

## Overview by Days

Monday 25. 8. 2014

9:00 – 9:45	Official Opening
9:45 – 10:30	<b>HS 3A</b> Plenary Talk P1: Eberhard Riedle <i>Understanding complex reactive molecular processes: from kinetics to comprehensive transient spectroscopy on all relevant time scales.</i>
10:30 – 11:00	Coffee Break
11:00 – 11:30	<b>HS 3A</b> Invited Talk I1: W. Leo Meerts <i>Novel strategies for solving highly complex NMR spectra of solutes in liquid crystals</i>
11:30 – 12:00	<b>HS 3A</b> Invited Talk I2: Giorgos Voyiatzis <i>Polarized raman spectra: opportunities &amp; challenges - What about polarized SERS?</i>
12:00 – 12:30	<b>HS 3A</b> Invited Talk I3: Maurizio Becucci <i>Non bonding interactions in molecular clusters</i>
12:30 – 13:00	<b>HS 3A</b> Invited Talk I4: Alexandre Dazzi <i>Infrared Nanoscopy Applied to Microbiology</i>
13:00 – 14:30	Lunch
<b>14:50 – 16:30</b>	<b>HS 3A Session 1    Spectroscopy of Isolated Molecules I</b>
14:50 – 15:10	<u>S. Schiller</u> <i>Precision Spectroscopy of the Simplest Molecules</i>
15:10 – 15:30	José Arturo Ruiz-Santoyo, Marcela Rodríguez-Matus, <u>Leonardo Álvarez-Valtierra</u> , José Luis Cabellos, Rafael Grande-Aztatzi, José Gabriel, Merino-Hernández, John T. Yi, and David W. Pratt <i>Rotationally Resolved Electronic Spectra of the Electronic Origin and Some Vibronic Bands of Guaiacol and Mequinol: Vibrational Assignment of Low-Frequency Bands</i>
15:30 - 15:50	<u>J. Laane</u> , E. J. Ocola, H. L. Sheu, H. J. Chun, P. Boopalachandran, and N. Meinander <i>Spectroscopic and Theoretical Investigations of Molecular Vibrations and Potential Energy Surfaces in Ground and Excited Electronic States</i>
15:50 – 16:10	<u>P. Hemberger</u> , A Trevitt, T. Gerber, E. Ross and G. da Silva <i>Isomer-Specific Product Detection of Xylyl Radical Rearrangement and Decomposition Using VUV Synchrotron Photoionization</i>
16:10 – 16:30	B. Stuhlmann, <u>F. Gmerek</u> and M. Schmitt <i>Determination of the Geometry Change of Benzimidazole upon Electronic Excitation</i>
<b>14:50 – 16:30</b>	<b>HS 3B Session 3    Environmental Applications in Spectroscopy</b>
14:50 – 15:10	<u>Albert van Oyen</u> , Jan Andries van Franeker, Uwe Oppermann, Marion Egelkraut-Holtus <i>Monitoring Plastic Waste Using FTIR Spectroscopy</i>
15:10 – 15:30	G. Renner, M. Egelkraut-Holtus, A. van Oyen and <u>J. Schram</u> <i>Characterization of Plastic Marine Litter Using FTIR Microscopy</i>

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- 15:30 - 15:50 I. R. Ivascu, C. E. Matei, M. Patachia, A. M. Bratu and D. C. Dumitras *Trace Gases Photoacoustic Detection for Monitoring of Some Air Pollutants*
- 15:50 - 16:10 G. Zerbi, M. Tommasini *Vibrational Spectroscopy of Anthropogenic Carbonaceous Particles: A Difficult Problem*
- 16:10 - 16:30 A. Bagheri Garmarudi, M. Khanmohammadi, Z. Haji Seyed Razi *Crude Oil Geochemical Evaluation by Infrared Spectroscopy and Chemometrics*
- 14:50 - 16:30** **HS 3C Session 5** **Medical Applications in Spectroscopy I**
- 14:50 - 15:10 S. Turrell, A. Uwimanimpaye, C. Kinowski, C. Masselot-Robbe, F. Cardon and O. Cristini *Sol-Gel Biocompatible Porous Materials for Local Controlled Drug Release in Treatment of Parkinson's Disease*
- 15:10 - 15:30 Iryna Goncharova, Sergey Orlov, Pavlina Novotná, Marie Urbanová *Determination of the ligand-protein binding parameters by combination of circular dichroism and fluorescence spectroscopy*
- 15:30 - 15:50 S. Tamosaityte, M. Pucetaite, V. Hendrixson, Z. A. Kucinskiene and V. Sablinskas *FT-Raman Spectroscopy as a Non-Destructive Tool for Determination of Chemical Composition of Urinary Sediments*
- 15:50 - 16:10 C. Paluszkiwicz, P. Chaniecki, W. M. Kwiatek, J. Lekki, M. Rękas *Natural Lenses with Cataracts Studied by FTIR Spectroscopy*
- 16:10 - 16:30 Thorsten Vahlsing and H. Michael Heise *Spectral Bandwidth Limitations of Tuneable External-Cavity Based Quantum Cascade Lasers for Clinical Biofluid Analysis with Different Multivariate Calibration Strategies*
- 14:50 - 16:30** **HS 3D Session 7** **Theory I**
- 14:50 - 15:10 Jörg Tatchen, Reuven Ianconescu, and Eli Polak *Semiclassical Computation of Vibronic and Vibrational Spectra Beyond the Harmonic Approximation*
- 15:10 - 15:30 Jan-M. Mewes, Vladimir Jovanović, Christel M. Marian and Andreas Dreuw *Electronic Structure and Molecular Mechanism of Non-Radiative Decay of Nitrobenzene*
- 15:30 - 15:50 Stavrov, Solomon *Relationship between Structure and Vibrational Spectra of A<sub>0</sub>, A<sub>1</sub>, and A<sub>3</sub> Conformational Substates of Carbonmonoxy Myoglobin*
- 15:50 - 16:10 Güneş Süheyla Kürkcüoğlu *Theoretical Studies on the Molecular Structure and Vibrational Spectra of 2-Pyridineethylamine*
- 16:10 - 16:30 Tony Ford *The Molecular Complexes of Boron Trifluoride with Nitrosyl Fluoride and Nitrosyl Chloride. Ion-Pair Formation*
- 16:30 - 17:00 Coffee Break
- 17:00 - 19:00** **HS 3A Session 2** **Spectroscopy of Isolated Molecules**
- 17:00 - 17:20 James. R. Durig and Bhushan S. Deodhar *The Utilization of Rare Gas Solution for Making Vibrational Assignments and Conformation Stability Determinations of Three Membered Rings*
- 17:20 - 17:40 A. Stamm, M. Weiler, A. Brächer, K. Schwing, M. Gerhards *Excited state proton transfer reactions in isolated hydroxychromones investigated by different IR/UV techniques*
- 17:40 - 18:00 A. Bouchet, M. Schütz, B. Chiavarioni, M-E. Crestoni, S. Fornarini, O. Dopfer *Binding Motifs of a Microhydrated Neurotransmitter: IR*

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- Spectroscopy of Rare Gas-Tagged Protonated Phenylethylamine and its Water Clusters*
- 18:00 – 18:20 A. N. Heays, J. M. Ajello, A. Aguilar B. R. Lewis and S. T. Gibson *Fluorescence of Electron-Excited N<sub>2</sub>*
- 18:20 – 18:40 Martin Wilke, Josefin Wilke and Michael Schmitt *Manipulation of Electronically Excited States of Indole*
- 17:00 – 18:40** ***HS 3B Session 4 New Materials I***
- 17:00 – 17:20 Sloufova I., Prochazka M., Vlckova B. *Charge-Transfer Resonance Mechanism Contribution to SERS of 2,2':6',2''-Terpyridine Chemisorbed on Ag Nanoparticles*
- 17:20 – 17:40 P. Smejkal, L. Hochmann, J. Pflieger, and I. Sloufova *SERS spectral probing of laser ablated nanoparticles prepared in alcohols*
- 17:40 - 18:00 Murat Taş, Mürsel Arıcı, Okan Zafer Yeşilel *Syntheses, Crystal Structures and Spectroscopic Properties of Cadmium(II) AND Manganese (II)-Azoxybenzenetetra-carboxylate Complexes with 1,2-Bis(Imidazole-1Yl-Methyl)Benzene*
- 18:00 – 18:20 B. Kutus, A. Pallagi, G. Peintler, A. Bíró, I. Pálinkó and P. Sipos *Structure and Equilibria of Ca(II)–Gulonate Complexes Forming in Aqueous Solutions from Multinuclear NMR Spectroscopy, Potentiometry, Conductometry and Freezing Point Depression*
- 18:20 – 18:40 Maria Buchholz, Peter G. Weidler, Chengwu Yang, Hikmet Sezen, Fabian Bebensee, Stefan Heissler, Alexei Nefedov and Christof Wöll *Polarization- and azimuth-dependent Infrared Reflection absorption spectroscopy of metal oxide single crystals*
- 17:00 – 18:40** ***HS 3C Session 6 Medical Applications in Spectroscopy II***
- 17:00 – 17:20 E.Y.M. Bonnist, P.D.A. Pudney, P.J. Caspers, G.J. Puppels, C. Marriott, L.A. Weddell, F.L. Baines, S. Paterson, J.R. Matheson *Raman Spectroscopic Studies of the Scalp Skin, In Vivo*
- 17:20 – 17:40 Said Mohammed El Amin, Dahmane El Montausie, Naubron Jean-Valère, Vanloot Pierre, Bombarda Isabelle, Vanthuyne Nicolas, Dupuy Nathalie, Roussel Christian *Chiral Study of Artemisia Herba Alba by Vibrational Circular Dichroism*
- 17:40 – 18:00 Gjorgji Petruševski, Tomče Runčevski, Marina Čačorovska, Sonja Ugarčević, Igor Micovski, Gordana Bogoeva-Gaceva, Gligor Jovanovski, Robert E. Dinnebier and Petre Makreski *Solvatomorphism and Crystal Structure of the Narcotic Analgesic Drug Codeine Phosphate Sesquihydrate*
- 18:00 – 18:20 M. Khanmohammadi, F. Mozaffari, A. Bagheri Garmarudi *Diagnosis of Cardiovascular Defect by Infrared Spectrometric Analysis of Blood Serum*
- 18:20 – 18:40 M.I. Oshtrakh, I.V. Alenkina, A.V. Vinogradov, T.S. Konstantinova and V.A. Semionkin *Mössbauer Spectroscopy of Liver and Spleen Tissues from Normal Human and Patients with Hematological Malignancies*
- 18:40 – 19:00 A.A. Kamnev, A.V. Tugarova, L.A. Kulikov, and Yu.D. Perfiliev *Emission Mössbauer Spectroscopy in Probing Cation-Binding Sites in Biocomplexes: from Small Biomolecules to Enzymes*

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<b>17:00 – 18:40</b>	<b><i>HS 3D Session 8 Theory II</i></b>
17:00 – 17:20	<i>A. El-Azhary, N. Al-Jallal Conformational and Vibrational Analysis of Dibenzo-18-Crown-6</i>
17:20 – 17:40	<i>Choi Jun-Ho<sup>a</sup> and Cho Minhaeng Numerical Simulation of Vibrational Spectrum Under Aqueous Solution: Protein and Bulk Water System</i>
17:40 – 18:00	<i>A. Wohler, M. Schmitt Franck-Condon Simulation of Hot Absorption Spectra at Arbitrary Temperatures</i>
18:00 – 18:20	<i>C. G. T. Feugmo, V. Liégeois, Y. Caudano, F. Cecchet and B. Champagne Toward modeling Infrared-Visible Sum-Frequency Generation (SFG) of organic monolayers on hydrogen-terminated Si(111)</i>
18:20 – 18:40	<i>Valery Andrushchenko, Ladislav Benda and Petr Bouř Improving the Precision of Ab Initio Spectra Modeling by Employing Molecular Dynamics Simulations</i>