

EUCMOS 2008 - CONGRESS SCHEDULE

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

- 11.00 - 13.00 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-d₀ and -d₅, 2-Fluoro- and 3-Fluoropyridine, and 1,3-Benzodioxan
- 11.40 - 12.00 E. Kleinpeter, A. Koch
Spatial Magnetic Properties of Trisannelated 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 Chloride, Bromide and Perchlorate
- 12.20 - 12.40 D.K. Breitinger, G. Brehm, M. Weil, S. Baumann
Vibrational Spectra of K₂[O(HgSO₃)₃] Containing a New Anionic Metallo-Oxonium Complex with a OHg₃ 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. Mantele
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. Tsentalovich, 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

Hall: Camelia 2

Topic 11. Time resolved spectroscopy & Topic 12. New instrumentation
(Chairs: I. Pálínkó, 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

Congress Hall

INVITED LECTURES

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 Nada 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 α -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 B₁₃ Complexes with Transition Metal Ions. The Role of Unusual Cu(II)··· π 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, G. Granozzi)

- 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
- 12.30 - 12.50 **V. Ličina**, A. Mogaš-Milanković, Ž. Skoko, S. Musić, M. Ivanda
Influence of Crystallization on the Electronic Conductivity of Iron Phosphate Glasses

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 $[Cu(biz)_2][Cu_2Br_4]$ 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 $CH_3Cl + H_2O$ and $NO + H_2O$ 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 **G.S. Kürkcüoğlu**, S. Aksay, I. Kavlak
FT-IR and FT-Raman Spectroscopic Studies of 2-Methylpyrazine Tetracyanonickelate Benzene Clathrates: $M(C_5H_6N_2)Ni(CN)_4 \cdot C_6H_6$ ($M = Mn, Cd, Co$ or Ni)
- 12.10 - 12.30 **R. Singh**, M. Kumar, R.A. Yadav
Theoretical Study of IR and Raman Spectra of 5-Hydroxy Uracil

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 TiO₂ 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

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 Matrices
- 16.30 - 17.00  Coffee break

POSTER PRESENTATIONS

17.00 - 19.00 Poster Session A - Topics 1-3, 11, 12

1. MOLECULAR STRUCTURE

S. Akyuz, T. Akyuz

Vibrational Spectroscopic Study of 4-Aminopyrimidine Complexes

L. Andreeva, F. Trajkovic, J. PetreskaInvestigation of the Vibrational Spectra of Some Partially Deuterated Cd(NH₃)₂Cl₂, Hg(NH₃)₂Cl₂, Pd(NH₃)₄Cl₂ Complexes**L.M. Babkov**, N.A. Davydova, K.E. Uspenskiy

2-Biphenylmethanol Vibrational Spectra and Their Interpretation Using Structural-Dynamical Model in Anharmonic Approximation

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

L.M. Babkov, I.I. Gnatyuk, G.O. Puchkovska, K.E. Uspenskiy

The Appearance of Conformational Mobility of Behenic Acid in IR Spectra

K. Balci, Y. Akkaya, S. Akyuz

A Theoretical Conformational Analysis and Vibrational Spectroscopic Investigation on Niflumic Acid

Gonul Basar, S. Akyuz, Gunay Basar, S. Kröger

Studies on Kyotorphin and D-Kyotorphin in Aqueous Solution by Raman Spectroscopy

C. Bayrak

Vibrational Spectroscopic Studies on the T_d -Type Clathrates: $M(N,N'$ -Dimethylethylenediamine) $M'(CN)_4.C_6H_6$ ($M = Mn, M' = Zn, Cd$ or Hg ; $M = Cd, M' = Cd$ or Hg)

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 α -ol

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 $CF_3CO_2CH_2CF_3$ from Electron Diffraction Data, Infrared Spectra and Quantum Chemical Calculation of Vibrational Properties

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

E. Benassi, P.S. Sherin

Combined Experimental and Theoretical Study on the Kynurenine

A. Borba, A. Gómez-Zavaglia, R. Fausto

Photochemistry and Vibrational Spectra of Matrix-Isolated Isoniazid

D.K. Breitinger, G. Brehm, J. Zürlbig, M. Weil, S. Baumann

Bis(sulfito)mercurates $M_2[Hg(SO_3)_2] \cdot xH_2O$ ($M = NH_4, Na, K$; $x = 0, 1, 2.25$). Vibrational Spectra of the Solids and of Aqueous Solutions.

D.K. Breitinger, M. Moll, G. Brehm

Sulfito Mercurate Complexes in Solution Studied by ^{199}Hg NMR Spectrometry

J. Ceponkus, D. Lesciute, V. Sablinskas

Association of Water with Small Monocarboxylic Acids. Matrix Isolation Infrared Absorption Study.

V. Chiş, R. Ştiufluic, N. Leopold

Molecular and Electronic Structure of PTCDI and Melamine-PTCDI Complex

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

A. Nikolić, B. Jović, E. Davidović, S. Petrović

N-H...O Hydrogen Bonding. FT-IR and NIR Study of N-Methylformamide-Ether Systems.

Z. Dega-Szafran, M. Szafran

Experimental and Theoretical Vibrational Spectra of Piperidine-2-carboxylic Acid

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

I. Despotović, Z.B. Maksić

Towards Organic Conductors - the Structure and Stability of Cyano-[n]-Radialenes and Their Dianions

M.E. Jamróz, M.H. Jamróz, J.E. Rode, J.Cz. Dobrowolski

Interpretation of Vibrational Spectra of Allyl Acrylate

K. Furić, B.-M. Kukovec, Z. Popović

Raman Study of Nickel(II) Complexes with 6-Methylpicolinic Acid

J. Polovková, A. Gatiaľ, M. Gróf, J. Kožíšek, V. Milata, N. Prónayová, P. Matějka

Isomerizational and Conformational Study of 3-Cyclopropylamino-2-Acetyl Propenenitrile (CpAAP) and 3-Cyclopropylamino-2-Methylsulfonyl Propenenitrile (CpASP)

I. Gocan, C. Nagy, M.M. Venter, V. Bercean, L. David

Spectral Investigations on Metal Complexes of Heterocyclic N,S-Donors

M. Gróf, A. Gatiaľ, J. Kožíšek, V. Milata, P. Matějka

Conformational Analysis of Aminomethylene- and Methylaminomethylene-Malonic Acid Dimethylester

M. Gróf, A. Gatial, J. Kožišek, V. Milata, P. Matějka

Conformational Analysis of Dimethylaminomethylene-Malonic Acid Dimethyl Ester

Ł. Hetmańczyk, J. Hetmańczyk, A. Migdał-Mikuli, E. Mikuli

Phase transition and H₂O motions in [Ba(H₂O)₄](ClO₄)₂ studied by differential scanning calorimetry, infrared spectroscopy and inelastic/quasielastic incoherent neutron scattering

I. Jelovica Badovinac, N. Orlić, C. Gellini, L. Moroni, P.R. Salvi

Micro-Raman and Computational Study of the Azoxybenzene Photorearrangement to 2-Hydroxybenzene

M. Juribašić, L. Stella, Ž. Marinić, M. Vinković, Lj. Tušek-Božić

Microwave Synthesis and Spectroscopic Study of 3-Quinoline-substituted α -Amino-phosphonates

M. Jurić, P. Planinić, D. Žilić, B. Rakvin, B. Prugovečki

A New Heterometallic (Ni²⁺ and Cr³⁺) Complex - Crystal Structure and Spectroscopic Characterization

A. Kocot, K. Merkel, J. Ziolo

Investigation of Liquid-Liquid Phase Transition for Trans-1,2 dichlorethylene

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

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

L. Macalik, M. Mączka, J. Hanuza, A.A. Kaminskii

Polarized Raman and IR spectra of the orthorhombic CaNb₂O₆:Pr³⁺ single crystal

W. Makulski, A. Wikiel

Nuclear Magnetic Shielding and Spin-spin Coupling Constants for Acetaldehyde from Gas-phase NMR Spectroscopy

K.M. Marzec, K. Malek, B. Gawel, W. Lasocha, L.M. Proniewicz

Structure Determination of Ag(I) Ion Complex of Rhodanine

K. Malek, M. Makowski, L.M. Proniewicz

Raman Spectroscopy in Studies on the Selected Dehydropeptides

K.M. Marzec, K. Malek, A. Kaczor, L.M. Proniewicz

Conformational and Vibrational Analysis of Selected Monoterpenoids by Using Density Functional Theory

S. Miljanić, Z. Meić, G. Keresztury

Polarized Vibrational Spectra of *p*-Substituted Nitro and Dinitro *cis*- and *trans*-Stilbenes

I. Movre Šapić, L. Bistričić, V. Volovšek, V. Dananić

DFT Study of Molecular Structure and Vibrations of 3-Glycidoxypropyltrimethoxysilane

P. Novak, K. Pičuljan, T. Hrenar, M. Rubčić, M. Cindrić

Solution State Structure of Methoxysalicylaldehyde Thiosemicarbazone Derivatives by NMR and DFT Methods

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

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

N. Peran, Z.B. Maksić

Calculating pK_a of Some α -Aminoacids Using Cluster-Continuum Model

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®

K. Pičuljan, P. Novak, K. Užarević, M. Cindrić, T. Hrenar, T. Jednačak

Hydrogen Bonding and Deuterium Isotope Effects in ¹³C NMR Spectra of Phenylene Enaminones Derived from Dehydracetic Acid

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

S. Rada, V. Maties, M. Rada, L. Pop, E. Culea
The Local Structure of Europium Lead-Borate Glasses and Glass Ceramics

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

M. Ristova, G. Petruševski, A. Raškova, B. Šoptrajanov
Vibrational Spectra of Hydrates of Some Metal(II) Malonates

J.Cz. Dobrowolski, M.H. Jamróz, R. Kołos, J.E. Rode, J. Sadlej
IR Low-temperature Matrix and *Ab Initio* Study on β -Alanine Conformers

D. Rusu, O. Baban, I. Hauer, L. David, M. Rusu
Synthesis and Physical Chemical Characterization of The Potassium 11-Tungstovanado(IV) Phosphate Anion

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

M. Sałdyka, B. Golec, Z. Mielke
Spectroscopy and Photochemistry of Glyoxal-Hydroxylamine Complexes. Matrix Isolation and Theoretical Study

M. Sitarz, Z. Fojud, Z. Olejniczak
Submicroheterogenous Structure of Silico-Phosphate Glasses Studied by ^{23}Na , ^{27}Al , ^{31}P NMR and FTIR

V. Smrečki, P. Novak, D. Vikić-Topić, Z. Meić
Deuterium Isotope Effects in ^{13}C NMR Spectra of *ortho*-, *meta*- and *para*-Deuterium Labelled Mono- and Binuclear Aromatic Compounds

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

D. Vojta, G. Baranović
Raman Study of Anharmonic Effects in Vibrational Spectra of Acetylenic Compounds

S.X. Zhou, D.T. Durig, J.R. Durig
Vibrational Spectra and Structural Parameter of Methyl and Ethyl Isocyanate

D. Vojta, B. Zimmermann, G. Baranović
Vibrational Analysis of Diacetylenic Aromatic Compounds

2. BIOSPECTROSCOPY

V. Andrushchenko, P. Bouř
Interpretation of Vibrational Spectra of DNA Fragments Interacting with Metal Ions

Gunay Basar, S. Kin, G. Temizkan, T. Gunel, S. Akyuz
Laser Tweezers Raman Spectroscopic Investigation of Geranylgeranyl Pyrophosphate Synthase in Recombinant *Schizosaccharomyces pombe* Cell

N.V. Belogurova, N.S. Kudryasheva, R.R. Alieva, A.G. Szykh
Upper Electron-Excited States in Coelenterate Bioluminescence

P. Carmona, M. Molina, A. Rodríguez-Casado
On the Hydrogen-Deuterium Exchange in Proteins and Nucleic Acids Monitored by Vibrational Spectroscopy

S. Cavalu, V. Simon, F. Banica
Dysprosium/Iron Aluminosilicate for Simultaneous Radiotherapy and Hyperthermia: Structural Investigation and Biocompatibility Evaluation

G. Doyle, D. Zerulla

Investigating the Kinetic Interactions between Protein and Nanoparticles via Mie Scattering Spectroscopy and Optical Trapping

A.V. Glushkov, S.V. Malinovskaya, S.V. Ambrosov, O.Yu. Khetselius

Spectroscopy and Structural Properties of Biogene Amines (Serotonine, Histamine, γ -amino oil acid) and Account for Laser and Neutron Capture Effects

V. Gombás, J. Mink

Chemometrics Methods Used by Spectroscopic of Biological Samples

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

R. Dědic, 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

Y. Ike, E. Hashimoto, S. Kojima

Micro-Brillouin Scattering Study of Low Temperature Elastic Properties of Protein Crystals

G. Keresztury, T. Sundius, T. Lóránd

Vibrational Spectroscopic Investigation of Bioactive Aminoalcohols

S. Kumar, A. Barth

Ligand induced conformational change of pyruvate kinase studied by ATR-FTIR spectroscopy

Z. Tarle, D. Škrtić, A. Knežević, D. Matošević, M. Ristić, K. Prskalo, S. Musić

Degree of Vinyl Conversion in Experimental ACP Composites

K. Merkel, A. Kocot, W. Pluskiewicz, A. Pyrkosz

Raman and FTIR Spectroscopy of the Keratin as a Potential Tool for Probing Bone Health

V. Mohaček Grošev, J. Grdadolnik, J. Stare, D. Hadži

Hydrogen Bonding in $(\text{COOH})_2 \cdot 2\text{H}_2\text{O}$ and $(\text{COOD})_2 \cdot 2\text{D}_2\text{O}$

A. Aranyi, Z. Csendes, J.T. Kiss, I. Pálínkó

Covalently Grafted, Silica Gel Supported C-protected Cysteine or Cystine Copper Complexes – Syntheses, Structure and Possible Surface Reaction Studied by FT-IR Spectroscopy

M. Lasalvia, N. L'Abbate, G. Perna, E. Mezzenga, V. Capozzi

Raman Spectroscopy Study of Cellular Damage in Human Keratinocytes Treated with Organophosphate Compounds

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

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

M. Rokita, M. Sitarz

Phosphate Layers on Titanium and Ti6Al4V Titanium Alloy - Comparison of Hydroxyapatite Layers Obtained During SBF Soaking

M. Śmiechowski, E. Gojto, J. Stangret

Systematic Study of Hydration Patterns of Phosphoric (V) Acid and Its Mono-, Di- and Tripotassium Salts in Aqueous Solution

J. Surmacki, B. Brożek-Płuska, H. Abramczyk, Z. Morawiec, M. Tazbir

Application of Raman Spectroscopy for Breast Cancer Diagnosis

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

A. Tinti, J. Domènech, S. Atrian, M. Capdevila, A. Torreggiani

Raman Spectroscopy Investigation on Metal-Metallothionein Complexes

3. NANOSTRUCTURED MATERIALS

M. Barczak, A. Dąbrowski

Spectroscopic Characterization of Polysiloxane and Bridged Polysilsesquioxane Xerogels

L. Bistričić, M. Leskovac, G. Baranović, E. Govorčin Bajsić

Linear IR dichroism of polyether-based polyurethane-silica nanocomposites

V. Canpean, S. Astilean

Subwavelength Metallic Nanohole Arrays as Multifunctional Plasmonic Substrates for SPR and SERS Sensors

E. Culea, L. Pop, M. Bosca

Novel Bismuth-Lead-Silver Glasses Doped with Neodymium Ions

V.G. de Resende, E. De Grave, A. Cordier, C. Laurent, A. Peigney, A. Weibel

Carbon Nanotube-Fe/Al₂O₃ Nanocomposites by CCVD Method: Formation of CNTs from α -(Al_{1-x}Fe_x)₂O₃ Oxide Powders that were Prepared by Oxinate Route

M. Didović, S. Valić, D. Klepac, A.P. Meera, S. Thomas

ESR Study of NR/Montmorillonite Nanocomposites

A. Fraczek, C. Paluszkiwicz, A. Weselucha-Birczynska, S. Blazewicz

The Influence of Carbon Nanotubes on PAN-based Fibers Properties

A. Gajović, S. Šturm, B. Jančar, M. Čeh

The Mechanism of BiFeO₃ Hydrothermal Synthesis

A.V. Glushkov, S.V. Malinovskaya, S.V. Ambrosov, O.Yu. Khetselius

Spectroscopy and Structural Properties of Biogene Amines (Serotonine, Histamine, γ -Amino Oil Acid) and Account for Laser and Neutron Capture Effects

T. Gumuła, C. Paluszkiwicz, S. Blazewicz

Study on Thermal Decomposition Processes of Polysiloxane Polymers - from Polymer to Nanosized Silicon Carbide

M. Iosin, F. Toderas, P. Baldeck S. Astilean

Study of Protein-Gold Nanoparticle Conjugates by Fluorescence and Surface Enhanced Raman Scattering

M.S. Sytnyk, Yu.B. Khalavka, O.V. Jovtiuk, O.O. Korovyanko

Morphological Dependence of Magnetite Nanocrystals under Different Growth Conditions

S. Krehula, S. Musić

Formation of Iron Oxides in a Highly Alkaline Medium in the Presence of Palladium Ions

D. Mikociak, C. Paluszkiwicz, R. Słowiak, M. Blazewicz

Vibrational Spectroscopy Applications to Study Carbonization Process of Fibrous Materials

E. Stodolak, C. Paluszkiwicz, M. Bogun, M. Blazewicz

Nanocomposite Fibres for Medical Applications

D. Mikociak, C. Paluszkiwicz, T. Gumuła, J. Michałowski, S. Błażewicz

FTIR Studies of Carbon Matrices Modified with Nanosized Hydroxyapatite

P. Pascuta, 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

V. Pashynska, A. Glamazda, A. Plokhotnichenko, E. Karpenko, T. Pokynbroda, V. Karachevtsev

Spectroscopic Investigations of Carbon Nanotubes in Aqueous Suspensions with Biosurfactants

R. Rémiás, A. Kukovecz, Z. Kónya, I. Kiricsi

A Spectroscopic Study on Noble Metal Nanoparticle Embedding into a SBA-15 Catalyst System

S. Musić, M. Ristić, S. Popović

Synthesis and Microstructure of Porous Mn-Oxides

S. Musić, A. Šarić, S. Popović, M. Ivanda
Formation and Characterization of Nanosize α -Rh₂O₃

Ž. Skoko, S. Popović, G. Štefanić
Thermal Behaviour of Al-Zn and Zn-Al Alloys

D. Sović, D. Iveković, B. Zimmermann
Modification of Titanate Nanotubes with Transition Metals and Transition Metal-1,10-phenanthroline Complexes

G. Štefanić, S. Musić, M. Ivanda
The Influence of Thermal Treatment on the Phase Development of ZrO₂-ZnO Precursors

D.S. Su, J. Zhang, X. Liu, J. Delgado, A. Gajović
Raman Spectroscopy of Nanocarbon Catalyst for Oxidative Dehydrogenation Reactions

F. Toderas, M. Baia, L. Baia, S. Astilean
Investigation of Annealed Gold Nanoparticles Self-Assembled on Solid Surface for Surface-Enhanced Raman Spectroscopy

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

K. Žagar, A. Gajović, S. Šturm, M. Čeh
BaTiO₃ Nanorods: New Insight by Raman Spectroscopy

M. Žic, M. Ristić, S. Musić
Precipitation of hematite from dense B-FeOOH suspensions with ammonium amidosulfonate adding

11. TIME RESOLVED SPECTROSCOPY

V. Dananić, K. Košutić, B. Kunst, D. Bosnar
Pore Size Distribution of NF/RO Composite Membranes by Positron Annihilation Lifetime Spectroscopy

A. Krzysztofowicz, V.I. Tomin
The Temporal Dipole Moment of the Solutes Undergoing Charge Transfer in the Excited State

12. NEW INSTRUMENTATION

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 (Chair: 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 S₂ 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-Pluska, 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. Kondepoti, 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

Topic 5. Optoelectronics and Semiconductor Materials, Topic 3. Nanostructured Materials & Topic 7. Spectroscopy Applied to Archaeology, Arts, Geology and Mineralogy

(Chairs: M. Ivanda, C. Paluszkiwicz)

- 10.30 - 10.50 **Z. Győri**, 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_x 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 **S. Rashev, D.C. Moule**
Theoretical Study of a Combined Electronic + Vibrational Relaxation Process in Thiophosgene $SCCl_2$
- 12.10 - 12.30 **A.V. Glushkov**
Raman Scattering of the Light on Metastable Levels of Diatomics: Consistent Energy Approach
- 12.30 - 12.50 **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 **Gaetano Granozzi**
TiO_x Nanostructures on Metallic Substrates: A Combined Spectroscopic and Theoretical Investigation
- 16.00 - 16.30 **Markku Räsänen**
Advances in Noble Gas Chemistry
- 16.30 - 17.00  **Coffee break**

POSTER PRESENTATIONS

17.00 - 19.00 Poster Session B - Topics 4-10

4. SPECTROSCOPY OF MACROMOLECULES

S. İde, A.B. Arıĝ, T. Trkeř, O. Mergen, S.H. Bayarı, . elik

Structural Investigation on Some Silk (Dragline, Hiding and Egg Coccon) Samples Weaved by Different Species Living in Turkey

L. Bistrii, V. Volovřek, V. Danani, I. Movre řapi, M. Leskovac

DFT Vibrational Study of Organic-Inorganic Hybrid Polymers Based on 3-Glicidoxy-propyltrimethoxysilane

T. Burova, G. Ten, A. Anashkin

Quantum-Mechanical Calculation of the Intensity Distribution in Resonance Raman Spectra of Derivatives of Uracil

E. Dřafi, O. Klein, W. Mntele

Monitoring of Hydrogen-Deuterium Exchange in Membrane Proteins using Attenuated Total Reflection Infrared (ATR-IR) Spectroscopy and a Microdialysis Perfusion-Cell

M. Handke, A. Kowalewska, W. Mozgawa

Spectroscopic Study of Preceramic Polymers Obtained by Hydrolytic Condensation of Ethoxycyclosiloxanes

M. Handke, A. Kowalewska

New POSS-Siloxane Materials of Ladder-Like Structure

S. Ilie, R. Setnescu

Characterization of Some Irradiated Materials Using Spectroscopic and Related Methods

D. Krilov, M. Balarin, M. Kosovi, O. Gamulin, J. Brnjas-Kraljevi

FTIR Spectroscopy of Lipoproteins - A Comparative Study

E.A. Minakova, E.B. Kruglova

Different Interaction Models for Explanation of Optical Properties of Ligand-Polynucleotides Systems

ř. Miti, G.S. Nikoli, M. Caki, P. Premovi, Lj. Ili

FTIR Spectroscopic Characterization of Cu(II) Coordination Compounds with Exopolysaccharide Pullulan and its Derivatives

I. Puci, B. Mihaljevi, M. Jakři

Concentration of Vapor Phase Corrosion Inhibitor in Anticorrosion Polymer Films - Correlation of Ion-Beam Analysis Results and UV-Vis Spectrophotometry

I. Puci, T. Jurkin γ -Irradiated Poly(Ethylene Oxide): Spectroscopic and Thermal Analysis**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

F. Torrens, G. Castellano

Binding of Water-Soluble, Globular Proteins to Anionic Model Membranes

V. Volovřek, K. Furi, L. Bistrii

Raman Spectroscopic Study of Siloxane Structures Developed Under Low Pressure

5. OPTOELECTRONICS AND SEMICONDUCTOR MATERIALS

B. Altiocka, S. Aksay, G.S. Kürkçüoğlu

FT-Raman and X-ray Diffraction Spectra of CuInS_2 Films by the Spray Pyrolysis at Different Substrate Temperatures

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

M. Fridrichová, I. Němec, P. Němec

Guanylurea(1+) Hydrogenphosphite - A New Material for Non-Linear Optics

T.M. Hammad

The Effect of Annealing on Electrical, Structural and Optical Properties of Sol Gel ITO Thin Films

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

D. Ristić, M. Ivanda, K. Furić

Application of the Phonon Confinement Model on the Optical Phonon Mode of Silicon Nanoparticles

N. Vedeanu, D.A. Magdas, O. Cozar, I. Ardelean

EPR Structural Investigation of $\text{CuO-V}_2\text{O}_5\text{-P}_2\text{O}_5\text{-CaO}$ Glass System for Optoelectronic Applications

D.A. Magdas, N. Vedeanu, O. Cozar, I. Ardelean

The Structural Changes Induced in Lead-Phosphate Glasses by Addition of Cooper Oxide

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

Y. Akkaya, K. Balci, S. Akyuz

IR and Raman and Density Functional Theory Studies on a Non-Steroidal Anti-Inflammatory Drug, Naproxen

B. Minčeva-Šukarova, L. Andreeva, O. Magdenovska, V. Manevska, N. Anevsk-Stojanovska

Raman and Infrared Spectroscopic Study of Pharmaceutical Tablets *DIPROL* and *CAFETINE COLD*, Products of *ALKALOID AD SKOPJE* (Republic of Macedonia)

K. Chruszcz-Lipska, M. Baranska, L.M. Proniewicz

Binding Ability of Fosfomycin towards Sodium and Calcium Ions

A. Baran, M. Baranska

Vibrational spectroscopy analysis of the anthraquinone pigment alizarin

M. Bartoszek, J. Polak, A. Kos, W.W. Sułkowski

Spectroscopic Study of Humic Substances Extracted From Bottom Sediment and Water

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

A.E. Yavuz, S.H. Bayar, N. Kazancı

Structural and Vibrational Study of Maprotiline

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

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

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

O. Cozar, F. Drăgan, C. Jelic, V. Chiş, N. Leopold, L. Szabó

Spectroscopic Investigation of Some Cu(II) Cardiovascular Complexes

M. Culea, O. Cozar, E. Culea

GC/MS as a Tool for Non-Invasive Diagnosis

M. Culea, S. Neamtu

Study of Amino Acid Transmembrane Transport

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

C. Farcau, S. Astilean

Single-Molecule Surface Enhanced Raman Scattering on Periodically Nanostructured Gold Films

M. Gotić, G. Koščec, S. Musić

A Study of the Reduction and Reoxidation of Substoichiometric Magnetite

A. Hacura, M. Jadamus-Hacura

Classification of Polish Honeys by Mid-Infrared Spectroscopy and Multivariate Statistical Analysis

I. Hannus, Sz. Mészáros, M. Búza, J. Halász

IR Spectroscopic Study of the Hydrodechlorination of Chlorobenzenes and Chlorophenols over Nobel Metal Containing Zeolites

I. Hannus, M. Búza, A. Beck, L. Guzzi

Catalytic Activity of Bimetallic Gold Containing Nanoparticles on Different Supports Investigated by IR Spectroscopy

A. Iordache, M. Culea, O. Cozar

Characterization of Allergens in Different Perfumes and Herbs

O. Klein, I. Klein, G. Oremek, W. Mänteles

Clinical Chemistry without Reagents? An Infrared Spectroscopic Technique for Determination of Clinically Relevant Constituents of Body Fluids

E. Kucharska, W. Sasiadek, H. Ban-Oganowska, M. Maćzka, J. Hanuza

Synthesis, Molecular Structure, IR and Raman Spectra as well as DFT Quantum Chemical Calculations for N-thiocyanopiperidine and its Methyl Derivatives

L. Kukoč Modun, Nj. Radić

Kinetic Spectrophotometric Determination of N-(2-Mercaptopropionyl)-glycine in Pharmaceuticals

J. Lorenc, B. Palasek, J. Hanuza, M. Maćzka, A. Waśkowska

Rotational Disorder in 2-Piperidyl-5-nitro-6-methylpyridine: Structural Phase Transition and its Vibrational Characteristics

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

M. Marković, T. Biljan, D. Škalec Šamec

Entacapone Isomer Quantification Using Raman Spectroscopy

J. Maurer, V. Vogel, W. Mänteles

Study of Heparin/Protamine Complexation by Means of Fluorescence Spectroscopy, Light Scattering and Analytical Ultracentrifugation

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

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

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

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

V. Balevicius, Z. Gdaniec, V. Sablinskas

2D NMR Study of Media Effects of Ionic Liquids on Hydrogen Bonding

S. Strazdaite, J. Ceponkus, V. Aleksa, V. Sablinskas

Structures of 1-Butene and 1-Heptene Primary Ozonides as Studied by Means of Matrix Isolation FTIR Spectroscopy

L. Szabó, V. Chiş, A. Pîrnău, N. Leopold, O. Cozar, Sz. Orosz

Vibrational, NMR and DFT Investigations of Amlodipine Molecule

L. Szabó, A. Pîrnău, N. Leopold, V. Chiş, O. Cozar

Vibrational, NMR and DFT Investigations of Ethylenediaminetetraacetic acid

A. Terczynska, K. Cholewa-Kowalska, M. Laczka

The Effect of Silicate Network Modifiers on Colour and Electron Spectra of Transition Metal Ions

V. Toteva, A. Georgiev, L. Topalova, S. Andreev

Estimation of the Desulphurization Degree in Light Cycle Oil Using FTIR Spectroscopy

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

G. Schäfer, W. Mäntele, G. Wille

Carboxylation Reactions Studied Using Caged CO₂

K. Vranić, V. Vojković

Spectrophotometric Studies of the Interaction of Ruthenium with Hesperetin

A. Zajac, M. Wandas, J. Hanuza

Synthesis, Molecular Structure and Vibrational Spectra of Bioactive Hybrid Materials Composed on Chitosan, Sodium Alginate and 1,6-Hexamethylene-di(aminocarboxy-sulfonate)

J. Zhang, A. Gajović, D. Su, R. Schlögl

Molecular Spectroscopy in Coke-free Carbon Catalysis

B. Trzcińska, J. Zięba-Paluś, 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

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

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)

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

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

N. Tomašić, A. Gajović, V. Bermanec
Raman Spectra and Luminescence of the Minerals with Aeschnite and Euxenite Crystal Structure

S. Gosay, M. Praisler, D.O. Dorohoi
Expert Systems Built for the Modeling of Small Molecular Structures Using a Concatenated Spectral Database

S. Gosay, M. Praisler
Optimisation of the Performances of a Hybrid Expert System Designed for the Elucidation of Molecular Structures

P. Makreski, G. Jovanovski, B. Kaitner
Minerals from Macedonia. XXIV. Spectroscopic and Structural Characterization of Tectosilicates

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

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)

W. Mozgawa, W. Jastrzębski
Vibrational Spectra of β -Cage Units in Different Silicate Structures

W. Mozgawa, M. Król
Application of IR Spectra in the Studies Heavy Metal Cations Immobilization on Natural Sorbents

A. Adamczyk, W. Mozgawa, M. Handke, E. Długoń, A. Ferensowicz
The FTIR Studies of Influence of Different Al_2O_3 and SiO_2 Precursors on Structure of Alumina-Silica Gels and Coatings

W. Mozgawa, J. Deja
The IR Spectroscopy Studies of Alkaline Activated Slag Geopolymers

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

M. Łodziński, M. Sitarz
Chemical and Spectroscopic Characterization of Some Phosphates Accessory Minerals from Pegmatites of the Sowie Mts (Owles Mts), SW Poland

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

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

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.

E. García-Fernández, M.A. Muñoz, C. Carmona, M. Balón
Ground state Isomerism and Dual Fluorescence of 2-Methylharminine Anhydronium Base (7-Methoxy-1, 2-dimethyl-2H-pyrido[3,4-b]indole) in Aprotic Solvents

J. Hetmańczyk, Ł. Hetmańczyk, E. Mikuli, A. Migdał-Mikuli
Phase Transition and 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

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

M. Rudbeck, S. Kumar, M. Blomberg, M.-A. Mroginski, A. Barth
PEP Vibrations from DFT

V.I. Tomín, 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

G.A. Akverdieva, N.M. Godjajev, S. Akyuz, N.E. Dogan, T. Akyuz
Molecular Mechanics Study of Antihypertensive Val-Tyr Dipeptide

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

S. Aydemir, M. Duran, E. Tasal, Halil Berber, C. Öğretir, M.S. Kılıçkaya
Ab Initio Calculations of pK_a Values for 7-Acetylcoumarin-3-Carboxylic Acid

P. Borowski, M. Fernández-Gómez, M.-P. Fernández-Liencres, T.P. Ruiz
An Effective Scaling Frequency Factor Method (ESFF) for Scaling of Harmonic Vibrational Frequencies

M.Q. Rincón, M. Fernández-Gómez, M.P. Fernández-Liencres, 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

O. Gamulin, M. Kosović, M. Balarin, D. Krilov, J. Brnjas-Kraljević
Denoising Raman Spectra of Biological Samples Using Wavelets

A.V. Glushkov, S.V. Malinovskaya, O.Yu. Khetselius
New Laser-Electron Nuclear Effects in the Nuclear γ Transition Spectra of Molecular Systems

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

D. Kirin, I. Lukačević, S.K. Gupta, P.K. Jha
Density Functional Calculation of Raman Intensity in High Pressure Phases of TiO₂ crystal

M. Szafarska, M. Woźniakiewicz, M. Pilch, J. Zięba-Palus, P. Kościelniak
Computer Analysis of ATR-FTIR Spectra of Paint Samples for Forensic purposes

J. Lamouroux, V.I.G. Tyuterev, L. Régalia-Jarlot, S.A. Tashkun
Comparison of Theoretical Intensity Calculations and Experimental Intensities Measurements for Non Linear Triatomic Molecules

I. López-Tocón, J.F. Arenas, S.P. Centeno, D. Pelaez, J.C. Otero
Correlating the Force Fields of Methylpyrazines: Vibrational Spectrum of Tetramethylpyrazine

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

G. Ogruc-Ildiz, S. Akyuz, A.E. Ozel
Experimental, *Ab Initio* and Density Functional Theory Studies on Sulfadiazine

R. Kępa, M. Ostrowska-Kopec
New Spectroscopic Studies of the Fourth-Positive ($A^1\Pi \rightarrow X^1\Sigma^+$) System Bands in ¹³C¹⁶O

A.E. Ozel, S. Celik, S. Akyuz
Vibrational Spectroscopic Investigation of Free and Coordinated 5-Aminoquinoline: The IR, Raman and DFT Studies

A. Padilla, J. Pérez
Hindered Rotation in the Infrared Spectra of HCl in Liquefied Rare Gases

R. Kępa, I. Piotrowska
New Analysis of the Comet-Tail ($A^2\Pi_r \rightarrow X^2\Sigma^+$) System Bands in ¹²C¹⁸O⁺

V.H. Rusu, J.B.P. da Silva, M.N. Ramos
A Theoretical Study of the Hydrogen Bonding between vic-, cis- and trans-C₂H₂F₂ Isomers and Hydrogen Fluoride

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 H₂C=CHX and HC≡CHX Molecules

P. Singh, S. Jaiswal, G. Srivastav, R.A.Yadav

Vibrational Spectroscopic Investigation on Vitamin P Using Ab Initio and DFT Method: Theoretical Study

E. Taşal, Y. Gülseven, İ. Sıdır, T. Önkol, C. Öğretir, M.S. Kılıçkaya

Experimental and Theoretical Studies on ^{13}C and ^1H NMR Spectra of 6-(2-fluoro-benzoyl)-3-(2-(4-(4-fluorophenyl) piperazin-1-yl)-2-oxoethyl)benzo[d]thiazol-2(3H)-one

E. Taşal, Y. Gülseven, İ. Sıdır, T. Önkol

Theoretical Studies on Molecular Structure and Some Molecular Properties of 6-(2-fluoro-benzoyl)-3-(2-(4-(4-fluorophenyl)piperazin-1-yl)-2-oxoethyl)benzo[d]thiazol-2(3H)-one

Y. Gülseven, E. Taşal, İ. Sıdır, C. Öğretir

Quantum Chemical Studies on Tautomerism and Acidity-Basicity Behaviours of Some 1,2,4-triazole Derivates

T. Wróblewski

DFT and Ab Initio Computational Study of Structural Properties and Vibrational Spectra for Protonated Water Clusters

G. Yapar, K. Balci

A Theoretical IR and Raman Spectroscopic Study on 1,2-Bis(o-carboxyphenoxy) ethane molecule

H. Yurtseven

Pippard Relations Modified by the Raman Frequency Shifts for the Phases I and II in NH_4I

H. Yurtseven

Calculation of the Raman Frequencies Using Volume Data Close to the Tricritical and Second Order Phase Transitions in NH_4Cl

10. SURFACE SPECTROSCOPIES

E. Akalin, S. Akyuz, T. Akyuz

Adsorption of Isoniazid onto Sepiolite-Palygorsgite Group of Clays: An IR and DFT Study

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

S. Bonora, M. Di Foggia, A. Maris

Surface Enhanced Raman Spectroscopy (SERS) Study of Diluted Solutions of Cimetidine and Some of its Metallocomplexes

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

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

M.R. Lopez-Ramirez, L. Roldán, J.V. Garcia-Ramos, S. Sanchez-Cortes

SERS Analysis of Herbicide Diquat on Nanostructured Metal Electrodes

M. Muniz-Miranda, E. Giorgetti, G. Margheri, S. Sottini, A. Giusti, G. Dellepiane

SERS Study of Self-Assembled Carbazolyl-Diacetylene Monolayers Chemisorbed on Gold Surfaces

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

E. Stodolak, C. Paluszkiwicz, M. Błażewicz

In vitro Biofilms Formation on Polymer Matrix Composites

C. Paluszkiwicz, W.M. Kwiatek, E. Długoń, A. Weselucha-Birczyńska, M. Piccinini

IR Mapping of Bio-Ceramic Layers on Titanium Substrate

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 **Closing Lecture (EUCMOS 2010)**

11.30 - 12.00 **Closing Ceremony**