate as corrosion products [5]. There, the reductive and adsorptive immobilization by Fe(II)-bearing minerals are the main mechanisms for the removal of redox-active selenium and iodine. Since the information on the mutual interactions of selenium or iodine and Fe(II)-bearing minerals is scarce, the main objective is to evaluate the state of the research and available spectroscopic techniques, such as XAS, providing information on the effects of redox properties of Fe(II)-bearing solids on selenium and iodine speciation. The iodine mobility studies will be shown regarding the coprecipitation and adsorption onto the iron mineral (magnetite) surfaces prevailing under anoxic conditions. Furthermore, iron compounds formed in the far-field area and their interaction with selenium were studied by Mössbauer spectroscopy.

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OL53

NICKEL-IRON AND ZINC-IRON BIMETAL OXALATES: PREPARATION, CHARACTERIZATION AND THERMAL DECOMPOSITION TO SPINEL FERRITES

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The in-situ investigation of Ni and Zn spinel ferrites preparation via oxalate route is presented. In recent years, both Ni and Zn ferrites have been reported for use in a number of applications, for example sensors [1,2], photocatalysis [3], battery cells [4], etc. Although the oxalate route in general is rather well-known, the detailed investigations of the decomposition reactions of the well-characterized bimetal oxalate precursors have been mostly omitted by the authors. The formation of the solid solution, i.e. the incorporation of both metals into the single oxalate crystal structure, is essential for the subsequent decomposition reaction and synthesis of spinel ferrites. The optimally prepared precursor decomposes in a single reaction step at relatively low temperatures, evading the undesirable sintering, and allowing the preparation of microporous/mesoporous ferrites with relatively high BET areas.

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OL54

MÖSSBAUER SPECTROMETRY OF METALLIC ALLOYS

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Mössbauer spectrometry is highly sensitive method for precise characterization of the nearest surroundings of the resonant atoms. It is capable of scanning hyperfine interactions between the nucleus and its electronic shell. In this way it provides information on the local microstructure of the investigated samples.

This contribution highlights the most important aspects of ^{57}Fe Mössbauer spectrometry in the study of metallic alloys. In particular, we focus on selected tool and construction steels. The effects of production treatment such as hardening and/or thermal annealing lead in the former to repositioning of the resonant atoms within their crystalline lattice. Consequently, variations in the chemical composition in the nearest neighborhoods of the resonant atoms occur. They result changes in the hyperfine interactions as shown by the analysis of the corresponding Mössbauer spectra.

Construction stainless steels are of immense practical interest due to their applications in nuclear industry. Mössbauer spectrometry can effectively unveil microstructural modification that are caused in the investigated steels by common mechanical treatment such as cutting, grinding, and polishing. In addition, differences in structural arrangement on their surface and in their bulk can be also determined. Before illustrating the possibilities of Mössbauer spectrometry in the identification of individual atomic sites, basic principles of this analytic method will be briefly presented.

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OL55

MÖSSBAUER SPECTROSCOPY STUDY OF TIN-CONTAINING METALLIC GLASSES

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^{119}Sn and ^{57}Fe Mössbauer spectrometry were used to investigate several Fe-Sn-B-type metallic glasses. Thin strips of $Fe_{78}B_{15}Sn_7$, $Fe_{81}B_{12}Sn_7$ and $Fe_{83}B_{12}Sn_5$ were prepared through the method of planar-flow casting. They were studied in the as-quenched state and also after annealing at 400 °C. During the annealing, nanocrystalline grains formed within the alloy. The effect of slight alteration of boron and tin content on the resulting microstructure was investigated. The results show advantageous soft-magnetic properties which have wide practical applications.

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OL56

APPROACHES TO EVALUATION OF MEASUREMENT UNCERTAINTY IN ICP-MS ANALYSIS

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Measurement uncertainty (MU) is a key parameter describing quality and reliability of measurement results. Its definition in the International Vocabulary of Metrology (VIM 3) non-negative parameter characterizing dispersion of the quantity values being attributed to a measurand, based on the information used emphasizes that information used for MU evaluation may significantly influence its value.

This contribution discusses two basic approaches used for MU evaluation, so called “bottom-up” as well as “top down” in ICP-MS analysis. Outcomes from our research will be shown on three practical applications. The first one deals with MU evaluation for bromine and iodine determination in mineral waters and implements “top-down” approach introduced by LGC [1]. More detailed insight describing using correlated validation data to estimate MU by “top-down” approach will be shown on the issue of determination of Pd as an elemental impurity in pharmaceutical products by ICP-MS [2]. The last application focuses on “bottom-up” approach to determination od elemental impurities in a nasal spray. In this example, the calibration process was studied, and linear regression and linear weighted regression implemented to acquire results [3]. The obtained values of MU by different approaches will be compared and crucial steps of MU evaluation identified.

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OL57

SEASONAL VARIATION OF DRINKING WATER QUALITY AND HUMAN HEALTH RISK ASSESSMENT: A CASE STUDY IN RURAL VILLAGE OF THE EASTERN CAPE, SOUTH AFRICA

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Contamination of drinking water by metal ions remains a global threat to living organisms. Therefore, the current study describes variations of metal occurrence, water quality and human health risk assessment between the dry and wet seasons of a rural village located in the Eastern Cape Province, South Africa. The concentration levels of major and trace metals (Al, As, Ca, Cd, Co, Cr, Cu, Fe, K, Mg, Mn, Ma, Ni, Pb, Sb, Se, Tl, V and Zn) were determined in the drinking water from the tap and windmill using inductively coupled plasma-optical emission spectrometry (ICP - OES). Moreover, physicochemical parameters, water quality index (WQI), total water hardness (TWH) and health risk assessment (hazard quotient: HQ and chronic daily intake: CDI) were evaluated seasonally. The TWH results showed that the water was very hard with water hardness values ranging between 415 and 442. The water also contained several metals and metalloids such as Al (2.18–3.36 mg l-1), As (0.17 – 0. 53 mg l-1), Cd (0.0068 – 0.0134 mg l-1), Cr (0.2481 – 0.2601 mg l-1), Mn (0.387 – 1.582 mg l-1), Pb (0.064 – 0.0802 mg l-1), Sb (0.0496 – 0.1391 mg l-1) and Se (0.075 – 0.148 mg l-1) that exceeded the SANS and WHO permissible limits in drinking water. The health risk assessment revealed that the water may cause non-carcinogenic health effects due to the presence of As, Cr, Sb, Tl and V in water samples, while the water quality index revealed that the water was of very poor quality.

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HIGH PRECISON MEASUREMENTS OF LEAD ISOTOPE RATIO WITHOUT MATRIX SEPARATION

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Knowledge of the isotopic composition is important for the understanding of many physical and chemical processes occurring in nature. Subtle isotopic changes are the result of the phenomenon of isotope fractionation, which is a division of different isotopes of a given element between coexisting phases.

One of the common problems in measuring isotope composition are the very complex sample preparation procedures. Simplification of these procedures, accompanied by the well fitted calibration strategy is currently one of the most important directions in the development of isotopes research. Different calibration methods have different robustness to matrix influences [1], thus by appropriate selection of the calibration strategy and optimizing measurement parameters, the sample preparation process can be reduced to a minimum [2].

In this work we compared the performance of Optimized Regression Model and internal standard method (Tl as an internal standard) for the isotope ratios of lead in heavy matrix samples. We have developed measurement approaches designed for the specific type of sample, using model samples with increasing matrix-to-analyte ratio (up to 30000:1). We optimized the spectrometer (Plasma II MC ICP MS) conditions, i.e. background correction method, analyte to standard ratio, etc. We tested the maximum concentrations of chosen interferents at which the calibration methods cease to give correct results. Then, we applied the developed measurement protocols to selected samples with known isotope ratios of lead. We have made every effort to ensure that the range of sample diversity is as wide as possible: archaeological objects (bronzes), pieces of works of art (pigments), geological materials (granite G2), oceanic water (NASS-2) spiked with Pb and street dust (NIST 1648). For any of the samples mentioned, neither purification nor isolation of Pb was applied. Finally, we demonstrated the accuracy of the simplified protocols for the isotopic ratio measurements.

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OL59

MAGNETIC FE_3O_4@MG/AL-LAYERED DOUBLE HYDROXIDE ADSORBENT FOR PRECONCENTRATION OF TRACE METALS IN WATER MATRICES

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A magnetic Fe_3O_4@MgAl-layered double hydroxide (MLDH) nanocomposite was successfully synthesized and applied as an effective adsorbent for preconcentration of trace As(III), Cd(II), Cr(III), Co(II), Ni(II), and Pb(II) ions from complex matrices. The quantification of the analytes was achieved using the inductively coupled plasma optical emission spectrometry (ICP-OES) technique. The nanocomposite was then characterized using BET, FTIR, SEM, and EDS. Due to its high adsorption surface area, compared to traditional metal oxide-based adsorbents, MLDH nanocomposite exhibited high extraction efficiency [1]. Several experimental parameters controlling the preconcentration of the trace metals were optimized using response surface methodology based on central composite design. Under optimum conditions, the linearity ranged from 0.1 to 500 µg L^{-1} and the correlation of coefficients (R^2) were higher than 0.999. The limits of detection (LODs) and quantification (LOQs) were 0.11–0.22 µg L^{-1} and 0.35–0.73 µg L^{-1}, respectively. The intra-day (n = 10) and inter-day precisions (n = 5 working days) expressed in the form of percent relative standard deviations (%RSDs) were below 5%. The proposed method was successfully applied for the analysis of the As(III), Cd(II), Cr(III), Co(II), Ni(II), and Pb(II) ions in different environmental water samples.

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IL24

SOME PERSPECTIVE SPECTROSCOPIC TECHNIQUES FOR ANALYSIS OF NANOPARTICLES USED IN STUDIES WITH SOILS, PLANTS AND FILAMENTOUS FUNGI

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Engineered nanoparticles are increasingly used in many varying areas of human endeavour. Thanks to the rise in their use, they may be accidentally or unintentionally released into the environment, or intentionally applied in agriculture as micronutrients, growth enhancers and pesticide formulas. Therefore, the development of techniques that can explain their behaviour in plants, fungi and soils is needed [1]. In recent years, different techniques using single-particle ICP-MS were directly used on the effluents from column experiments or used together with laser ablation on soil and plant samples, where the evaluation of the concentration and the form (dissolved vs particulate) is important, and in case of laser ablation, a more precise location of nanoparticles can be discerned within the sample. Other more exotic techniques were also used to either discern the nanoparticulate character within the sample. Mössbauer spectroscopy [2,3] can be used for Fe-based nanoparticles to discern their crystallinity and also nanoparticulate character. Characterisation of nanoparticles and their location is mostly done by different techniques of electron microscopy. More exotic techniques, such as nano-XRF, XAS, XANES, and SAXS that use synchrotron radiation, can be applied to find specific information about the behaviour of nanoparticles in plants, fungi, or soil.

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IL25

APPLICATION OF ANALYTICAL TECHNIQUES IN THE STUDY OF BIOLOGICAL SYSTEMS

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Iron is the most important metal in human body and can be associated with neurogedenerative disease. Postmortem brain tissues samples from human *globus pallidus* were investigated by the light (LM), scanning (SEM) and transmission electron microscopy (TEM), electron diffraction, SQUID magnetometry and Mössbauer spectroscopy (MS). Large accumulation of micrometer-sized Fe^{3+} ions LM by was identified. TEM with diffraction revealed magnetite Fe_3O_4 and hematite α-Fe_2O_3 with the size 50 – 3000 nm. The SQUID magnetometry reveals three groups: dominating diamagnetism (I), dominating paramagnetism (III), and the intermediate class (II). MS shows a number of iron oxide minerals (ferritin, magnetite, hematite) in all samples. Endogenous magnetic field of magnetic biominerals can influence the function of the cells in the human brain.

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OL60

SPECIATION OF IRON IN MICROBIAL BIOMASS AND NATURAL OCHRIC PRECIPITATES AS AFFECTED BY FUNGAL ACTIVITY

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Since iron participates in various vital metabolic processes in the cell, it is an essential micronutrient for microorganisms. It serves as a cofactor in various microbial metabolic pathways. Thus, organisms have developed various mechanisms for its uptake and storage [1]. This includes redox transformation and chelation, which also affects stability of natural ferric/ferrous precipitates (e.g., ochres). However, the determination of the exact mineral forms and speciation of iron is always challenging, especially in the case of biomass where the iron concentration is usually low [2,3]. Therefore, we have collected various biogenic materials, and studied the prospects of various spectroscopic methods (e.g., Mössbauer spectroscopy [4,5]) to analyze the iron in such complex matrices [6].

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IL26

UNRAVELLING NEW ISOTOPIC DIMENSIONS OF NITROUS OXIDE BY QUANTUM CASCADE LASER ABSORPTION SPECTROSCOPY

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Nitrous oxide (N_2O) is one of the most important greenhouse and ozone-depleting gases. Due to anthropogenic activities, its atmospheric abundance has been rising with unprecedented speed. However, mitigation of N_2O emissions is challenging since its source and sink processes have not been understood yet.[1] We will present a method for analysis of doubly isotopically substituted molecules of N_2O based on quantum cascade laser absorption spectroscopy (QCLAS). These "clumped isotopes" are expected to be new tracers for the characterization of the global N_2O budget and the nitrogen biogeochemical cycle.

The first goal was to set up and optimize the QCLAS method for simultaneous analysis of clumped ($^{14}N^{15}N^{18}O$, $^{15}N^{14}N^{18}O$, $^{15}N^{15}N^{16}O$) and singly substituted species ($^{14}N^{15}N^{16}O$, $^{15}N^{14}N^{16}O$, $^{14}N^{14}N^{17}O$, $^{14}N^{14}N^{18}O$), including the most abundant unsubstituted species ($^{14}N^{14}N^{16}O$).[2] Next, a calibration scheme for quantification of the clumped species was introduced. The method was validated against another QCLAS method using an established isotope-ratio calibration and an isotope-ratio mass spectrometry (IRMS) method.[3]

In addition, we are going to demonstrate the applicability of the method on a natural N_2O source (denitrification by bacteria *Pseudomonas aureofaciens*) and a natural N_2O sink (stratospheric UV photolysis) on samples prepared in the laboratory. By that, we have opened unexplored possibilities for research on N_2O in the nitrogen cycle.

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IL27

TUNABLE OPTICAL METASURFACES BASED ON VO_2

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Artificially nanostructured flat optical elements (called metasurfaces) can influence propagation of light beams with much broader range of possibilities than what is commonly available using their conventional macroscopic counterparts. Not only do metasurfaces greatly reduce the optical thickness required, for example, to focus light through a lens, they also allow control over other parameters of the light beam, such as polarization, phase, or orbital angular momentum. My contribution will be devoted to implementation of tunability into the realm of metasurfaces. I will focus on one material – vanadium dioxide (VO_2) – which can play the role of a versatile tunable element. More specifically, I will describe our recent work in this area [1]-[3] and address future challenges which remain to be tackled in this emerging field.

IL32

FINDING OF NEEDLE IN A HAYSTACK - NONTARGETED MASS SPECTROMETRY ANALYSIS OF ENVIRONMENTAL SAMPLES

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One of the biggest problems in the analysis of environmental and biological samples is their complexity, because they contain many organic substances with different physico-chemical properties. In addition, contaminants found in complex samples are often unknown, or arise as a result of various degradation/transformation biotic and abiotic processes of the original substance and are often present at very low concentration levels. In this context, combination of liquid chromatography and high-resolution mass spectrometry (LC-HRMS), due to its high resolution and high selectivity, and on the other hand, the recording of MS spectra with high accuracy of mass determination allows the identification and quantification of a large number of known and, moreover, unknown compounds. From an analytical point of view, there are three approaches to LC-HRMS analysis of environmental samples, namely (i) targeted analysis, (ii) suspect screening and (iii) non-targeted analysis. Especially, nontargeted HRMS data are complex and challenging in identification of compounds of interest and consequently in interpretation of the presence of identified compounds toward the biological effect of the sampled mixture.

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IL28

COMPLEMENTARITY OF LASER-INDUCED BREAKDOWN SPECTROSCOPY AND LASER ABLATION INDUCTIVELY COUPLED PLASMA MASS SPECTROMETRY IN CANCER TISSUES ANALYSIS

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It has been shown that cancerous tissues change the chemical composition of cells **Error! Reference source not found.**. These changes in elemental composition can be observed using Laser-Induced Breakdown Spectroscopy (LIBS) or Laser Ablation Inductively Coupled Plasma Mass Spectrometry (LA-ICP-MS), where imaging of biotic (e.g., C, P, Ca, Mg) and trace (e.g., Zn, Cu) elements provides information about the distribution of soft tissue elements and, consequently, the location of cancerous tissue.

This paper deals with a correlative study using LIBS and LA-ICP-MS in a sample of healthy human skin, four samples of malignant tumours (squamous cell carcinoma, malignant melanoma, basal cell carcinoma, and epithelioid angiosarcoma), and one sample of a benign tumour (pigmented nevus). Analysis was performed using both techniques for all these samples, and spatial distributions of selected elements were constructed. This work aims to show the potential of correlation of data obtained from both analytical methods, which could be used for the possible diagnosis of cancer as a complementary technique to classical histological examination.

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IL29

UNDERSTANDING THE CORRELATION OF LIBS AND ACOUSTIC MEASUREMENTS OF ROCKS AND SOILS FOUND IN THE TRAVERSE OF THE PERSEVERANCE ROVER ACROSS THE JEZERO CRATER, MARS

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The SuperCam instrument of the NASA MARS 2020 Perseverance rover combines a suite of atomic and molecular spectroscopies intended for an extensive description of rocks, soils and minerals in the surroundings of the landing site of the mission – the Jezero crater. The microphone installed on the SuperCam instrument allows the acquisition of acoustic signals resulting from the expansion of laser-induced plasmas towards the atmosphere. Apart from being affected by the propagation characteristics of the Mars atmosphere, the acoustic signal has an additional component related to the properties of the target including surface morphology, hardness, deformation parameters, and elasticity, among others. This information is currently being investigated as a complementary resource for characterization of the ablated material and may well supplement the LIBS data gathered from coincident laser shots. This talk will present SuperCam acoustic data of rocks and minerals found in the traverse of the Perseverance rover and will discuss its correlation with LIBS spectra.

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OL62

LASER INDUCED BREAKDOWN SPECTROSCOPY IMAGING OF URANIUM ORES

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Laser-induced breakdown spectroscopy (LIBS) was applied to create images revealing the distribution and possible migration of elements in samples of uranium ore. Compared to SEM or LA-ICP-MS, fast LIBS scanning made it possible to perform analysis across the big sample area containing different mineral phases of uranium ores including associated minerals. However, the imaging of some associated elements is due to rich spectra and low contents still challenging. Moreover, compromise conditions have to be often set to reach the required spatial resolution, speed of scanning and sensitivity. Generally, higher resolution is paid for by the loss of sensitivity and vice versa. Nevertheless, there are some possibilities for improvement in both instrumentation and spectral data processing. Different effects such as the role of the introduction of noble gas, influence of laser wavelength or double pulse methods will be discussed.

The investigated geological samples represent U-mineralisation from a former deep uranium mine. Obtained elemental images help to reveal and distinguish different phases such as massive uraninite and carbonate vein or metasomatite. Additionally, the signal correlation of some elements (correlation between different emission lines) helps with the identification of other associated minerals.

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OL63

LIBS APPLICATIONS OF ONLINE MONITORING AND 2D/3D MAPPINGS FOR ADVANCED CONTROL OF INDUSTRIAL PROCESSES

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Advanced monitoring and control methods are significant in the industrial processes. Laser-induced breakdown spectroscopy (LIBS) is an analytical detection technique based on atomic emission spectroscopy to measure the elemental composition, which has been widely applied in various fields [1]. In this study, LIBS applications of online monitoring and 2D/3D mappings were demonstrated for advanced control of industrial processes.

A collinear long and short DP-LIBS method (LS-DP-LIBS) was developed to improve the detection ability and measurement accuracy by the control of the plasma cooling process using the long pulse-width laser radiation[2]. The plasma generated by the short pulse-width laser is stabilized and maintained at high temperature during the plasma cooling process by long pulse-width laser radiation. C, Al, Si, S, Ti, Cr, Ni, Cu, Nb, Mo, Mn, and B concentration measurements in molten steel samples were performed using LS-DP-LIBS. It demonstrates the feasibility of multi-element concentration measurements in iron and steel making processes and this will lead to the advanced monitoring and control methods in these processes.

The analysis of elemental composition distribution is indispensable to ensure the quality of various materials production. In this regard, 2D/3D mapping techniques using LIBS are widely used in various fields. In many LIBS studies, lasers with ns pulse widths are used, and the spatial resolution of 2D LIBS mapping is usually several to several tens of micrometers. In this study, a spatial resolution of 1 µm was achieved by using a laser with a pulse width of 9 ps. This LIBS mapping system consists of a picosecond laser, lens, spectrometer, ICMOS camera, and XYZ stage. The LIBS system was applied to steel and Li-ion battery electrodes for 2D elemental distribution analysis. The steel sample has a structure with Zn coating around the steel at the µm level, and this LIBS mapping system was able to detect the Zn distribution around the steel at the µm level. This result was in good agreement with the SEM-EDS measurement. LIBS has the advantage of elemental composition mapping without the need for high vacuum conditions and has many advantages when applied to industrial processes. In the future, the LIBS analysis speed is improved to 1 kHz and the LIBS system is utilized for elemental composition mapping in industrial processes.

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IL30

NANOPARTICLES IN PLASMA SPECTROSCOPY: DETECTION AND SIGNAL ENHANCEMENT IN GASEOUS, LIQUID AND SOLID SAMPLES

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Nanoscience has advanced greatly in the last two decades. Due to their special optical, mechanical, magnetic and energetic properties, nanoparticles (NPs) are nowadays exploited in many industrial, scientific and medical fields. The continuous development of nanomaterials as well as their increasing presence in the environment and biological systems also necessitates the development of such analytical methods that are capable of the sensitive detection and characterization of NPs in various sample matrices. Such methods often built on the application of laser induced breakdown spectroscopy (LIBS) or single particle inductively coupled plasma mass spectrometry (spICP-MS). At the same time, plasma spectroscopy techniques – LIBS included – also can benefit from using NPs to enhance their analytical signals. Therefore the development of NPs and plasma spectroscopy are strongly intertwined fields.

In this contribution, some recent results of the research group of the author obtained using LIBS and spICP-MS methods will be presented. It will be demonstrated, how various characteristics (composition, concentration, structure, size distribution, porosity, aspect ratio, etc.) of inorganic NPs and nanocomposites dispersed in aqueous liquid samples can be assessed using novel spICP-MS methodologies. The LIBS detection and characterization of NPs suspended in a gas medium and occurring in plant samples will also be described. Results on LIBS signal enhancement effectuated with the application of NPs for gas, liquid and solid samples via the exploitation of plasmonic and electron field- or thermoemission mechanisms will also be presented.

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IL31

ENHANCING THE SENSITIVITY OF LASER-INDUCED BREAKDOWN SPECTROSCOPY FOR THE DETECTION OF NANOPARTICLE-LABELED CANCEROUS TISSUES

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Fluorescent labels, based on conjugates of antibodies with various nanoparticles, are popular because of their broad detection posibilities (plate readers, microscopes). However, fluorescence is a limiting factor in e.g. multiplexing; only a limited number of dyes can be detected due to the overlaps of dye spectra or optical filters. Thus, novel readout methods are necessary to overcome such limitations. Laser spectroscopy – namely Laser-Induced Breakdown Spectroscopy (LIBS) – is a prospective option in nanoparticle detection [1]. LIBS provides superior performance in terms of throughput and repetition rate enabling large-scale elemental imaging in combination with high lateral resolution. In this talk, we will demonstrate the feasibility of LIBS as a readout method in immunochemical assays and imaging of cancer tissues (breast cancer) through the indirect detection of upconversion nanoparticles (UCNPs) [2]. The LIBS scanning enabled detecting the characteristic elemental signature of yttrium as a principal constituent of UCNP, thus indirectly providing a reliable way to differentiate between HER2-positive BT-474 cells and HER2-negative MDA-MB-231 cells. The comparison of results with upconversion optical microscopy and luminescence intensity scanning confirmed that LIBS is a promising alternative for the readout of immunohistochemical samples. Moreover, we have deployed the collinear double-pulse arrangement for enhanced sensitivity and detection capability, Fig. 1.

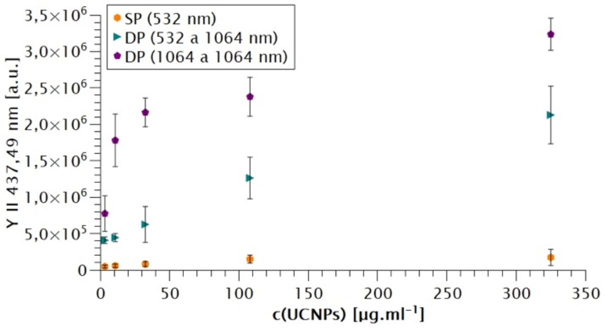

Fig. 1. Signal of Y II 437.49 nm spectral line enhanced by collinear DP arrangement

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OL64

OPTIMIZED ROLAND CIRCLE ALIGNMENT CONCEPT (ORCA)

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The lecture will discuss a spectrometer that is competitive in ICP spectrometers to ECHELLE type spectrometers. The ECHELLE optical system is very often used in ICP spectrometers, which has its advantages (in particular, it is small in size), but also a number of disadvantages, especially the very variable spectral resolution.

The company SPECTRO A.I. Kleve, Germany uses Paschen-Runge type spectrometers in their manufactured instruments. This lecture discusses these spectrometers.

Paschen-Runge spectrometers use the Rowland circle system. They are generally larger in size than ECHELLE spectrometers, but they have a number of advantages, among which the main ones include constant and uniform spectral resolution and smaller (weaker) scattered light than in ECHELLE spectrometers.

The Optimized Roland Circle Alignment Concept (ORCA), as SPECTRO AI calls its patented spectrometer system, is based on the Paschen-Runge spectrometer system.

In this system, the spectral resolution is determined only by the diameter of the Rowland circle and the dispersion of the grating used (number of scratches/1mm). The larger the diameter of the Rowland circle and the number of scratches of the dispersion grating, the better the spectral resolution. But this cannot be increased to infinity because the light intensity decreases with the square of the distance. At twice the distance, there is a fourfold decrease in light. Therefore, a reasonable compromise must be chosen.

OL65

AEROSOL ANALYSIS WITH LASER-INDUCED BREAKDOWN SPECTROSCOPY: SAMPLING APPROACHES AND RECENT APPLICATIONS

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This talk describes how laser-induced breakdown spectroscopy (LIBS) became a viable analytical tool for aerosol analysis through advances in sampling and data analysis strategies, as well as deployment applications. The analysis of aerosols is a challenging task due to the wide variation of aerosol particles characteristics (e.g., source, size, chemical composition) and measurements requirements (e.g., chemical determination, sizing, number density), however, LIBS has demonstrated to perform well analyzing both the aerosol particles and the gaseous phase, specially, in harsh conditions where other techniques are simply not applicable. By coupling the point-to-point sampling nature of laser-induced plasmas with the discrete nature of aerosols particles and selective spectra analysis (i.e., Conditional Analysis) a considerable increase in LIBS sensitivity can be achieved. Finally, an overview of aerosol LIBS applications in industrial and laboratory setting are presented to showcase the versatility and in situ applicability of LIBS with recent data, including the applications of heavy metals high temperature effluents, gas and particulate emissions from battery cells at high temperature, and vapors and aerosols from molten salts.

POSTER ABSTRACTS

MP1

NANOSCALE INFRARED SPECTROSCOPY OF PROTEINS

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Nanoscale Fourier-transformed infrared (nano-FTIR) spectroscopy is a powerful tool which combines scattering-type scanning near-field optical microscopy (s-SNOM) and FTIR spectroscopy. This technique provides the spatial resolution on the level of atomic force microscopy (AFM) and the chemical information of the sample is acquired together with the topography. Obtained absorption spectra are comparable to macroscopic FTIR spectra. By this technique is possible to detect e.g. individual macromolecules and also single monolayers[1,2].
Proteins belong to the most important cell components. They are the essence of all living organisms. One of the most fundamental issue of the life science is to understand their structures together with their functions. The most interesting and important are peptide bonds associated with the amide's stretching and bending vibrational modes, which reflect the structure of the proteins together with the surrounding environment[2].
The main scope was to obtain spectra of single protein. Pyruvate kinase, an enzyme involved in the last step of glycolysis, was chosen as a model sample. Aqueous solution of pyruvate kinase was dried on the silicon or gold-coated silicon wafers. The nano-FTIR spectra were recorded in the full fingerprint spectral region focusing on the region included amide I and II absorption bands. Different parts of the films brought various sizes (and shapes) of particles, which was also reflected in the spectra. Round particles with heights around 10 nm were preferred, because they could be single proteins. Spectra were collected at several parts of the dried film layers - inside the rim, in the rim and nearby to the outside of the rim under the various settings (e.g. tapping amplitude, spectral resolution, integration time). A comparison and evaluation of the spectra acquired from the silicon and gold-coated silicon wafers at different conditions was performed as well as spectra obtained at different harmonics of the tip oscillation frequency.

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MP2

THE EFFECT OF FARNESOL AND TYROSOL TREATMENT FOR THE INTRACELLULAR METAL CONTENT OF *CANDIDA AURIS*

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Nowadays, alternative treatments using quorum sensing molecules (QSM) are increasingly attractive, especially for difficult-to-treat multidrug-resistant pathogens such as *Candida auris*. Metals are essential for the survival of pathogenic microorganisms, as well as to maintain their virulence. Recent transcriptomic data have demonstrated that farnesol treatment affected the transcription of iron homeostasis-related genes, as well as the iron, manganese, zinc, and copper contents of *C. auris* [1]. Based on these data, the purpose of our experiments was to measure the changes in intracellular metal content induced by farnesol (FAR) and tyrosol (TYR) treatment with ICP-OES technology in *C. auris*.

The fungal pathogen was treated with FAR and TYR for 2 and 4 hours, after that the metal contents of the samples were measured with ICP-OES following atmospheric wet digestion. Spectrophotometric measurements demonstrated that adding FAR and TYR to preincubated cells resulted in a remarkable growth inhibition which was further confirmed by changes in measured dry cell mass. From the results of the elemental analysis we calculated the average metal content of the samples. 2 hours of FAR treatment caused a reduction in intracellular iron, manganese, and zinc content compared to untreated control cells, whereas the level of intracellular copper showed increase. TYR exposure of the same duration resulted in a decrease in the intracellular contents of the four elements. After 4 hours of FAR and TYR treatment we experienced similar results except for the intracellular manganese content.

Presents study indicates that FAR and TYR affect the growth and intracellular metal content of *C.auris*. Our results suggest, that these QSMs may be promising candidates in alternative treatment regimens against the multidrug-resistant microbe.

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MP3

THE PROCESS OF PHOTOPOLYMERIZATION OF ACRYLATED SOYBEAN OIL BASED EPOXIDES INVESTIGATED BY POSITRON ANNIHILATION LIFETIME SPECTROSCOPY

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The lifetime spectra of positrons annihilating in polymer matrices based on acrylated epoxidized soybean oil (AESO) were measured. The chemical structure of the polymer series AESO and AESO/VDM was investigated by NIR spectroscopy. The semi-empirical quantum mechanical model Tao-Eldrup was used to estimate the sizes of individual free volumes in these matrices. Investigation of free-volume properties of polymer matrices based on natural oils, which are intended for the construction of amperometric biosensors, allows a better understanding of the relationship between the crosslinking densities of the matrices, i. e. microscopic characteristics, and the main operating parameters of the biosensors. The free volumes of the investigated matrices before, during and after the photopolymerization process were determined. The effect of vanillin-dimetacrylate (VDM) and photoinitiator (PI) concentrations on the final microstructural properties of the investigated matrices was determined.

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MP4

QUANTITATIVE DETERMINATION OF SUPRAMOLECULAR COMPLEX STABILITIES USING COLLISION-INDUCED DISSOCIATION AND FOURIER TRANSFORM ION CYCLOTRON RESONANCE MASS SPECTROMETRY

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The gas-phase stabilities of non-covalent complexes between native cyclodextrins (α, β, γ) and tetracycline derivates were investigated using electrospray ionization (ESI) with Fourier transform ion cyclotron resonance mass spectrometry (FT-ICR-MS) combined with collision-induced dissociation (CID) studies. The CID-MS methods developed were further applied to complexes of glycopeptide antibiotics and the bacterial cell-wall precursor peptide H-L-Lys-D-Ala-D-Ala-OH, and an artificial carbohydrate receptor and β-D-glucopyranosides. The collision energy CE_{50} for 50 % dissociation of the corresponding supramolecular complex was obtained from dissociation profiles (as described by Gabelica et al. [1]) and used as a semi-quantitative valuation standard for complex stability. The CID results show that the recorded CE_{50} values depend on the ion mode, the charge state and adduct type of the respective complex ion, as well as the hexapole flight time set on the mass spectrometer. The investigations extend the informative value of already existing liquid-phase and theoretical data and thus help to clarify the understanding of the interaction of the different complex partners with each other. Furthermore, determination of relative gas-phase binding affinities is useful for rapid screening of pharmaceutical relevant non-covalent complexes.

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MP5

DROP COATING DEPOSITION RAMAN SPECTROSCOPY OF LIPOSOMES ON NANOSTRUCTURED FLUOROCARBON FILM

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Raman spectroscopy represents a widely used analytical technique providing unique information about the vibrational motion of molecules. The great advantage in the study of biological molecules and their interaction is the absence of any markers or probes with undesirable effects. Unfortunately, the conventional Raman spectroscopy approach is limited to highly concentrated solutions or suspensions. To overcome this problem, a drop coating deposition Raman (DCDR) method can be used. DCDR is based on the evaporation of a solvent from a small droplet of a studied solution or suspension. The evaporation of a droplet deposited on a hydrophobic substrate with a pinned contact line leads due to a capillary flow to the solute accumulation in the ring-shaped pattern. The Raman spectra are then acquired from this pre-concentrated ring by a confocal Raman microspectrometer. Owing to this, the DCDR technique enables to measure Raman spectra from small sample volumes at very low initial concentrations in comparison with the conventional Raman measurements from solutions. Final dried patterns (and a spectral sensitivity as well) are influenced not only by the properties of the solution, but it also depends on the substrate characteristics such as wettability and roughness that governs the droplet drying dynamics.

We focused our attention on the spherical membrane structures – liposomes – often used as real membrane models. Liposome suspensions dried on nanostructured hydrophobic substrates with different roughness were studied by DCDR method. The preparation of the substrates is based on the nanostructuring of magnetron sputtered hydrophobic C:F films by a base layer of metallic nanoparticles (Cu or Ag) that were fabricated employing a gas aggregation source of the original construction. The nanoroughness, as well as the wettability of produced coatings, are controlled by a number of nanoparticles in the base layer, including an option of a gradient surface coverage. It was shown that in the case of liposome suspension, the nanoroughness leads to stronger pre-concentration as well as to the reduction of the ring diameter, i.e. two parameters crucial for desirable and effective DCDR measurements [1].

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MP6

DETERMINATION OF THE IMPACT OF LA-ICP-MS PARAMETERS DURING SOFT MATERIAL ANALYSIS

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The trace metal determination in tissue samples by laser ablation inductively coupled plasma mass spectrometry (LA-ICP-MS) has become important in life science research. Therefore, a lot of development was made to improve the setup and the capabilities of the instrument. Additionally, many reactions and physical effects during the measurement process were observed, but there is still a lack of publications that address how the various parameters influence these effects. Some effects such as surface re-sampling and the wash out time have been studied by Woodhead et al. [1] for geologic samples. All effects usually influence the decision on the selected measurement conditions. The intensity should usually be high in order to be able to measure as sensitively as possible. The washout time should be as small as possible to avoid carryover from areas of high concentration. Furthermore, the area of the surface re-sampling effect determines how close individual line scans can be for imaging measurements so that they do not influence each other.

However, the behavior of the sample material during ablation can be very different, depending on the sample matrix. Therefore, this work deals with the estimation of these effects for the examination of tissue samples. For this purpose, systematic investigations on a polymeric reference material with contents of various elements in the trace concentration range were carried out.

The influence of the gas flows (carrier gas flow and markup gas flow), spot size, fluence, scan speed and repetition rate of laser pulses were considered to find out under which conditions the signal intensities are highest and to estimate the wash out time and in which area surface re-sampling takes place.

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MP7

COMPARISON OF RADIATION SOURCES FOR ATOMIC FLUORESCENCE SPECTROMETRY

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Atomic fluorescence spectrometry (AFS) coupled with hydride generation is an extremely sensitive method suitable for ultra-trace element analysis. The emitted fluorescence intensity is proportional to the excitation radiation intensity and the commercial AFS instruments are usually equipped with boosted-discharge hollow cathode lamps (Superlamps) [1], whereas the electrodeless discharge lamps (EDLs) are mainly used in experimental laboratory setups of AFS [2]. EDLs are said to provide higher radiation intensities, however, the direct comparison of both sources in AFS has never been reported. In this work, our laboratory-made non-dispersive atomic fluorescence spectrometer [3] was successfully adjusted so that both sources could be compared using bismuth as a model analyte. Resonance fluorescence lines at 222.8 nm and 223.1 nm were selected for detection by means of an interference filter situated in front of the solar-blind channel photomultiplier [2,3]. The miniature diffusion flame was used for the atomization of bismuthane generated by the acid/$NaBH_4$ reaction. The radiation source is used in a modulated mode, which helps to reduce the background signal caused by the flame of the atomizer [2]. The optimized parameters included the modulation frequency, the duty cycle and the power supply. The emission spectra of both lamps were recorded and their radiation intensities were measured using an optical power meter. The sensitivity obtained with the EDL was almost 5 times higher, which is given by its higher radiation intensity at the excitation wavelengths, and is reflected in LODs of 1.8 ng/L while LOD of 11 ng/l was obtained with the Superlamp. To the best of our knowledge, this is the first direct comparison of two radiation sources used in AFS.

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MP8

METHOD DEVELOPMENT FOR THE ANALYSIS OF HIGHLY SALINE SAMPLES USING TXRF

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Total reflection X-ray fluorescence (TXRF) is becoming a more and more popular method for the analysis of heavy metals in environmental and industrial sample systems.[1-3] However, there is still a need for optimisation for the fast and precise analysis of highly saline liquid samples. In this study, a variety of different elements were analysed in the matrices lithium carbonate (Li_2CO_3), lithium hydroxide (LiOH) and artificial seawater (mainly NaCl). Different sample preparation methods were compared with each other in order to achieve the highest possible reproducibility and signal-to-noise ratios. Parameters such as the drying process, temperature or measuring time were varied. The use of additives such as Triton® X-100 and solid phase extraction as sample preparation were also examined in more detail. The relative standard deviation (RSD) was used as a measure of reproducibility, whereby 3 sample carriers were analysed in each case. Furthermore, one carrier was rotated several times by 90° each in order to examine the homogeneity of the sample on the carrier. A multi-element standard solution was used, whereby the concentration of each of the 23 analytes ranged between 200 and 1000 µg/L. The concentration of the matrix was 1000 mg/L (Li_2CO_3, LiOH) and 24000 mg/L (NaCl in artificial seawater), resulting in matrix-analyte ratios up to 120000:1. Samples without a highly saline matrix achieved high reproducibility, i.e. very low RSD values. By using Triton, RSD values below 5% could also be achieved for the samples with high matrix concentrations, whereby the optimal additive concentration and sample preparation method is partly element-specific.

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MP9

MOBILIZATION OF POTENTIALLY TOXIC ELEMENTS FROM MINE DRAINAGE OCHRES BY ASPERGILLUS SPECIES

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In this study we described the ability of precipitated ferrous ions (ochres) from acid mine drainage outflow to removal potentially toxic elements from water-bodies in mining sites [1,2]. The roentgenogram of XRD revealed their amorphous character, however based on the Mössbauer spectra, we assume that the minerals are goethite and ferrihydrite. The suspensions of ochres were inoculated with fungal spores of *Aspergillus niger*, *A. clavatus*, *A. versicolor*, which was followed by static 14-day incubation. The non-dissolved residue, ochres and biomass samples were digested in PTFE pressure vessels using concentrated HNO_3 and H_2O_2. Subsequently, the culture media filtrates, digested biomass and insoluble residue were analyzed for total antimony, arsenic, zinc and iron content by flame atomic absorption spectrometry with deuterium background correction [3]. Our results highlighted that due to extensive leaching of iron from ferric ochres, filamentous fungi were capable of bioextracting arsenic and antimony from this naturally occurring precipitate. Thus, our outcomes underline the relevance of *Aspergillus* strains' activity and the composition of fungal community *in situ* for the mobilization of contaminants associated with ferric ochres at abandoned mining sites.

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MP10

REALISATION OF A LIBS METHOD TO DETERMINE THE DEGREE OF IMIDIZATION OF POLYIMIDES

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Due to their excellent chemical and physical properties, polyimides are widely used in industrial applications including automotive, aerospace and electronics. Because they are non-soluble and due to their high thermal stability, the shaping is done via a chemical reaction or thermal treatment of a soluble precursor, the poly(amic acid). During this treatment the conversion of the amic acid group into imide is achieved, which is reflected in the degree of imidization. The degree of imidization of a polyimide is also closely related to the final properties of the polymer. IR is a well-established technique to determine this characteristic feature but lacks the possibility of analyzing depth profiles. As a consequence, polymerization studies are limited to the sample surface.

In this work, we present a LIBS method for the investigation of the imidization degree of a self-synthesized poly(4,4'-oxydiphenylene-pyromellitimide) (PMDA-ODA). To confirm the LIBS method, IR measurements served as a reference and a good agreement between those two techniques was found. Furthermore, the investigation of variably imidized samples is shown as an example of use.

MP11

THE EVALUATION OF SOLID STATE OF RICE FLOUR BY IR AND NIR SPECTROSCOPY

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Rice flour is a starch-based biopolymer that forms a compound grain structure, and it has an ordered / disordered structure with hierarchical scale. The physical treatment such as milling are aimed to control solid properties of rice flour by production of the disordered structure. When the rice flour is exposed to a high humidity condition for long period, the caking occurs. Thus, the water sorption is also an important to control the food quality. In our previous research, it is found that the surface structure of starch grain changed during water sorption process. Six rice flours with crystalline was produced by dry and wet milling procedure. The α-formed sample was also prepared by shear and heat milling method. Each rice flour was kept in desiccators with saturated salt solution at 25°C until water sorption equilibrium. The sample was dried at 105°C for 72 h. The water activity of the rice flours was controlled in the 0.11–0.98 a_w range and water contents were measured at each water activity. Attenuated total reflectance (ATR)-IR spectra of each sample in the 4000–100 cm^{-1} region and NIR spectra in the 10000-4255 cm^{-1} were measured during water sorption process. A band at around 1740 cm^{-1} due to lipids or oils occurred in the spectra of the rice flour with a crystalline structure. This band disappeared at high a_w values for these rice flours, whereas it was not observed for the α-formed sample in the whole a_w range. Therefore, it is very likely that starch disorder occurred not only due to milling, but also due to the sorption process. The lipid band at around 1740 cm^{-1} can be used for the evaluation of the solid state of rice. The band at 990 cm^{-1} shifted to a higher wavenumber above $a_w = 0.7$. It was thought that the band shift at 990 cm^{-1} corresponded to the change caused by the water molecule during the intramolecular interaction of COH and O in glucose. The behavior of the bands at 990 cm^{-1} indicated the glass–rubber transition of starch due to water sorption.

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MP12

NOVEL CELL FOR TRANSCORNEAL PERMEATION STUDIES USING VIBRATIONAL SPECTROSCOPY TECHNIQUES

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The cornea is an important barrier to the penetration of ophthalmic drugs into the anterior segment of the eye. The drug must pass through all corneal structures, especially the epithelium, stroma and endothelium.[1] The corneal epithelium is relatively impermeable compared to other epithelial tissues.[2] The epithelium and stroma have the greatest influence on the rate of passage of substances during the transcorneal penetration.[3] In vitro experiments are used to determine the apparent permeability coefficient. In this experiment, the isolated cornea is placed in a diffusion cell that allows the studied formulations to penetrate the cornea.[2] Studies simulating transcorneal permeation use mathematical models[3], diffusion cells made for other purposes[4], or specially made cells for a specific experiment[5].

The aim of the work was to design a transcorneal diffusion cell which would be suitable for the first experiment in the development of ophthalmic drugs. The corneas used in the experiments were characterized by vibrational spectroscopy methods. A FTIR spectrometer with an ATR attachment was used to monitor changes in corneal structure induced by eye drop permeation. A confocal Raman spectrometer with a microscopic adapter was used to characterize drug penetration through the cornea.

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MP13

APPLICATION OF EMISSION SPECTROSCOPIC SOLID SAMPLING METHODS ON BIOMASS SAMPLES FOR CO-COMBUSTION

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Due to the processing of many biomass samples, composting is not an option, since those samples often include environmentally harmful elements. For example, wood from construction sites is usually coated or painted or might be infested with vermin. Materials such as sewage sludge contain, next to hazardous components, elements, which must be recovered like phosphorous. Since those waste products serve as energy sources, they are lead to combustion and/or material usage. Whether they are added to coal-fired power plants or thermally utilized in other incinerators, the chemical composition needs to be known to achieve a high combustion temperature without slagging and fouling. Furthermore, some elements are problematically to meet emission limits.

To analyze the elemental contents of biomass samples in the combustion process, a fast and direct method for the analysis of solids is required. As robust solid sample methods, the laser-induced breakdown spectroscopy (LIBS) as well as the electrothermal vaporization (ETV) as a sample introduction system for inductively coupled plasma optical emission spectrometry (ICP-OES) were found to be qualified.

Applying LIBS, the influences of various parameters, such as grain size, water content or the use of an inert gas on the analytical figures of merit were analyzed. A suitable strategy for evaluating the data using various emission lines and normalization procedures is also needed to be optimized for each element. In case of ETV-ICP-OES, the optimization includes the selection of a suitable reaction gas, plasma parameters, temperature programs and emission lines. Due to the high variation of the matrix, a method for calibrating the systems had to be found, to be able to analyse as many different sample types as possible applying the same calibration. By optimizing the various parameters, a simultaneous determination of all relevant elements from main constituents to trace elements can be achieved with one measurement. The method development and the optimization approach for different matrices described above is presented in this work and open problems are addressed.

MP14

EFFICIENCY OF CHEMICAL VAPOR GENERATION OF ZINC

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Chemical vapor generation (CVG) has been repeatedly proposed as a method for increasing the sensitivity of zinc determination compared to liquid nebulization.[1–3] However, increasing efficiency of nebulization systems in modern instrumentation raises the question, if the CVG of zinc species is still a more efficient introduction technique. We thus set out to answer the question by using the overall generation efficiency, i.e. the amount of zinc transported into the detector. We used two approaches: i) comparison of sensitivity of CVG with nebulization and ii) radioactive isotope of zinc and radiometry. The overall generation efficiency was determined as 2.7 % (comparison with nebulization) and 3.1 % (radiometry) at the optimum conditions, which included neutral to basic pH of the reaction mixture, i.e., 0.1M HCl and 0.5% (m/V) $NaBH_4$ prepared in 0.1M NaOH. Radiometry uncovered low generation efficiency as the main source, because over 90 % of Zn remained unreacted in the liquid waste; the losses of generated volatile species were relatively low. The CVG was carried out in a custom made reactor with high resolution continuum source atomic absorption (HR-CS-AAS) detection. The influence of various reaction modifiers was studied prior to determination of generation efficiency and substantial improvement (approx.18-times) was achieved with 8-hydroxyquinoline and a blank limited LOD of 4 ng mL^{-1} was obtained.

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MP15

MULTIELEMENTAL SPECIATION ANALYSIS OF CD^{2+}, PB^{2+} AND $(CH_3)_3PB^+$ IN HERB ROOTS BY ADVANCED HYPHENATED TECHNIQUE HPLC/ICP-DRC-MS

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The high risk of including elements that induce toxic effects in the food chain is caused by the poor physiological barrier of plants and the absorption of toxic elements, as well as the development of high tolerance to their high level and a poor reaction to stress initiated by the presence of metals. An important problem in the speciation analysis of lead and cadmium together with their organic and inorganic compounds is the stability of these compounds throughout the analytical process and the availability of appropriate certified reference materials (CRMs), which are necessary for the validation of the analytical procedure. The main concept of the research was to develop and validate the sensitive analytical procedure for the determination of Pb^{2+}, $(CH_3)_3Pb^+$ and Cd^{2+} in samples of Chinese herbs. The object of the study were roots in which lead and cadmium accumulate in significant amounts, according to previous studies. The advanced high performance liquid chromatography combined with inductively coupled plasma mass spectrometry equipped with a dynamic reaction chamber – HPLC/ICP-DRC-MS, was applied to the analysis of environmental samples. Separation of species was achieved using a column IonPac CS5A 2x250-mm, and the composition of the mobile phase: 40 mM EDTA, 20 mM TMAH, 20 mM oxalic acid, which allowed for a short analysis time, less than 2 minutes. The method allowed very low levels of LOQ: 0.10, 0.29, 0.30 µg L^{-1} for Cd^{2+}, Pb^{2+} and $(CH_3)_3Pb^+$, respectively. Then, the method was applied to the herbs samples in which the share of contents of the determined species is on average 59% for Cd, and 58% for Pb. The content of Cd^{2+} in the extracts was in the range 3.3 – 107 µg kg^{-1}, and for Pb^{2+} 5.1 – 23 µg kg^{-1}, however no $(CH_3)_3Pb^+$ was detected in the samples.

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MP16

SOIL IODINE FRACTIONATION BY SEQUENTIAL EXTRACTION FOLLOWED BY ICP-MS DETERMINATION

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Iodine is an essential micronutrient that enters the food chain from soil primarily via plant root absorption. [1]. In this work we have evaluated the total and soil fraction iodine content extracted from soils by single and sequential extraction methods [2-5] followed by ICP-MS determination. Most of the iodine was extracted from organically rich soils with more than 2.5 $mg.kg^{-1}$ of iodine. The correlation analysis highlighted that organic matter content, amorphous and weakly crystalline forms of aluminum, clay fraction content, aluminum and iron minerals plays the most important role in soil iodine retention [6,7]. The water-soluble fraction contained only 4.4% of the total iodine on average. Our results highlight the significance of soil chemistry for iodine distribution and agricultural research.

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MP17

SPECTROSCOPIC METHODS IN THE ANALYSIS OF WEAR PARTICLES

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Detailed characteristics wear particles formed in various brake pads were done. We tried to identify structure and chemical composition of powder particles released by brake abrasion. The experimental studies were carried out using Mössbauer spectroscopy, X-ray powder diffraction, scanning electron microscopy and magnetic measurements. Structure and chemical composition of the original brake pads and disc samples were compared with the results obtained for wear particles. The chemical and phase composition of wear particles is in large part similar to composition of the original brake pads. Wear particles contained mainly various types of iron oxides, iron an iron carbon metallic particles. Their magnetic state at room temperature are prevailing is paramagnetic. The low temperature Mössbauer and magnetic measurements indicate their transition to magnetically ordered states – ferro / antiferromagnetic.

MP18

3D RAMAN MAPPING AS AN INVESTIGATION TOOL FOR PARTICLE COATING THICKNESS

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The coating of pharmaceutical solid dose forms (SDFs) is often used for modified release of API. In other cases, coating might be functional for light protection of photosensitive molecules present in tablets, taste masking or improving the mechanical properties of SDFs [1].

Confocal Raman microscopy provides the possibility of examination of the inner layers of SDFs, without the need for sample destruction before measurement [2]. The resolution of images produced by Raman mapping can be high, even in the micrometer range [3].

For the present work, paracetamol particles (100 -800 µm) were dry-coated with carnauba wax. The size and outer surface morphology were examined by SEM. A novel quantitative method was developed to measure the coating thickness of particles via Raman mapping. Three different fractions were examined; 100 µm -200 µm, 200 µm -400 µm and 400 µm -800 µm. The average thickness was 5.3 ± 3.7 µm, 6.2 ± 4.9 µm and 6.5 ± 3.5 µm for each size fraction, respectively. The morphology and thickness of coating were associated with the dissolution profiles of coated particles and tablets containing those. For particle dissolution it was found that as the particle size increases the API release is slower, while tableting not only decreases the dissolution rate but also destroys the morphology of the coated particles, providing unpredictable dissolution profiles.

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MP19

OVERVIEW OF XRF VERSUS ICP APPLICATIONS IN ELEMENTAL ANALYSIS OF GLASS MATERIALS

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Determination of the chemical composition of the glasses doped with therapeutic ions is a crucial part of the development of materials with bioactive properties. This work deals with a comparison of two conventional analytical techniques as X-ray fluorescence (XRF) and inductively coupled plasma spectrometry (optical ICP-OES and mass spectrometry ICP MS) where advantages and disadvantages of each of these elemental techniques are discussed to verify the composition of glasses reflecting the chemical composition commercially available 45S5 Bioglass®. The ICP OES can be applied for the analysis of major and minor elements, while ICP MS facilitates the determination of elements < 500 ppm to complete compositional information about the sample 0. The microwave digestion of glass samples using aqua regia with the addition of hydrofluoric acid (HF) at the temperature of 230°C was done before the elemental analysis 0. The addition of HF in the decomposition process makes the quantitative determination of Si in Si-based materials inaccurate due to the formation of volatile SiF_4 **Error! Reference source not found.**.

The X-ray fluorescence (XRF) is a non-destructive method covering the determination of a wide range of elements in silicate-based glass materials. The phosphorus-based bioactive glasses tend to crystallize during the fusion of beads, or inhomogeneity within the glass sample occurs using various dopants (Ag, B, Ce, Co, Cu, Sr, Y, Zn) with therapeutic effects in concentrations reaching the trace amount. Using a larger amount of powder sample and preparation of pressed pellets can be a solution, as well as the main restriction of XRF analysis.

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MP20

TWO EXTRACTION PROCEDURES COUPLED TO ETAAS QUANTIFICATION EMPLOYED FOR SPECIATION OF INORGANIC ANTIMONY

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In this work, two extraction procedures were optimized for speciation of inorganic antimony in natural waters [1,2]. Quantification of the analyte was done by electrothermal atomic absorption spectrometry (ETAAS). In dispersive solid phase extraction (dSPE), nano-TiO_2 as a solid sorbent was used for separation of total inorganic antimony (iSb). After adsorption of iSb onto TiO_2, TiO_2-slurry was directly injected into the graphite furnace. In cloud point extraction (CPE), ammonium pyrrolidine dithiocarbamate (APDC) was used as a chelating agent and octyl phenoxy polyethoxy ethanol (Triton X-114) was used as an extracting agent. The CPE procedure was utilized for selective separation of Sb(III). In both extraction procedures, systematic study of all experimental conditions was made.

In the dSPE procedure, the pH of a sample solution (100 ml) was adjusted to 3.0 ± 0.1 and placed into a HDPE bottle containing 100 mg of nano-TiO_2. After that, the mixture was shaken for 10 min at lab temperature. Subsequently, the mixture was centrifuged at 4000 rpm for 10 min. The bulk aqueous phase was decanted and 5 ml of DW was added to the remaining solid phase to prepare a slurry sample. Finally, the slurry was injected into the graphite furnace.

In the CPE procedure, aliquots of 10 ml of a sample solution (pH 5.5 ± 0.1) containing 0.02 % APDC and 0.08 % Triton X-114 were incubated in a water-bath at 45 °C for 5 min. After that, the mixture was centrifuged at 4000 rpm for 5 min. Subsequently, an ice-bath was used for 10 min. The bulk aqueous phase was decanted and the SRP obtained was diluted by 0.2 M HNO_3 in methanol. Finally, the methanol solution was injected into the graphite furnace.

In the both cases, improvement of quantification limits for ETAAS was achieved.

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MP21

ANOTHER PERSPECTIVE AT THE ORIGIN OF ALIEN BANDS IN THE SURFACE-ENHANCED RAMAN SPECTRA OF 4-AMINOBENZENETHIOL

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4-Aminobenzenethiol (4-ABT) is a substance which is often used as a model probe for newly prepared SERS substrates and which SERS spectra have been discussed many times. The discussion is especially focused on the sources of bands not resembling the signals of 4-ABT in non-enhanced Raman spectra and various 4-ABT SERS spectra have been observed. The features found in the SERS spectra can be assigned (i) to the enhanced signal of 4-ABT (visible also in the non-enhanced spectra), moreover (ii) to the modes which are forbidden from point of view of the basic selection rules in SERS spectroscopy. However, some other works explain the presence of “alien” signals by the photochemical reaction taking place on the surface after illumination; there is still no complete consensus describing the nature of these bands. Although the sources of additional bands in the 4-ABT spectra are not unambiguously known, spectrum itself has been established as a SERS spectrum of 4-aminobenzenthiol.

Here we present new observations, which could contribute to clarify the abundance and the origin of the above-mentioned phenomenon. The relevant measurements were performed using a Raman microscope enabling the use of excitation radiation from the visible region, supplemented by spectra from an FT-Raman spectrometer. Parameters related to the properties of the studied plasmonic surfaces were assessed by electron microscopy and visible spectroscopy in the reflection mode.

MP22

LASER ABLATION SYNTHESIS OF TELLURIUM CLUSTERS

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Laser ablation synthesis of nano-tellurium and tellurium clusters Te_m (m = 1, 6) from bulk tellurium was developed. For a generation of tellurium nanoparticles in liquids (e.g. ethanol) Nd: YAG laser at 1064 nm was used while for the clusters synthesis the Nd: YAG laser at 355 nm on a commercial mass spectrometer was applied. Mass spectrometric characterization of synthesized product using Matrix Assisted Laser Desorption Ionization Time of Flight (MALDI-TOF) was done. It was found that nano-tellurium produced in ethanol rapidly aggregates and precipitate. The aggregation can be stopped (or diminished) via cooling to low temperature (approx. 5 °C) or complexing Te nanoparticles in a β-cyclodextrin forming supramolecular complex.

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MP23

A NOVEL STANDARD ADDITION APPROACH FOR MATRIX-MATCHED CALIBRATION WITH LA-ICP-MS VIA SPRAY DEPOSITION

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For more than 30 years, Laser Ablation – Inductively Coupled Plasma – Mass Spectrometry has become a powerful technique for the determination of natural and synthetic specimens' elemental or isotopic composition. It offers vast applicability for direct solid sampling analysis with minimal sample preparation, analyzing major, minor, and trace constituents over a wide elemental range, and performing laterally- and depth-resolved microanalysis without requiring vacuum or conducting samples. Therefore, LA-ICP-MS finds application in various research fields, i.e., on biological, medical, geological, and technological samples. However, reliable quantification requires matrix-matched calibration standards due to matrix- and elemental fractionation effects.

Because certified reference materials are only available for a small selection of materials and sample types, their usability as matrix-matched calibration standard is rather limited. The preparation and characterization of matrix-matched standards is a very laborious and time consuming procedure. This makes it indispensable to develop methods that work with in-house prepared pseudo-matrix matched standards using aqueous standard solutions. Already proven methods in the LA-ICP-MS community are "Dried Droplet Quantification", "Micro Groove Quantification" or "Micro Well Quantification", each having individual benefits and drawbacks regarding their applicability to specific sample types.

In this work, a new approach for matrix-matched calibration was developed. A layer with a sufficiently homogeneous distribution of the elements of interest was obtained by deposition of liquid standards onto the sample surface with a commercial spraying system, which provides almost instant solvent evaporation. Following, LA-ICP-MS measurement of the sample including deposited surface layer enables quantitative analysis. The method was applied using various elements on different substrate materials to demonstrate its universal applicability. The results were verified by the determination of sulfur in a commercial Kapton® polyimide film. A comparison of the results showed good agreement with a reference method's determination, carried out using microwave-assisted acid digestion of the samples followed by liquid ICP-MS determination with external calibration. The developed method represents a promising new approach for quantitative trace determination with LA-ICP-MS.

MP24

CHEMILUMINESCENT DETERMINATION OF VITAMIN B12 USING AUTOMATIC SEQUENTIAL INJECTION ANALYSIS

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Automatic sequential injection analysis (SIA) with chemiluminescent (CL) detection is presented for the determination of vitamin B12 in pharmaceutical formulations. The determination is based on the chemiluminescent reaction when luminol is oxidized by hydrogen peroxide in a basic medium. This reaction is catalyzed by Co(II) ions after their quantitative release from the molecules of cobalamin [1]. The CL intensity, corresponding to the Co(II) ions concentration, was measured as an analytical signal using a spectrofluorometric detector.
Several experimental parameters were optimized to get the highest sensitivity of the determination. The sample flow rate (5.0 ml min^{-1}), volumes of sample and reagent solution (**550 µl : 50 µl)**, hydrogen peroxide concentration (**0.5% w/w)**, luminol concentration (17.5 mmol dm^{-3}), and the pH of reaction media (9.0) were found as optimal.
The developed method for determining Co(II) ions was successfully applied to the determination of vitamin B12 in several pharmaceutical formulations. The analytical procedure includes the sample decomposition based on the UV irradiation in the presence of potassium persulfate (1.5 mmol dm^{-3}). The recovery was up to 95±3 %. The calibration equation was established in a dynamic range of 0.01–25 mg dm^{-3} for the visible detection at 425 nm. The limit of quantitation was 0.04 mg dm^{-3}. The sample throughput was estimated at 35 h^{-1}.
The interference study demonstrates that from a wide range of interfering ions only Ni(II) and Zn(II) ions significantly affect the CL signals from the concentration above 50 mg dm^{-3}. The advantages of the presented SIA method are its complete automation, speed, very low reagent consumption, and a wide dynamic range of analyte concentrations.

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MP25

DETERMINATION OF RARE EARTH ELEMENTS IN GEOLOGICAL SAMPLES BY ICP-MS

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The Rare earth elements (REE) are a group of 17 elements with similar chemical and physical properties. Due to their unique properties they have become essential in many technologies. During the last three decades, there has been an explosion in the applications of REE in several technology devices such as computer memory, DVDs, rechargeable batteries, autocatalytic converters, super magnets, mobile phones, LED lighting, superconductors, glass additives, fluorescent materials, phosphate binding agents, solar panels and magnetic resonance imaging agents [1]. With such a wide and increasing range of applications their determination in environment has also become important.

In environmental monitoring, REE have been used as geochemical fingerprints, giving information on rock formation and geochemical processes occurring in the Earth's crust and in meteorites, as well as indicator of anthropogenic sources, giving information about origin and production techniques of archeological samples [2].

In this study we report determination of selected rare earth elements (dysprosium (Dy), erbium (Er), europium (Eu), gadolinium (Gd), holmium (Ho), lutetium (Lu), neodymium (Nd), praseodymium (Pr), samarium (Sm), terbium (Tb), thulium (Tm), ytterbium (Yb)) in geological samples by ICP-MS. Previously used technic – ICP-OES was not sufficient enough mainly because of spectral interferences caused by iron, manganese and other REE present in geological samples. Interferences in ICP-MS are reduced thanks to its high resolution, collision reaction interface with helium, ion mirror and low noise double off-axis quadrupole. The method was tested by analyses of the geochemical reference materials such as AGV-1 and AGV-2. Limits of quantification were in the range of 0.02 – 0.05 mg.kg^{-1}. Every year we also participate in the GeoPT proficiency testing programme.

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MP26

SUITABLE METHODS OF HEAVY METALS DETERMINATION IN WINES BY ETA-AAS

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Grape must and wine always contain relatively large amounts of heavy metals come from vines and grapes, but most of it originates from sprays used to treat vines, from soil, from agricultural insecticide or atmospheric pollution. Most of heavy metals (Fe, Pb, Cu, Cd) in the grapes precipitate during fermentation into the sediments. Therefore it is lower content of them in the wine than in the must. Some heavy metals are indispensable for us in very small quantities essential minerals like Cu, Al, F, Co, Pb, Zn. The article presents the heavy metal content in red and white wines with protected designation of origin (PDO) “Južnoslovenská” from south Slovakia. The white wine variety “Rizling vlašský”vintage 2007 (Riesling blanc) was determined by „Stripping chronopotentiometry“ as well as the red variety “Frankovka modrá” vintage 2007 (Blaufrankisch). The amounts of Pb were 59 µg/l and 73 µg/l respectively. The Cd content was 1,60 µg/l and 1,79 µg/l respectively and content of Cu was 183µg/l and 262µg/l respectively. In the white wine variety “Rizling rýnsky” vintage 2020 (Rheinriesling) were determined by ETA-AAS metals Pb, Cu, Fe and the amounts were 10 µg/l, 220 µg/l and 390 µg/l respectively. In the red wine variety “Frankovka modrá” vintage 2020 was determined 66 µg/l Pb, 420 µg/l Fe and 195 µg/l Cu by AAS. Both methods enables the determination of heavy metals in wine at very low concentration levels (LOD≤1µg/l). The main advantages of this analytical methods are automatic analysis including the calibration. Compendium of International methods of wine and musts analysis by OIV was used for determination.

MP27

OVERVIEW AND EXAMPLES OF THE USE OF SELECTED SPECTROMETRIC TECHNIQUES IN THE CUSTOMS TECHNICAL LABORATORY

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The poster presents the Customs Technical Laboratory (CTL) of the Czech Customs Administration and gives a brief overview of the spectrometric methods including some examples of their applications. At present, the CTL consists of a central laboratory in Prague and detached units in Hradec Králové, Olomouc, Ostrava and Ústí n/L., currently employs around 60 people. Its activities are carried out in accordance with standards EN ISO/IEC 17025 and EN ISO 9001 as for laboratory testing and analysis of samples of goods for customs, tax and other inspection purposes (as regards safety, health and environmental protection). CTL is also involved in the methodology of sampling and mobile diagnostics, including the operation of the vehicle mobile laboratory. Approximately 6-8 thousand samples are received annually, on which a total of 20-30 thousand tests are usually carried out. Spectral analyses account nearly a third of all these analyses. The specific applications of spectrometric methods in the CTL are as follows. Nuclear Magnetic Resonance (NMR), Isotope-Ratio Mass Spectrometry (IRMS), Gas Chromatography-Mass Spectrometry (GC-MS), Liquid Chromatography-Mass Spectrometry (LC-MS), Liquid Scintillation Counting (LSC), X-Ray Fluorescence (XRF), Inductively Coupled Plasma-Optical Emission Spectrometry (ICP-OES), Infrared (IR), and Raman Spectrometry (RS). The NMR technique is mainly used in CTL to determine the structure of unknown organics and to quantify them. In addition, NMR spectrometry, together with IRMS, are used e.g. for the determination of the botanical origin of ethanol in alcoholic and sugars in non-alcoholic beverages, for the determination of added sugars in honey. Also geographical origin of wines, can be determined. The MS is also an indispensable method and is used coupled with liquid (LC-MS) or gas (GC-MS) chromatography, in various configurations. This are used to analyze food and food supplements, tobacco and tobacco products, spirits and beverages, industrial samples such as washing powder and gel, wood and plant materials (CITES control), narcotics and psychotropic substances, pharmaceuticals, peptides and peptide hormones, petroleum products. The XRF spectrometry is mainly used for the identification of elements in inorganic materials and chemicals, in petroleum products, waste, metals and alloys above all. In addition, XRF can provide a comparison of the elemental profiles of tobacco samples, and XRF-microscopy is used for elemental 2D-maping to detect counterfeit jewelry, pearls, bijouterie and examination of rough diamonds. By application of FTIR and RS mainly organic substances, like pure chemicals, plastics, food preparations and unknown samples are determined. In the fuel analysis the unwanted admixtures can be detected as well as the other, such as bio-compounds, octane number, aromatic content etc. Finally, ICP-OES is used for example, to determination of some heavy metals in wines and food.

MP28

EVALUATION OF TOXICITY AND BIOACCUMULATION OF METALS FROM TRANSPORT AND THEIR EFFECT ON THE MINERAL COMPOSITION OF GREEN ALGA DESMODESMUS SUBSPICATUS USING ICPMS/MS

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Ecotoxicological tests on green algae *Desmodesmus subspicatus* are used to determine the toxicity of environmental samples. Since green algae are among the primary producers in most of aquatic food chains, harmful pollutants accumulated in the algae can be transmitted to higher trophic levels. A method for analysing the bioaccumulation of Cr, Zn, K, P, S by unicellular algae *Desmodesmus subspicatus* using ICP – MS/MS has been optimized. Cr and Zn were selected as elements originating from transport; K, P, and S are among the basic mineral elements.

Bioaccumulation was monitored during a 72-hour ecotoxicological test (in accordance with EN ISO 8692), $K_2Cr_2O_7$ and aqueous extract of contaminated sediment were selected for testing in such concentration to include algae growth inhibition in the range of approximately 0–90%. After the end of the ecotoxicological tests and the determination of cell density, the samples were filtered through the 0.22 µm membrane filter from a mixture of cellulose esters (Merck – Millipore, Germany) catching the algae cells. Together with samples, blank filters and the certified reference material Green Algae (Metranal 08, Analytika, CZ) were digested in nitric acid (sub-boiled) and hydrogen peroxide suprapure (Analytika, CZ) in a microwave system SW-4 (Berghof, Germany) and analysed together with the filtered solutions using 8800 ICP – MS/MS (Agilent, Japan). ^{53}Cr, ^{65}Zn and ^{39}K were analysed on mass in single quadrupole collision mode using He. $^{32\text{-}48}$S and $^{31\text{-}47}$P were analysed using MS/MS reaction mass shift mode in O_2. Since cell density was known for the individual dilutions, the resulting values of the content of elements (after blank subtraction) in algal cells were recalculated per one algal cell. This value represents the ammount of elements that are adsorbed on the surface of the cells and accumulated directly in the cells, which made it possible to assess the relationship between sample toxicity, accumulation of pollutants in algae and a change in the content of selected elements in algal cells.

It was found that with increasing concentrations of the toxicant, the concentration of Cr and Zn in the algal cells increased, with the most significant increase being observed at the EC50 concentration corresponding to a 50% growth inhibition; on the other hand, the content of K in cells gradually decreased to zero at the highest concentrations of the toxicant. For sulphur, the concentration in the cells was increased up to the EC50 concentration and then decreased; the content of P in cells increased with the increasing toxicant concentration.

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MP29

DETECTION OF BIOMOLECULES LABELED WITH PHOTON-UPCONVERSION NANOPARTICLES BY LASER-INDUCED BREAKDOWN SPECTROSCOPY

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In immunohistochemistry (IHC) and immunocytochemistry (ICC) various labels are used to identify cancerous cells. However, some of widely used labels (e.g., enzymes or fluorophores) have their limitations especially in short-term stability, time-consuming signal development or narrow possibility of multiplexing [1]. Thus, there is a need for alternative readout techniques. Laser-induced breakdown spectroscopy (LIBS) is analytical technique providing multi-elemental analysis of the biological sample surface. Recently so-called Tag-LIBS approach was used as a readout method for HER2 biomarker labeled with photon-upconversion nanoparticles (UCNPs). Although clear differentiation between HER2-positive and HER2-negative cell pellets was shown by yttrium signal detection, further optimization is still necessary [2]. In this work we investigate the laser ablation with the use of different laser pulse wavelengths (266, 532, and 1064 nm) and fluences. Moreover, single pulse (SP) and double pulse (DP) LIBS arrangements were compared with respect to the enhancement of the readout sensitivity. We have deployed a simplified sample preprocessing when focusing solely on the analysis of UCNPs dopped with erbium and ytterbium deposited on microscope slide. The combination of collinear DP LIBS setting with both laser pulses operating at 1064 nm wavelength shown the best yttrium signal-to-noise ratio and lateral resolution trade-off. Thus, better analytical sensitivity compared to the case of SP and DP LIBS with other combination of wavelength. Obtained results suggest a great potential to meet IHC and ICC readouts needs.

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MP30

EVALUATION OF HETEROTROPHIC LEACHING OF ARSENIC IN MULTICOMPONENT HUMIC ACID / AMORPHOUS FERRIC OXOHYDROXIDE / BENTONITE SYSTEM USING ATOMIC SPECTROMETRY

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Heterotrophic microorganisms have shown exceptional ability to leach metals and metalloids from minerals via their surface interactions with microbial acidic and chelating extracellular metabolites [1]. Furthermore, microorganisms can alter the speciation of elements in the environment effectively via methylation and precipitation, thus, affecting their bioavailability [2,3]. Therefore, these processes have been addressed in our experiments of heterotrophic bacterial (Pseudomonas spp., Rhodococcus sp.) and fungal interactions (Aspergillus niger) with prevalent soil components (aluminosilicates, amorphous oxohydroxides and humic substances) on arsenic distribution during static cultivation of selected microbial species. The data obtained in culture media using atomic spectrometry [4] indicated that the bentonite component in the humic acid/amorphous ferric oxohydroxide composite decreased the efficiency of arsenic(V) leaching by heterotrophic microorganisms. This highlights the significance of multicomponent system analysis as a more realistic approach for evaluation of arsenic mobility in complex matrices, e.g., soils and sediments.

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MP31

POSITRON ANNIHILATION SPECTROSCOPY AS A TOOL FOR EXAMINING MICROSTRUCTURAL PROPERTIES

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The photopolymerization process of the liquid material takes place under specific and controllable conditions. Most photopolymers react to radiation in the wavelength range of the UV region or the visible light region, where they undergo a reaction and become solid. Such cured polymers are often used in the biomedical field, orthopedics and in dentistry to fill and seal grooves and prevent cavities. The 2M liquid samples are mixtures of UDMA and D_3MA monomers with added photo initiator at two different concentrations. The microstructural properties of the materials were measured by positron annihilation spectroscopy. It is a capable technique for investigation of the local free volume at the atomic level by measuring the lifetime of positrons and positronium. Through the lifetime of ortho-positronium (*o*-Ps) ($\tau 3$) from the complex annihilation time spectrum, it is possible to monitor the influence of various chemical and physical parameters on the change of local free volume. 2M samples with two concentrations of photo initiator were periodically illuminated and lifetime spectra were measured during the interrupted reaction in dark. Each sample was cured and crosslinked after a specific time, when a constant lifetime of *o*-Ps as well as local free volume was reached. With a higher concentration of photo initiator, the crosslinking is faster, the lifetimes and the sizes of the free volumes are reduced. The final cured and crosslinked samples were also measured by near-infrared spectroscopy to determine the conversion of monomers and its mutual relationship with microstructure.

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MP32

POLYPROPYLENE TREATED BY ATMOSPHERIC PLASMA JETS: CORELLATING PLASMA CHEMISTRY WITH SURFACE MODIFICATIONS

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Atmospheric pressure plasma discharges are a promising alternative to standard wet chemical surface treatment methods; the main advantages of plasma are low running costs, eco-friendliness, and the possibility of automation. Their disadvantage lies in the unpredictability of the plasma treatment process, as the outcome depends on both the surface and plasma properties. In this work, we correlate the plasma chemistry of four different atmospheric pressure plasma jets with the changes induced on treated polypropylene (PP) strip surfaces. The three industrial jets (Plasmatreat rotating plasma jet, AFS plasma jet, and SurfaceTreat gliding arc) utilized air as their working gas. The home-built RF plasma slit jet used Ar. The gas chemistry was studied mainly using optical emission spectroscopy (OES). Spectra of all discharges contained OH, N_2 optical bands, and O atomic lines of different intensities. Decomposition of N_2 molecule and subsequent formation of NO or NO_2^+ species was observed only for jets running in dry air with higher gas temperatures. The surface chemistry was assessed by water contact angle and X-ray photoelectron spectroscopy. The plasma of the AFS jet was too hot and destroyed the surface of PP strips. The smallest number of functional groups were attached on surfaces treated by RF plasma slit jet where mainly scission of polymer chains by Ar species occurred. The two remaining jets running in the air (Plasmatreat plasma jet and SurfaceTreat gliding arc) were similarly effective, which is reflected by the similarities of their OES spectra.

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MP33

APPLICATION OF X-RAY DIFFRACTION AND SCANNING ELECTRON MICROSCOPY TO CLAY MINERALS

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Clay minerals can occur as secondary minerals, especially in sediments. They are aluminosilicates with layered structure. Their structure consists of tetrahedral and octahedral sheets connected to each other into one layer in two possible ways. In the first case, one tetrahedral and one octahedral sheet join by apical oxygens and create a 1:1 or T:M layer (e.g. kaolinite or serpentinite). In the second case, the octahedral sheet is located between two tetrahedral sheets and creates a 2:1 or T:M:T layer (e.g. smectite or illite). All layers are stacked one by one along a c-axis. The main structural differences between clay minerals are the type of layers and the distance between the layers.

Particles of clay minerals are usually very small (< 2 µm), therefore, it is impossible to study them with optical microscopy. The most used method of studying clay minerals is X-ray powder diffraction. The similarities in the structure of individual minerals mean that it is not sufficient for the sample used for their identification to be ground only and measured as in other cases.

At first, the clay-size particles were separated by size by centrifugation in demineralized water and particles in suspension were dropped on laboratory slide to obtain preferred orientation along 0 0 l during sedimentation. Then the sample was measured after it air dried, then also after it was saturated by ethylene glycol and also after it was fired at 400 °C. Some clay structures have the ability to absorb molecules of ethylene glycol, and different structures have different resistance to high temperatures. Results from X-ray diffraction show changes in the position of the diffraction lines (structure changes) which can enable the determination of the specific clay mineral [1]. For example, smectite structure can absorb molecules of ethylene glycol into its interlayer space and it moves the diffraction line (0 0 1) from 15 Å to 17 Å.

Other useful methods for identifying clay minerals are the Scanning Electron Microscope (SEM), which allows the study of crystal morphology, and Electron Probe Microanalysis (EPMA) with energy dispersive detector, which provides information on the chemical composition. These methods are also very helpful in identifying associated minerals needed for quantification. All the mentioned methods are best combined with X-ray diffraction because that way we better identify individual minerals. Study of clay minerals is a very important field of geology; they can cause a lot of problems in the construction industry, but they can be very useful in pharmacy or other industries where their ability of absorption is utilized.

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MP34

TABLETOP CμXRF SPECTROMETER FOR NONDESTRUCTIVE DEPTH-RESOLVED ELEMENT ANALYSIS

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Tabletop CμXRF units have been introduced only recently and are the subject of studies by various research groups during the last years. The in-depth sensitivity of the spectrometer is based on a defined three-dimensional probing volume which is formed by the confocal arrangement of two polycapillary lenses in the excitation and the detection channel. The spectrometer used in this study is a modified commercial tabletop μXRF spectrometer (M4 TORNADO) by Bruker Nano GmbH. The setup is based on research results obtained by the Kanngießer group at TU Berlin. [1] The commercial μXRF setup is equipped with a polycapillary fulllens with a spot size of ≤ 20 μm (Mo-Kα) for X-ray focusing and a 30 mm^2 silicon drift detector (SDD). Due to the modification a polycapillary halflens was installed perpendicular to the first one in front of a 60 mm^2 SDD.

Nondestructive CμXRF analysis provides micro-scalic resolved measurements of sample volumes due to its in-depth sensitivity by e.g. depth profiles and stacked elemental distribution images. The strengths, challenges and potential of the CμXRF tabletop spectrometer for nondestructive and depth-sensitive element analysis will be illustrated by various fields of application, like measuring the three-dimensional element distribution of Ca and Br in *I. basta* demosponge skeletal after different solvent treatments, [2] examining the spatial distribution of Cu within a spongin-atacamite composite due to mineralization [3] and analysis of mineral inclusions. Moreover, the implementation and verification of polymeric multi-layer systems as stratified inhouse standards for organic samples will be introduced.

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MP35

TRACING NEW POTENTIAL CHEMOTERAPEUTICS USING ICP-MS AND LA-ICP-MS

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Cancer is the second leading cause of death from any disease for which chemotherapy is the most widely used treatment. The medical treatment often relies on an application of platinum-based anticancer drugs characterized with low efficiency and large number of unsolicited side effects, which significantly affects the life quality of cancer patients. This is a wide broad issue and there is a growing effort to find new drugs that have tumor-cell specificity, better efficiency and fewer negative side effects for oncological patients. The well-known and frequently used chemotherapeutic agents are cisplatin and other derived platinum derivatives such as oxaliplatin and carboplatin. However, these compounds are highly cytotoxic and many tumors are resistant to the use of this cytostatics. In recent years, metallocene-based drugs containing a central metal atom in their structure have been gaining interest. These drugs show better selectivity and can alter platinum-based drugs in case of more resistant tumors. Moreover, they show controlled activation of their cytotoxic properties to some extent (activation only upon interaction with cancer cells). Our research is focused on the investigation of the distribution and efficiency of newly synthesized metallocenes with ruthenium, hafnium or zirconium as a central atom in their structure towards lung cancer cell lines A549 and H1299. The behaviour of these cells was monitored in relation to the presence or absence of the gene *Anterior GRadient 2* (*AGR2*) to investigate its impact on the sensitivity of these cells to administered drugs. Determination of the amount of new potential chemotherapeutic agents present in the cells was performed by inductively coupled plasma mass spectrometry (ICP-MS) and in conjunction with laser ablation (LA-ICP-MS). Metal distributions within the single cells and 2D-imaging was also studied.
Based on the experiment conducted, the greatest potential was found for ruthenium-based drugs, which showed the highest permeability, exhibited the highest cytotoxicity, and since entered the cells in the large amount.

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MP36

SYNTHETIC CANNABINOIDS: STRUCTURE DETERMINATION AND CHARACTERIZATION BY MOLECULAR SPECTROSCOPY

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An increasing number of products containing synthetic cannabinoids pose a growing crisis to public health worldwide [1]. Recently, a rising number of cases of serious adverse health effects, intoxications, and death cases associated with synthetic cannabinoids were reported [2, 3]. The current study represents the comprehensive structural analysis of three synthetic cannabinoids (AB-, ADB- and AMB-FUBINACA) in solution investigated by electronic and vibrational circular dichroism together with the conventional methods of infrared and ultraviolet absorption spectroscopy, all supported by the density functional theory (DFT) calculations. The best level of theory to reproduce the experimental wavenumbers and wavelengths was found to be the B3LYP method with a 6-311++G(d,p) basis set including the solvent effects. Very good agreement between the experimental and simulated spectra allowed us to determine the absolute configuration and a detailed interpretation of all spectra of AB-, ADB- and AMB-FUBINACA. In addition, the HOMO and LUMO electronic transitions were calculated.

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MP37

SIMULATED STABILITY OF SELECTED ELEMENTS IN TRIS BUFFER SOLUTION

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The development of novel bioactive glasses relies on an understanding of the dissolution mechanism of these materials in a biological buffer solution simulating the body environment. The (hydroxymethyl)aminomethane (TRIS) is a buffer commonly used in aqueous solutions simulating human plasma. Such solutions were developed for testing *in vitro* reactivity of bioactive glasses [1] to which dopants (named *therapeutic ions*) are incorporated in the glass structure to increase their antibacterial property and to provoke osteogenic and angiogenic effects to start bone regeneration [2,3,4]. The stability of selected elements: Ag, Ca, Cu, Sr, Zn, and Y in 0.05M TRIS was investigated in this study. These ions at certain concentrations might trigger precipitation or complexation reactions during the storage of samples. The resulting information about the amount of ions released from a glass at a particular time can be misleading. These elements were separately spiked in the TRIS solution with the final concentration of elements: 0.5, 2, and 5 mg/L. The 3 parallels were prepared for each dose of dopants, each parallel was divided into two parts, one was stabilized to pH ~ 2 using concentrated ultrapure nitric acid and another one was left without stabilization. TRIS solution without spiked metals was prepared as the comparative *blank* solution and tested under the same conditions to check the leaching of the ions from the bottles used in the tests. The solutions were stored at the temperature of 4°C in the fridge. Quantitative analysis was done immediately after spiking the elements in the TRIS solution and at the time interval of 3 and 7 days using an optical emission spectrometer with inductively coupled plasma (ICP-OES). The obtained results show that copper in the measured concentration range reports very low reactivity in TRIS solution for 3 days. The determination of copper in the leachates from testing of Cu-containing bioactive glass in TRIS-based solutions could be done without stabilization in the studied time interval. The measured concentrations of Ag show that stabilization of Ag-containing solutions with the nitric acid may lead to the formation of silver nitrate. Further studies are ongoing for selecting suitable stabilization agents for solutions containing silver. The instability of other investigated dopants in TRIS solution was observed already from the early stage.

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MP38

ENHANCEMENT OF LUMINESCENCE SIGNAL OF TETRACYCLINES ANTIBIOTICS BY DEUTERATED WATER

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While deuterated water has been known to alter molecular luminescence emission for over 60 years, only a few analytical applications were described in the literature. When H_2O is merely substituted for D_2O, an increase of both fluorescence intensities and lifetimes can reach units to hundreds of percent. Employment of D_2O may theoretically increase the signal of all methods relying on luminescence detection, which can lead to lower detection limits and dye concentrations. The molecules potentially profiting from such an enhancement include many dyes, biomolecules, or pharmaceuticals. Selected antibiotics from the class of tetracyclines have been analyzed using a spectrofluorometer, liquid chromatography with fluorescence detection, and liquid chromatography with mass spectrometric detection on a core-shell C18 column. As the majority of systems nowadays rely on reversed-phase columns with water being the main component of the mobile phase, a simple replacement of H_2O with D_2O in the mobile phase enhanced the sensitivity for selected compounds. Another way to increase the fluorescence intensity lay in the production of complex compounds of the tetracycline molecules and Mg^{2+} ions. The combination of the mentioned phenomena can lead to a decrease in detection limit from $1.3\cdot10^{-10}$ mol·l^{-1} (H_2O mobile phase) to $8.8\cdot10^{-12}$ mol·l^{-1} (mobile phase with D_2O and Mg^{2+}) for minocycline, from $1.3\cdot10^{-9}$ mol·l^{-1} to $7.1\cdot10^{-12}$ mol·l^{-1} for tetracycline and from $1.5\cdot10^{-9}$ mol·l^{-1} to $2.1\cdot10^{-11}$ mol·l^{-1} for doxycycline.

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MP39

PLASMA-MEDIATED VAPOR GENERATION BY DIELECTRIC BARRIER DISCHARGE: DIRECT ANALYSIS OF MERCURY BY AAS

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Dielectric barrier discharge (DBD) is a device which refers to a plasma formed between two electrodes separated by at least one dielectric barrier. In recent years, the DBD reactors have been used as a plasma-mediated vapor generation technique (PMVG) alternatively to the more common chemical vapor generation (CVG). A thorough optimization of the DBD reactor for Hg^{2+} and $MeHg^{+}$ determination based on PMVG from a single drop without any reagents and subsequent AAS detection was the main goal of this work. A lab-made volume discharge DBD reactor was designed with the dielectric barrier consisting of a 1.5 mm thick flat bottom glass tube. An aluminum foil electrode was placed beneath its bottom. The second electrode was a stainless steel grid positioned 4 mm below the glass surface. Both electrodes were coupled to a lab-made high voltage uni-directional power supply. The procedure consists of opening the DBD reactor and introducing the sample (2 µL) on the dielectric barrier. Then, the reactor is closed and the power supply is synchronized with the spectrometer for signal acquisition. Preliminary experiments have revealed an interesting and significant improvement of peak shape and peak area for Hg^{2+} and $MeHg^{+}$ when was the glass dielectric barrier covered by a piece of polymeric film (Parafilm). After that, the matrix influence (HCl or HNO_3) was investigated. A significant signal decrease was observed with concentrations higher than 0.001 and 0.1 mol L^{-1} for HCl and HNO_3, respectively. The effect of discharge gas identity was studied. Higher intensities for both Hg species were observed using He, compared to pure Ar or Ar:H_2 (10:1). Additionally, when using Ar:O_2 (200:1) a spectral interference was observed, probably due to O_3 generated inside the reactor. Under optimized conditions, which included the use of 23 W, 38 kV, and 150 mL min^{-1} He, both Hg species yielded similar sensitivity. The volatilization efficiency quantified by a mercury analyzer was above 82% for both Hg species. The proposed PMVG method and the conventional CVG provided similar sensitivity. Limit of detection of 100 µg L^{-1} (200 pg in absolute mass) was obtained. In conclusion, the proposed DBD reactor was proven to perform a successful PMVG as a one-step process comprising Hg volatilization and atomization from a single drop. The key point is that no reagents are required.

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MP40

ULTRASENSITIVE DETERMINATION OF CADMIUM BY ATOMIC SPECTROMETRY

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Chemical vapor generation (CVG) of cadmium was optimized in the presence of Cr^{3+}/KCN modifiers in a four-channel CVG system in a flow-injection mode, reaching generation efficiency of 60% [1]. The optimized CVG was subsequently coupled with atomic fluorescence spectrometry (AFS) with atomization in a miniature diffusion flame (MDF) as well as flame-in-gas-shield (FIGS). The interference from hydride forming elements (Sn, Sb, Se, Bi, As and Pb) and Hg was investigated using both atomizers. There were no serious interferences up to concentration of 100 ng ml^{-1} except Pb. The FIGS atomizer provided a limit of detection (LOD) of 0.4 pg ml^{-1} Cd (0.06 pg absolute) and was chosen for real sample analysis (water and rice). For comparison, the LOD achieved with AAS and atomization in the QTA was 56 pg ml^{-1} (8.4 pg absolute). Another approach to improve LOD involved a preconcentration. A simple Cd preconcentration step in the gas phase, after CVG, was developed employing a modular trap-and-atomizer device [2,3]. The inner surface of the trap (emptied, cleaned quartz tube-commercially used with an amalgamator filling) was modified by a solution of gold nanoparticles (AuNPs, 60nm) to enhance preconcentration efficiency. Key parameters such as trapping and volatilization temperature, the composition and flow rate of carrier gas were optimized as well as the amount of AuNPs (8 µg Au). In this preconcentration arrangement LOD of 13 pg mL^{-1} was reached being approximately 5-times better than in the on-line mode without preconcentration step. The efficiency of Cd preconcentration step at optimized conditions with AuNPs was preliminarily estimated as 70%.

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MP41

STRUCTURAL INVESTIGATION OF A/G-HYBRID PEPTIDE OLIGOMERS

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Peptide-like foldamers consisting of alternating α,β,γ-triamino acids 3-amino-4-(aminomethyl)-2-methylpyrrolidine-3-carboxylate (AAMP) and natural amino acids glycine and alanine were synthesized and their secondary structure was determined. We demonstrate that both non-amide bond forming amino groups present in AAMP contribute to secondary structure formation in α,γ-oligopeptides and induce new folding patterns. The relatively stable secondary structures of all oligomers containing AAMP units are supported by both ECD and VCD spectroscopies. VCD investigations point to a handeness of constituted structures.

MP42

MULTIELEMENTAL ANALYSIS OF TANTALUM ORES BY ICP-OES

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The main goal of this work is to design an analytical procedure for determining the content of tantalum and niobium in ore concentrates with variable content of these elements. In nature, tantalum deposits rarely have a concentration of more than 0.05 wt. % Ta_2O_5 (usually 0.01 - 0.04 wt.%). Primary Ta (and Nb) mineralization is mainly related to igneous rocks, so-called rare element pegmatites. Moreover, depending on the nature of the deposit the ore may contain a wide range of accompanying minerals. For the evaluation of ore from an economic point of view, the tantalum oxide content determination is the most important. Nevertheless, knowledge of the concentrations of accompanying elements, such as tin, silicon, uranium, thorium, titanium, manganese, sulfur, sodium, potassium, is crucial for choosing the technological procedure of further processing [1,2].

The following types of decompositions have been previously developed and can be found in the available literature: 1) microwave decomposition in various mineral acids; 2) alkaline melting; 3) decomposition with HF; 4) melting with Na_2O_2. Nevertheless, some of these decomposition methods do not reliably achieve 100% recovery, are time-consuming, the used chemicals contain also the elements of interest or there is an increased risk of contamination.

Melting with lithium borax and subsequent dissolution in a mixture of acids has been found as an optimal method for tantalum ores sample preparation with variable content of the above-mentioned elements. Depending on the origin and type of the ore the contents of Ta, Nb, Sn, Si, Ti, Mn, S, Na, K and other elements were determined by ICP-OES. The optimization of the decomposition method was verified using the standard X1808 or by the samples analyzed in an accredited laboratory by the XRF method. Verification of the results by the sum to 100% was also applied.

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MP43

LIBS ANALYSIS OF *CANNABIS SATIVA* AFTER LONG-TERM EXPOSITION IN CADMIUM-CONTAMINATED SOIL

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Heavy metal contamination of a soil is a significant problem that we face nowadays. The accumulation of heavy metals in soil is a big concern because of the effects of heavy metals on food safety, crop growth and health of soil organisms [1]. The content of cadmium in soil is 0.01-1.1 mg per 1 kg of soil (i.e., ppm level) [2]. *Cannabis sativa* is a plant that has a high tolerance to heavy metal contaminants in soil and could be used for phytoremediation [3].

Determination of exact distribution of heavy metals in plants is important for an assessment of toxicity and possible health risks. Laser-Induced Breakdown Spectroscopy (LIBS) is capable of the detection of broad range of elements. Additionally, it gives us information about spatial distribution of studied elements in the sample which enables a retrospective study of pollutant migration within the plant. It is possible to map the whole plants or only chosen parts of plant samples [4].

In this study, *Cannabis sativa* was grown in man-made cadmium contaminated soil. The content of cadmium in soil was 50 mg/kg. Plants were grown for 1, 2 and 4 weeks, in contaminated soil as well as control soil without contaminants. Toxicity of cadmium in soil was assessed on the basis of macroscopic toxicological endpoints. LIBS was used to demonstrate the spatial distribution of cadmium in plants. We found out that the cadmium was preferentially accumulated in the roots.

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MP44

MICROSCOPIC AND NANOSCOPIC STUDY OF POLYMER MEMBRANES

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Nowadays, there are many kinds of polymers with various functions and properties, and new polymers are still being developed. Although the chemical structure is usually known, the spatial arrangement of individual molecules is only supposed and estimated. In this study, we focused on two types of polymers, namely polyvinylidene difluoride (PVDF) and polydopamine (PDA), which both of them do not exhibit toxic properties and can be employed for special surface treatment. The second polymer studied in this work, PDA, is commonly used as a protective layer in biomedicine [1], however, its sorption mechanism is still not completely understood. The various chemical bonds in the network of molecules in the polymers were studied from the microscopic and nanoscopic point of view using infrared microscopy together with scanning near-field infrared microscopy, which enables a detailed analysis of the polymer membranes below with nanoscale resolution.

PVDF blend membranes including cationic/zwitterionic polymeric parts were studied using both methods and it was observed that the side chains play an important role in the mechanism of networking.

The PDA layers were adsorbed on silicon, titanium and gold substrates at various times of polymerization and the adsorption mechanism was investigated. It was observed that the mechanism depends not only on the time of polymerization, which was expected, but also on the surface material. It was found out that in the case of silicon and titanium surfaces, the PDA is adsorbed via quinone units, whereas in the case of gold, it is rather adsorbed *via* the aromatic system [2].

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MP45

MULTITECHNIQUE DETERMINATION OF HALOGENS AND SULFUR IN HUMAN HAIR

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Halogens and sulfur in human biological samples are associated with diet, environmental exposure, health problems, medicines or supplements taken [1]. These elements have been determined by several analytical tools – using direct solid sampling or after performing a sample preparation [1]. However, determining all of them in solid or complex matrices using a single analysis is not an easy analytical task [1]. Ion chromatography with suppressed conductivity and mass spectrometry detection (IC-CD-MS), inductively coupled plasma mass spectrometry (ICP-MS), inductively coupled plasma optical emission spectrometry (ICP OES) and ion selective electrode (ISE) are alternatives but requiring a suitable sample preparation. Nevertheless, halogens can be lost in their volatile species during sample preparation, especially by wet digestion using concentrated acids, and the presence of organic matter and high acidity in final solution can compromise the accuracy of the results. Thus, an effective sample preparation method for further halogens and sulfur determination in human hair by multitechniques has been developed by our research group [2-5]. Human hair was efficiently digested based on combustion reaction to obtain compatible solutions with IC-CD-MS, ICP-MS, ICP OES and ISE analysis. Using microwave-induced combustion (MIC), masses ranging from 50 to 300 mg of human hair [2,3] were efficiently digested. A diluted solution fully compatible with all determination techniques (100 mmol L^{-1} NH_4OH) was used for the absorption of all analytes. Trueness was evaluated by analysis of certified reference material (results did not differ significantly from those described in the certificate) and by recovery tests (mean recoveries ranged from 92% to 105%). Relative standard deviations were always lower than 8%. Final digests were fully compatible with multiple determination techniques and proposed method presents several advantages compared to the others reported in the literature. Other analytical parameters and halogens and sulfur concentration range in human biological samples can be accessed in our studies present in the literature [2-5].

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TP1

INSTRUMENTAL CONFIGURATION EFFECT ON THE LIBS ACOUSTIC SIGNAL RESPONSE

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During years, the potential of acoustic shockwaves from laser-induced plasmas has been tried to exploit as a standardization score to the optical emission properties, mainly to correct/normalize shot-to-shot plasma inherent instabilities. However, nowadays its in-depth study is revealing that its benefits can go even further, by physically characterizing the studied samples and allowing the enhancement of the discriminative power between spectrally similar samples via data fusion strategies.[1,2]

As is well known, the instrumentation used for the generation of the plasma and the subsequent spectroscopic detection of the light it emits, significantly conditions the analytical information obtained. In this sense, and considering the associative character of the plasma with the acoustic wave recorded, in this work, research is intended to evaluate how the instrumentation affects the recorded acoustic signal; Nd:YAG lasers operating at 1064 nm and 266 nm and miscellaneous types of microphones (commercially available and ad-hoc built, varying in sensitivity, frequency response, …) have been considered.

In parallel with multi-elemental LIBS imaging, given the simultaneity of the optical and acoustic phenomena, surface acoustic mapping from different samples performance was evaluated. Results revealed that the first peak-to-peak acoustic amplitude in the sound wave recorded finely describes the morphological characteristics of the interrogated surface; the information that can contribute to a much more complete characterization of the sample under study.

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TP2

BIORECOGNITION TOOLS

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This work deals with the development of molecularly imprinted polymers on the surface of magnetic particles (Mag-MIP/NIP) for metallothionein detection by LA-ICP-MS. After the successful optimization of the preparation of Mag-MIP/NIP based on dopamine, the developed method was tested on the extraction of metallothionein from a real sample, which was a melanoma of the MeLiM minipig. Subsequently, the potential of molecularly imprinted polymers as a direct antibody replacement for subsequent imaging of metallothionein in tissues was investigated. The procedure was optimized using dot-blot experiments.

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TP3

GRAPHENE ANALYSIS BY ICP-OES: THE IMPORTANCE OF SAMPLE PREPARATION

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Carbon nanostructures, such as nanotubes or graphene, have become widely studied materials. Recent studies suggest that some of the properties originally attributed to these materials (e.g. electrocatalysis) in fact originate from their contamination with other elements, mostly metals used to catalyze synthesis of the material [1]. Therefore, there is a need to reliably determine impurities in these materials. Inductively coupled plasma optical emission spectroscopy (ICP-OES) is one of promising methods for the purpose as it provides multielement analysis with low detection limits and is relatively tolerant to sample matrix. Unfortunately, carbon nanostructures are extremely difficult samples in terms of sample preparation [2], and many commonly used sample preparation techniques, such as microwave assisted digestion, struggle to completely dissolve the sample, raising doubts about thoroughness of the process and reliability of results.

This work presents an experimental comparison of several sample preparation techniques applied to a graphene sample. Microwave assisted acid digestion and Schöniger method are used as well as direct sample introduction into plasma using electrothermal vaporization unit. Impurities contents determined by ICP-OES after each of these procedures are compared to assess how successful these techniques are at dissolving graphene sample, or leaching impurities from graphene structure.

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TP4

VORTEX ASSISTED LIQUID-LIQUID MICROEXTRACTION FOR EXTRACTION OF SELENIUM IN FOOD SAMPLES USING ALCOHOL BASED-DES PRIOR TO ICP-OES: ONE STEP CLOSER TO ACHIEVING GREEN ANALYTICAL CHEMISTRY

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New generation of solvents termed the deep eutectic solvents (DESs) are attracting increasing attention as green solvents in analytical chemistry. This present study proposes a novel, eco-friendly, simple, and low-cost approach for the extraction of total selenium from food samples using alcohol-based DES vortex assisted liquid- liquid microextraction (DES-VA-LLME) prior to Inductively coupled plasma optical emission spectrometry (ICP-OES) detection. Central composite design (CCD) combined with surface response methodology was used to optimize the method parameters and obtain the desirable optimum operating conditions for DES-VA-LLME. The obtained optimum conditions for the microextraction process are as follow: Volume of DES, mass of sample, temperature (T), acid concentration (AC) and extraction time (ET) should be 4 ml, 50 mg, 125 °C, 3.4 M and 2.8 min, respectively. In addition, the DES-VA-LLME technique achieved LOD, LOQ and linearity of 2.137 µg/g, 7.555 µg/g and 7.555-250 µg/g, respectively, under the optimum conditions. Relative standard deviation was 1.2% and 2.5% for inter-day and intraday respectively. The obtained analytical results showed that the proposed method achieved important features such as simplicity, eco-friendly, quick, efficient, and low cost which made it attractive for the efficient extraction and determination of total Selenium (Se) in food samples. Finally, the developed DES-VA-LLME method was successfully applied to real food samples.

Keywords
Alcohol DES; Selenium; Vortex assisted liquid-liquid microextraction; ICP-OES; Food samples; Green analytical chemistry

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TP5

REARRANGEMENT OF INTRACELLULAR CRYSTALLINE GUANINE AS AN ADAPTATION FOR VARIOUS ILLUMINATION LEVELS

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It is well known that biogenic guanine crystals are widely used by various animals to manipulate light. Because of extremely high refraction index and plate-like arrangement, multiple arrays of guanine crystals can act as diffuse scatterers, broad- and narrowband reflectors, tunable photonic crystals, and image-forming mirrors. Crystalline inclusions composed of guanine or related purines were recently identified also in different phylogenetically unrelated photosynthetic microalgae. In the case of dinoflagellate *Amphidinium carterae* they were shown to serve as a long-term, high capacity store of nitrogen [1]. However, nitrogen storage does not exclude other roles, and light manipulation was already speculated for photosynthetic eukaryotes.

A confocal Raman microscopy was used for visualization of crystalline guanine within intact cells of *A. carterae* cultivated under low light (5 μmol(photons)$\cdot$m$^{-2}\cdot$s^{-1}) and high light (200 μmol(photons)$\cdot$m$^{-2}\cdot$s^{-1}) conditions.

We show that location of guanine crystals in *A. carterae* depends on the intensity of illumination. When the cells are cultivated under continuous supply of inorganic nitrogen but exposed to low light intensity, their adaptation consists of increasing amount of plastids and synthesis of guanine crystals situated behind the plastids, closer to the center of the cell. Acting as photonic mirrors or diffusers for redirecting untrapped photons back to plastids, guanine crystals might increase efficiency of photosynthesis. In the case of high light intensity, extensive layers of guanine crystals are organized between the cell wall and plastids, shielding plastids from the excessive illumination.

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TP6

ANALYSIS OF NON-METALS IN TECHNOLOGICALLY RELEVANT MATERIALS USING LASER-INDUCED BREAKDOWN SPECTROSCOPY (LIBS)

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To overcome the challenges of the 21st-century, material science has made tremendous progress in the last years. Novel high-performing materials (e.g., complex metal oxide (CMO), C- and N-based coatings) are crucial for developing improved technology for energy production and storage (e.g., solar cells, fuel cells, and batteries) and systems exposed to high temperatures, corrosive milieus, or mechanical impact (e.g., machining, aerospace industry). Since crucial material properties are determined by the elemental composition from the bulk stoichiometry down to unwanted impurities or dopant levels, a precise analytical characterization is inevitable to establish a connection between composition and function. In particular, for thin films or coatings also, knowledge about the distribution of the prevailing elements within the sample is essential.

For this purpose, direct solid sample techniques like EPMA (electron probe microanalysis), LA-ICP-MS (laser-ablation inductively-coupled-plasma mass spectrometry), or SIMS (secondary ion mass spectrometry) can be used as analytical techniques to characterize high-performance materials. Another method, which gained increased attention recently in the field of material science is LIBS (laser-induced breakdown spectroscopy). The main advantage of LIBS compared to other solid sampling methods is a high sample throughput and the possibility to detect almost every element of the periodic table.

In this work, a new ablation chamber for a 193nm ArF-excimer LA-ICP-MS system is introduced, enabling LIBS measurements; the methods can be used separately or in tandem. The applicability of this setup will be demonstrated by the analysis of ceramic materials focusing on challenging elements like carbon, oxygen and nitrogen, which are usually not measurable with LA-ICP-MS, showing the improved information obtained by this new measurement setup.

TP7

THE DISTRIBUTION OF POTENTIALLY TOXIC AND RISK ELEMENTS IN THE ORGANS OF *RUMEX ALPINUS*

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The Monk's rhubarb, *Rumex alpinus* is a native plant in the mountains of Europe and its distribution has partly been affected by its utilization as a vegetable and medicinal herb. The distribution of potentially toxic and risk elements in its organs is so far not well-studied. This makes the safety of *R. alpinus* consumption questionable. The study examined the safety of consuming *Rumex alpinus* from the Krkonoše Mountains, the Czech Republic, and the Alps (Austria and Italy). The total and plant-available concentrations of Fe, Zn, Cu, Mn, Cr, Al, As, Ni, Pb, and Cd in the soil and total concentration in organs (rhizome, emerging, mature and senescent leaves, stem, and petioles) of *Rumex alpinus* were determined using *aqua regia* and Mehlich-3 extractions, respectively, followed by inductively coupled plasma optical emission spectrometry. The uptake and distribution of elements by the plant in all localities were characterized by bioaccumulation (BF) and translocation (TF) factors. The level of the elements accumulated by *Rumex alpinus* is considerably different, depending on local geological substrates and environmental conditions. The result indicated that *Rumex alpinus* has considerable tolerance to Zn, Cu, As, Cr, and Ni, with an easy accumulation strategy. The high Al and Cd concentrations in belowground biomass (rhizome) indicate a defensive mechanism for them. Although the aboveground biomass (emerging, senescent, mature leaves, and petiole) has some degree of accumulation of risk elements, the results revealed that *Rumex alpinus* is an excluder. *Rumex alpinus* does not accumulate Al, As, Cr, Ni, Pb, and Cd in organs (leaf and petiole) that are consumed based on the permissible limit according to World Health Organization (2001) and can therefore be used without concern. However, caution must, therefore, be taken in the consumption of these organs in highly contaminated soils.

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TP8

WHERE CADMIUM ACCUMULATES AFTER INHALATION OF CADMIUM-BASED NANOPARTICLES

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Cadmium and its toxic effects are a very current issue at this time, as poisoning by this element can cause serious health problems or death. Long-termed exposure to cadmium can lead to cancer and adverse effects on organ systems (skeletal, reproductive, cardiovascular, central and nervous etc.). *Cadmium is transported through the bloodstream and is found in a wide range of tissues.* We monitor the distribution of cadmium in the lungs and kidneys. We also monitor whether the distribution of cadmium in the tissues will affect the content of biogenic elements (copper, zinc, iron etc.*)* [1]

The distribution of the elements was monitored in the tissues of mice that inhaled either clean air or air contaminated with cadmium nanoparticles. The mice were sacrificed and their organs were removed. The organs were placed on a microscope slide in the form of a thin cryosection, which was analyzed by laser ablation in combination with inductively coupled plasma mass spectrometry. Distribution maps of cadmium and other elements of interest were created from the measured data. In our poster, the distribution maps of the kidneys and lungs of mice that inhaled clean air and mice that inhaled air contaminated with cadmium nanoparticles are compared.

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TP9

IN-SITU TRAPPING OF VOLATILE SPECIES IN DBD ATOMIZERS: NEW APPROACH TO PRECONCENTRATION OF CADMIUM AND SELENIUM

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Cadmium is one of the most toxic metal elements with high accumulative capability. On the contrary, selenium is considered essential for human health. It can cause diseases by deficiency while is toxic at levels less than an order of magnitude above those required for health. Their accurate ultratrace detection is thus perceived as a priority task. Introduction efficiency of both elements into atomic spectrometric detectors can be significantly enhanced by chemical vapor generation (CVG). Selenium is converted to SeH_2 by the $NaBH_4$ reduction. Cd is reduced by the same reagent but in the presence of reaction modifiers (Cr^{3+}/KCN) to a mixture of free Cd atoms and most probably CdH_2. The latter method has intensively been studied at our laboratory recently yielding overall generation efficiency of 70%.
A way to improve the limit of detection (LOD) of a given atomic spectrometric detector is to combine the use of the CVG step with a subsequent analyte preconcentration in the gas phase. Efficient preconcentration of analyte hydrides directly in the novel dielectric barrier discharge (DBD) plasma atomizers prior to detection by atomic absorption spectrometry (AAS) was proven feasible. In this arrangement, the DBD plasma regulates analyte trapping, release and atomization. An addition of low O_2 flow rates to the discharge gas (Ar) results in quantitative analyte retention. After a given preconcentration period, O_2 flow is switched off while the DBD discharge as well as CVG of the blank is kept running, the latter serving as a source of co-generated H_2 which is essential for analyte volatilization and atomization. Trapped analyte species are efficiently released under these conditions. There is no need to change the high voltage/power settings between the trapping and volatilization steps. Preconcentration of As and Sb hydrides has been investigated with AAS detection so far providing 100% efficiency and LODs around 10–20 pg mL^{-1}. In-situ preconcentration of SeH_2 in a planar DBD plasma atomizer was optimized with AAS detection in this work. The use of ^{75}Se radiotracer revealed efficient analyte trapping (90%) in a small spot in the central part of the DBD optical arm whereas incomplete volatilization was found responsible for 70% preconcentration efficiency. Volatile Cd species can be preconcentrated after the CVG step in the same apparatus in a similar manner. Optimal O_2 flow rate added to Ar discharge gas was 3.5 ml min^{-1} resulting in complete Cd trapping. Volatilization efficiency was estimated to 80% with tailing signal peaks observed. The effect of alternative experimental arrangements including the DBD with sputtered electrodes or a power supply source with square wave modulation of high voltage on preconcentration efficiency of Se and Cd, signal profiles and analytical figures of merit will be discussed. The mechanism of preconcentration processes will be outlined.

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TP10

SELECTED SPECTROMETRIC METHODS FOR DETERMINATION OF IODINE IN BIOLOGICAL SAMPLES

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This article compares different methods for determination of iodine in biological samples. Most frequently, indirect methods are applied in clinical practice. Sandell-Kolthoff spectrophotometric method of iodine determination [1] ranks among the most widely used ones; researchers also developed other modifications of the above method. Regarding direct determination, the following methods are considered the most suitable ones: emission spectrometry with inductively coupled plasma (ICP-OES), electrochemical methods, mass spectrometry with inductively coupled plasma (ICP-MS), and nuclear activation analysis (NAA) [2]. The ICP-MS and NAA are costly, but iodine can be analyzed directly regardless of its form, oxidation state, and isotopic distribution of iodine [3]. On the contrary, electrochemical, and ICP-OES determinations can be complicated with remarkable spectral interferences and also with dependence on possible presence of various forms and oxidation states of iodine in samples [4].

We compared three most frequently used methods for determination of iodine in selected biological materials: Sandell-Kolthoff spectrophotometric determination, ICP-OES and ICP-MS techniques [5]. The samples of biological materials such as foods and food supplements corresponding to content of iodine in urine were selected (Jooste and Strydom 2010). A NIST-SRM-1549 Milk powder certified reference material (CRM) with certified iodine concentration (3.38±0.6 mg/kg) was used to control the accuracy of the total iodine determination. The least accurate results were obtained by ICP-OES in analyses of given CRM (5.64±0.39 mg/kg), better results were acquired by spectrophotometric method (4.53±0.23 mg/kg) and the most accurate results were provided by ICP-MS method (3.36±0.12 mg/kg of iodine).

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TP11

MÖSSBAUER STUDY OF THERMAL BEHAVIOR OF CL20ES AND CL50WS STEEL POWDERS USED IN SELECTIVE LASER MELTING

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Selective laser melting (SLM) is an additive manufacturing technique (AM) used primarily for rapid prototyping. In SLM, the surface of the metal powder on the bed is melted by a laser, which scans the cross sections based on a 3D model of the part being manufactured. Once the cross section is fully scanned, the bed is lowered to allow a new layer of powder to be placed on the previous cross section. The laser rescans this layer and the whole process is repeated until the entire 3D model is scanned and the part is completed. SLM is suitable for the production of parts from Mg, Ni and Ti alloys, stainless and hard tool steels and various metal composites. Various experimental techniques (X-ray diffraction - XRD, scanning electron microscopy - SEM, energy dispersive spectroscopy - EDS) were used to improve the SLM process and to inspect the properties (surface morphology, microstructure, phase and elemental composition) of components produced by SLM. Mössbauer spectroscopy (MS) is a suitable method for examining iron-based components. The phase composition of stainless steel metal powders (CL20ES) and maraging steel powders (CL50WS) during annealing was studied in the temperature range of 500 - 1100 °C in air and in an inert atmosphere. No changes in the Mössbauer spectrum were identified when the stainless steel powder (CL20ES) was annealed in a nitrogen atmosphere at all temperatures. Mössbauer spectra were fitted with a doublet with parameters IS = (-0.8 ± 0.02) mm/s and QS = (0.16 ± 0.03) mm/s. These parameters correspond to austenitic steel, the presence of which has been confirmed by XRD. No changes in phase composition were observed during air annealing at 500 and 600 °C. At annealing temperatures of 700 and 800 °C, the stainless steel powder oxidizes and a sextet corresponding to α-Fe_3O_3 was identified in the Mössbauer spectrum with IS = (0.36 ± 0.02) mm/s, ε = (-0.18 ± 0.02) mm/s and B = (51.0 ± 0.5) T. At a temperature of 1000 °C outside the oxidation, TMS identified the transformation of the austenitic phase to a ferritic phase. The ferritic phase was fitted with a sextet with IS = (0.0 ± 0.01) mm/s and a hyperfine magnetic field distribution with a mean value of B = 29.8 T. Furthermore, two sextets and a doublet were identified in the Mössbauer spectrum of powder annealed at 1100 °C. The sextets correspond to two positions of iron in the Fe_3O_4 crystals with IS = (0.28 ± 0.01) and (0.48 ± 0.03) mm/s and B = (48.1 ± 0.5) and (43.2 ± 0.5) T. The doublet corresponds to wüstitu with IS = (0.90 ± 0.05) mm/s and QS = (0.64 ± 0.10) mm/s. All phases were also identified by XRD.The Mössbauer spectrum of maraging steel powder (CL50WS) consists of two subspectra. The first corresponds to the austenitic phase with IS = (-0.06 ± 0.02) mm/s and QS = (0.16 ± 0.02) mm/s, the second subspectrum corresponds to the ferritic phase with IS = (0.02 ± 0.02) mm/s and the distribution of the hyperfine magnetic field distribution with a mean value of B = (31.7 ± 0.5) T. When annealing in a nitrogen atmosphere, the ratio of austenitic and ferritic phases varies from 8 : 92 for unannealed powder through 48 : 52 at an annealing temperature of 700 °C to 0 : 100 at annealing temperatures greater than 900 °C. The content of the austenitic phase gradually decreases with the annealing temperature in the oxidizing atmosphere, and at temperatures higher than 900 °C, the austenite completely disappears. Simultaneously, with increasing annealing temperature, oxides Fe_3O_4, α-Fe_2O_3 and wüstit are formed. The parameters of the Mössbauer oxide spectra are close to their parameters given above for the case of CL20ES powder annealing. All phases were also identified by XRD.

TP12

RAMAN SPECTROSCOPIC STUDY OF MINERALS IN GRANITIC ROCKS

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Granite occurs in large quantities only on Earth and is the primary rock that makes up the continental crust. The study of the formation process of granite helps us to understand the evolution of the continental crust. Granite mainly consists of plagioclase, K-feldspar, quartz, biotite and hornblende. Plagioclase is a major component mineral of granite and is a solid solution of albite ($NaAlSi_3O_8$) and anorthite ($CaAl_2Si_2O_8$). The proportions of albite and anorthite in plagioclase are important data for understanding the formation of granites. These proportion data have generally been measured by electron probe micro analyzer (EPMA). However, the EPMA instrument is not available in all laboratories due to cost issues. Therefore, a simpler alternative method is needed. In recent years, Raman spectroscopy has been actively used in the field of petrology or earth sciences, e.g., [1][2][3]. A wide variety of information, such as the chemical composition of minerals, can be obtained in the microscopic region of the mineral by measuring with a microscopic laser Raman spectrometer. In this study, the Ohata granodiorite pluton in Hyogo Prefecture, southwestern Japan, was selected as a case study. Rock thin sections of granite samples were prepared, and plagioclase minerals were analyzed by a microscopic laser Raman spectrometer. The wavelength of the laser used for the measurement was 532 nm. A correlation was found between the Ca content in plagioclase and the band at approximately 280 cm^{-1}. Calibration curves were created for this band and the Ca concentration in plagioclase based on literature data. This indicates that the spectrum shifts toward lower wavelengths as the percentage of Ca in plagioclase increases. In the future, more data on the calibration curve may allow for a more accurate composition determination of plagioclase.

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TP13

THE LUMINESCENCE OF NIR-EXCITED UP-CONVERTING NANOPARTICLES IN THE BLOOD SOLUTION

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The use of near-infrared excitation provides low photodamage of biological materials, autofluorescence reduction, and deeper light penetration depth than in the case of UV and visible light [1]. Therefore, much attention has been paid to obtaining up-converting nanoparticles (UCNPs) doped with lanthanide ions (Ln^{3+}), which show intense luminescence even in biological fluids such as blood [2]. Nowadays, many blood experiments are carried on to determine, e.g., light penetration depth and the presence of markers for some diseases [3]. The main goal of our research was to determine the whole human blood penetration depth based on the luminescence of multi-mode NIR laser-excited UCNPs. The high-quality core/shell materials were obtained using precipitation in high-boiling-point solvents and then transferred to the water by acid treatment [4,5]. The different RE ions were used as light sensitizers: Yb^{3+} ions for 975 nm, Er^{3+} for 808, 975, and 1532 nm, or Tm^{3+} for 1208 nm covering the optical transparency windows, important for medicine. The emissions of ligand-free UCNPs were registered in the water and whole human blood at different sample depths. The effect of light absorption and scattering of blood components was observed. The conducted research allowed us to estimate the depth to which the excitation radiation penetrates the sample and how thick a layer of blood allows to observe the emission.

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TP14

SPECTROSCOPIC ANALYSIS OF LASER ABLATION PLASMA IN LIQUID DURING NANOPARTICLES SYNTHESIS

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On-line and real time monitoring of the nanoparticles (NPs) production process is one of the most important tasks for fabrication of NPs with the desired parameters. In the present work, the experiments demonstrating the feasibility of the laser-induced breakdown spectroscopy (LIBS) as a monitoring technique for the NPs detection in solution including the control of NPs stoichiometry were carried out. LIBS was used in two different ways: (i) for the spectroscopic analysis of laser ablation plasma and (ii) for the determination of the formed NPs composition. The laser ablation experiments were carried out by using the radiation of a Nd:YAG laser (LOTIS TII, LS2134D), operating in a double-pulse mode at 1064 nm (energy 80 mJ/pulse, pulse duration 8 ns). Plasma emission spectra were detected using a grating spectrometer equipped with an ICCD linear array.

As the examples, the LIBS spectra of Ag, Si and Zn NPs in colloidal solutions formed during laser ablation were examined enabling the chemical identification and stoichiometry analysis of the formed compound NPs. The NPs were characterized on-line directly in the solution. The limit of detection (LOD) for Ag particles was estimated to be around 50 ppm of silver. Stoichiometry identification was achieved by using the comparative analysis of spectral line intensities related to the particles components and calculating the elemental composition of a sample in comparison with the analogous certified sample ablated in the same conditions. The quantitative values obtained correlated well with the results derived from the energy dispersive X-ray spectroscopy analysis.

Spectroscopic analysis of the laser ablation plasma during Si NPs preparation allowed elucidating the possible mechanisms of SiC NPs formation in the mixture of Si and C colloids, that can be associated with the interaction of either silicon and carbon NPs in the mixture [1] or silicon species with ethanol and its decomposition products. Optical emission spectra showed that laser ablation in ethanol resulted in the observation of mainly silicon atomic (390.55 nm) and ionic (385.61 nm, 413.10 nm, 505.61 nm) lines while the intensities of the molecular lines of ethanol decomposition products (e.g. C_2 Swan bands) were low.

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TP15

CHARGE ORDERING AND HYPERFINE INTERACTIONS IN MAGNETITE AT LIQUID HELIUM TEMPERATURE

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Magnetite as a typical representative of ferrimagnetic iron oxides is a material with mixed valence. Its cubic crystal lattice of the Fd-3m space group contains 8 formula units in the elementary cell. Its formal valence composition can be written as $(Fe^{3+})A[Fe^{3+}\ Fe^{2+}]BO_4$, in which A denotes the tetrahedral and B the octahedral sublattices of the spinel structure. Around the Verwey temperature TV ~ 125 K, a phase transition occurs, which was detected, e.g., as an anomaly in the temperature dependence of specific heat, a jump in the temperature dependence of magnetization and a jump of two orders of magnitude in the temperature dependence of electrical conductivity [1]. When studying magnetite above TV using 57Fe NMR [3], no difference was observed between Fe^{3+} and Fe^{2+} ions in the B-sites of the crystal lattice, which indicates a delocalized character of charge carriers and is in agreement with previous NMR experiments and Mössbauer spectroscopy [2].

We collected 57 Fe NMR and Mössbauer spectra of a monocrystalline plate of magnetite with a diameter of ~3 mm and thickness of ~40 µm at liquid helium temperature. In the Mössbauer spectroscopy experiments, the sample was cooled at zero external magnetic fields and in the field of 6 T. After cooling without the applied field, the magnetization is perpendicular to the plane of the sample, i.e., parallel to the direction of the γ-rays, which results in the suppression of the intensity of the 2nd and 5th line of the sextets. The NMR spectra provide higher resolution and enable determination of the hyperfine fields of all inequivalent iron crystallographic sites of magnetite in the Cc structure below the Verwey transition (8 A and 16 B-sites) [4]. These values were used in the analysis of the Mössbauer spectra as fixed parameters, which allowed us to determine the isomer shift and quadrupole splitting of the three sextets with the lowest hyperfine fields.

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TP16

ZN AND FE IN VEGETABLES: SIMULTANEOUS DETERMINATION USING HR-CS GF-AAS

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As the most often deficient elements in human diet, Fe and Zn have stayed in the spotlight of both nutritionists and analytical chemists. Knowledge of their content in foodstuffs is very important and so are the methods for their determination.

Here we present a new method for simultaneous determination of Zn and Fe using high-resolution continuum source (HR-CS) graphite furnace AAS in a single shot.

Unlike the traditional line-source AAS, this technique monitors not only the spectral line of the analyte, but also its surroundings. This allows monitoring multiple nearby lines at once. Here, secondary lines of Zn and Fe at 307.588 and 307.572 nm, respectively, were chosen for the co-determination. The temperature program was optimized to be short (90 seconds) and yet to atomize both analytes under optimal conditions due to two-step atomization.

As the selected lines are rather weak, sensitivity in terms of characteristic concentration was 125 $\mu g.L^{-1}$ for Zn and 500 $\mu g.L^{-1}$ for Fe. Such sensitivity actually corresponds to the typical concentration of the elements in the digests of many foodstuffs, including vegetables.

We applied the method to the set of samples of vegetables obtained from private gardeners and also from local markets. Some digests of the samples were analyzed also with ICP-MS for checking the trueness of the developed method. According to the results, the mean content of Fe in lettuce (n=52) was 6.8 ± 3.0 $mg.kg^{-1}$ (fresh weight) and 3.5 ± 1.6 $mg.kg^{-1}$ in the case of Zn. Although the variances were slightly wider among samples of home-grown vegetables compared to store-bought, the difference was not statistically significant, nor was the difference in total contents of the elements.

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TP17

ALKALOID FAGARONINE AND ITS INTERACTION WITH NON-CANONICAL DNA STRUCTURES

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Fagaronine is a rare member of the benzo[c]phenanthridine alkaloid family that can be extracted from the roots of the *Fagara zanthoxyloïdes* plant or produced synthetically. Several benzo[c]phenanthridine alkaloids have already been shown to have a stabilizing effect on non-canonical structures, in particular on g-quadruplexes, which are secondary DNA structures occurring on guanine-rich sequences, especially at the ends of telomeres. Increasing the stabilization of these structures can inhibit DNA replication or transcription, which can result in a significant reduction in cell division. For this reason, g-quadruplexes have become a popular target in the search for new anticancer drugs.[1]

In this work, the interactions of fagaronine with parallel, antiparallel and hybrid g-quadruplexes were measured, some of which occur on human telomeres. We measured that fagaronine significantly stabilized all 3 types of g-quadruplexes, while parallel G4s were stabilized by up to 30 °C, which is our highest stabilizing effect measured so far.

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TP18

SIMULATIONS RADIOFREQUENCY FIELD OF MULTIPLE-REFLECTION TIME-OF-FLIGHT MASS SPECTROMETER

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Multiple-reflection time-of-flight mass spectrometer (MR-TOF MS) is being built in Flerov Laboratory of Nuclear Reactions in Joint Institute of Nuclear Research in Dubna. MR-TOF MS will help to determine mass of superheavy elements produced there. To measure mass of produced superheavy nuclei, those nuclei have to be slowed down first. This is done using cryogenic gas stopping cell (CGSC). After stopping the ions are then guided from the CGSC to the MR-TOF MS using a radiofrequency (RF) funnel. RF funnel is an ion guide that consists of 76 individual ring electrodes with a decreasing inner diameter from 266 mm to 5 mm towards the extraction nozzle. Between neighboring electrodes, a 180° phase-shifted radio frequency is applied that creates a repulsive electric field force to prevent the ions from hitting the electrodes [1]. At the end of RF funnel there located extraction radio-frequency quadrupole (RFQ) consisting of 86 individual electrodes, which extracts the ions from the RF funnel. This paper deals with development of RF funnel and extraction RFQ. Optimal RF field in RF funnel and RFQ was simulated using COMSOL Multiphysics and NI Multisim. Circuit layout was then designed and optimized using data from simulations.

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TP19

A BRIEF STUDY OF PLASMA PLUME PARAMETERS FROM LASER ABLATION OF MICA UNDER ARGON AMBIENT

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Laser-Induced Breakdown Spectroscopy (LIBS), one of the prime techniques for elemental analysis, is here used to study the plasma plume parameters for mica, as the technique requires no sample treatment and is relatively fast to analyze [1].

The plasma plume generated by a Nd-YAG laser (at 532 nm) by ablating the mica sample was studied using a broadband echelle spectrometer (ME5000, Andor) equipped with an ICCD camera (iStar DH743, Andor). The chosen gate delays were ranging from 300 ns to 3000 ns. The measurements were carried out at 8 different spots on the sample surface with an accumulation of 50 spectra in each of them. An argon gas flow was maintained for a better quality of the emission spectral signals.

The present study analyses the plasma temperature using Boltzmann plots, and determines the electron density using the Stark Broadening method for various elements (K at 766nm, Al at 396 nm, Si at 288 nm, and Si at 390 nm) as a function of the gate delay for a precise calibration-free LIBS analysis [2]

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TP20

MERCURY IN VARIOUS TOBACCO PRODUCTS

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The toxicity of various types of mercury, as well as the risk of its decomposition in the environment, have been widely described in the scientific literature. As a result, Hg can be found in a variety of natural products, such as food. Tobacco deserves special attention due to the high toxicity of mercury vapor and its reported emission during combustion processes. Smoking conditions appear to be particularly favorable for the release and targeted delivery of volatile Hg into the lungs of consumers. This study examined a wide range of inhaled tobacco products, including 37 cigars, 5 cigarette, 4 pipe tobacco and 5 bidi brands. Cold vapor - atomic absorption spectrometry was employed to perform the analysis, which was done on a solid homogenized sample. The amounts of Hg in the studied materials ranged from 8.4 to 41 µg/g. Cigarettes were also identified as one of the tobacco products with the highest mercury levels among those analyzed. The majority of samples contained more than 20 µg/g of Hg. It was estimated that such concentrations could contribute significantly to total consumer exposure since it is believed that all mercury would be released to smoke.

TP21

APPLICATION OF SPECTROSCOPIC METHODS FOR ANALYSIS OF HUMIC ACIDS' INTERACTIONS WITH ALUMINIUM(III)

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Humic acids are surface reactive and redox active component of soils and sediments that affect the mobility and speciation of various metals and metalloids, as well as non-humous organic compounds [1-3]. Since humic acids are insoluble in acidic solutions, their ability to complex aluminium(III) from solutions has been challenged under these conditions. Highly heterogenous and rich in oxygen-containing groups (e.g., carboxyl, hydroxyl and carbonyl) [4], humic acids showed great affinity towards aluminium at pH 3, achieving the sorption equilibrium after 500 min with reaction order of 3.6. Spectral properties of purified humic acids did not show any significant deviation from those obtained commercially (Sigma-Aldrich). The data on non-complexed, free aluminium concentration in solution obtained using flame atomic absorption spectrometry indicated up to 67% separation efficiency by humic acids when initial concentration of aluminium in solution was below 10 mg.L^{-1}. Thus, the surface phenomenon of chemisorption most likely plays significant role in aluminium mobility in acidic natural matrices containing humic acids.

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TP22

TEMPERATURE DEPENDENT LUMINESCENCE OF $FS_2@NAYF_4:YB^{3+}/ER^{3+}$ NANOCOMPOSITES

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Temperature is one of the fundamental physical properties that influence investigated materials' optical properties. Iron sulfides are semiconducting materials composed of world abundant elements, i.e. Fe and S. Iron sulfides can be present in several different types in nature, i.e. troilite (FeS), pyrrhotite ($Fe_{(1-x)}S$, x=0-0,2), pyrite (FeS_2), marcasite (FeS_2), or greigite (Fe_3S_4) with different composition, crystal structure, and physicochemical properties [1]. Different iron sulfide materials can be easily obtained via the optimized hydrothermal method. These materials absorb light in a broad range of the spectrum from UV-NIR. Additionally, nano-sized iron sulfides exhibit weak plasmonic properties that can be utilized in novel optoelectronic materials.

Sodium yttrium fluoride is a well-known matrix for luminescent materials. After doping with a pair of Yb^{3+} and Er^{3+} ions, the material shows great upconversion (UC) luminescence properties. β-$NaYF_4$ is superior in UC due to the low phonon energy responsible for the non-radiative relaxation. UC is an energy conversion process where one high-energy photon is emitted after excitation with two or more low-energy photons. Here, after excitation with Yb^{3+} ions with $\lambda = 975$ nm laser, characteristic emission bands of Er^{3+} ions can be observed. The Er^{3+} ions have thermally coupled levels (TLC), which intensity is temperature-dependent. The intensity of the band at $\lambda \approx 525$ nm increases relatively with increasing temperature [2].

Here, the $NaYF_4$: Yb^{3+}/Er^{3+} nanocrystals and $FS_2@NaYF_4:Yb^{3+}/Er^{3+}$ nanocomposite were synthesized. The photophysical properties of both materials were compared. The FeS_2 absorption properties and UC luminescence of $NaYF_4$: Yb^{3+}/Er^{3+} were combined. The influence of temperature on the UC luminescence properties for both materials was investigated. The presented results show the potential application of obtained nanocomposites as novel luminescent contactless thermometers.

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TP23

ISOTOPIC LABELING OF MICROALGAE: RAMAN STUDY

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Autotrophic microalgae can produce a number of substances such as polysaccharides, lipids, proteins, carotenoids, polyphosphates, or crystalline purines directly from inorganic sources. Different microalgal species are used for the economic production of high-value products. Due to their autotrophic nature, microalgae can biosynthesize complex isotopically labeled biomolecules from simple isotopically labeled inorganic substances. Analysis of the chemical composition of microalgae by means of chemical-analytical methods is relatively complex, time-consuming, and laborious. Confocal Raman microscopy (CRM) represents practical optical method by which the biosynthesis of isotopically labeled compounds can be monitored *in situ*, i.e. directly within intact cells [1]. The CRM combining confocal optical microscopy with Raman spectroscopy enables fast and non-destructive analysis of the chemical composition of substances in the investigated objects, including the effect of isotopic labeling. The chemical composition of the investigated objects is reflected by their Raman spectra, in the case of Raman mapping of microscopic objects by their chemical maps.

In this work, two specific cases of isotopic labeling were studied, namely the effect of heavy water (deuteration) and ^{15}N-enrichment of biomolecules in living cells of the marine dinoflagellate *Amphidinium carterae*. The main result was the detection of variously deuterated and ^{15}N-enriched forms of crystalline guanine depending on the ratio of D_2O/H_2O and $^{15}N/^{14}N$-labelled nitrates in the culture medium and the determination of the mean degree isotopic labeling by comparison of the biosynthesized guanine with synthetically prepared isotopic forms of guanine. An interesting and valuable discovery, which was not originally the intention of this work, was the finding of unexpected persistence against the dissolution of nanocrystalline guanine even in highly diluted solutions.

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TP25

SYNTHESIS OF GOLD NANOPARTICLES USING TETRAHYDROXY-1,4-BENZOQUINONE OXOCARBON AS A CAPPING AGENT

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The field of nanotechnology deals with the knowledge and issues associated with materials and objects usually smaller than 100 nm. Nanoparticles are basic building blocks of nanomaterials. Research of their structure, optical properties, method of preparation and processing leads to their incorporation into several areas of practical application. The interest in nanoparticles is mainly in the field of biology and medicine [1], but also in photovoltaics, photonics, computer engineering, quality control, forensic science, cosmetics, the automotive industry or materials engineering [2]. Gold nanoparticles (AuNPs) exhibit interesting optical properties due to the interaction of light with electrons located on their surface. This phenomenon is called localized surface plasmon resonance (LSPR) [3]. As a result, we can observe a strong absorption peak in the visible light region, which allows us to study nanoparticles using spectroscopic methods.

In the present study, we focused on the preparation of surface modified gold nanoparticles using tetrahydroxy-1,4-benzoquinone (THBQ) as a capping agent. We approached the synthesis by bottom-up method where nanoparticles are formed from simple inorganic precursors, most often by reducing salts containing metal atoms. The result is the successful preparation and characterization of the metal gold nanoparticles (AuNPs@THBQ). By changing some important factors during the synthesis, it is possible to control their size precisely. Using THBQ as a stabilizing and reducing agent, we obtained 45-110 nm nanoparticles that proved to have high stability even after three months. We achieved the best results and stability under the following conditions: basic environment ($pH > 8$), synthesis during boiling ($t > 95$ °C) and rapid stirring of the reaction mixture. We also determined the pK_a dissociation constants of THBQ - $pK_{a1} = 4{,}718 \pm 0{,}016$ and $pK_{a2} = 6{,}656 \pm 0{,}026$ spectrophotometrically.

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TP26

ARSENIC SPECIES IN THE AIR OF BRNO CITY PARK

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City parks are considered as a quiet green zone in contrast to the surrounding urban environment. Important and frequently discussed aspect of urban parks is their ability to purify air via deposition of particulate matter (PM) on leaves of vegetation. In this study was for monitoring of air quality chosen park Lužánky in the center of Brno, Czech Republic. PM samples were collected during two campaigns (summer and winter) in 2020. Special attention was focused on the arsenic content in PM_{10}.
Arsenic is in trace amounts always present in the environment. Because of its well-known toxicity is the total content in the air limited by law (201/2012 Sb). This limit, 6 ng/m^3 per year, applies only to the total content of arsenic and neglects the various toxicity of its different species. Inorganic species of arsenic are considered about 100times more toxic than the organic ones, whereas As^{5+} is about 6times less toxic than As^{3+}. Therefore, content of arsenic species monomethylarsonite (MA), dimethylarsinite (DMA), trimethylarsine oxide (TMAO), As^{3+} and As^{5+} captured in fraction PM_{10} were also monitored.
For determination of total arsenic content were halves of the nitrocellulose filters with captured PM_{10} digested in Teflon tubes with HNO_3 using an SW-4 microwave system (Berghof, Germany).and analyzed by inductively coupled plasma mass spectrometer Agilent 8800 (ICP-MS/MS). For separation of arsenic species were used the second halves of the filters extracted with ultra-pure water[1]. Separation was performed via high performance liquid chromatography (HPLC) 1260 Infinity II (Agilent Technologies) with anion-exchange column Hamilton PRP-X100 (250 × 4.6 mm, 5 µm pore size, PEEK), connected directly to ICP-MS/MS for detection. Because As^{3+} and TMAO coelute, was their concentration calculated by subtraction of two chromatograms of the same sample - before and after oxidation of As^{3+} to As^{5+} by H_2O_2.
The total arsenic content was in a good agreement with the sum of all determined arsenic species confirming their high water solubility during the extraction. The most abundant specie was As^{5+}. In trace amounts also As^{3+} and TMAO were detected. In samples collected during the summer period trace amounts of DMA were detected. Concentrations of MA were bellow DL in all samples.

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TP27

ATOMIZATION OF TELLURIUM HYDRIDE IN A DIELECTRIC BARRIER DISCHARGE AND ITS IN-SITU TRAPPING FOR ATOMIC ABSORPTION SPECTROMETRY

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Tellurium is an element quite rare in nature but increasingly used and vital for modern technologies such as those needed for modern communication, computing and the production of clean energy. Increased use also brings increasing demand for analytical methods for Te determination.

In this work, atomization of volatile tellurium hydride (TeH_2) in dielectric barrier discharge (DBD) atomizers was investigated using hydride generation for analyte introduction and atomic absorption spectrometry (AAS) for detection. The performance of a new DBD atomizer with sputtered electrodes coupled with power sources generating either sinusoidal or square waveform functions was optimized and compared to that of a DBD with glued electrodes supplied with sinusoidal waveform function [1]. Very similar analytical performance in terms of sensitivity (in s ng–1) was obtained for both DBD atomizers regardless of the power source waveform function used and it was also comparable to that achieved with a standard quartz tube atomizer heated to 900 °C. Similarly, the tolerance towards interferences from hydride forming elements (As^{3+}, Sb^{3+}, Bi^{3+}, Se^{4+} and Hg^{2+}) was comparable for both DBD atomizers. The limit of detection (LOD) for the coupling of flow injection HG with the DBD with glued electrodes and detection with high-resolution continuum-source AAS reached 56 ng L^{-1} while the repeatability at 5 μg L^{-1} Te^{4+} level reached 2.8% for 15 replicates of peak area evaluated from 3 pixels. A feasibility of in-situ trapping of TeH_2 in the DBD atomizer was also studied to substantially decrease LOD. Using little amount of O_2 added to the discharge gas, a collection efficiency of 50% was obtained, which seems to be promising for further studies.

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TP28

ANALYSIS OF CHEMOTHERAPEUTICS IN EXTRACELLULAR VESICLES

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Extracellular vesicles are membranous vesicles involved in many physiological and pathological cellular processes and appears to be a type of cell-to-cell communication. Vesicles are classified into exosomes and ectosomes according to the mechanism of biogenesis. Exosomes are also released by tumor cells, which can also result in response to treatment.

This pilot study was designed to investigate the possibility of detecting platinum in extracellular vesicles by ICP-MS and, in case of positive results, to determine its content. This research deals with platinum derivatives, namely cisplatin, carboplatin and oxaliplatin. These drugs are commonly used in the treatment of various types of cancer, including ovarian cancer.

Three ovarian cancer cell lines showing different sensitivity to cisplatin were used for the experiment; the naturally resistant SK-OV-3, the sensitive A2780, and the derived resistant A2780cis. The greatest extent of all excreted platinum chemotherapeutics incorporated in exosomes were detected in case of the naturally resistant line SK-OV-3. On the other hand, the lowest Pt efflux was determined in A2780cis, which has resistance acquired. However, considering the amount of platinum taken up by the cell, it turned out that sensitive A2780 cell line secreted the lowest platinum amounts.

The ICP-MS method proved to be appropriate for further research on cell-to-cell communication. From our results we may conclude that the naturally resistant SK-OV-3 cell line probably uses the mechanism of chemotherapeutic drug excretion from the cells by exosomes. In comparison, A2780cis cells also seemed to secrete exosomes abundantly, but at the same time with lower influx efficiency. Based on this fact, it can be assumed that A2780cis has a different resistance mechanism compared to SK-OV-3.

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TP29

RISK ELEMENTS IN SOILS IN SELECTED AREAS OF NORTHWESTERN BOHEMIA

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This work deals with the pollution of soils in the NW Bohemia with risk elements with special emphasis on As, Be, Cd, and Sb, as well as organic pollutants, especially polycyclic aromatic hydrocarbons (PAH) produced by coal combustion. The area of northwestern Bohemia was chosen both for its great geological diversity and also for its changes caused by extensive anthropogenic activities in the past. Agricultural land in that area has elevated concentrations As and Be, however, it is not clear if these have resulted from anthropogenic contamination or from natural anomalies in the bedrock. Contamination of NW Bohemia can come from both ore mining and processing and coal mining and combustion. In the case of coal mining and utilization, contamination by atmospheric fallout (As, Cd, Sb) could have occurred in a diffuse manner over vast areas and regardless of the bedrock, while contamination from ore mining and processing (As, Sb) can be expected to have smaller spatial impact around historical mines and smelters; both should increase upward in soil profiles. Geogenic anomalies should result in association of elevated concentrations with geological units and be homogenous in soil depth profiles. The analysis of organic pollutants will serve as a proxy for the impact of coal combustion in the area and the approximate dating of sediments.

So far, several soil profiles have been sampled in the Teplice region and in the Ore Mountains and the reference locality NW of Lovosice. The analytical methods in this work include acid extractions and analysis by ICP-MS, HPLC-MS as well as total analyses by XRF. Analyses show that many samples in the study areas have elevated arsenic concentrations, that up to now seems to point to geogenic control. The aim of this work is to distinguish natural contamination from the bedrock and the consequences of anthropogenic activities.

TP30

ALNUS GLUTINOSA SHORT ROTATION COPPICE FOR HCH CONTAMINATED AREA - CHEMICAL AND MICROBIOLOGICAL EVALUATION

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Background: Phytoremediation is one of the possibilities for removing persistent compounds like organochlorine pesticides hexachlorocyclohexane (HCH). The principle of this method is removal, stabilization, or deactivation using plants and plant-associated microorganisms [1,2]. HCH has been one of the most extensively used pesticides of the last century. The extensive production and application have led to HCH global contamination [3]. This study aimed at monitoring *Alnus glutinosa's* changes in phytohormone profiles, HCH phytoaccumulation, and rhizospheric bacterial consortia to discriminate between HCH-induced and pruning-induced stresses.

Methods: The plants of different ages (one-year and two-years-old) growing in the contaminated soil were used for this experiment. Half of the plants were pruned to simulate establishing a shrub culture. HCH isomers were determined in the plant biomass by an established method using GC/ECD. Plant hormones analysis was performed using the optimized (LOD, LOQ, linearity, repeatability, recovery, and matrix effect) LC/HRMS method.

Results and conclusion: The obtained phytohormone results are highly variable and revealed significant differences among age- and HCH- influenced groups. The accumulation of HCH in biomass is negligible, although there are significant differences depending on the age and pruning of the plants. However, the presence of the plant promotes the removal of pesticides from the soil by affecting the rhizosphere microbiota. In conclusion, according to the chemical and microbiological results, the annual plants are suitable for use as part of wetland systems with the possibility of establishing shrub culture.

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TP31

RECOGNITION OF PROTEINS USING METAL-BASED NANOPARTICLES

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The work aimed to create conjugates of antibodies with gold and silver nanoparticles with a size of 10 and 60 nanometers and apply them in multiplex analysis. The functionality of the conjugates was verified by dot-blot and visualization was performed by laser ablation with ICP-mass spectrometry.

In the experimental part, it was shown that the binding between the antibody and the metal nanoparticle does not impair its ability to recognize and bind antigen. A direct relationship between the size of the nanoparticle used and the intensity of the measured signal was also found.

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TP32

SPECIATION ANALYSIS OF TELLURIUM IN WATER SAMPLES BY SELECTIVE HG-ICP-MS/MS WITH TICL$_3$ AS PRE-REDUCING AGENT

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Tellurium is an element quite rare in the nature, however, it is gaining attention due to its use in modern technologies and concerns about increasing content in the environment. Unfortunately, determination of Te and its relevant species, tellurite (Te^{IV}) and tellurate (Te^{VI}) at concentration levels of ng L^{-1} present in natural waters has been so far a considerable challenge even for the most modern instrumentation such as ICP-MS, simply because of insufficient limits of detection (LOD). Te is an element which is poorly ionized in the plasma due to a high ionization potential, it is distributed into a number of natural isotopes and the most abundant ones, ^{128}Te and ^{130}Te, suffer from an overlap with isotopes of Xe and Ba.

Tellurium forms volatile hydride via reaction with $NaBH_4$ in acid media. Thus, hydride generation (HG) can help to increase sensitivity by improving the introduction of the analyte into the detector in the gas phase and, at the same time, separate most of the matrix. Only Te^{IV} is “hydride active”, which means that pre-reduction of Te^{VI} is needed to obtain total content. This selectivity encourages HG to be used also for Te^{IV}/Te^{VI} speciation.

A method for Te analysis in water samples based on HG-ICP-MS/MS is presented. Optimization of ICP-MS/MS parameters was performed to achieve the best possible sensitivity and minimum background. Measurement at m/z 128→128 in O_2 reaction mode (40% O_2 reaction gas with addition of 4 mL min^{-1} He for improved sensitivity) was chosen and LOD of 2.3 ng L^{-1} was obtained for conventional sample solution nebulization. Xe interference was eliminated in O_2 mode.

HG was performed from 3M HCl by 2% $NaBH_4$. A setup using a standard autosampler and ISIS-3 flow injection unit allowed fast automated Te determination. Hydride was selectively generated from Te^{IV} or sum of Te^{IV+VI} was measured after pre-reduction of Te^{VI}. For Te^{VI} prereduction, $TiCl_3$ was found a fast and efficient pre-reducing agent. An optimization of $TiCl_3$ concentrations and kinetic study of pre-reduction involving the common agents used for sample stabilization (HNO_3, HCl and EDTA) was performed. Under optimal conditions, this method reached a LOD of 0.013 ng L^{-1} Te and an intra-day repeatability of 5.2% (5 ng L^{-1}, n=10).

The method was applied to the speciation analysis of CRMs of river and sea water (SLRS-4, SLRS-6, AQUA-1, NASS-7, CASS-5 and CASS-6), bottled mineral waters and samples taken from Lake Geneva. Our results in the single to sub ng L^{-1} Te range appear to be on the lower side of the wide spread of so far published values for natural waters.

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TP33

ANALYSIS OF HIGH-MOLECULAR SELENIUM SPECIES IN LACTIC ACID BACTERIA

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Selenium's nutritional deficiency in many countries leads to the various ideas of how to eliminate it as naturally as possible. One of the ways is the preparation of functional foods containing selenium. In our work we focus on the preparation of fermented dairy products enriched with selenium and our approach is based on the strategy "one yoghurt a day" instead of "one pill a day" is more pleasant for the consumer, considering the average consumption of milk and dairy products is around 250 kg per person, per year in the Czech Republic.

Lactic acid bacteria (LAB), such as *Lactobacillus*, *Streptococcus*, *Enterococcus* and *Lactococcus* strains has shown the ability to accumulate and transform the inorganic selenium into organic forms, such as selenoaminoacids and its derivatives. These low-molecular weight selenium species obtained from samples by enzymatic extraction are widely studied, but the original proteins have not been much described yet. In addition to proteins, selenium can also be bound to polysaccharides, which form another category of high-molecular selenium species. Preliminary data aimed at characterization of high-molecular selenium species produce by LAB are presented.

The species fractionation was realized by size exclusion chromatography (Superdex 200 column) and selenium was detected using inductively coupled plasma mass spectrometry. The fractionation revealed four major fractions with approximate masses of 12 kDa, 26 kDa, 57 kDa and 120 kDa if water and surfactant-assisted extraction were used. Alkali-assisted extraction lead to higher extraction efficiency, but only two fractions outside the column separation range (>600 kDa and <10 kDa) were observed. Individual fractions were isolated and characterized in terms of its selenoamino acids profile.

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TP34

RAMAN SPECTROSCOPY OF METAL OXALATES

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Oxalic acid (ethanedioic acid) is a reducing agent, and its conjugate base, oxalate, is a common chelating agent for cations, especially metal ions. Metal oxalates can be either synthesized or are a common product of biochemical processes in organisms. In recent years, many new natural oxalate biominerals were discovered and several new oxalate compounds were synthesized [1]. To support the progress of discovering new oxalate species, both in natural and laboratory environments, this work was aimed at obtaining Raman spectra of chosen metal oxalates (Ca, Mg, Fe, Cu, Al, Ni, and Co).
In our study, all synthetic materials were purchased from Alfa Aesar. The purity of materials was not checked by X-Ray diffraction. Raman spectra of synthetic oxalates were obtained by DXR3xi Raman Imaging Microscope (Nicolet) equipped with a 785 nm laser. Strong signals in the region 1400-1600 cm^{-1} of Raman shift are generally considered the most diagnostic feature of oxalate compounds. The positions of the strongest signals of studied metal oxalates in the 1400-1600 cm^{-1} region were: calcium(II) oxalate monohydrate [1464 cm^{-1}], magnesium(II) oxalate dihydrate [1473 cm^{-1}], iron(II) oxalate dihydrate [1469 cm^{-1}], copper(II) oxalate hydrate [1513 cm^{-1}], aluminum(III) oxalate [1441 cm^{-1}], nickel(II) oxalate dihydrate [1477 cm^{-1}], and cobalt(II) oxalate anhydrous [1505 cm^{-1}]. Spectra were interpreted raw without any post-process. Band positions of calcium, magnesium, iron, and copper oxalates are in decent agreement when compared with Raman band positions of their natural analogues [2].
The clarification of metal oxalate band positions can assist in the progress of new metal oxalate biomineral species discoveries.

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TP35

THE SPECTROSCOPIC STUDY OF KINETIC PROPERTIES OF Pb(II) COMPLEXES WITH PHOSPHONIC ACID DERIVATIVE LIGANDS

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Pb(II) has been gaining popularity in various scientific fields – for example, in biomedicine for its potential to be a cancer-treating theranostic agent (in which ^{203}Pb can be used for tumor visualization and ^{212}Pb for tumor treatment) in the form of Pb(II) complexes of macrocyclic ligands. Macrocyclic ligands containing pendant arms with phosphonic/phosphinic acid-based groups enable greater structural variability of the macrocyclic complex as well as variability in the physico-chemical properties of the Pb(II) complex. In order to develop macrocyclic complexes with the desired properties for medicinal purposes, the kinetics and thermodynamics of the complexes must be well-understood. This poster presents a detailed kinetic and thermodynamic study of Pb(II) complexes with cyclen-based macrocycles containing one (DO3AP^{ABn}, DO3AP^{PrA}, DO3AP) or four (DOTP, DOT^{Ph}, DOTP^{Ph}, DOTP^{OEt}) phosphonic acid derivative pendant arms. The ligand DOTA, which contains four acetic acid pendant arms, is used as a comparison.

The kinetics of formation and dissociation of Pb(II) complexes in various pH conditions were monitored using conventional molecular absorption spectroscopy at $\lambda = 260$nm, while for very fast reactions (on the order of seconds), stopped-flow instrumentation was employed. The results for the formation kinetics indicated that complexes with ligands with one phosphonic-acid pendant arm had similar rate constants, while the formation of complexes with all four phosphonic-acid based ligands was slightly faster. The mechanism of formation was determined by doing studies with excess Pb(II) and is presented – in general, the complex is formed first as an out-of-cage complex with the pendant arms coordinating to the Pb(II) ion, which is then incorporated into the cavity through a second, slower step. The kinetic inertness of the complexes follows the order DOTA > DO3AP^{ABn} ≈ DO3AP^{PrA} > DO3AP > complexes with all four phosphonic-acid derivative pendant arms. Preliminary computational studies were done to determine any relationship between structural parameters (such as bond length) and kinetic parameters. Overall, complexes with a longer Pb-N bond length had a faster rate of formation; those with a longer Pb-O bond length had a slower rate of dissociation.

Acknowledgements
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TP36

EVALUATION OF CURRENT BENCHTOP ENERGY DISPERSIVE XRF INSTRUMENTATION IN COMPARISON TO WAVELENGTH DISPERSIVE XRF

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X-ray Fluorescence (XRF) is one of the major techniques used for elemental analysis and can be applied to many different sample matrices. XRF instruments can be divided into energy dispersive (ED-XRF) and wavelength dispersive instruments (WD-XRF), in which the ED-XRF systems generally have lower power X-ray sources and less possibilities in terms of sample introduction. Over the past years, however, the technology of benchtop XRF systems has improved tremendously leading to enhanced performance and better detection limits.

In this work, the capabilities of recent benchtop ED-XRF systems are evaluated and compared to WD-XRF systems mainly focused on quantitative analyses. A variety of elements, both light and heavier, in different polymer matrices are investigated using ED- and WD-XRF instruments and the results are critically compared on sensitivity, robustness, matrix effects, etc. Next to this, the different sample introduction options are explored, including sample preparation techniques.

This evaluation of benchtop ED-XRF instrumentation currently available in the market will help gaining insight in the possibilities of the latest instrumentation for low level quantitative analysis in polymer matrices.

TP37

DESIGN OF NEW MICROEXTRACTION PROCEDURE FOR AMMONIUM DETERMINATION

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Nessler's reagent is widely used for the ammonium determination in environmental samples, the main interfering compounds being S^{2-}, substances affecting turbidity and color of water samples and some organic compounds. Many metal ions also cause severe interference in the classical Nessler's reagent method. Various masking agents as well as separation procedures are used to improve selectivity, but this significantly complicates the determination [1]. In addition, this reagent is extremely toxic. To reduce these limitations, a new procedure based on headspace liquid-phase microextraction with optical immersion probe HS-LPME-OIP for the determination of ammonia has been proposed. 5 mL sample solution was heated firstly up to 50^{o}C. Then NaOH with the final concentration of 0.15 M in the donor phase was added with the help of the syringe to start NH_3 evaporation. Mixing speed was fixed at 1000 rpm. A plastic vial with immersed optical probe in 200 µL diluted Nessler reagent was fixed in the cork. Microextraction completely ended in 30 minutes. The linear range was from 0.7 to 15 mg/L, RSD ranged from 2.47% to 5.25%, analytical wavelength was equal to 400 nm.
Main ions present in the water samples, like SO_4^{2-}, HPO_3^{2-}, K^+, Na^+, Ca^{2+}in equal or more than 1000 times access, Br^-, NO_3^-, NO_2^- in 100 times access, do not cause serious interference on the microextraction. Alcohols and urea do not interfere at concentrations 2500-, and 100-times higher than ammonium present respectively for both classical method and HS-LPME-OIP. Fe^{3+} and Fe^{2+} interfere already at concentrations 10 times lower than ammonium present in the sample, microextraction procedure increases their tolerant limits 50 times. Tolerant limits for Mg^{2+} and Zn^{2+} were increased with microextraction 5 times. Propylamine does not bring serious interference at concentrations 50 times higher than ammonium present. Sulfides also affect the Nessler reagent stability at concentrations higher than 10^{-6} M, microextraction procedure completely removes this influence. HS-LPME-OIP was successfully tested on CRM, fertilizer, tap and natural water samples.

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TP38

IS DIGITAL SCANNER SUITABLE AS CHEAPER ALTERNATIVE OF A SPECTROPHOTOMETER?

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Arrays and microarrays have become increasingly popular as tools for biological research using different capture agents in arrays in order to detect DNA/RNA, proteins, carbohydrates, *etc.* [1]. This concept was also enlarged to identification and sensing of other chemical entities, *e.g.*, ions, vapours, small organic molecules, *etc.* [1,2]. Technological advances such device miniaturization in combination with CCD technology (*e.g.*, digital scanner/camera or cell phone) have enabled to measure the experimental datasets by easier way using available hardware and software tools than in lab on spectrophotometer [1].

In this contribution, it is demonstrated how the digital scanner could be employed for fast and routine analysis of some analytes in biological samples. The parameters for procedure of scanning by digital scanner have been optimized in order to treat the experimental data by newly developed software ScanQuant2. The determination of Cu(II) and ammonium ions with commercial analytical strip papers as well as 96-well plates using digital scanner shows that it can be employed as suitable alternative for classical spectrophotometer. In addition, the methodology developed for analysis of ammonium ions was also utilized for enzymatic determination of urea.

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TP39

THE ELEMENTAL ANALYSIS OF THE MUMMIES OF VÁC, HUNGARY

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Present study considers the elemental analysis of bone remains received from the Hungarian Natural History Museum. During routine restoration of the Dominican church of Vác in 1994, workers discovered a crypt that had been bricked up for over 200 years with naturally mummified bodies placed in coffins. The primary artifacts were studied by inductively coupled plasma optical emission spectrometric (ICP-OES) method that was tested previously on the bones found at the earth coal mine of Bükkábrány, Hungary. According to our preliminary results the technique is suitable for the quantitative measurement of bone remains.

Samples were photo documented and weighed prior to sample pre-treatment process, which was carried out by wet digestion at high pressure and temperature. As expected, Ca and P were found in the highest concentration and no significant different occurred regarding the macroelements. However, the microelements showed statistically different results among the groups: the levels of Mn and Ba for instance were remarkably higher compared to the others, which can indicate dietetic habits based on vegetal nutrients.

In case of the separately evaluated metals (Al, Fe, Pb, Zn) we experienced significant divergence between the samples: the female bones of Vác pointed higher concentration values than the male ones, especially for Fe, Pb, Zn. The complement of the Pb detected in the remains probably originate from occupational disease in default of protective pieces of equipment. There was an overconcentration of Al and Fe belonging to bones originating from the lignite mine, which can be explained by burial traditions, environmental effects or diagenesis. Results of present work highly contribute to the investigation of the mummies of Vác, supporting the interdisciplinary science of anthropology.

Acknowledgements

We highly acknowledge the Hungarian Natural History Museum for providing the samples. The research was supported by the GINOP-2.3.2- 15-2016-00054 and EFOP-3.6.3-VEKOP-16-2017-00008 projects. We acknowledge the Agilent Technologies and the Novo-Lab Ltd. (Hungary) for providing the ICP-OES 5100 instrument for the elemental analysis. The research was supported by the EU and co-financed by the European Regional Development Fund under the project GINOP-2.3.2-15-2016. E. Baranyai is grateful for the financial support of the János Bolyai Research Scholarship of the Hungarian Academy of Sciences and for the support of the ÚNKP-20-5 (Bolyai+) New National Excellence Program of the Ministry of Innovation and Technology from the source of the National Research, Development and Innovation Fund of Hungary.

TP40

FEATURE ENGINEERING TO IMPROVE CLASSIFICATION IN LIBS

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The high dimensionality of the modern LIBS data combined with the rapid advances in the machine learning field have resulted in an ever-greater motivation to employ advanced machine learning tools in the LIBS-based classification. Despite the ability of these methods to capture the complex data relationships, their black-box nature often leads to a low chemical interpretability of the resulting classifiers. Concurrently, employing the entire spectral information in the modelling often results in high sensitivity of the classifiers to measurement changes. Whereby a manual encoding and/or pre-selection of the problem-relevant information by a domain expert might represent an ultimate solution to these issues, considering the great number of spectral variables generated by the high-resolution instruments, the time and effort required for their processing and a great diversity of the LIBS classification problems, such an approach is simply not feasible.

Powered by a vision that an approach fusing the two worlds - expert understanding and the power of artificial intelligence - might provide a great enhancement in the current state of the art, we investigate the possibility of developing a universally appliable method for handling (high dimensional) LIBS classification data based on automatic feature engineering. The insights obtained and lessons learned in the process will be shared during the poster session.

TP41

DETERMINATION OF K AND N WITHIN FUNCTIONALIZED POLYSTYRENE BEADS FOR GLYCAN PURIFICATION

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Glycans are essential biomolecules that serve a great range of purposes in living organisms. They participate in the regulation of various physiological processes and have also proved to be associated with a number of diseases. Therefore, qualitative and quantitative analysis of structurally diverse glycans from biological samples represents an essential field for the investigation of their structure-function correlations. A straightforward method for isolation of glycans from complex samples is the usage of sulfonyl hydrazine-functionalized polystyrene (SHPS) beads. Starting from sulfonated polystyrene (PS) ion exchanger beads, production in large amount and high yield is possible. The manufacturing process involves various steps, whereat the product and all intermediate steps are usually measured by IR spectroscopy.

As IR only sustains bulk information, a LIBS method was implemented to further improve the characterization of the individual reaction products. LIBS was used to investigate single beads, especially to differentiate between shell and core of the samples. This allowed spatially resolved measurements of the elements Potassium und Nitrogen within single PS beads, which exhibit a diameter of approx. 200 µm, and serves as a prerequisite for further improvement of the synthesis procedure.

TP42

CONTRIBUTION OF THE CHEMICAL MECHANISM TO THE OVERALL ENHANCEMENT IN THE SURFACE-ENHANCED RAMAN SPECTRA OF METHYLENE BLUE

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Since its first observation, the surface-enhanced Raman scattering phenomenon has been inextricably linked to atypical behavior. To a large extent, this behavior is associated with the physical nature of this spectroscopic technique which provides the huge amplification of the observed signal of molecules. The origin of the enhancing mechanism itself is due to its complexity even after almost fifty years since its discovery not quite unambiguously deciphered. However, it can be said with certainty that on the total amplification of the observed signal of molecules adsorbed on metals, substrates are involved in several sub-mechanisms, of which the most important role is standardly assigned to the electromagnetic mechanism. This one is related, for example, to the material properties and morphology of metal substrates. On the other hand, only a minor function is attributed to the chemical mechanism, although in some specific cases, its contribution can be significant, for example in the case of molecule resonant effect. This work aims at the examination of the variability of recorded enhanced spectra of methylene blue deposited on the surfaces of gold, copper and finally composite Au-Cu structures and the assessment of the extent of each amplification mechanism to the overall observed response of the model probe.

For the listed purposes, the prepared enhancing substrates were characterized by electron microscopy, energy-dispersive X-ray spectroscopy, and visible spectroscopy. Following the adsorption of methylene blue, these described substrates were measured using a Raman microscope with three different excitation wavelengths (532, 633, and 785 nm), as well as an FT-Raman spectrometer with near-infrared excitation (1064 nm). Depending on the assumptions, characteristic manifestations of individual enhancement mechanisms were observed in the spectra, depending on specific experimental conditions such as studied surface and used excitation wavelength, with a significant degree of effect of the chemical enhancement mechanism.

TP43

NANOSCOPIC INVESTIGATION OF WOOD CELL WALLS

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One of the important raw materials in the industry is wood which is popular for its outstanding properties (e.g., strength-to-weight ratio), natural and sustainable character. The strength of the woody material comes from the micro-structure which is given by cells surrounded by their walls. Several thin layers build the cell walls and contain variable amounts of cellulose fibrils embedded in a matrix of hemicellulose and lignin. The deeper knowledge of the arrangement of the individual components within the cell wall is important for understanding the relations between how the wood behaves, growths, gets its structure and its final properties.

For wood cell walls studies, vibrational spectroscopic techniques are commonly used because they allow chemical mapping of a material; however, they are not able to reach a spatial resolution on the nanoscopic level as they are diffraction limited. To distinguish individual cell wall layers, nowadays, we can utilize the nanoscopic techniques. This group is based on the near-field approaches coupling advantages of scanning probe and infrared microscopies into one. The nano-FTIR technique works by focusing an infrared laser beam at the sharp metallic tip, which concentrates the radiation at the apex of the tip and acts as an antenna that induces a near-field between the tip and the sample surface and scatters the incident infrared radiation. To employ such nanoscopic techniques for the investigation of cell walls is a crucial step for determining the cell wall structure, monitoring of the mutual interactions between biopolymers and their cross-linkage.

Our study is aimed at the examination of cell walls of natural and different types of genetically modified aspen, especially at monitoring of the distribution and abundance of main constituents (cellulose, hemicellulose, and lignin) in their specific layers. Reference spectra of pure components were collected on the macroscopic and nanoscopic level in several spectral ranges and we reached a good resemblance between them. To compare the obtained data set, the characteristic wavenumbers were found for each biopolymer to differentiate them from each other. Possessing this knowledge, we can highlight areas rich on individual components employing imaging mode. Moreover, from the nanoscopic spectra using the multivariate statistical evaluation we are able to visualize variables between the studied samples.

TP44

MÖSSBAUER STUDY OF THE STAINLESS STEEL SURFACE AFTER ANNEALING IN THE TEMPERATURE RANGE 700 - 1000 °C

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Mössbauer conversion electron spectroscopy (CEMS) and secondary conversion X-ray spectroscopy (CXMS) were used as the main method for studying the surface of specimens made from CL20ES steel powder by selective laser melting. Other study methods were X-ray diffraction (XRD), scanning electron microscopy (SEM), and energy dispersive spectroscopy (EDS). Samples measuring 25x25x2 mm3 were prepared on a Concept Laser M2-cusing system (Concept Laser, Germany). After 3D printing, the samples were sandblasted with corundum powder and annealed at 700°C - 1000°C for 0.5, 1, 2, 4, 8, 16 and 32 hours in air with the step 100°C. The CXMS spectra (e.g., samples annealed for 0.5 hours in Fig. 1 (left)) of all samples contained only the singlet line of the corresponding austenitic stainless steel. These CXMS spectra are identical to the Mössbauer spectra of the starting metal powder (CL20ES) registered in the transmission geometry of the Mössbauer experiment. Changes related to oxidation in the surface layer with a thickness of about 0.5 µm were identified in the CEMS spectra. These changes were observed, for example, in the CEMS spectra of the annealed samples for 0.5 hours (Fig. 1(right)). Note that the CEMS spectra did not register on all samples. This is related to the diffusion of alloying elements to the surface of the samples where they oxidize. This process is associated with an affinity of the alloying elements (Cr, Mn) for oxygen that is greater than the affinity of iron for oxygen. A thin surface layer formed by oxides of alloying elements is formed. This layer prevents the exit of conversion electrons formed during deexcitation of 57Fe nuclei. The passage of these electrons in the material is less than 0.5 mm and the corresponding surface layer does not contain iron. Therefore, CEMS cannot be registered. A doublet with IS = 0.33 mm/s and QS = 0.55 mm/s appears in the CEMS spectra. According to the isomeric shift, this doublet corresponds to Fe3+.Using the SEM method, it was found that a new oxide layer forms on the surface of the sample due to temperature annealing. At the same time, EDS confirmed an increase in the concentration of alloying elements (Cr and Mn). XRD identified Cr2O3 and Mn2NiO4 on the surface for samples annealed at 1000°C. According to the literature, Cr in Cr2O3 may be partially substituted for iron, which may cause the existence of a doublet (IS = 0.33 mm/s and QS = 0.55 mm/s) in the CEMS spectrum. SEM showed an inhomogeneity of the emerging surface layer, which unfortunately results in difficulties in the registration of CEMS spectra. CEMS spectra could not be recorded at all in some samples, and the shape of these spectra shows a certain chaos.

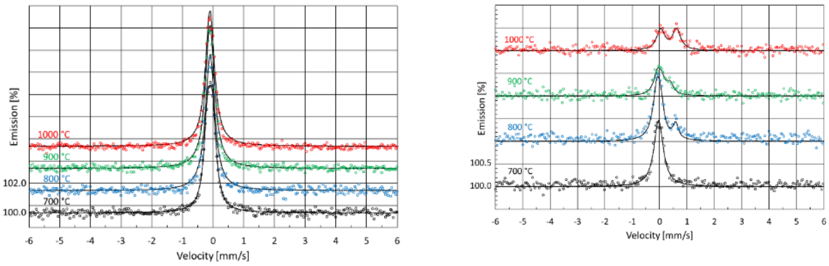

Figure 1. CXMS spectra of annealed samples for 0.5 hours at different temperatures (left) and CEMS spectra of annealed samples for 0.5 hours at different temperatures (right).

TP45

LASER-INDUCED BREAKDOWN SPECTROSCOPY IN ANALYSIS OF ALGAE CONTAMINATION ON THE FILTER

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The heavy metal contamination of algae on a filter was directly monitored with laser-induced breakdown spectroscopy (LIBS) as a demonstration of LIBS capabilities. To enhance the LIBS sensitivity, single or double pulse arrangements employing 1064 and 532 nm lasers, noble gasses or nanoparticles were tested. Liquid samples of the green alga Desmodesmus subspicatus were intentionally contaminated with chromium, nickel or zinc, incubated, filtered, and the filters with the algae were analysed. Also laser ablation inductively coupled plasma mass spectrometry (LA-ICP-MS) was used for comparison and (ICP-MS) was used as a reference method. One half of the filter with the algae was dissolved and analysed as a solution with ICP-MS and the second half was subjected to the LIBS and LA-ICP-MS analysis. The metals were attributable to the algae contamination and detectable with LIBS. The results from the LIBS provided almost equivalent information about the relative changes of the contaminants concentration in the algae. The LIBS sensitivity with a Czerny-Turner spectrometer was fully comparable with the ICP-MS procedure. The LIBS trends were more similar to the LA-ICP-MS ones. The algae growth inhibition in dependence on the contaminant content, number of cells and the rate of cell contamination can be alternatively monitored with LIBS instead of the complicated procedure in ICP-MS analysis.

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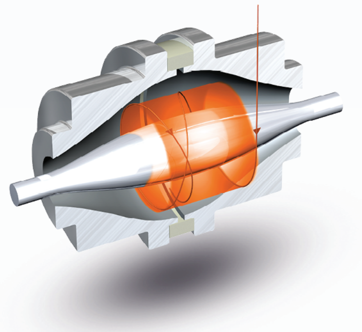

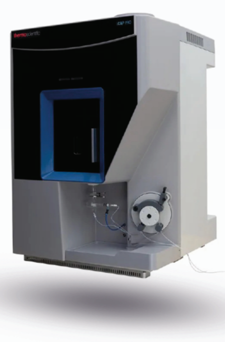

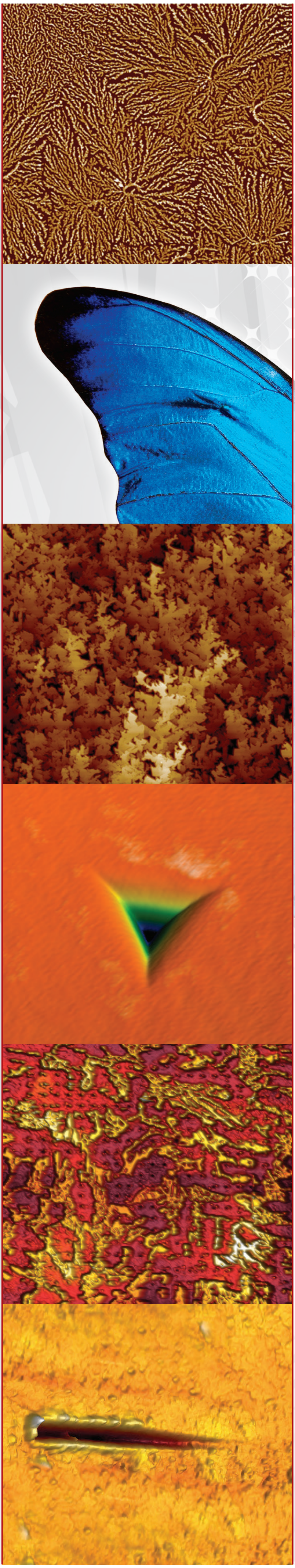

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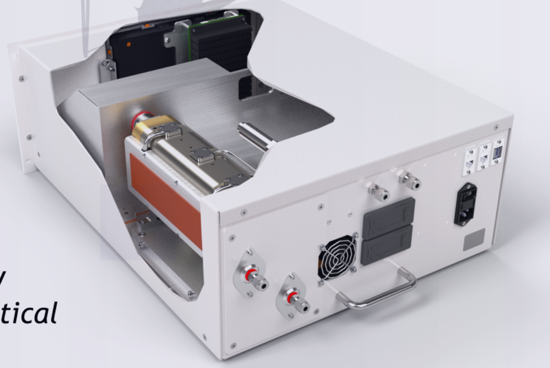

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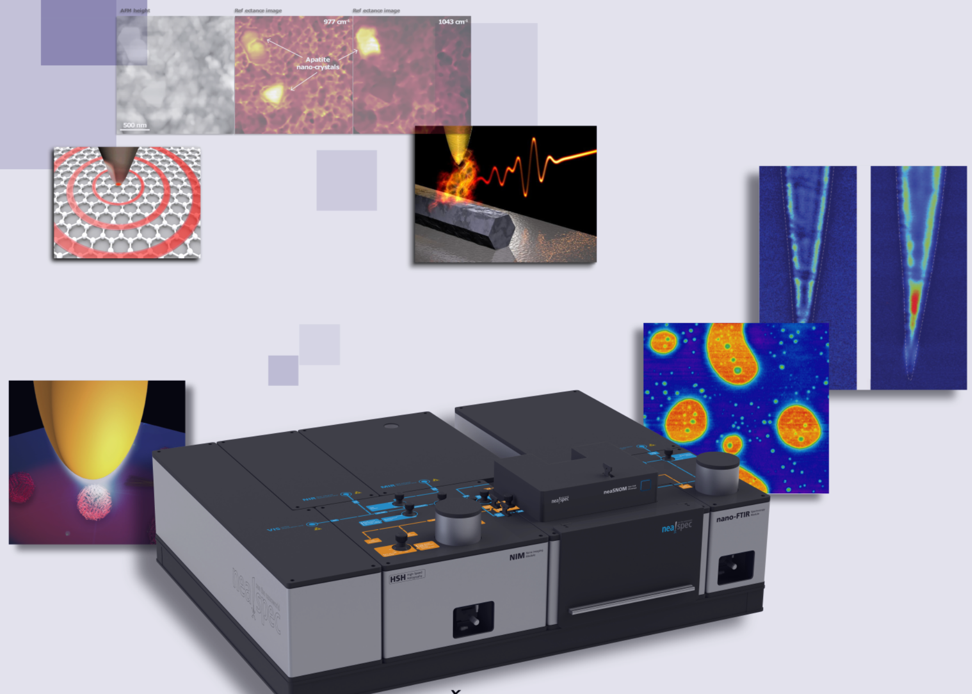

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- Prostorové rozlišení až 0.2 μm

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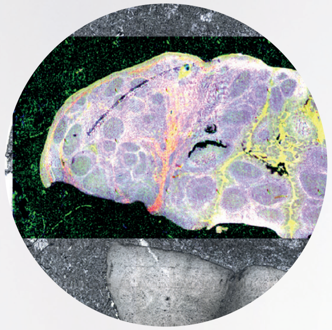
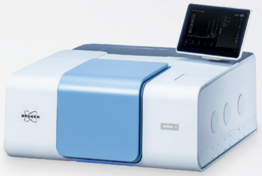
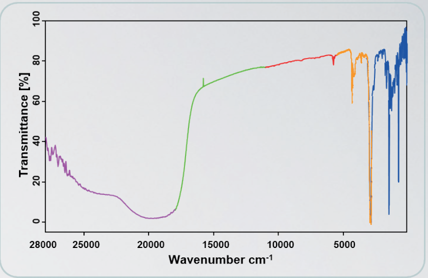


Flexibilní multispektrální analýza (spektrometr INVENIO-X)

- Kombinace až 3 děličů, 4 zdrojů a 7 detektorů na jednom zařízení
- Automatizované měření a přepínaní mezi komponentami v regionech UV, VIS, NIR, MIR, FIR
- Automatické spojování spekter z různých regionů

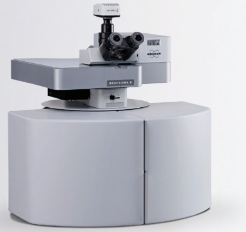


FTIR spektrometr INVENIO-X a multispektrální měření

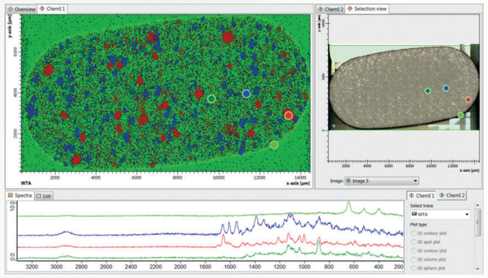


Hybridní Ramanův mikroskop (SENTERRA II)

- Kombinace disperzní a FT-Ramanovy spektrometrie na 1 zařízení
- Kombinace až 4 různých laserů
- Rychlé mapování až 100 spekter/s



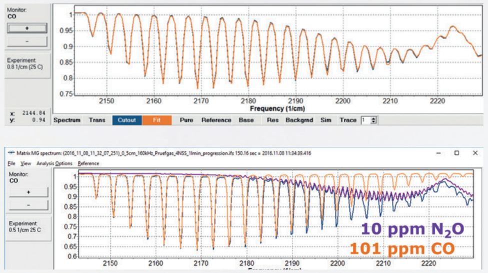
Mapování tablety Ramanovým mikroskopem SENTERRA II



Bezkalibrační analýza plynů (analyzátory MATRIX-MG a OMEGA)

- Unikátní software OPUS GA s algoritmem nelineárního fitování
- Přesná kvantifkace plynů na základě 1 referenčního spektra
- Referenční spektra 300 nejčastějších plynů součástí přístroje

Analyzátor OMEGA a bezkalibrační kvantifikace CO



Monitor: CO

Experiment: 0.8 1/cm (25 C)

x: 2144.84
y: 0.94

Matrix MG spectrum: (2016_11_08_11_32_07_251)_0_5cm_160kHz_Pruefgas_4NSS_1lmin_progression.ifs 150.16 sec = 2016.11.08 11:34:39.416

Monitor: CO

Experiment: 0.5 1/cm 25 C

10 ppm N_2O

101 ppm CO

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PerkinElmer, leader v oblasti anorganické analýzy metodou ICP-MS, představil v roce 2020 první multi-kvadrupólové ICP-MS NexION 5000. Tento unikátní přístroj se čtyřmi kvadrupóly doplnil portfolio pro prvkovou analýzu o nejvýkonnější nabízené ICP-MS na trhu. Historie ICP-MS v PerkinElmer začíná v roce 1983 prvním komerčním přístrojem ELAN 250. S inovacemi přicházely další modely, až po nejnovější 4Q NexION 5000. V průměru tedy PerkinElmer představuje nový model ICP-MS po méně než 5-ti letech.

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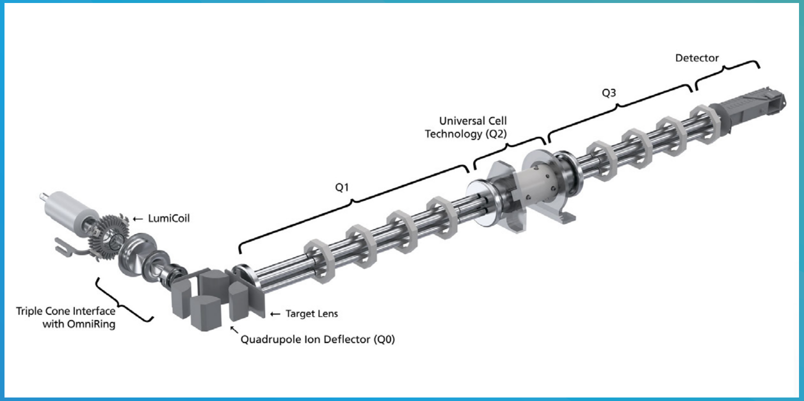
- Minimální údržba

První 4Q ICP-MS

NexION 5000



Avio 550 Max ICP-OES

Inovovaná řada ICP-OES Avio Max Series přináší unikátní funce pro kvalitnější a rychlejší měření, úsporu provozních nákladů nízkou spotřebou argonu a minimální údržbou.

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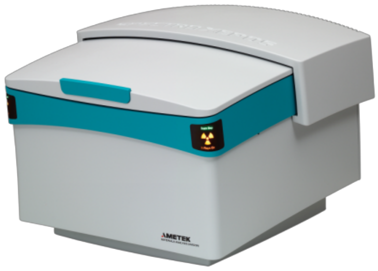

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- Malé množství vzorku pro analýzu
- Měření všech prvků v rozsahu Na - U

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- Různé typy pohledů radial, axial, DSOI
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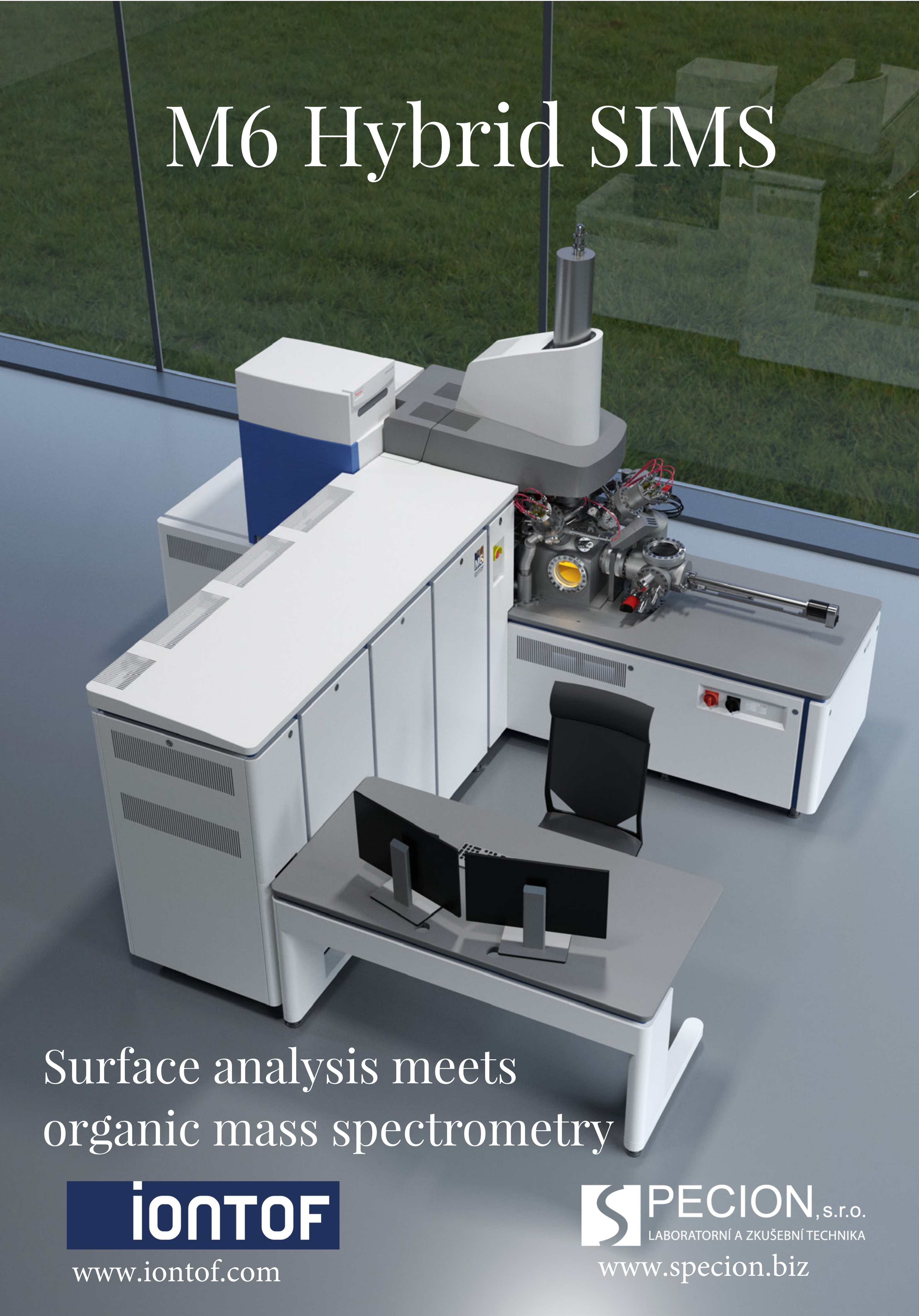

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IN MEMORIAM

On the following pages we would like to remember all colleagues and friends, excellent scientists who have left us in recent years. Although their loss is irreplaceable, at least in this form we show respect for their lives, which partly dedicated to science.

Prof. Ing. Eduard Plško, DrSc. (1930-2021)

We mourn the loss of Prof. Ing. Eduard Plško, DrSc., one of the last Czechoslovak spectroscopy pioneers, who passed away on December 7th, 2021 at the age of 91. He will be remembered as a dear friend, warm-hearted man, a distinguished scientist and respectable university teacher, founder of Bratislava Spectroscopy School, who was internationally recognized as a renowned expert in the field of atomic spectrometry. He became a member of the Commission on Spectrochemical and Other Optical Procedures for Analysis at the International Union of Pure and Applied Chemistry and served on the editorial boards of prestigious journals in analytical chemistry and spectroscopy, including Spectrochimica Acta Part B – Atomic Spectroscopy and Journal of Analytical Atomic Spectrometry. He was an honorary member of the Slovak Spectroscopic Society, Ioannes Marcus Marci Spectroscopic Society and Serbian Chemical Society. He is laureate of the Nicolaus Konkoly-Thege Medal, the Medal of Jan Marek Marci from Kronland and the Török Tibor Medal. He was an astounding polyglot with knowledge of Latin, English, German, French, Russian and Hungarian languages. Besides his professional field, he was interested in music and visual arts and well-versed in history, mathematics and astronomy, which he often implemented in his original and provocative positions on both scientific and philosophical issues.

* * *

Dr. Bohumil Dočekal (1950-2021)

Our colleague and friend Bob Dočekal lost his struggle with a serious illness and untimely passed away. Born in 1950, he graduated from the Faculty of Science of the Masaryk University in Brno in 1974 and received his Ph.D. in 1988. He spent most part of his scientific career at the Institute of Analytical Chemistry of the Czech Academy of Sciences in Brno. His work was focused on the trace element analysis in variety of materials for a broad spectrum of applications. He put a lot of effort to development of new atomic spectrometry methods including solid sampling techniques, to investigation of electrothermal devices and related trapping, vaporization and atomization processes and to investigation of toxicity of nano-particles. Bob took part in conferences all over the world to present his work and to maintain relationships with his colleagues and friends abroad. In the course of his numerous scientific stays at recognized laboratories, mainly in Germany, he was receiving high credit from the cooperating parties. He was deeply engaged in activities of the Ioannes Marcus Marci Spectroscopic Society serving as a deputy-chair and as a head of the Atomic Spectroscopy Section. Among awards he received were the Ioannes Marcus Marci Medal and a honorary membership of the Slovak Spectroscopic Society. Also his pedagogical activities should not be omitted: teaching courses at universities in Brno and in Prague, receiving associate professor degree, supervision of numerous MSc and PhD students. Bob was a wonderful person and excellent scientist. He is leaving a big gap in our spectroscopic community and is sorely missed but his legacy certainly remains.

* * *

Prof. Tibor Kántor (1930-1921)

Tibor Kántor graduated from the Technical University of Budapest as chemical engineer in 1953. His first employment was at the Central Institute of Physics, Department of Spectroscopy (1953-1959), then he received a status as research coworker in the Academic Research Group of the Technical University of Budapest, Department of General and Analytical Chemistry. From 1970, he got the rank of senior research worker and was nominated as the leader of the Spectrochemical Research Group until 1990, when he was retired officially. However, from 1991, he continued the research at the Eötvös Loránd University, Department of Inorganic and Analytical Chemistry and further at the Department of General and Inorganic Chemistry (1998-2006), financed by the Hungarian Research Foundation. He was a honorary coworker at the Spectroscopic Laboratory of Geological and Geophysical Institute of Hungary. He received doctor technicus (MSc) title in 1965, PhD in 1976, DSc (doctor of science) in 1987, and the Professor title from the Technical University of Budapest in 1990. Stipendiums in abroad were 12 months stay at the University of Houston (Texas), 1973-74 and 6 months stay at the University of Florida (USA), 1981-82. The most significant scientific results might be: the vaporization process in the emission spectroscopy (1969-1974); Introduction of: the graphite-arc vaporization technique for sample introduction into flames (1973), laser ablation into flames (1976), new interpretation of the releasing effect in flame spectrometry (elimination of aluminium interference on calcium) (1987), halogenation reactions with halocarbon vapors in d.c. arc (1980), flame (1983), graphite furnace (1983), ICP (1994) and combinations of these sources, interpretation of the aerosol formation in the electrothermal vaporization and in part laser ablation (1987). He is a member of the Editorial Advisory Board of Spectrochimica Acta Part B from 1987, chairman of the Spectrochemical Association of the Hungarian Chemical Society (1995, 1996). He was granted with the Tibor Török Award by the Hungarian Spectrochemical Association (2002), with the Jerzy Fijalkowski Award by Committee of Analytical Chemistry of Polish Academy of Sciences (2009) and with the Nicolaus Konkoly Thege Award by the Slovak Spectroscopic Society (2010). We all keep him in our memories with respect and love.

* * *

RNDr. Zdeněk Slovák, CSc. (1937-2019)

RNDr. Zdeněk Slovák, CSc., an excellent all-round analyst and spectroscopist, started studying chemistry in 1955 in Brno at the Faculty of Science of (today's) Masaryk University. As part of an academic student Exchange from 1956 to 1961, he studied chemistry in Germany at the University of Leipzig as a graduate chemist. After his return, he was awarded the degree of "prom. chem." at the University of Brno in 1961. His first internship was at the Research Institute of Macromolecular Chemistry in Brno in the Analytical Chemistry Department, where he developed unique coulometric methods for the determination of water and strongly reducing substances under the supervision of Ing. M. Pribyl, CSc. In 1963-1966, this topic then became the focus of his external postgraduate studies with Prof. Dr. A. Okáč at the University of Brno, where, after graduation, he received the title of RNDr. together with the title of CSc. In 1962-1965, he also completed a special postgraduate course in analytical chemistry at the University of Chemical Technology under the guidance of Prof. Dr. F. Čůta as a "specialist engineer". From 1966 until his retirement he worked at the Research Institute of Pure Chemicals (Lachema Brno), in the department of analytical chemistry. He worked on the characterization of reagents for spectrophotometry, he studied analytical properties of selective sorbents based on glycol methacrylate gels with target-bound analytical functional groups, except AAS, OES and the analysis of materials for microelectronics and modern ceramics, in etching baths, in the production of platinum cytostatics and testing of clinical materials, in intermediate products of precious metals and rare earth processing, in hazardous waste, etc. He has served on the SSJMM main committee and presidency, and has organized courses, seminars and conferences. In October 2002 he suffered a stroke with permanent consequences. He died in January 2019.

* * *

Prof. Bernhard Welz (1936 - 2018)

It was unexpected and bad news that was hard to cope with: on June 2, Prof. Bernhard Welz died in a hospital in Florianópolis from health complications following his car accident in April 2018. Bernhard was born in Augsburg and graduated in chemistry from the University of Stuttgart in 1966. His professional career was from the outset linked to atomic spectrometry and the Perkin Elmer Überlingen company located near Lake Constance. From 1982 he worked for 16 years as director of the company's applied research department. After a major reorganization of the company in 1998, he refused to become a contented retiree and at a ripe age started a new phase of his life on a new continent - first as a visiting professor at the universities in the Brazilian states of Santa Catarina and Bahia and since 2003 as an outstandingly successful "Voluntary Professor" at the Federal University of Florianópolis (Santa Catarina). During his scientific career, Bernhard has left his imprint on a number of atomic spectrometry disciplines, contributing to the development of a commercial graphite atomizer, collaborating on the development of the STPF concept for use with this atomizer, including the design of a universal modifier, and the coupling of flow injection analysis with AAS. His contribution to the development of hydride generation cannot be overlooked. Even before his move to Brazil, he recognized the potential of a continuous radiation source for high-resolution AAS and has spent the last twenty years mainly on applications of this technique, including its extension to molecular absorption spectroscopy. Without wishing to slide into scientometrics, it is worth adding that Bernhard was the author of a huge number of widely cited publications. In particular, he came to the attention of the wider scientific community by authoring the basic monograph on AAS (latest edition 1997, together with M. Sperling) and also by co-authoring (together with the group of H. Becker-Rosse) the first monograph on AAS with a continuous source in 2005. In 1988, his contribution to the development of spectroscopy in general and in our country in particular was awarded with the Jan Mark Marci of Kronland Medal. This was the first of many important international awards he received.

* * *

RNDr. Jiří Toman (1935-2016)

Jiří Toman studied chemistry at the Faculty of Science, University of Brno (1953-58), specializing in analytical chemistry. From 1958, as an assistant to Professor Rudolf Jirkovský, he was engaged in the analysis of metallurgical materials using optical analytical methods at the Department of Analytical Chemistry of the Faculty of Metallurgy of the Mining University in Ostrava. He taught at the VŠB for two years after his departure to Moravian Chemical Works, n.p. Ostrava in 1962. In the research centre of semiconductor materials and products of qualified chemistry of the Nový Bohumín plant, he specialised as an independent researcher in spectrochemical analysis of raw materials, intermediates and auxiliary substances for the production and treatment of semiconductor silicon and ferrites. He was also involved in spectrochemical analysis during his work at the Research Institute of Pure Chemicals (VÚČCH) Lachema, n.p., in Nový Bohumín in 1965-70 by analysing ferritic materials, battery materials and materials for nuclear technology. He also did postgraduate studies in special analytical chemistry with a focus on optical and separation methods (1965-66). Since 1970 he worked in the Analytical Chemistry Department at VÚČCH Lachema, n. p. Brno, developing methods for determination of impurities in pure preparations for analytical purposes using emission spectrography and AAS. With his colleague Dr. Zdeněk Slovák he was developing ETA-AAS for the determination of impurities in materials for advanced technologies (luminophors and auxiliaries of special purity for semiconductors, monocrystals, selective sorbents on the basis of Spheron in inorganic analysis), in Geological Survey Ostrava, Brno Branch (GPO), since 1977 he developed e.g. the first generally available atlas of rare earth element line coincidences for medium dispersion spectrometers, a gas hydride generator for both AAS and ICP-OES, and developed instrumentation and methods for ICP-OES determinations. Since 2000, Dr. Toman has worked as a consultant for LABTECH, s.r.o. for inorganic analysis and as a consultant for Jobin-Yvon ICP-OES users in the Czech and Slovak Republics. From 1962 to 2003 he served as a representative of the members of the company in the Czechoslovak Spectroscopic Society and Ioannes Marcus Marci Spectroscopic Society. He organized courses and seminars on plasma spectroscopy in cooperation with MU Brno. He was an external member of the State Final Examination Committee at the Faculty of Science of MU.

* * *

Ing. Miloslav Vobecký, CSc. (1929 - 2019)

Our long-time colleague and friend Ing. Miloslav Vobecký, CSc., founder and long-time chairman of the instrumental radioanalytical methods group, long-time member of the main committee and vice-chairman of the SSJMM in 1993-1999, has passed away in June 2019. At the turn of the 1950s and 1960s, he laid the foundations of the activation analysis group at the Department of Nuclear Spectroscopy at the Institute of Nuclear Physics of the CAS in Řež and led it until the early 1970s. Their results were recognized by the world scientific community and in 1969 they were among the prestigious laboratories entrusted with the analysis of rare rock samples from the American Apollo 11 and 12 lunar expeditions. After his forced departure from Řež in the early 1970s, he worked at the Geological Institute and later at the Institute of Nuclear Biology and Radiochemistry of the Czechoslovak Academy of Sciences. Later he worked simultaneously at the Institute of Technical and Experimental Physics of the Czech Technical University in Prague, right from its foundation in 2002. As part of his organizational activities at the SSJMM, he founded the Instrumental Radioanalytical Methods Group in 1971 and organized the IAA conference under its auspices, which brought together both local and foreign experts in the field of radioanalytical methods. The outstanding scientific achievements of Ing. M. Vobecký, CSc. in the field of instrumental radioanalytical methods and his contribution to the domestic development of this field as well as his further professional and organizational activities were recognized by both societies with the award of the Jan Marek Marci of Kronland Medal in 1980 and the Vladimir Majer Medal in 2015.

ESAS-CSSC 2022 BOOK OF ABSTRACTS

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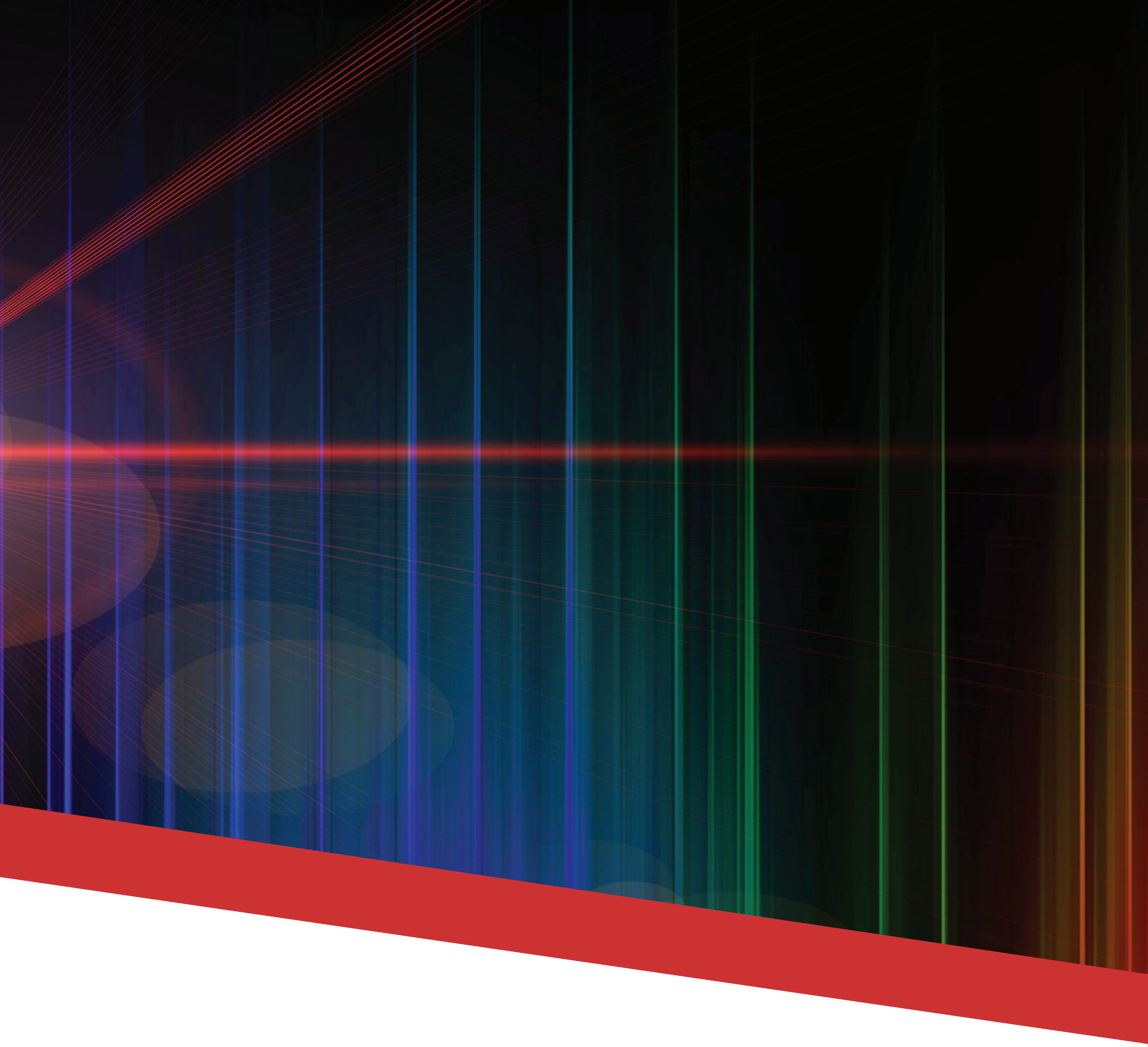

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