

August 31<sup>st</sup> – September 5<sup>th</sup> 2008 | Grand Hotel Adriatic, Opatija, Croatia



**EUCMOS 2008**

**XXIX European Congress on Molecular Spectroscopy**

**P R O G R A M M E**

# EUCMOS 2008 - CONGRESS PROGRAMME

**Sunday, August 31**

14.00 - 19.00 Registration

20.00 - 22.00 Welcome Reception

**Monday, September 1**

**MORNING SESSION**

08.30 - 09.00 Opening Ceremony

## PLENARY LECTURES

09.00 - 09.45 Austin Barnes  
EUCMOS - Past, Present and Future

09.45 - 10.30 Vincenzo Schettino  
Spectroscopy and Monitoring of High Pressure Phenomena

10.30 - 11.00  Coffee break

## ORAL PRESENTATIONS

Congress Hall

### Topic 1. Molecular Structure (Chairs: S. Akyuz, A. Loewenschuss)

11.00 - 11.20 G. Keresztury, M. Rogojerov, T. Sundius  
Polarized IR Spectroscopy and Transition Dipole Moment Determinations in Structural Studies

11.20 - 11.40 J. Laane, P. Boopalachandran, K. McCann, M. Wagner  
Spectroscopic Studies of the Electronic Excited States of Pyridine-d<sub>0</sub> and -d<sub>5</sub>, 2-Fluoro- and 3-Fluoropyridine, and 1,3-Benzodioxan

11.40 - 12.00 E. Kleinpeter, A. Koch  
Spatial Magnetic Properties of Trisannulated Benzenes and Cyclobutadiene Dianion Derivatives Subjected to Aromaticity

12.00 - 12.20 M. Szafran, I. Kowalczyk, E. Bartoszak-Adamska, Z. Dega-Szafran  
X-Ray diffraction, FTIR and NMR Spectra, and DFT Calculations of 2-Aminopyridine Betaine and 1-*H*-2-oxo-2,3-dihydroimidazo[1,2-*a*] Pyridinium

12.20 - 12.40 D.K. Breitinger, G. Brehm, M. Weil, S. Baumann  
Vibrational Spectra of K<sub>2</sub>[O(HgSO<sub>3</sub>)<sub>3</sub>] Containing a New Anionic Metallo-Oxonium Complex with a OHg<sub>3</sub> Core

12.40 - 13.00 A. Viridi  
X-ray crystallographic, spectroscopy and quantum chemical studies on 3, 3, 6-trimethyl-3, 4-dihydroiso-coumarin

**Topic 2. Biospectroscopy (Chairs: M. Heise, A. Barth)**

- 11.00 - 11.20 G. Schäfer, M.-K. Verhoefen, S. Shastri, I. Weber, C. Glaubitz, J. Wachtveitl, W. Mäntele  
Low Temperature FTIR Difference Spectroscopy Reveals New Insights on the Proton Pathway of Proteorhodopsin at Different pH Values
- 11.20 - 11.40 J. Grdadolnik  
Preferential Conformations of Blocked Amino Acids in Water
- 11.40 - 12.00 N.S. Kudryasheva, N.V. Belogurova  
Energy Conversion in Bioluminescent Reactions
- 12.00 - 12.20 P.S. Sherin, O.A. Snytnikova, Yu.P. Tsentlovich, E. Vauthey  
The excited-state dynamics of kynurenine - UV filter of the human eye
- 12.20 - 12.40 B.R. Wood, T. Chenenko, U. Bernhard, C. Jayne, A. Bramble, A.O. Trounson, D. McNaughton, O. Lacham-Kaplan  
Synchrotron FTIR Spectroscopy Reveals New Insights into Mouse Oocyte Maturation
- 12.40 - 13.00 Y. Ike, Y. Seshimo, S. Kojima  
Crystallization and Vitrification of Cryoprotectants Studied by Raman Scattering, Brillouin Scattering and THz-TDS


**Topic 11. Time resolved spectroscopy & Topic 12. New instrumentation (Chairs: I. Pálinkó, V. Ivanovski)**

- 11.00 - 11.20 C. Niezborala, F. Hache  
Ultrafast Conformational Dynamics of (R) - 1,1'-Bi-2-naphthol Measured with Time-Resolved Circular Dichroism
- 11.20 - 11.40 C. Krejtschi, O. Ridderbusch, R. Huang, T.A. Keiderling, K. Hauser  
Site-Specific Folding Dynamics of Peptides Studied by Time-Resolved Infrared-Spectroscopy
- 11.40 - 12.00 D. McNaughton, R. Tuckermann, L. Puskar, B. Wood, J. Popp, T. Frosch  
Raman Spectroscopic Analysis in Acoustically Levitated Drops
- 12.00 - 12.20 J. Mink, J. Mihály, Z. Bacsik, V. Gombás, X. Zhou  
New Application of Infrared Microscopy and Imaging in Difficult Sample Analysis

**AFTERNOON SESSION****INVITED LECTURES**

Congress Hall

Chairs: G. Keresztury, V. Schettino

- 15.00 - 15.30 Z. Meić, T. Hrenar  
Vibrational Assignment of 1,4-(E,E)-Distyrylbenzene Supported by Isotopic Shifts and DFT Calculations
- 15.30 - 16.00 Ruth Signorell  
Intrinsic Particle Properties in Infrared Spectra of Aerosols
- 16.00 - 16.30 Nađa Došlić  
Multidimensional Quantum Dynamics of Large Amplitude Motion
- 16.30 - 17.00  Coffee break

Congress Hall

## Topic 1. Molecular Structure (Chairs: J. Laane, M. Szafran)

- 17.00 - 17.20 C. Öğretir  
The Hydrogen Bonding in Life and Society
- 17.20 - 17.40 B. Tolnai, J.T. Kiss, K. Felföldi, I. Pálkó  
C-H...F Hydrogen Bonds as the Organising Force in F-substituted  $\alpha$ -phenyl Cinnamic Acid Aggregates Studied by the Combination of FTIR Spectroscopy and Computations
- 17.40 -18.00 D. Michalska, K. Hernik, R. Wysokiński, W. Zierkiewicz, A. Pietraszko  
Structures of Vitamin B<sub>13</sub> Complexes with Transition Metal Ions. The Role of Unusual Cu(II)··· $\pi$  Interaction and Hydrogen Bonds.
- 18.00 - 18.20 J.G. Philis  
UV R2PI Spectra of p-difluorobenzene van der Waals Complexes
- 18.20 - 18.40 A.K. Singh, V. Mukherjee, V.B. Singh, B. Singh, A.N. Singh  
Spectroscopic Investigation of the Vibrational Spectra of the Benzoxazine
- 18.40 - 19.00 S. Mishra, D. Chaturvedi, P. Tandon, V.P. Gupta, A.P. Ayala, S.B. Honorato, H.W. Siesler  
Molecular Structure and Vibrational Spectroscopy investigation of Secnidazole using Density-Functional Theory

Hall: Camelia 2

## Topic 6. Spectroscopy in Chemical, Pharmaceutical and Environmental Analyses (Chairs: O. Cozar, I. Hannus)

- 17.00 - 17.20 O. Abbas, R. Codony, C. von Holst, V. Baeten  
Assessment of the Discrimination of Animal Fat by FT-Raman Spectroscopy
- 17.20 - 17.40 J. Barbillat, S. Sobanska, J. Rimetz, S. Scolaro, J. Laureyns, D. Petitprez, C. Brémard  
Raman and AFM Imaging of Marine Aerosol Particles
- 17.40 -18.00 T. Frosch, J. Popp  
Vibrational Spectroscopic Investigation of Drug-Target-Interactions in Malaria Research
- 18.00 - 18.20 M. Watanabe, T. Kurabayashi, T. Tanno, N. Kikuchi  
Significance of Terahertz Spectrometry for Detecting Molecular States of Chemicals

## WORKSHOP

- Time \ Hall Camelia 1
- 17.00 - 19.30 **HORIBA Jobin Yvon**  
Latest Innovations in Raman Microscopy for Ultra Fast Raman Imaging and Macro-mapping
- 21.00 - 22.00 **Concert**


# Tuesday, September 2

## MORNING SESSION

### PLENARY LECTURES

Congress Hall

Chairs: I. P. Suzdalev, M. Oshtrakh

- 08.30 - 09.15 **Philip Gütlich**  
Mössbauer Spectroscopy - A Powerful Tool In Molecular Magnetism
- 09.15 - 10.00 **Eddy De Grave**, V.G. de Resende, C. Van Cromphaut, Ch. Laurent, L. Presmanes, R.E. Vandenberghe  
Integral Low-Energy Electron Mössbauer Spectroscopy (ILEEMS): Methodology and Recent Applications in Material Research
- 10.00 - 10.30  Coffee break

### ORAL PRESENTATIONS

Congress Hall - **Topic 3. Nanostructured Materials (Chairs: E. De Grave, E. Culea)**

- 10.30 - 10.50 **I.P. Suzdalev**, Yu.V. Maksimov  
Magnetic Phase Transitions in Nanoclusters and Nanostructures
- 10.50 - 11.10 **S.N.B. Bhaktha**, O. Robbe-Cristini, K. Raulin, B. Capoen, M. Bouazaoui, **S. Turrell**, J. Habinshuti, B. Grandidier, C. Kinowski  
Use of Spectroscopic Techniques for Synthesis Optimisation and for the Characterisation of Optical Properties of Semiconductor Nanoparticles
- 11.10 - 11.30 **R. Holomb**, **V. Mitsa**  
Ring-, Branchy-, and Cage-Like  $As_nS_m$  Nanoclusters in the Structure of Amorphous Semiconductors: *ab initio* and Raman Study
- 11.30 - 11.50 **S.K. Gupta**, **P.K. Jha**  
Vibrational Quantization in Semiconductor Nanocomposites
- 11.50 - 12.10 **O. Robbe-Cristini**, K. Raulin, B. Capoen, M. Bouazaoui, S. Turrell  
Spectroscopic Studies of Energy Transfer between Semiconductor Nanoparticles and  $Eu^{3+}$  Ions in Silica Gels
- 12.10 - 12.30 **D. Gracin**, A. Gajović, M. Ceh, K. Juraić, D. Meljanac, P. Dubček, S. Bernstorff  
Structural Analysis of Thin Amorphous- Nano-Crystalline Thin Films by HRTEM, GISAXS and Raman Spectroscopy

## Hall: Camelia 1 - Topic 1. Molecular Structure (Chairs: D.K. Breitinger, J. Philis)

- 10.30 - 10.50 P. Drożdżewski, M. Kubiak  
Crystal Structure and Vibrational Spectroscopy of Mixed-valence [Cu(biz)<sub>2</sub>][Cu<sub>2</sub>Br<sub>4</sub>] Complex Formed After *In Situ* Oxidation of 2-Hydrazino-2-Imidazoline to Bisimidazoline (biz) by Copper(II) Ions
- 10.50 - 11.10 L. Krim, N. Dozova, E. Alikhani, N. Lacombe  
Infrared Spectra of CH<sub>3</sub>Cl + H<sub>2</sub>O and NO + H<sub>2</sub>O Isolated in Solid Neon at 5 K
- 11.10 - 11.30 N. Biliškov, G. Baranović  
Infrared Spectroscopy of Liquid Water-*N,N*-dimethylformamide Mixtures
- 11.30 - 11.50 Y. Kawashima, Y. Tanaka, A. Sato, E. Hirota  
Fourier Transform Microwave Spectra of Isobutylmercaptan and Normal Butylmercaptan
- 11.50 - 12.10 R. Singh, M. Kumar, R.A. Yadav  
Theoretical Study of IR and Raman Spectra of 5-Hydroxy Uracil

## Hall: Camelia 2 - Topic 2. Biospectroscopy (Chairs: W. Pohle, V. Mohaček Grošev)


- 10.30 - 10.50 A.A. Kamnev  
Application of Mössbauer and FTIR Spectroscopic Techniques in Structural Research Related to Microbial Signalling and Cellular Responses to Environmental Factors
- 10.50 - 11.10 M. Di Foggia, C. Fagnano, P. Taddei, A. Torreggiani, M. Dettin, S. Sanchez-Cortes, A. Tinti  
Vibrational Characterization of Self-Assembling Oligopeptides for Tissue Engineering on TiO<sub>2</sub> Surfaces
- 11.10 - 11.30 P. Matějka, L. Mrnka, H. Tokárová, M. Vosátka, K. Volka  
Effect of Different Fungal Associates on the FT Raman Spectral Characteristics of Norway Spruce Needles
- 11.30 - 11.50 I. Piantanida, L. Mašić, G. Rusak  
Structure-Activity Relationship in Interactions of Quercetin and its Analogues with Double Stranded DNA/RNA and Single Stranded RNA
- 11.50 - 12.10 A. Zwielly, J. Gopas, G. Brkic, S. Mordechai  
Identification of Drug Resistant Melanoma Cell Lines Using Vibrational Spectroscopy
- 12.10 - 12.25 M. Egelkraut-Holtus, U. Oppermann (Shimadzu)  
"State of the Art" Spectroscopy in Food Analysis

## AFTERNOON SESSION

## PLENARY LECTURES

Congress Hall

Chairs: S. Turrell, M. Ceppatelli

- 15.00 - 15.45 Mile Ivanda, D. Ristić, K. Furić, S. Musić, M. Ristić, M. Gotić, G. Štefanić, Z. Crnjak Orel, M. Bitenc, M. Montagna, M. Ferrari, A. Chisaera, Y. Jestin  
Low-Frequency Raman Scattering in Materials Research
- 15.45 - 16.30 Thomas Bally  
Electronic and Vibrational Spectroscopy of Radical Cations in Argon
- 16.30 - 17.00  Coffee break

17.00 - 19.00

Poster Session A - Topics 1-3, 11, 12

## 1. MOLECULAR STRUCTURE

- P1-1 S. Akyuz, T. Akyuz  
Vibrational Spectroscopic Study of 4-Aminopyrimidine Complexes
- P1-2 L. Andreeva, F. Trajkovic, J. Petreska  
Investigation of the Vibrational Spectra of Some Partially Deuterated  $\text{Cd}(\text{NH}_3)_2\text{Cl}_2$ ,  $\text{Hg}(\text{NH}_3)_2\text{Cl}_2$ ,  $\text{Pd}(\text{NH}_3)_4\text{Cl}_2$  Complexes
- P1-3 L.M. Babkov, N.A. Davydova, K.E. Uspenskiy  
2-Biphenylmethanol Vibrational Spectra and Their Interpretation Using Structural-Dynamical Model in Anharmonic Approximation
- P1-4 L.M. Babkov, I.I. Gnatyuk, G.A. Puchkovska, S.V. Truckhachev  
The Investigation of 4-n-butyl-4'-cyanobiphenyl Conformational Mobility by IR Spectroscopy Methods
- P1-5 L.M. Babkov, I.I. Gnatyuk, G.O. Puchkovska, K.E. Uspenskiy  
The Appearance of Conformational Mobility of Behenic Acid in IR Spectra
- P1-6 K. Balci, Y. Akkaya, S. Akyuz  
A Theoretical Conformational Analysis and Vibrational Spectroscopic Investigation on Niflumic Acid
- P1-7 Gonul Basar, S. Akyuz, Gunay Basar, S. Kröger  
Studies on Kyotorphin and D-Kyotorphin in Aqueous Solution by Raman Spectroscopy
- P1-8 C. Bayrak  
Vibrational Spectroscopic Studies on the  $T_d$ -Type Clathrates:  $M(\text{N}, \text{N}'\text{-Dimethyl-ethylenediamine})\text{M}'(\text{CN})_4 \cdot \text{C}_6\text{H}_6$  ( $M = \text{Mn}$ ,  $M' = \text{Zn}$ ,  $\text{Cd}$  or  $\text{Hg}$ ;  $M = \text{Cd}$ ,  $M' = \text{Cd}$  or  $\text{Hg}$ )
- P1-9 I. Iriepa, J. Bellanato, E. Gálvez, A.I. Madrid  
Synthesis, Structural and Conformational Study of Some Esters Derived from 3-Methyl 3-azabicyclo[3.2.1]octan-8 $\alpha$ -ol
- P1-10 M.E. Defonsi Lestard, M.E. Tuttolomondo, E.L. Varetti, D.A. Wann, H.E. Robertson, D.W.H. Rankin, A. Ben Altabef  
Experimental Structure of  $\text{CF}_3\text{CO}_2\text{CH}_2\text{CF}_3$  from Electron Diffraction Data, Infrared Spectra and Quantum Chemical Calculation of Vibrational Properties
- P1-11 E. Benassi, I. Baraldi, S. Ciorba, I. Škorić, M. Šindler-Kulyk, A. Spalletti  
New Organic Fluorophores for Optical and Spectroscopic Applications: 2,3- and 2,5-Distyrylfuran
- P1-12 E. Benassi, P.S. Sherin  
Combined Experimental and Theoretical Study on the Kynurenine
- P1-13 A. Borba, A. Gómez-Zavaglia, R. Fausto  
Photochemistry and Vibrational Spectra of Matrix-Isolated Isoniazid
- P1-14 D.K. Breitingner, G. Brehm, J. Zürbig, M. Weil, S. Baumann  
Bis(sulfito)mercurates  $M_2[\text{Hg}(\text{SO}_3)_2] \cdot x\text{H}_2\text{O}$  ( $M = \text{NH}_4$ ,  $\text{Na}$ ,  $\text{K}$ ;  $x = 0, 1, 2.25$ ). Vibrational Spectra of the Solids and of Aqueous Solutions.
- P1-15 D.K. Breitingner, M. Moll, G. Brehm  
Sulfito Mercurate Complexes in Solution Studied by  $^{199}\text{Hg}$  NMR Spectrometry
- P1-16 J. Ceponkus, D. Lesciute, V. Sablinskas  
Association of Water with Small Monocarboxylic Acids. Matrix Isolation Infrared Absorption Study.
- P1-17 V. Chiş, R. Ştiuşiuc, N. Leopold  
Molecular and Electronic Structure of PTCDI and Melamine-PTCDI Complex
- P1-18 K. Cholewa-Kowalska, M. Laczka, Z. Olejniczak  
Effect of Organic Modifiers on the Solution Viscosity, Gelation Time and Progress of Hydrolysis/Condensation Reactions during Hybrid Gels Formation

- P1-19 **A. Nikolić, B. Jović, E. Davidović, S. Petrović**  
N-H···O Hydrogen Bonding. FT-IR and NIR Study of N-Methylformamide-Ether Systems.
- P1-20 **Z. Dega-Szafran, M. Szafran**  
Experimental and Theoretical Vibrational Spectra of Piperidine-2-carboxylic Acid
- P1-21 **Z. Dega-Szafran, A. Katrusiak, M. Szafran**  
Molecular Structure of the Hydrated Complex of 1,4-dimethylpiperazine di-betaine with L-tartaric Acid Studied by X-ray Diffraction and FTIR
- P1-22 **I. Despotović, Z.B. Maksić**  
Towards Organic Conductors - the Structure and Stability of Cyano-[n]-Radialenes and Their Dianions
- P1-23 **M.E. Jamróz, M.H. Jamróz, J.E. Rode, J.Cz. Dobrowolski**  
Interpretation of Vibrational Spectra of Allyl Acrylate
- P1-24 **K. Furić, B.-M. Kukovec, Z. Popović**  
Raman Study of Nickel(II) Complexes with 6-Methylpicolinic Acid
- P1-25 **J. Polovková, A. Gatial, M. Gróf, J. Kožišek, V. Milata, N. Prónayová, P. Matějka**  
Isomerizational and Conformational Study of 3-Cyclopropylamino-2-Acetyl Propenenitrile (CpAAP) and 3-Cyclopropylamino-2-Methylsulfonyl Propenenitrile (CpASP)
- P1-26 **I. Gocan, C. Nagy, M.M. Venter, V. Bercean, L. David**  
Spectral Investigations on Metal Complexes of Heterocyclic N,S-Donors
- P1-27 **M. Gróf, A. Gatial, J. Kožišek, V. Milata, P. Matějka**  
Conformational Analysis of Aminomethylene- and Methylaminomethylene-Malonic Acid Dimethylester
- P1-28 **M. Gróf, A. Gatial, J. Kožišek, V. Milata, P. Matějka**  
Conformational Analysis of Dimethylaminomethylene-Malonic Acid Dimethyl Ester
- P1-29 **Ł. Hetmańczyk, J. Hetmańczyk, A. Migdał-Mikuli, E. Mikuli**  
Phase transition and H<sub>2</sub>O motions in [Ba(H<sub>2</sub>O)<sub>4</sub>](ClO<sub>4</sub>)<sub>2</sub> studied by differential scanning calorimetry, infrared spectroscopy and inelastic/quasielastic incoherent neutron scattering
- P1-30 **I. Jelovica Badovinac, N. Orlić, C. Gellini, L. Moroni, P.R. Salvi**  
Micro-Raman and Computational Study of the Azoxybenzene Photorearrangement to 2-Hydroxybenzene
- P1-31 **M. Juribašić, L. Stella, Ž. Marinić, M. Vinković, Lj. Tušek-Božić**  
Microwave Synthesis and Spectroscopic Study of 3-Quinoline-substituted  $\alpha$ -Aminophosphonates
- P1-32 **M. Jurić, P. Planinić, D. Žilić, B. Rakvin, B. Prugovečki**  
A New Heterometallic (Ni<sup>2+</sup> and Cr<sup>3+</sup>) Complex - Crystal Structure and Spectroscopic Characterization
- P1-33 **A. Kocot, K. Merkel, J. Ziolo**  
Investigation of Liquid-Liquid Phase Transition for Trans-1,2 dichlorethylene
- P1-34 **N. Kuş, S. Breda, E.M.S. Eusébio, T.M.R. Estronca, R. Fausto**  
Matrix Isolation Spectrum, UV-Induced Photochemistry ( $\lambda > 215$  nm) and Differential Scanning Calorimetry Analysis of 3-(N-Acetamide)-Coumarin
- P1-35 **S. Lopes, A. Gómez-Zavaglia, C. M. Nunes, T.M.V.D. Pinho e Melo, R. Fausto**  
Photochemistry and Vibrational Spectra of Matrix Isolated Methyl 4-Chloro-5-Phenylisoxazole-3-Carboxylate
- P1-36 **L. Macalik, M. Maćzka, J. Hanuza, A.A. Kaminskii**  
Polarized Raman and IR spectra of the orthorhombic CaNb<sub>2</sub>O<sub>6</sub>:Pr<sup>3+</sup> single crystal

- P1-37 **W. Makulski, A. Wikiet**  
Nuclear Magnetic Shielding and Spin-spin Coupling Constants for Acetaldehyde from Gas-phase NMR Spectroscopy
- P1-38 **K.M. Marzec, K. Malek, B. Gawel, W. Lasocha, L.M. Proniewicz**  
Structure Determination of Ag(I) Ion Complex of Rhodanine
- P1-39 **K. Malek, M. Makowski, L.M. Proniewicz**  
Raman Spectroscopy in Studies on the Selected Dehydropeptides
- P1-40 **K.M. Marzec, K. Malek, A. Kaczor, L.M. Proniewicz**  
Conformational and Vibrational Analysis of Selected Monoterpenoids by Using Density Functional Theory
- P1-41 **S. Miljanić, Z. Meić, G. Keresztury**  
Polarized Vibrational Spectra of *p*-Substituted Nitro and Dinitro *cis*- and *trans*-Stilbenes
- P1-42 **I. Movre Šapić, L. Bistričić, V. Volovšek, V. Dananić**  
DFT Study of Molecular Structure and Vibrations of 3-Glycidoxypropyltrimethoxysilane
- P1-43 **P. Novak, K. Pičuljan, T. Hrenar, M. Rubčić, M. Cindrić**  
Solution State Structure of Methoxysalicylaldehyde Thiosemicarbazone Derivatives by NMR and DFT Methods
- P1-44 **P. Forgó, G. Dombi, K. Felföldi, I. Pálinkó**  
Conformations of Z-2(3'-pyridyl)-3-phenyl Propenoic Acid in Various Solvents - an NMR Study Supplemented with Computations
- P1-45 **I. Pálinkó, J. Mink**  
Determining the Positions of Aromatic Hydrogens in (ar)C-H...X (X = O or F) Hydrogen Bonded Assemblies of Phenyl-phenyl, Phenyl-furyl Substituted Propenoic Acids and Esters from Their FTIR Spectra
- P1-46 **N. Peran, Z.B. Maksić**  
Calculating pK<sub>a</sub> of Some  $\alpha$ -Aminoacids Using Cluster-Continuum Model
- P1-47 **G. Petruševski, P. Naumov, G. Jovanovski**  
Fourier Transform Infrared Spectroscopic Analysis of the Solvates and Polymorphs of Sodium Valproate, Active Component of the Anticonvulsant Drug Epilim<sup>®</sup>
- P1-48 **K. Pičuljan, P. Novak, K. Užarević, M. Cindrić, T. Hrenar, T. Jednačak**  
Hydrogen Bonding and Deuterium Isotope Effects in <sup>13</sup>C NMR Spectra of Phenylene Enaminones Derived from Dehydracetic Acid
- P1-49 **M. Randić, K. Mehulić, D. Vukičević, T. Pisanski, D. Vikić-Topić, D. Plavšić**  
Graphical Representation of Proteins as Four-Color Maps and Their Numerical Characterization
- P1-50 **S. Rada, V. Maties, M. Rada, L. Pop, E. Culea**  
The Local Structure of Europium Lead-Borate Glasses and Glass Ceramics
- P1-51 **S. Rada, M. Barlea, D. Chicea, E. Culea**  
Structural properties of Gadolinium Borate-Tellurate Glasses and Glass Ceramics Inferred from FTIR spectroscopy and DFT Studies
- P1-52 **M. Ristova, G. Petruševski, A. Raškowska, B. Šoptrajanov**  
Vibrational Spectra of Hydrates of Some Metal(II) Malonates
- P1-53 **J.Cz. Dobrowolski, M.H. Jamróz, R. Kołos, J.E. Rode, J. Sadlej**  
IR Low-temperature Matrix and *Ab Initio* Study on  $\beta$ -Alanine Conformers
- P1-54 **D. Rusu, O. Baban, I. Hauer, L. David, M. Rusu**  
Synthesis and Physical Chemical Characterization of The Potassium 11-Tungstovanado(IV) Phosphate Anion

- P1-55 **S.G. Sagdinc, B. Köksoy, F. Kandemirli, S.H. Bayari**  
Spectroscopic and Theoretical Studies of 5-Fluoro-isatin-3-(N-cyclohexylthiosemi-carbazone) and Its Metal Complexes
- P1-56 **M. Sałdyka, B. Golec, Z. Mielke**  
Spectroscopy and Photochemistry of Glyoxal-Hydroxylamine Complexes. Matrix Isolation and Theoretical Study
- P1-57 **M. Sitarz, Z. Fojud, Z. Olejniczak**  
Submicroheterogenous Structure of Silico-Phosphate Glasses Studied by  $^{23}\text{Na}$ ,  $^{27}\text{Al}$ ,  $^{31}\text{P}$  NMR and FTIR
- P1-58 **V. Smrečki, P. Novak, D. Vikić-Topić, Z. Meić**  
Deuterium Isotope Effects in  $^{13}\text{C}$  NMR Spectra of *ortho*-, *meta*- and *para*-Deuterium Labelled Mono- and Binuclear Aromatic Compounds
- P1-59 **İ. Sıdır, E. Taşal, Y. Gülseven, R. Fausto, T. Önkol**  
Molecular Structure, Infrared Spectra and Some Molecular Properties of 5-Chloro-6-(4-chlorobenzoyl)-2-benzothiazolinone
- P1-60 **D. Vojta, G. Baranović**  
Raman Study of Anharmonic Effects in Vibrational Spectra of Acetylenic Compounds
- P1-61 **S.X. Zhou, D.T. Durig, J.R. Durig**  
Vibrational Spectra and Structural Parameter of Methyl and Ethyl Isocyanate
- P1-62 **D. Vojta, B. Zimmermann, G. Baranović**  
Vibrational Analysis of Diacetylenic Aromatic Compounds
- P1-63 **S. Rada, P. Pascuta, M. Culea, M. Pica, E. Culea**  
Vibrational Spectroscopic and DFT Studies of Gadolinium Vanado-Tellurite Glasses and Glass Ceramics
- P1-64 **V. Stefov, A. Cahil, B. Šoptrajanov, M. Najdoski, F. Spirovski, B. Engelen, H.D. Lutz, V. Koleva**  
Fourier Transform Infrared and Raman Spectra of Hexagonal  $\text{MgCsPO}_4 \cdot 6\text{H}_2\text{O}$

## 2. BIOSPECTROSCOPY

- P2-1 **V. Andrushchenko, P. Bouř**  
Interpretation of Vibrational Spectra of DNA Fragments Interacting with Metal Ions
- P2-2 **Gunay Basar, S. Kin, G. Temizkan, T. Gunel, S. Akyuz**  
Laser Tweezers Raman Spectroscopic Investigation of Geranylgeranyl Pyrophosphate Synthase in Recombinant *Schizosaccharomyces pombe* Cell
- P2-3 **N.V. Belogurova, N.S. Kudryasheva, R.R. Alieva, A.G. Sizykh**  
Upper Electron-Excited States in Coelenterate Bioluminescence
- P2-4 **P. Carmona, M. Molina, A. Rodríguez-Casado**  
On the Hydrogen-Deuterium Exchange in Proteins and Nucleic Acids Monitored by Vibrational Spectroscopy
- P2-5 **S. Cavalu, V. Simon, F. Banica**  
Dysprosium/Iron Aluminosilicate for Simultaneous Radiotherapy and Hyperthermia: Structural Investigation and Biocompatibility Evaluation
- P2-6 **G. Doyle, D. Zerulla**  
Investigating the Kinetic Interactions between Protein and Nanoparticles via Mie Scattering Spectroscopy and Optical Trapping
- P2-7 **A.V. Glushkov, S.V. Malinovskaya, S.V. Ambrosov, O.Yu. Khetselius**  
Spectroscopy and Structural Properties of Biogene Amines (Serotonin, Histamine,  $\gamma$ -amino oil acid) and Account for Laser and Neutron Capture Effects
- P2-8 **V. Gombás, J. Mink**  
Chemometrics Methods Used by Spectroscopic of Biological Samples

- P2-9 **A. Gómez-Zavaglia, A. Kaczor, R. Almeida, M.L.S. Cristiano, R. Fausto**  
Different Conformational Ground States of a *Pseudosaccharin* Ether in the Gaseous Phase and in Solid Krypton
- P2-10 **R. Dedic, V. Vyklický, A. Svoboda, J. Hála**  
Phosphorescence of Singlet Oxygen and 5,10,15,20-tetrakis(1-methyl-4-pyridinio)por-phyrin: Time and Spectral Resolved Study
- P2-11 **Y. Ike, E. Hashimoto, S. Kojima**  
Micro-Brillouin Scattering Study of Low Temperature Elastic Properties of Protein Crystals
- P2-12 **G. Keresztury, T. Sundius, T. Lóránd**  
Vibrational Spectroscopic Investigation of Bioactive Aminoalcohols
- P2-13 **S. Kumar, A. Barth**  
Ligand induced conformational change of pyruvate kinase studied by ATR-FTIR spectroscopy
- P2-14 **Z. Tarle, D. Škrčić, A. Knežević, D. Matošević, M. Ristić, K. Prskalo, S. Musić**  
Degree of Vinyl Conversion in Experimental ACP Composites
- P2-15 **K. Merkel, A. Kocot, W. Pluskiewicz, A. Pyrkosz**  
Raman and FTIR Spectroscopy of the Keratin as a Potential Tool for Probing Bone Health
- P2-16 **V. Mohaček Grošev, J. Grdadolnik, J. Stare, D. Hadži**  
Hydrogen Bonding in  $(\text{COOH})_2 \cdot 2\text{H}_2\text{O}$  and  $(\text{COOD})_2 \cdot 2\text{D}_2\text{O}$
- P2-17 **A. Aranyi, Z. Csendes, J.T. Kiss, I. Pálinkó**  
Covalently Grafted, Silica Gel Supported C-protected Cysteine or Cystine Copper Complexes – Syntheses, Structure and Possible Surface Reaction Studied by FT-IR Spectroscopy
- P2-18 **M. Lasalvia, N. L'Abbate, G. Perna, E. Mezzenga, V. Capozzi**  
Raman Spectroscopy Study of Cellular Damage in Human Keratinocytes Treated with Organophosphate Compounds
- P2-19 **D.R. Gauger, E. Mrazkova, P. Hobza, W. Pohle**  
Disentangling Infrared CH Bands Arising from Polar and Apolar Domains of Phospholipids: Headgroup CH Moieties are Involved in Water Binding
- P2-20 **O. Ryazanova, I. Voloshin, I. Dubey, L. Dubey, V. Zozulya**  
Spectroscopic Studies on Binding of Cationic Pheophorbide-a Derivative to Double-stranded and Quadruplex Polynucleotides
- P2-21 **M. Rokita, M. Sitarz**  
Phosphate Layers on Titanium and Ti6Al4V Titanium Alloy - Comparison of Hydroxyapatite Layers Obtained During SBF Soaking
- P2-22 **M. Śmiechowski, E. Gojło, J. Stangret**  
Systematic Study of Hydration Patterns of Phosphoric (V) Acid and Its Mono-, Di- and Tripotassium Salts in Aqueous Solution
- P2-23 **J. Surmacki, B. Brożek-Płuska, H. Abramczyk, Z. Morawiec, M. Tazbir**  
Application of Raman Spectroscopy for Breast Cancer Diagnosis
- P2-24 **R. Tamaian, I. Ștefănescu, R. Ionete**  
Investigations on Deuterium's Grade of Substitution in the Swiss Mice's Body at the Administration of Deuterium Depleted Mediums
- P2-25 **A. Tinti, J. Domènech, S. Atrian, M. Capdevila, A. Torreggiani**  
Raman Spectroscopy Investigation on Metal-Metallothionein Complexes

### 3. NANOSTRUCTURED MATERIALS

- P3-1 **M. Barczak, A. Dąbrowski**  
Spectroscopic Characterization of Polysiloxane and Bridged Polysilsesquioxane Xerogels
- P3-2 **L. Bistričić, M. Leskovac, G. Baranović, E. Govorčin Bajsić**  
Linear IR dichroism of polyether-based polyurethane-silica nanocomposites
- P3-3 **V. Canpean, S. Astilean**  
Subwavelength Metallic Nanohole Arrays as Multifunctional Plasmonic Substrates for SPR and SERS Sensors
- P3-4 **E. Culea, L. Pop, M. Bosca**  
Novel Bismuth-Lead-Silver Glasses Doped with Neodymium Ions
- P3-5 **V.G. de Resende, E. De Grave, A. Cordier, C. Laurent, A. Peigney, A. Weibel**  
Carbon Nanotube-Fe/Al<sub>2</sub>O<sub>3</sub> Nanocomposites by CCVD Method: Formation of CNTs from  $\alpha$ -(Al<sub>1-x</sub>Fe<sub>x</sub>)<sub>2</sub>O<sub>3</sub> Oxide Powders that were Prepared by Oxinate Route
- P3-6 **M. Didović, S. Valić, D. Klepac, A.P. Meera, S. Thomas**  
ESR Study of NR/Montmorillonite Nanocomposites
- P3-7 **A. Fraczek, C. Paluszkiwicz, A. Weselucha-Birczynska, S. Blazewicz**  
The Influence of Carbon Nanotubes on PAN-based Fibers Properties
- P3-8 **A. Gajović, S. Šturm, B. Jančar, M. Čeh**  
The Mechanism of BiFeO<sub>3</sub> Hydrothermal Synthesis
- P3-10 **T. Gumuła, C. Paluszkiwicz, S. Blazewicz**  
Study on Thermal Decomposition Processes of Polysiloxane Polymers - from Polymer to Nanosized Silicon Carbide
- P3-11 **M. Iosin, F. Toderas, P. Baldeck S. Astilean**  
Study of Protein-Gold Nanoparticle Conjugates by Fluorescence and Surface Enhanced Raman Scattering
- P3-12 **M.S. Sytnyk, Yu.B. Khalavka, O.V. Jovtiuk, O.O. Korovyanko**  
Morphological Dependence of Magnetite Nanocrystals under Different Growth Conditions
- P3-13 **S. Krehuła, S. Musić**  
Formation of Iron Oxides in a Highly Alkaline Medium in the Presence of Palladium Ions
- P3-14 **D. Mikociak, C. Paluszkiwicz, R. Słowiak, M. Blazewicz**  
Vibrational Spectroscopy Applications to Study Carbonization Process of Fibrous Materials
- P3-15 **E. Stodolak, C. Paluszkiwicz, M. Bogun, M. Blazewicz**  
Nanocomposite Fibres for Medical Applications
- P3-16 **D. Mikociak, C. Paluszkiwicz, T. Gumuła, J. Michałowski, S. Błażewicz**  
FTIR Studies of Carbon Matrices Modified with Nanosized Hydroxyapatite
- P3-17 **P. Pascuța, S. Rada, G. Borodi, M. Bosca, L. Pop, E. Culea**  
Influence of Europium Ions on Structure and Crystallization Properties of Bismuth-Alumino-Borate Glasses and Glass Ceramics
- P3-18 **V. Pashynska, A. Glamazda, A. Plokhotnichenko, E. Karpenko, T. Pokynbroda, V. Karachevtsev**  
Spectroscopic Investigations of Carbon Nanotubes in Aqueous Suspensions with Biosurfactants

- P3-19 **R. Rémiás, A. Kukovecz, Z. Kónya, I. Kiricsi**  
A Spectroscopic Study on Noble Metal Nanoparticle Embedding into a SBA-15 Catalyst System
- P3-20 **S. Musić, M. Ristić, S. Popović**  
Synthesis and Microstructure of Porous Mn-Oxides
- P3-21 **S. Musić, A. Šarić, S. Popović, M. Ivanda**  
Formation and Characterization of Nanosize  $\alpha$ -Rh<sub>2</sub>O<sub>3</sub>
- P3-22 **Ž. Skoko, S. Popović, G. Štefanić**  
Thermal Behaviour of Al-Zn and Zn-Al Alloys
- P3-23 **D. Sović, D. Iveković, B. Zimmermann**  
Modification of Titanate Nanotubes with Transition Metals and Transition Metal-1,10-phenanthroline Complexes
- P3-24 **G. Štefanić, S. Musić, M. Ivanda**  
The Influence of Thermal Treatment on the Phase Development of ZrO<sub>2</sub>-ZnO Precursors
- P3-25 **D.S. Su, J. Zhang, X. Liu, J. Delgado, A. Gajović**  
Raman Spectroscopy of Nanocarbon Catalyst for Oxidative Dehydrogenation Reactions
- P3-26 **F. Toderas, M. Baia, L. Baia, S. Astilean**  
Investigation of Annealed Gold Nanoparticles Self-Assembled on Solid Surface for Surface-Enhanced Raman Spectroscopy
- P3-27 **V. Vogel, T. Pisternik, M. Holzer, K. Langer, W. Mäntele**  
Study of Controlled Release of Model Proteins from Poly (D,L lactic-co-glycolic) Acid Nanoparticles by Fluorimetry and Analytical Ultracentrifugation
- P3-28 **K. Žagar, A. Gajović, S. Šturm, M. Čeh**  
BaTiO<sub>3</sub> Nanorods: New Insight by Raman Spectroscopy
- P3-29 **M. Žic, M. Ristić, S. Musić**  
Precipitation of hematite from dense  $\beta$ -FeOOH suspensions with ammonium amidosulfonate adding

## 11. TIME RESOLVED SPECTROSCOPY

- P11-1 **V. Dananić, K. Košutić, B. Kunst, D. Bosnar**  
Pore Size Distribution of NF/RO Composite Membranes by Positron Annihilation Lifetime Spectroscopy
- P11-2 **A. Krzysztofowicz, V.I. Tomin**  
The Temporal Dipole Moment of the Solutes Undergoing Charge Transfer in the Excited State

## 12. NEW INSTRUMENTATION

- P12-1 **V. Ivanovski, T.G. Mayerhöfer, J. Popp**  
Employing Polyethylene as Contacting Agent Between ATR-crystals and Solid Samples with Hard Surfaces


# Wednesday, September 3

## MORNING SESSION

### PLENARY LECTURES

Congress Hall

Chairs: H. Abramczyk, T. Bally

- 08.30 - 09.15 Hiro-o Hamaguchi  
Time- and Space-Resolved Raman Spectroscopy of Single Living Cells
- 09.15 - 10.00 Rui Fausto  
Search for Missing Conformers: Matrix-Isolation SWAT
- 10.00 - 10.30  Coffee break

### ORAL PRESENTATIONS

Congress Hall - **Topic 8. Chemical Dynamics (Chairs: R. Fausto, G. Patonay)**

- 10.30 - 10.50 M. Ceppatelli, A. Serdyukov, R. Bini, H.J. Jodl  
FTIR Study of the Reactivity of Solid CO at High Pressure
- 10.50 - 11.10 V.I. Tomin, R. Jaworski  
ESIPT from the S<sub>2</sub> Singlet State in the 3-Hydroxyflavone
- 11.10 - 11.30 M. Pasquini, N. Schiccheri, G. Piani, G. Pietraperzia, E. Castellucci, M. Becucci  
Studies on Microsolvation in the Gas Phase by HR-LIF and REMPI-TOF Spectroscopy
- 11.30 - 11.50 A.S. Bali, A. Viridi  
Kinetics and Mechanistic Studies of the Dissociation of Anthranilic-diacetato-2,2'-dipyridyl Chromium (III) Dihydrated in Acidic Media

Hall: Camelia 1 - **Topic 10. Surface Spectroscopies (Chair: M. Muniz-Miranda)**

- 10.30 - 10.50 S. Astilean, M. Baia, D. Maniu, F. Toderas, C. Farcau, M. Iosin, V. Canpean  
Multifunctional Plasmonic Nanostructures for Surface-Enhanced Spectroscopies
- 10.50 - 11.10 M. Nullmeier, I. Zawisza, S.E. Pust, R. Boukherroub, S. Szunerits, G. Wittstock  
Structural Studies of Lipid Bilayers on Titania Surfaces by Means of Polarization Modulation Infrared Reflection Absorption Spectroscopy
- 11.10 - 11.30 P. Taddej, A. Tinti, M.G. Gandolfi, F. Siboni, C. Prati  
Vibrational Study on the Bioactivity of Portland Cement-Based Materials for Endodontic Use
- 11.30 - 11.50 B. Vlckova, K. Siskova, M. Prochazka, J. Stepanek, P. Smejkal, P.-Y. Turpin  
Surface-enhanced Resonance Raman Scattering of Free-base Porphyrins for Ultrasensitive Spectral Detection and Surface Probing

Hall: Camelia 2 - **Topic 4. Spectroscopy of Macromolecules (Chair: M. Handke)**

- 10.30 - 10.50 M.M. Vorob'ev  
Microwave Hydration Measurements in Aqueous Systems of Proteins and Synthetic Polymers
- 10.50 - 11.10 T. Burova, G. Ten, A. Anashkin  
Quantum-Mechanical Analysis of Intensity Distribution in Resonance Raman and Two-Photon Absorption Spectra of Nucleic Acid Base Pairs
- 11.10 - 11.30 Olesya V. Stepanenko, I.M. Kuznetsova, V.V. Verkhusha, V.N. Uversky, K.K. Turoverov  
The Structural Changes of Green Fluorescent Protein Induced by Small Guanidine Hydrochloride Concentrations
- 11.30 - 11.50 Olga V. Stepanenko, I.M. Kuznetsova, K.K. Turoverov, V. Scognamiglio, M. Staiano, S. D'Auria  
The Structural Changes of D-Galactose/D-Glucose-Binding Protein Induced by Calcium Depletion

**13.00 - 20.00 Conference Excursion**


# Thursday, September 4

## MORNING SESSION

### PLENARY LECTURES

Congress Hall

Chairs: H. Hamaguchi, M. Grodzicki

- 08.30 - 09.15 Halina Abramczyk, I. Placek, B. Brożek-Płuska, J. Surmacki, Z. Morawiec, M. Tazbir  
From Femtosecond Dynamics to Breast Tissue Diagnosis by Raman Spectroscopy
- 09.15 - 10.00 Dieter Naumann, H. Fabian, P. Lasch  
FT-IR Spectroscopy of Cells and Tissues
- 10.00 - 10.30  Coffee break

### ORAL PRESENTATIONS

Congress Hall

#### Topic 2. Biospectroscopy (Chairs: P. Matejka, S. Mordechai)

- 10.30 - 10.50 G. Patonay, L. Strekowski, M. Henary, J.-K. Seok  
Near-Infrared Fluorescence in Bioanalytical and Medical Applications
- 10.50 - 11.10 A. Barth  
Ligand Binding to Proteins Studied by Infrared Spectroscopy
- 11.10 - 11.30 H.M. Heise, U. Damm, V.R. Kondepati, J.K. Mader, F. Feichtner, M. Ellmerer  
Infrared Spectroscopy in Clinical Chemistry: From Lab to Bed-Side Applications
- 11.30 - 11.50 S.S. Stavrov  
The FeCO Unit Vibrations as a Probe of the Structure of the Active Site of Heme Proteins: Combined Quantum Chemical, Vibronic and Spectroscopic Study
- 11.50 - 12.10 S. Madathil, K. Fahmy  
Cross-Correlation of Fluorescence-Quenching and Infrared Absorption in the Study of Protein Ligand Binding Sites
- 12.10 - 12.30 W. Pohle, D.R. Gauger, V. Andrushchenko, P. Bour, H. Boehlig  
New Insights into the Structural Biophysical Chemistry of Amphiphiles with 18-Carbon Chain Length as Provided by FTIR Spectroscopy
- 12.30 - 12.50 L. Puskar, M. Tobin, P. Heraud, B. Wood  
The New Infrared Beamline: Australian Synchrotron Infrared Microscopy at the Single Cell Level
- 12.50 - 13.10 P. Heraud, E. Ng, B. Wood, T. Frosch, D. McNaughton, E. Stanley, A. Elefanty  
Early Stages of Human Embryonic Stem Cell (HESC) Differentiation Characterized by FT-IR Spectroscopy

## Hall: Camelia 1

## Various Topics (Chairs: M. Ivanda, C. Paluszkiwicz)

- 10.30 - 10.50 Z. Györi, D. Tátrai, F. Sarlós, G. Szabó, A. Kukovecz, Z. Kónya, I. Kiricsi  
Laser-induced Fluorescence Measurements On CdSe Quantum Dots
- 10.50 - 11.10 G. Kozma, Á. Kukovecz, Z. Kónya  
Spectroscopic Characterization of Mechanochemically Synthesized Cr/SnO<sub>x</sub> Nanocomposites
- 11.10 - 11.30 K. Raulin, O. Cristini, P. Baldeck, S. Turrell, B. Capoen, M. Bouazaoui  
Spectroscopic Characterization of Two-photon Generated CdS Nanoparticles in Sol-gel Zirconia Thin Films
- 11.30 - 11.50 M. Darányi, Á. Kukovecz, Z. Kónya, I. Kiricsi  
Characterization of Carbon Thin Films Prepared by the Thermal Decomposition of Spin Coated PAN Films
- 11.50 - 12.10 A. Gajović, I. Friščić, M. Plodinec, D. Iveković  
High Temperature Raman Spectroscopy of Titanate Nanotubes
- 12.10 - 12.30 G. Trettenhahn  
In situ FTIR Spectroelectrochemical Investigations and two-dimensional Correlation Spectroscopy of the Hexacyanoferrate-II/-III Redox Couple
- 12.30 - 12.50 V.A. Karachevtsev  
Spectroscopy of Nanohybrids Formed by Carbon Nanotubes and Biomolecules
- 12.50 - 13.10 B. Davarcioglu  
Spectral Characterization of Kolsuz Area (Ulukisla-Nigde) Clays, Central Anatolian Region, Turkey

## Hall: Camelia 2

## Topic 9. Theoretical Spectroscopy and Computer Methods (Chairs: D. Kirin, K. Balci)

- 10.30 - 10.50 T.A. Ford  
*Ab initio* Molecular Orbital Calculations of the Structures and Vibrational Spectra of Some Molecular Complexes Containing Sulphur Dioxide
- 10.50 - 11.10 T.P. Živković  
Vibrational Isotope Effect by the Low Rank Perturbation Method
- 11.10 - 11.30 S. Lebernegg, G. Amthauer, M. Grodzicki  
Single-centre Molecular Orbital Theory of Transition Metal Complexes
- 11.30 - 11.50 E. Benassi  
New Features in Theoretical Description of Electronic Energy Transfer: Mechanisms and Matrix Element Calculation
- 11.50 - 12.10 A.V. Glushkov  
Raman Scattering of the Light on Metastable Levels of Diatomics: Consistent Energy Approach
- 12.10 - 12.30 V. Mukherjee, N.P. Singh, R.A. Yadav  
FTIR and Raman Spectra of Some Tetra Substituted Benzenes

## AFTERNOON SESSION

### INVITED LECTURES

Congress Hall

Chairs: V. Mitsa, A.A. Kamnev

- 15.00 - 15.30 Michael Oshtrakh, V.A. Semionkin, O.B. Milder, E.G. Novikov  
Mössbauer Spectroscopy with High Velocity Resolution: New Possibilities in Biomedical Research
- 15.30 - 16.00 Markku Räsänen  
Advances in Noble Gas Chemistry

16.00 - 16.15 J. Sikola, G. Zachmann, M. Huber (Bruker Optik GmbH)  
The New Vacuum FT-IR Spectrometer: Design Advances and Research Application

16.15 - 16.30 Don McNaughton  
An invitation to Australia for the 5th International Conference on Advanced Vibrational Spectroscopy

16.30 - 17.00  Coffee break

### POSTER PRESENTATIONS

17.00 - 19.00 Poster Session B - Topics 4-10

#### 4. SPECTROSCOPY OF MACROMOLECULES

- P4-1 S. İde, A.B. Arıĝ, T. Türkeş, O. Mergen, S.H. Bayarı, Ö. Çelik  
Structural Investigation on Some Silk (Dragline, Hiding and Egg Cocoon) Samples Weaved by Different Species Living in Turkey
- P4-2 L. Bistričić, V. Volovšek, V. Dananić, I. Movre Šapić, M. Leskovic  
DFT Vibrational Study of Organic-Inorganic Hybrid Polymers Based on 3-Glicidoxy-propyltrimethoxysilane
- P4-3 T. Burova, G. Ten, A. Anashkin  
Quantum-Mechanical Calculation of the Intensity Distribution in Resonance Raman Spectra of Derivatives of Uracil
- P4-4 E. Džafić, O. Klein, W. Mäntele  
Monitoring of Hydrogen-Deuterium Exchange in Membrane Proteins using Attenuated Total Reflection Infrared (ATR-IR) Spectroscopy and a Microdialysis Perfusion-Cell
- P4-5 M. Handke, A. Kowalewska, W. Mozgawa  
Spectroscopic Study of Pre-ceramic Polymers Obtained by Hydrolytic Condensation of Ethoxycyclosiloxanes
- P4-6 M. Handke, A. Kowalewska  
New POSS-Siloxane Materials of Ladder-Like Structure
- P4-7 S. Ilie, R. Setnescu  
Characterization of Some Irradiated Materials Using Spectroscopic and Related Methods
- P4-8 D. Krilov, M. Balarin, M. Kosović, O. Gamulin, J. Brnjac-Kraljević  
FTIR Spectroscopy of Lipoproteins - A Comparative Study

- P4-9 **E.A. Minakova, E.B. Kruglova**  
Different Interaction Models for Explanation of Optical Properties of Ligand-Polynucleotides Systems
- P4-10 **Ž. Mitić, G.S. Nikolić, M. Cakić, P. Premović, Lj. Ilić**  
FTIR Spectroscopic Characterization of Cu(II) Coordination Compounds with Exopolysaccharide Pullulan and its Derivatives
- P4-11 **I. Pucić, B. Mihaljević, M. Jakšić**  
Concentration of Vapor Phase Corrosion Inhibitor in Anticorrosion Polymer Films - Correlation of Ion-Beam Analysis Results and UV-Vis Spectrophotometry
- P4-12 **I. Pucić, T. Jurkin**  
 $\gamma$ -Irradiated Poly(Ethylene Oxide): Spectroscopic and Thermal Analysis
- P4-13 **J. Striova, M. Camaiti, A. Sansonetti, A. deCruz, R. Palmer, E.M. Castellucci**  
Spectroscopic Study of Ablated Organic Substances by a Pulsed Er:YAG Laser
- P4-14 **F. Torrens, G. Castellano**  
Binding of Water-Soluble, Globular Proteins to Anionic Model Membranes
- P4-15 **V. Volovšek, K. Furić, L. Bistričić**  
Raman Spectroscopic Study of Siloxane Structures Developed Under Low Pressure

## 5. OPTOELECTRONICS AND SEMICONDUCTOR MATERIALS

- P5-1 **B. Altiocka, S. Aksay, G.S. Kürkçüoğlu**  
FT-Raman and X-ray Diffraction Spectra of CuInS<sub>2</sub> Films by the Spray Pyrolysis at Different Substrate Temperatures
- P5-2 **M. Balarin, O. Gamulin, M. Ivanda, M. Kosović, D. Ristić, M. Ristić, S. Musić, K. Furić, D. Krilov, J. Brnjas-Kraljević**  
Structural, Optical and Electrical Characterization of Porous Silicon Prepared on Thin Epitaxial Layer
- P5-3 **M. Fridrichová, I. Němec, P. Němec**  
Guanylurea(1+) Hydrogenphosphite - A New Material for Non-Linear Optics
- P5-4 **T.M. Hammad**  
The Effect of Annealing on Electrical, Structural and Optical Properties of Sol Gel ITO Thin Films
- P5-5 **I. Kavlak, G.S. Kürkçüoğlu, T. Arslan**  
Theoretical and Experimental Investigation of Vibrational (FT-IR and Raman) Spectra and Electronic Transitions of Di-p-tolylamine
- P5-6 **D. Ristić, M. Ivanda, K. Furić**  
Application of the Phonon Confinement Model on the Optical Phonon Mode of Silicon Nanoparticles
- P5-7 **N. Vedeanu, D.A. Magdas, O. Cozar, I. Ardelean**  
EPR Structural Investigation of CuO-V<sub>2</sub>O<sub>5</sub>-P<sub>2</sub>O<sub>5</sub>-CaO Glass System for Optoelectronic Applications
- P5-8 **D.A. Magdas, N. Vedeanu, O. Cozar, I. Ardelean**  
The Structural Changes Induced in Lead-Phosphate Glasses by Addition of Cooper Oxide
- P5-9 **E. Wolarz, E. Mykowska, T. Martyński, R. Stolarski**  
Spectral Properties of New Tetrafluoro-pentenyl-perylene in Isotropic Solvents, Liquid Crystal Layers, and LB Films

## 6. SPECTROSCOPY IN CHEMICAL, PHARMACEUTICAL AND ENVIRONMENTAL ANALYSES

- P6-1 Y. Akkaya, K. Balci, S. Akyuz  
IR and Raman and Density Functional Theory Studies on a Non-Steroidal Anti-Inflammatory Drug, Naproxen
- P6-2 B. Minčeva-Šukarova, L. Andreeva, O. Magdenovska, V. Manevska, N. Anevska-Stojanovska  
Raman and Infrared Spectroscopic Study of Pharmaceutical Tablets *DIPROL* and *CAFETINE COLD*, Products of *ALKALOID AD SKOPJE* (Republic of Macedonia)
- P6-3 K. Chruszcz-Lipska, M. Baranska, L.M. Proniewicz  
Binding Ability of Fosfomycin towards Sodium and Calcium Ions
- P6-4 A. Baran, M. Baranska  
Vibrational spectroscopy analysis of the anthraquinone pigment alizarin
- P6-5 M. Bartoszek, J. Polak, A. Kos, W.W. Sułkowski  
Spectroscopic Study of Humic Substances Extracted From Bottom Sediment and Water
- P6-6 J. Polak, M. Bartoszek, M. Kantor, W.W. Sułkowski  
Spectroscopic Comparison of the Physico-Chemical Properties of Humic Acids Extracted from Sewage Sludge and Bottom Sediment
- P6-7 A.E. Yavuz, S.H. Bayar, N. Kazancı  
Structural and Vibrational Study of Maprotiline
- P6-8 A.E. Ledesma, J. Zinzuk, J.J. López González, A. Ben Altabef, S.A. Brandán  
Structural and Vibrational Study of 4-(2'-Furyl)-1-Methylimidazole
- P6-9 B. Bojko, A. Sułkowska, M. Maciążek-Jurczyk, J. Równicka, D. Pentak, W.W. Sułkowski  
Comparison of the Influence of Myristic Acid on Acetaminophen and Acetylsalicylic Acid Binding with Serum Albumin
- P6-10 P.Ciacka, A. Jarota, B. Brożek-Płuska, H. Abramczyk  
Transient Absorption, Low-Temperature Raman, Fluorescence Quantum Yield and Stationary Absorption Studies of Various Metal Phthalocyanines and Their Sulfonated Derivatives
- P6-11 O. Cozar, F. Drăgan, C. Jelic, V. Chiş, N. Leopold, L. Szabó  
Spectroscopic Investigation of Some Cu(II) Cardiovascular Complexes
- P6-12 M. Culea, O. Cozar, E. Culea  
GC/MS as a Tool for Non-Invasive Diagnosis
- P6-13 M. Culea, S. Neamtu  
Study of Amino Acid Transmembranar Transport
- P6-14 T. Dziembowska, Z. Rozwadowski, M. Szafran  
NMR and DFT Study of the Enol Imine  $\leftrightarrow$  Enaminone Tautomeric Equilibrium in Schiff Bases in Some Organic Solvents
- P6-15 C. Farcau, S. Astilean  
Single-Molecule Surface Enhanced Raman Scattering on Periodically Nanostructured Gold Films
- P6-16 M. Gotić, G. Koščec, S. Musić  
A Study of the Reduction and Reoxidation of Substoichiometric Magnetite
- P6-17 A. Hacura, M. Jadamus-Hacura  
Classification of Polish Honeys by Mid-Infrared Spectroscopy and Multivariate Statistical Analysis

- P6-18 I. Hannus, Sz. Mészáros, M. Búza, J. Halász  
IR Spectroscopic Study of the Hydrodechlorination of Chlorobenzenes and Chlorophenols over Nobel Metal Containing Zeolites
- P6-19 I. Hannus, M. Búza, A. Beck, L. Guzzi  
Catalytic Activity of Bimetallic Gold Containing Nanoparticles on Different Supports Investigated by IR Spectroscopy
- P6-20 A. Iordache, M. Culea, O. Cozar  
Characterization of Allergens in Different Perfumes and Herbs
- P6-21 O. Klein, I. Klein, G. Oremek, W. Mäntele  
Clinical Chemistry without Reagents? An Infrared Spectroscopic Technique for Determination of Clinically Relevant Constituents of Body Fluids
- P6-22 E. Kucharska, W. Szaśiadek, H. Ban-Oganowska, M. Mączka, J. Hanuza  
Synthesis, Molecular Structure, IR and Raman Spectra as well as DFT Quantum Chemical Calculations for N-thiocyanoacetyl piperidine and its Methyl Derivatives
- P6-23 L. Kukoč Modun, Nj. Radić  
Kinetic Spectrophotometric Determination of N-(2-Mercaptopropionyl)-glycine in Pharmaceuticals
- P6-24 J. Lorenc, B. Palasek, J. Hanuza, M. Mączka, A. Waśkowska  
Rotational Disorder in 2-Piperidyl-5-nitro-6-methylpyridine: Structural Phase Transition and its Vibrational Characteristics
- P6-25 Ž. Marinić, P. Trošelj, M. Eckert-Maksić, D. Margetić  
Spectroscopic and Quantum-Chemical Assignments of Stereochemistry of Products Obtained by 1,3-dipolar Cycloaddition Reactions of Substituted 1,3,4-oxadiazoles With Norbornenes
- P6-26 M. Marković, T. Biljan, D. Škalec Šamec  
Entacapone Isomer Quantification Using Raman Spectroscopy
- P6-27 J. Maurer, V. Vogel, W. Mäntele  
Study of Heparin/Protamine Complexation by Means of Fluorescence Spectroscopy, Light Scattering and Analytical Ultracentrifugation
- P6-28 V. Pandurić, Z. Tarle, Z. Hameršak, I. Stipetić, D. Matošević, K. Prskalo, V. Negovetić-Mandić  
Detection of HEMA in Self-etching Adhesive Systems Using High Performance Liquid Chromatography
- P6-29 A. Pîrnău, V. Chiş, L. Szabo, O. Cozar, M. Vasilescu, O. Oniga, R.A. Varga  
Experimental and Theoretical Investigation of 5-para-nitro-benzylidene-thiazolidine-2-thione-4-one Molecule
- P6-30 J. Równicka, A. Sułkowska, M. Maciążek-Jurczyk, B. Bojko, J. Pożycka, W.W. Sułkowski  
Fluorescence Analysis of Sulfasalazine Bound to Defatted Serum Albumin in the Presence of Denaturing Factors
- P6-31 M. Maciążek-Jurczyk, A. Sułkowska, B. Bojko, J. Równicka, W.W. Sułkowski  
Fluorescence Analysis of Interaction of Phenylbutazone and Methotrexate in Binding to Serum Albumin in Combination Treatment in Rheumatology
- P6-32 V. Balevicius, Z. Gdaniec, V. Sablinskas  
2D NMR Study of Media Effects of Ionic Liquids on Hydrogen Bonding
- P6-33 S. Strazdaite, J. Cėponkus, V. Aleksa, V. Sablinskas  
Structures of 1-Butene and 1-Heptene Primary Ozonides as Studied by Means of Matrix Isolation FTIR Spectroscopy
- P6-34 L. Szabó, V. Chiş, A. Pîrnău, N. Leopold, O. Cozar, Sz. Orosz  
Vibrational, NMR and DFT Investigations of Amlodipine Molecule

- P6-35 L. Szabó, A. Pîrnău, N. Leopold, V. Chiş, O. Cozar  
Vibrational, NMR and DFT Investigations of Ethylenediaminetetraacetic acid
- P6-36 A. Terczynska, K. Cholewa-Kowalska, M. Laczka  
The Effect of Silicate Network Modifiers on Colour and Electron Spectra of Transition Metal Ions
- P6-37 V. Toteva, A. Georgiev, L. Topalova, S. Andreev  
Estimation of the Desulphurization Degree in Light Cycle Oil Using FTIR Spectroscopy
- P6-38 N.U. Perišić-Janjić, Gy.Gy. Vastag, J.D. Janjić, B.Ž. Jovanović  
Organic Solvents Influence on Electronic Absorption Spectra of 4-R-phenyl 5-carboxyethyl-6-methyl-3,4-dihydropyrimidine-2-thione Derivatives. Ionization Constants Determination.
- P6-39 G. Schäfer, W. Mäntele, G. Wille  
Carboxylation Reactions Studied Using Caged CO<sub>2</sub>
- P6-40 K. Vranić, V. Vojković  
Spectrophotometric Studies of the Interaction of Ruthenium with Hesperetin
- P6-41 A. Zając, M. Wandas, J. Hanuza  
Synthesis, Molecular Structure and Vibrational Spectra of Bioactive Hybrid Materials Composed on Chitosan, Sodium Alginate and 1,6-Hexamethylene-di(aminocarboxylsulfonate)
- P6-42 J. Zhang, A. Gajović, D. Su, R. Schlögl  
Molecular Spectroscopy in Coke-free Carbon Catalysis
- P6-43 B. Trzcińska, J. Zięba-Palus, P. Kościelniak  
Application of Microspectrometry in Visible Range to Differentiation of Car Solid Paints for Forensic Purposes

## 7. SPECTROSCOPY APPLIED TO ARCHAEOLOGY, ARTS, GEOLOGY AND MINERALOGY

- P7-1 S. Akyuz, T. Akyuz, S. Basaran, I. Kocabas, A. Gulec, H. Cesmeli  
FT-IR and EDXRF Analysis of Wall Paintings of Ancient Ainos Hagia Sophia Church
- P7-2 L. Darchuk, Z. Tsybriy, E.A. Stefaniak, C. Vazquez, O.M. Palacios, A. Worobiec, F. Sizov, R. Van Grieken  
Application of Molecular Spectroscopy to Study the Composition of Prehistoric Pigments from Excavations (Argentina)
- P7-3 E. del Puerto, Z. Jurasekova, S. Sánchez-Cortés, J.V. García-Ramos, C. Domingo, A. Roquero  
Towards a Surface-Enhanced Raman Spectra Database of Dyed Textiles
- P7-4 M.L. Franquelo, A. Duran, L.K. Herrera, M.C. Jimenez de Haro, J.L. Perez-Rodriguez  
Comparison between Two Molecular Spectroscopy Techniques as Analytical Tools in the Characterization of Pigments in Southern Spain Cultural Heritage: Micro Raman and Micro-FTIR Spectroscopy
- P7-5 N. Tomašić, A. Gajović, V. Bermanec  
Raman Spectra and Luminescence of the Minerals with Aeschynite and Euxenite Crystal Structure
- P7-6 S. Gosav, M. Praisler, D.O. Dorohoi  
Expert Systems Built for the Modeling of Small Molecular Structures Using a Concatenated Spectral Database
- P7-7 S. Gosav, M. Praisler  
Optimisation of the Performances of a Hybrid Expert System Designed for the Elucidation of Molecular Structures

- P7-8 P. Makreski, G. Jovanovski, B. Kaitner  
Minerals from Macedonia. XXIV. Spectroscopic and Structural Characterization of Tectosilicates
- P7-9 N.F.C. Mendes, I. Osticioli, C. Lofrumento, A. Zoppi, E.M. Castellucci  
Combined Fluorescence-LIBS and Raman Spectroscopy Setup for Applications in the Field of Cultural Heritage
- P7-10 J. Mihály, J. Mink, V.T. Dobosi, S.F. Parker, J. Tomkinson  
FTIR and INS Study of Lower Palaeolithic Burned Animal Bones from Vértesszőlős (Hungary)
- P7-11 W. Mozgawa, W. Jastrzębski  
Vibrational Spectra of  $\beta$ -Cage Units in Different Silicate Structures
- P7-12 W. Mozgawa, M. Król  
Application of IR Spectra in the Studies Heavy Metal Cations Immobilization on Natural Sorbents
- P7-13 A. Adamczyk, W. Mozgawa, M. Handke, E. Długoń, A. Ferensowicz  
The FTIR Studies of Influence of Different  $\text{Al}_2\text{O}_3$  and  $\text{SiO}_2$  Precursors on Structure of Alumina-Silica Gels and Coatings
- P7-14 W. Mozgawa, J. Deja  
The IR Spectroscopy Studies of Alkaline Activated Slag Geopolymers
- P7-15 L.A. Pérez-Maqueda, A. Duran, P.E. Sánchez Jiménez, M.L. Franquelo, J.L. Perez-Rodriguez  
Study of the Dehydroxylation-Rehydroxylation of Pyrophyllite by Spectrometric and Thermal Analysis Methods
- P7-16 M. Łodziński, M. Sitarz  
Chemical and Spectroscopic Characterization of Some Phosphates Accessory Minerals from Pegmatites of the Sowie Mts (Owles Mts), SW Poland
- P7-17 A. Van Alboom, V.G. De Resende, E. De Grave, M.D. Dyar, J.A.M. Gómez  
Low Temperature Mössbauer Spectra of Rozenite and Szomolnokite

## 8. CHEMICAL DYNAMICS

- P8-1 L.M. Babkov, N.A. Davydova, K.E. Uspenskiy  
Vibrational Spectra of the 2-, 4-Bromo- and 4,4'-Chlorobenzophenones and Their Interpretation Using Structural-dynamical Models
- P8-2 C. Carmona, J. Hidalgo, A. Sánchez-Coronilla, M.A. Muñoz, M. Balón  
Betacarboline Tautomerism Induced by Temperature. Dual Emission of Betacarboline Self-Associated Hydrogen Bond Aggregates.
- P8-3 E. García-Fernández, M.A. Muñoz, C. Carmona, M. Balón  
Ground state Isomerism and Dual Fluorescence of 2-Methylharmine Anhydronium Base (7-Methoxy-1, 2-dimethyl-2H-pyrido[3,4-b]indole) in Aprotic Solvents
- P8-4 J. Hetmańczyk, L. Hetmańczyk, E. Mikuli, A. Migdał-Mikuli  
Phase Transition and  $\text{NH}_3$  Motions in Polycrystalline  $[\text{Ca}(\text{NH}_3)_6](\text{ClO}_4)_2$  Studied by Infrared Spectroscopy and Inelastic/Quasielastic Incoherent Neutron Scattering
- P8-5 O.Yu. Khetselius  
Laser Photo-Ionization (Dissociation) of Molecules in the Isotopes Separation and Relativistic Calculating the Hyperfine Structure Parameters in Heavy-Element Chemistry and Spectroscopy
- P8-6 M. Rudbeck, S. Kumar, M. Blomberg, M-A. Mroginski, A. Barth  
PEP Vibrations from DFT
- P8-7 V.I. Tomin, S. Oncul, G. Smolarczyk, A.P. Demchenko  
Dynamic Quenching as a Simple Test for the Mechanism of Excited-State Reaction

## 9. THEORETICAL SPECTROSCOPY AND COMPUTER METHODS

- P9-1 **G.A. Akverdieva, N.M. Godjayevev, S. Akyuz, N.E. Dogan, T. Akyuz**  
Molecular Mechanics Study of Antihypertensive Val-Tyr Dipeptide
- P9-2 **S. Aydemir, M. Duran, E. Tasal, Halil Berber, C. Öğretir, M.S. Kılıçkaya**  
*Ab Initio* Calculations of  $pK_a$  Values for Some 6-Methyl-2-Pyridine Carboxaldehyde Derivatives
- P9-3 **S. Aydemir, M. Duran, E. Tasal, Halil Berber, C. Öğretir, M.S. Kılıçkaya**  
*Ab Initio* Calculations of  $pK_a$  Values for 7-Acetoxy coumarin-3-Carboxylic Acid
- P9-4 **P. Borowski, M. Fernández-Gómez, M.-P. Fernández-Liencre, T.P. Ruiz**  
An Effective Scaling Frequency Factor Method (ESFF) for Scaling of Harmonic Vibrational Frequencies
- P9-5 **M.Q. Rincón, M. Fernández-Gómez, M.P. Fernández-Liencre, T.P. Ruiz, P. Borowski**  
Analysis of the Vibrational Spectrum of P-Methyl Styrene Based on IR, Raman and INS Data and *Ab Initio* and DFT Calculations
- P9-6 **O. Gamulin, M. Kosović, M. Balarin, D. Krilov, J. Brnjas-Kraljević**  
Denoising Raman Spectra of Biological Samples Using Wavelets
- P9-7 **A.V. Glushkov, S.V. Malinovskaya, O.Yu. Khetselius**  
New Laser-Electron Nuclear Effects in the Nuclear  $\gamma$  Transition Spectra of Molecular Systems
- P9-8 **O.Yu. Khetselius, A.V. Glushkov, E.P. Gurnitskaya, A.V. Loboda**  
Spectroscopy of Hadronic Molecules and Molecules with Superheavy Elements: Spectra, Energy Shifts and Widths for Different Nuclear Models
- P9-9 **D. Kirin, I. Lukačević, S.K. Gupta, P.K. Jha**  
Density Functional Calculation of Raman Intensity in High Pressure Phases of  $TiO_2$  crystal
- P9-10 **M. Szafarska, M. Woźniakiewicz, M. Pilch, J. Zięba-Palus, P. Kościelniak**  
Computer Analysis of ATR-FTIR Spectra of Paint Samples for Forensic purposes
- P9-11 **J. Lamouroux, VI.G. Tyuterev, L. Régalia-Jarlot, S.A. Tashkun**  
Comparison of Theoretical Intensity Calculations and Experimental Intensities Measurements for Non Linear Triatomic Molecules
- P9-12 **I. López-Tocón, J.F. Arenas, S.P. Centeno, D. Pelaez, J.C. Otero**  
Correlating the Force Fields of Methylpyrazines: Vibrational Spectrum of Tetramethylpyrazine
- P9-13 **C.M. Nunes, S. Lopes, T.M.V.D. Pinho e Melo, R. Fausto**  
Matrix Isolation FTIR Spectroscopic and Theoretical Study of Dimethyl 2,2-Dioxo-1*H*,3*H*-Pyrazolo[1,5-*c*][1,3]Thiazole-6,7-Dicarboxylate
- P9-14 **G. Ogruc-Ildiz, S. Akyuz, A.E. Ozel**  
Experimental, *Ab Initio* and Density Functional Theory Studies on Sulfadiazine
- P9-15 **R. Kępa, M. Ostrowska-Kopeć**  
New Spectroscopic Studies of the Fourth-Positive ( $A^1\Pi \rightarrow X^1\Sigma^+$ ) System Bands in  $^{13}C^{16}O$
- P9-16 **A.E. Ozel, S. Celik, S. Akyuz**  
Vibrational Spectroscopic Investigation of Free and Coordinated 5-Aminoquinoline: The IR, Raman and DFT Studies
- P9-17 **A. Padilla, J. Pérez**  
Hindered Rotation in the Infrared Spectra of HCl in Liquefied Rare Gases
- P9-18 **R. Kępa, I. Piotrowska**  
New Analysis of the Comet-Tail ( $A^2\Pi_i \rightarrow X^2\Sigma^+$ ) System Bands in  $^{12}C^{18}O^+$

- P9-19** V.H. Rusu, J.B.P. da Silva, M.N. Ramos  
A Theoretical Study of the Hydrogen Bonding between vic-, cis- and trans-C<sub>2</sub>H<sub>2</sub>F<sub>2</sub> Isomers and Hydrogen Fluoride
- P9-20** M.N. Ramos, K.C. Lopes, V.H. Rusu, R.C.M.U. Araújo  
Effects of Wave Function Modifications on Calculated HC and CC Stretching Frequencies in H<sub>2</sub>C=CHX and HC≡CHX Molecules
- P9-21** P. Singh, S. Jaiswal, G. Srivastav, R.A. Yadav  
Vibrational Spectroscopic Investigation on Vitamin P Using Ab Initio and DFT Method: Theoretical Study
- P9-22** E. Taşal, Y. Gülseven, İ. Sıdır, T. Önkol, C. Öğretir, M.S. Kılıçkaya  
Experimental and Theoretical Studies on <sup>13</sup>C and <sup>1</sup>H NMR Spectra of 6-(2-fluorobenzoyl)-3-(2-(4-(4-fluorophenyl) piperazin-1-yl)-2-oxoethyl)benzo[d]thiazol-2(3H)-one
- P9-23** E. Taşal, Y. Gülseven, İ. Sıdır, T. Önkol  
Theoretical Studies on Molecular Structure and Some Molecular Properties of 6-(2-fluorobenzoyl)-3-(2-(4-(4-fluorophenyl)piperazin-1-yl)-2-oxoethyl)benzo[d]thiazol-2(3H)-one
- P9-24** Y. Gülseven, E. Taşal, İ. Sıdır, C. Öğretir  
Quantum Chemical Studies on Tautomerism and Acidity-Basicity Behaviours of Some 1,2,4-triazole Derivates
- P9-25** T. Wróblewski  
DFT and Ab Initio Computational Study of Structural Properties and Vibrational Spectra for Protonated Water Clusters
- P9-26** G. Yapar, K. Balci  
A Theoretical IR and Raman Spectroscopic Study on 1,2-Bis(o-carboxyphenoxy) ethane molecule
- P9-27** H. Yurtseven  
Pippard Relations Modified by the Raman Frequency Shifts for the Phases I and II in NH<sub>4</sub>I
- P9-28** H. Yurtseven  
Calculation of the Raman Frequencies Using Volume Data Close to the Tricritical and Second Order Phase Transitions in NH<sub>4</sub>Cl

## 10. SURFACE SPECTROSCOPIES

- P10-1** E. Akalin, S. Akyuz, T. Akyuz  
Adsorption of Isoniazid onto Sepiolite-Palygorskite Group of Clays: An IR and DFT Study
- P10-2** S. Aksay, G.S. Kürkçüoğlu, A.Ş. Aybek, M. Kul, E. Turan, T. Özer, Hüseyin Berber, Halil Berber, M. Zor  
FT-IR and FT-Raman Spectra of SnS Film Deposited by Chemical Bath Deposition Method
- P10-3** S. Bonora, M. Di Foggia, A. Maris  
Surface Enhanced Raman Spectroscopy (SERS) Study of Diluted Solutions of Cimetidine and Some of its Metallocomplexes
- P10-4** C. Domingo, L. Guerrini, S. Sánchez-Cortés, J.V. García-Ramos  
Fabrication and Functionalization of Core-Shell Au/Ag Nanoparticles with Advanced Physico-Chemical Properties: Application to the Detection of Pollutants by Surface-Enhanced Raman Scattering

- P10-5 J.V. García-Ramos, L. Guerrini, I. Izquierdo, C. Domingo, S. Sánchez-Cortés  
Building Highly Selective Hot Spots in Ag Nanoparticles Using Bifunctional Diamines with Variable Length: Application to the Detection of Pollutants by Surface-Enhanced Raman Scattering
- P10-6 M.R. Lopez-Ramirez, L. Roldán, J.V. Garcia-Ramos, S. Sanchez-Cortes  
SERS Analysis of Herbicide Diquat on Nanostructured Metal Electrodes
- P10-7 M. Muniz-Miranda, E. Giorgetti, G. Margheri, S. Sottini, A. Giusti, G. Dellepiane  
SERS Study of Self-Assembled Carbazoyl-Diacetylene Monolayers Chemisorbed on Gold Surfaces
- P10-8 M. Muniz-Miranda, B. Pergolese, A. Bigotto  
Study of the Adsorption of 2-Mercaptobenzoxazole on Gold Colloidal Nanoparticles by Means of Surface Enhanced Raman Scattering
- P10-9 E. Stodolak, C. Paluszkiwicz, M. Błażewicz  
*In vitro* Biofilms Formation on Polymer Matrix Composites
- P10-10 C. Paluszkiwicz, W.M. Kwiatek, E. Długoń, A. Weselucha-Birczyńska, M. Piccinini  
IR Mapping of Bio-Ceramic Layers on Titanium Substrate
- P10-11 M. Sladkova, B. Vlckova, K. Siskova, I. Pavel, M. Moskovits, M. Slouf  
Surface-enhanced Raman Scattering from a Single Molecularly-bridged Silver Nanoparticle Aggregate

## 20.00 Conference Dinner

### Friday, September 5

#### MORNING SESSION

#### PLENARY LECTURES

Congress Hall

Chairs: A. Barnes, S. Musić

- 09.00 - 09.45 Boris Galabov  
Spectroscopic and Theoretical Parameters In Predicting Hydrogen Bond Strength, Conformational Stability and Chemical Reactivity
- 09.45 - 10.30 Henry H. Mantsch  
The Globalization of Science and its Impact on the Transition Countries in Europe

10.30 - 11.00  Coffee break

#### CLOSING LECTURE

11.00 - 11.30 EUCMOS 2010 Lecture

11.30 - 12.00 Closing Ceremony