WELCOME TO TURCMOS 2015

On the behalf of the Scientific Committee and Organizing Committee, we would like to welcome you all to the “International Turkish Congress on Molecular Spectroscopy (TURCMOS2015)”. The scope of the congress is to encourage the exchange of ideas and future collaborations all around the world, introduce new techniques and instruments, and present recent developments in this field of research. In the congress, all aspects of spectroscopic methods as well as related computational and theoretical approaches will be considered. Contacts between young researchers (M.Sc. and Ph.D.) and prominent experts will be particularly stimulated, aiming at the development of future collaborations.

We hope that the congress will provide you intellectual and social experience. We wish you enjoyable week in Antalya.

Ozan ÜNSALAN  
President

Gülce ÖĞÜRÜÇ ILDIZ  
Vice President
Topics

The congress will include the scientific topics below:

1. Vibrational (IR and Raman) Spectroscopic Techniques
2. Electron Spin Resonance (ESR) Spectroscopy
3. Mössbauer Spectroscopy
4. Fluorescence Spectroscopy
5. Microwave Spectroscopy
7. Matrix Isolation Infrared Spectroscopy and Low Temperature Spectroscopy
8. Theoretical and Computational Methods
9. Spectroscopy in Drug Design and Drug Discovery

Organizing Committee:

Ozan ÜNSALAN (University of Istanbul, Istanbul, Turkey) (President)
Gülce ÖĞRÜÇ ILDIZ (Istanbul Kültür University, Istanbul, Turkey) (Vice President)
Sevgi BAYARI (Hacettepe University, Ankara, Turkey)
Erol EROĞLU (Akdeniz University, Antalya, Turkey)
Serpil KILIÇ (Akdeniz University, Antalya, Turkey)
Murat KILIÇ (Akdeniz University, Antalya, Turkey)
Nuri YORULMAZ (Akdeniz University, Antalya, Turkey)
Zekkiye Eda BOYLÜĞ (Akdeniz University, Antalya, Turkey)
Ersin KAYGISIZ (University of Istanbul, Istanbul, Turkey)
Hayrunnisa Nur KABUK (Istanbul Kültür University, Istanbul, Turkey)
Samet KIZILKAYA (University of Istanbul, Istanbul, Turkey)
Furkan Ali KÜÇÜK (University of Istanbul, Istanbul, Turkey)
Duhan KULUNÇKIRAN (Istanbul Kültür University, Istanbul, Turkey)
Burçay YAVAŞ (Istanbul Kültür University, Istanbul, Turkey)
Burkay AYTÜRK (Istanbul Kültür University, Istanbul, Turkey)
Sefa SAYLAN (Istanbul University, Turkey)
İpek ŞAHİN (Ege University, Turkey)
Çisem ALTUNAYAR (Ege University, Turkey)
Scientific Committee:

Rui FAUSTO  
*(Coimbra University, Portugal)*

Sevgi BAYARI  
*(Hacettepe University, Ankara, Turkey)*

Weitao YANG  
*(Duke University, USA)*

Maral SÜNNETÇIOĞLU  
*(Hacettepe University, Ankara, Turkey)*

Semra IDE,  
*(Hacettepe University, Ankara, Turkey)*

Alpaslan Hamdi KUZUCUOĞLU  
*(Yeniyiyzyl University, Istanbul, Turkey)*

Juergen POPP  
*(Institute of Photonics Technology, Germany)*

Michael OSHTRAKH  
*(Ural Federal University, Russian Federation)*

Cuauhtemoc Araujo ANDRADE  
*(Autonomous University of Zacatecas, Mexico)*

Mustafa ÇULHA  
*(Yeditepe University, Turkey)*

Mustafa KURT  
*(Ahi Evran University, Turkey)*

Sibel TUNÇ  
*(Akdeniz University, Antalya, Turkey)*

Nihal KUS  
*(Anadolu University, Turkey)*

Mustafa BÖYÜKATA  
*(Bozok University, Yozgat, Turkey)*

Eser Ercan ALP  
*(Argonne National Laboratory, Illinois, USA)*

Jadson C. BELCHIOR  
*(Universidade Federal de Minas Gerais, BH, BRASIL)*

Nadide KAZANCı  
*(Ege University, Turkey)*

Invited Speakers:

Prof. Dr. Peter VANDENABEELE  
University of Gent, Belgium

Prof. Dr. Rui FAUSTO  
Coimbra University, Portugal

Prof. Dr. Philippe COLOMBAN  
Pierre & Marie Curie University, France

Dr. Parvez HARIS  
De Montfort University, Leicester, UK

Prof. Dr. Harold LINNARTZ  
Leiden Observatory, Sackler Laboratory for Astrophysics, Netherlands

Prof. Dr. H. Michael HEISE  
University of Applied Sciences of South-Westphalia Interdisciplinary Center for Life Sciences, Germany

Prof. Dr. Mustafa ÇULHA  
Yeditepe University, Turkey

Dr. Emre ERDEM  
University of Freiburg, Germany

Prof. Dr. Weitao YANG  
Duke University, USA

Prof. Dr. Jadson C. BELCHIOR  
Universidade Federal de Minas Gerais, BH, BRASIL
Scientific Program
<table>
<thead>
<tr>
<th>Time</th>
<th>Event</th>
<th>Details</th>
</tr>
</thead>
<tbody>
<tr>
<td>08:00 - 08:50</td>
<td>Registration</td>
<td></td>
</tr>
<tr>
<td>09:00 - 09:30</td>
<td>OPENING CEREMONY</td>
<td>Session Chair: Rui Fausto</td>
</tr>
<tr>
<td>09:30 - 10:20</td>
<td>PL-01 - Philippe Colomban</td>
<td>On-site Raman analysis of Cultural Heritage artefacts and materials with mobile instruments: drawbacks and success</td>
</tr>
<tr>
<td>10:20 - 11:10</td>
<td>PL-02 - Harold Linnartz</td>
<td>The Molecular Universe - Spectroscopy as a tool to unravel interstellar chemistry</td>
</tr>
<tr>
<td>11:10 - 11:30</td>
<td>COFFEE BREAK</td>
<td></td>
</tr>
<tr>
<td>11:30 - 12:20</td>
<td>PL-03 - Mustafa Çulha</td>
<td>Surface-enhanced Raman Scattering from Protein Detection to Cancer Diagnosis</td>
</tr>
<tr>
<td>12:20 - 14:00</td>
<td>LUNCH BREAK</td>
<td></td>
</tr>
<tr>
<td>14:00 - 14:20</td>
<td>O-01 - Calculation of transient absorption spectra for the intramolecular electron transfer / Vladislav V. Yudanov, Serguei V. Feskov</td>
<td></td>
</tr>
<tr>
<td>14:20 - 14:40</td>
<td>O-02 - Measurement of air quality from greenhouses based on photoacoustic spectroscopy / Ioana Ruxandra Ivascu, Consuela Elena Matei, Mihai Patachia, Ana Maria Bratu, Dan Constantin Dumitras, Ovidiu Jerca</td>
<td></td>
</tr>
<tr>
<td>14:40 - 15:00</td>
<td>O-03 - Theoretical calculation of the optical and spin-hamiltonian parameters for the rhombic Cu^{2+} center in [Cd(sac)<em>{2}(HydEt-en)</em>{2}] powders / Emel Kalfaoğlu</td>
<td></td>
</tr>
<tr>
<td>15:00 - 15:20</td>
<td>COFFEE BREAK</td>
<td></td>
</tr>
<tr>
<td>15:20 - 15:40</td>
<td>O-04 - The challenge of static corrections in high dune areas / Wesam Elboaishi Elboaishi, Ziad Siad Aiob</td>
<td>NOT ATTENDED</td>
</tr>
<tr>
<td>15:40 - 16:00</td>
<td>O-05 - Comparison of spectral properties of 7-diethylamino-3-thienoyl coumarin and 7-diethylamino coumarin / Sanjay Kumar</td>
<td>NOT ATTENDED</td>
</tr>
<tr>
<td>16:00 - 16:20</td>
<td>O-06 - Interaction of 6-methoxyquinoline with anionic sodium dodecylsulfate micelles: Photophysics and rotational relaxation dynamics at different pH / Tej Varma Yenupuri, Debi D Pant</td>
<td></td>
</tr>
<tr>
<td>18:00 - 22:00</td>
<td>COCKTAIL - (WELCOME PARTY)</td>
<td></td>
</tr>
<tr>
<td>Time</td>
<td>Session</td>
<td>Title</td>
</tr>
<tr>
<td>------------</td>
<td>---------</td>
<td>----------------------------------------------------------------------</td>
</tr>
<tr>
<td>09:00 - 09:50</td>
<td>PL-04</td>
<td>Rui Fausto: An Excursion on Molecular Conformational Landscapes: Discovering Rare Species in the Highlands</td>
</tr>
<tr>
<td>09:50 - 10:40</td>
<td>PL-05</td>
<td>Peter Vandenabeele: Raman spectroscopy in archaeometry: in situ and in vitro investigations of art and archaeology objects</td>
</tr>
<tr>
<td>10:40 - 11:00</td>
<td>OE</td>
<td>COFFEE BREAK</td>
</tr>
<tr>
<td>11:00 - 11:50</td>
<td>PL-06</td>
<td>Jadson C. Belchior: Genetic algorithms coupled with quantum mechanical calculations applied to parametrize force fields to describe ribonucleosides - glicosidic energies as a case study</td>
</tr>
<tr>
<td>11:50 - 12:10</td>
<td>OE</td>
<td>O-07: Multi-Electron Transfer in Ruthenium-4H-Imidazole based Black Absorbers</td>
</tr>
<tr>
<td>12:10 - 12:30</td>
<td>OE</td>
<td>O-08: Near-Infrared Fluorescence Studies of Long Wavelength Carbocyanines</td>
</tr>
<tr>
<td>12:30 - 14:00</td>
<td>OE</td>
<td>LUNCH BREAK</td>
</tr>
<tr>
<td>14:00 - 14:20</td>
<td>OE</td>
<td>O-09: Using of egyptian greensand in drinking water purification (removal of iron and manganese)</td>
</tr>
<tr>
<td>14:20 - 14:40</td>
<td>OE</td>
<td>O-10: New pyrano[2,3-d:6,5-d']dipyrimidine derivatives - Synthesis, in vitro cytotoxicity and computational studies</td>
</tr>
<tr>
<td>14:40 - 15:00</td>
<td>OE</td>
<td>COFFEE BREAK</td>
</tr>
<tr>
<td>15:00 - 15:20</td>
<td>OE</td>
<td>O11: Relativistic DFT Study of Highly Selective N-Ligands for Lanthanides(III)/Actinides(III) Separation</td>
</tr>
<tr>
<td>15:20 - 15:40</td>
<td>OE</td>
<td>O12: Interaction of protonated 6-methoxyquinolone with anionic micelles: Effect of hydrophobic chain length</td>
</tr>
<tr>
<td>16:00 - 18:00</td>
<td>P-001</td>
<td>POSTER SESSION 1</td>
</tr>
<tr>
<td>Time</td>
<td>Session Chair</td>
<td>Speaker/Seminar Title</td>
</tr>
<tr>
<td>--------------</td>
<td>-----------------------</td>
<td>---------------------------------------------------------------------------------------</td>
</tr>
<tr>
<td>09:00 - 09:50</td>
<td>H. Michael Heise</td>
<td>PL7 - Weitao YANG Fractional Perspectives of DFT and Local Scaling Corrections</td>
</tr>
<tr>
<td>09:50 - 10:40</td>
<td>H. Michael Heise</td>
<td>PL8 - Parvez HARIS Application of FTIR spectroscopy in proteomics and metabolomics - potentials and challenges</td>
</tr>
<tr>
<td>10:40 - 11:00</td>
<td></td>
<td>COFFEE BREAK</td>
</tr>
<tr>
<td>11:00 - 11:20</td>
<td>Mustafa Çulha</td>
<td>O-13 - Calculation of The EPR and Ground State Wavefunction for VO$^{2+}$ ion in KH$_2$PO$_4$ and KH$_3$C$_4$O$<em>8$.H$</em>{20}$ Powders by Theoretical Methods / Emel Kalfaoğlu</td>
</tr>
<tr>
<td>11:20 - 11:40</td>
<td>Mustafa Çulha</td>
<td>O-14 - Use of Fluorescence, Synchronous Fluorescence and Circular Dichroism Spectroscopic Techniques in Protein-Herbicide Interactions: Binding of Dichlorprop and Diquat Dibromide to Human Serum Albumin Sibel Tunc, Osman Duman, Inanç Soylu, Bahar Kancı Bozoğlan</td>
</tr>
<tr>
<td>11:40 - 12:00</td>
<td>Mustafa Çulha</td>
<td>O-15 - A New Developing Spectroscopy Software and Constructing a Database / Sefa Saylan, Murat Gezer, Ozan Unsalan</td>
</tr>
<tr>
<td>12:00 - 13:00</td>
<td></td>
<td>LUNCH BREAK</td>
</tr>
</tbody>
</table>

EXCURSION
<table>
<thead>
<tr>
<th>Time</th>
<th>Session Chair</th>
<th>Session #</th>
<th>Title</th>
<th>Speaker(s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>09:00 - 09:50</td>
<td>Philippe COLOMBAN</td>
<td>PL-09</td>
<td>H. Michael Heise: Recent advances in ATR-sensor development based on silver halide fibers for infrared spectrometric process analysis and applications in microbiology and medicine</td>
<td>H. Michael Heise</td>
</tr>
<tr>
<td>09:50 - 10:40</td>
<td>Emre Erdem</td>
<td>PL-10</td>
<td>Advanced EPR studies in functional nano-materials: From ferroelectrics to semiconductors</td>
<td>Emre Erdem</td>
</tr>
<tr>
<td>10:40 - 11:00</td>
<td></td>
<td></td>
<td>COFFEE BREAK</td>
<td></td>
</tr>
<tr>
<td>11:00 - 11:20</td>
<td>Cuauhtémoc Araujo-Andrade</td>
<td>O-16</td>
<td>Accounting for Environment and Dynamics in Modeling of Vibrational Spectra in Condensed Phase</td>
<td>Valery Andrushchenko, Petr Bouř</td>
</tr>
<tr>
<td>11:20 - 11:40</td>
<td></td>
<td>O-17</td>
<td>NOT ATTENDED</td>
<td>Kaabar Wahiba</td>
</tr>
<tr>
<td>11:40 - 12:00</td>
<td></td>
<td>O-18</td>
<td>General Non-Markovian Dynamics of Open quantum systems and spectral density of complex systems using Exceptional Orthogonal Polynomials</td>
<td>Mahmoud Mahdian</td>
</tr>
<tr>
<td>12:00 - 13:30</td>
<td></td>
<td></td>
<td>LUNCH BREAK</td>
<td></td>
</tr>
<tr>
<td>13:30 - 13:50</td>
<td>Hamit Yurtseven</td>
<td>O-19</td>
<td>Bioremoval of crystal violet dye from egyptian textile effluent</td>
<td>Samah Saleh Abdallah, Khaled Abdel Aal Selim, Nagui Aly Abdel Khalek, Samah Mohamed El Sayed</td>
</tr>
<tr>
<td>13:50 - 14:10</td>
<td></td>
<td>O-20</td>
<td>The Kinetic of Biogas Production Rate from Dairy Wastewater in Batch Mode «Effect of Starting pH in mesophilic Phase »</td>
<td>Bani Kheiredine, Derbal Kerroum, Benchikhiievoucine Mosaab</td>
</tr>
<tr>
<td>14:10 - 14:30</td>
<td></td>
<td>O-21</td>
<td>Comparative study of liver and spleen tissues from healthy human and patients with some hematological malignancies using magnetization measurements and Mössbauer spectroscopy</td>
<td>Irina V Alenkina, Michael I Oshtrakh, Israel Felner, Alexander V Vinogradov, Tatiana S Konstantinova, Vladimir A Semionkin</td>
</tr>
<tr>
<td>14:30 - 14:50</td>
<td></td>
<td>O-22</td>
<td>Variation of the iron-bearing mineral content and the 57Fe hyperfine parameters in Chelyabinsk LL5 meteorite fragments revealed using the high velocity resolution Mössbauer spectroscopy</td>
<td>Alevtina A Maksimova, Michael I Oshtrakht, Zoltan Klencsár, Andrey V Chukin, Evgeniy V Petrova, Victor I Grokhovsky, Erno Kuzma, Zoltan Homonnay, Vladimir A Semionkin</td>
</tr>
<tr>
<td>14:50 - 15:10</td>
<td></td>
<td></td>
<td>COFFEE BREAK</td>
<td></td>
</tr>
<tr>
<td>15:10 - 15:30</td>
<td>Sibel Tunç</td>
<td>O-23</td>
<td>Calculation Of The Soft-Mode Frequency For The α-β Transition In Quartz</td>
<td>Hamit Yurtseven, Ozlem Tari</td>
</tr>
<tr>
<td>15:30 - 15:50</td>
<td></td>
<td>O-24</td>
<td>The effect of Ni2+ in the Fe3+ local microenvironment in both tetrahedral and octahedral sites on the 57Fe hyperfine field in NiFe2O4 nanoparticles</td>
<td>Mikhail V Ushakov, Baskar Senthilkumar, R. Kalai Selvan, Michael I Oshtrakh</td>
</tr>
<tr>
<td>16:00 - 18:00</td>
<td></td>
<td></td>
<td>POSTER SESSION 2</td>
<td>P-068 - P-135</td>
</tr>
<tr>
<td>19:00 - 23:30</td>
<td></td>
<td></td>
<td>CONFERENCE DINNER</td>
<td></td>
</tr>
<tr>
<td>Session Chair</td>
<td>Time</td>
<td>Paper ID</td>
<td>Title</td>
<td>Authors</td>
</tr>
<tr>
<td>------------------------</td>
<td>---------------</td>
<td>----------</td>
<td>----------------------------------------------------------------------</td>
<td>----------------------------------------------</td>
</tr>
<tr>
<td>Nihal Kuş</td>
<td>09:00 - 09:20</td>
<td>O25</td>
<td>Structural investigations of Some Sb2O3-Na2O-ZnO glasses by mean of FTIR, Raman and Er3+ probe</td>
<td>Toufik Mohamed Soltani, Majda Hamzaoui, Ronan Lebullenger, Alain Moreac, Marcel Poulain</td>
</tr>
<tr>
<td></td>
<td>09:20 - 09:40</td>
<td>O26</td>
<td>Pressure Dependence Of The Raman Frequency Of An Optical Mode In Cubic Gauche Nitrogen</td>
<td>Hamit Yurtseven, Ozgecan Tiryak</td>
</tr>
<tr>
<td></td>
<td>09:40 - 10:00</td>
<td>O27</td>
<td>Phonon spectral density of the FMO light-harvesting complex with associated and generalized jacobi polynomials</td>
<td>Mahmoud Mahdian</td>
</tr>
<tr>
<td></td>
<td>10:00 - 10:20</td>
<td></td>
<td>COFFEE BREAK</td>
<td></td>
</tr>
<tr>
<td></td>
<td>10:40 - 11:00</td>
<td>O29</td>
<td>Electronic Properties of the Transition Metal (1-phenylazo-2-naphthol) complexes: A TD-DFT Electronic Spectra Study</td>
<td>Bachir Zouchoune, Lakhdar Mansouri</td>
</tr>
<tr>
<td></td>
<td>11:00 - 11:20</td>
<td>O30</td>
<td>How Does Hyperforin (HYP) Interact with DPPC Membranes?: EPR Spin Labeling and DSC Study</td>
<td>Dilek Yonar, Maral M. Sünnetçioğlu</td>
</tr>
<tr>
<td></td>
<td>11:30 - 11:40</td>
<td></td>
<td>CLOSING CEREMONY</td>
<td></td>
</tr>
</tbody>
</table>
POSTER LIST
<table>
<thead>
<tr>
<th>Abs-Ref</th>
<th>Pub-Num</th>
<th>Abstract Title</th>
</tr>
</thead>
<tbody>
<tr>
<td>0001</td>
<td>P-001</td>
<td>TD-DFT Calculations of Visible Spectra and Structural Studies of Ibuprofen Inclusion Complex With β-Cyclodextrin Madi Fatiha</td>
</tr>
<tr>
<td>0004</td>
<td>P-002</td>
<td>The Redox Behavior of Uranium Complexes. A relativistic DFT/ZORA study Belkhiri Lotfi, Khireche Moncef, Zaiter Abdellah, Ephritikhine Michel, Boucekkine Abdou</td>
</tr>
<tr>
<td>0005</td>
<td>P-003</td>
<td>Measurement of Heavy Gases and Vapors by Means of a Conventional RGA Jamshid Soltan Mohammadi, Rudolf Dobrozemsky</td>
</tr>
<tr>
<td>0008</td>
<td>P-004</td>
<td>Theoretical and Experimental Vibrational Spectroscopic Studies of Sulphur Containing Diketopiperazines Ahsan Ali Khan, Babur Zahurridin Chowdhry, Andrew Paul Mendham, Trevor John Dines, Perry Devo</td>
</tr>
<tr>
<td>0010</td>
<td>P-005</td>
<td>Impact of Iron-complex (Fe(III)-Malonate) on Photoinduced Degradation of Ibuprofen in Aqueous Solution Debbache Nadra, Dekiche Besma, Ghoul Imene, Ars Khadirjda, Adala Amina</td>
</tr>
<tr>
<td>0011</td>
<td>P-006</td>
<td>Total Cross Sections for the Double Ionization of Water Molecule Dahbia Oubaziz, Christophe Champion, Michele Arcongolo Quinto, Zakia Aitelhadjali</td>
</tr>
<tr>
<td>0012</td>
<td>P-007</td>
<td>Computational Investigation of Trans-Pt(II) Ozone Complexes Koray Sayin, Duran Karakaş</td>
</tr>
<tr>
<td>0013</td>
<td>P-008</td>
<td>Spectroscopic Characterization of Carburized Surface of Fe20MnCr5 steel Fatima Zohra Benlahreche, El Amine Nouicer, Lazhar Yahia</td>
</tr>
<tr>
<td>0014</td>
<td>P-009</td>
<td>Corrosion Behaviour of Titanium Alloy in Alkaline Solution Using Spectroscopic Techniques El Amine Nouicer, Fatima Zohra Benlahreche, Lazhar Yahia</td>
</tr>
<tr>
<td>0015</td>
<td>P-010</td>
<td>A New Preconcentration Procedure to Quantify Total Acid Hydrolyzed Fluoride in Selected Beverages and Foods by Spectrophotometry Nail Altunay, Ramazan Gürkan, Ulaş Orhan, Emre Yıldırım, Sema Korkmaz</td>
</tr>
<tr>
<td>0017</td>
<td>P-011</td>
<td>Double Ionization if the Hydrogen Sulfide Molecule by Electron Impact: Influence of The Target Orientation on the Fivefold Differential Cross Sections Noura Imadouchene, Hocine Aouchiche, Christophe Champion</td>
</tr>
<tr>
<td>0019</td>
<td>P-012</td>
<td>Modeling of Photocatytic Removal of Cresol Red Using Box-Behnken Experimental Design Razika Zouaghli, Roumaysa Zerti, Narimène Hadi Brahimi</td>
</tr>
<tr>
<td>0022</td>
<td>P-013</td>
<td>Photochemical Degradation of the Phenol Red Induced by Goethite in the Aqueous Solution Debbache Nadra, Belattar Sara, Ghoul Imene, Seraghih Nassira</td>
</tr>
<tr>
<td>0025</td>
<td>P-014</td>
<td>Crystal Structure, Spectroscopic (FT-IR and UV-Vis) and DFT studies on (E)-N-[4-bromo-2- (trifluormethoxy)phenyl]-1-[(3-nitrothiophen-2-yl)methanimine Hasan Tanak, Figen Koyak, Erbil Agar</td>
</tr>
<tr>
<td>0026</td>
<td>P-015</td>
<td>Photodegradation of Paracetamol (PC) Induced by Goethite (α-FeOOH) In Aqueous Solution Up On Irradiation at 365 nm and by Solar Light Yazid Mameri, Nadra Debbache, Sarah Belattar, Taha Sehili</td>
</tr>
<tr>
<td>0027</td>
<td>P-016</td>
<td>Spectroscopic Characterisation of 6-Phosphogluconate Dehydrogenase Enzyme Purified from the Van Cat Erythrocytes Serpil Kilic, Fikret Karataş</td>
</tr>
<tr>
<td>0028</td>
<td>P-017</td>
<td>Investigation of Solvent Effect on Biological Reactivity, UV-VIS and NMR Analyses of Zn(II) Complexes with Pentaaza Macro cyclic Schiff-base Ligand Koray Sayin, Duran Karakaş, Nihat Karakaş, Sultan Erkan Kariper, Tuba Alagon Sayin</td>
</tr>
<tr>
<td>0029</td>
<td>P-018</td>
<td>Spectroscopic Characterization and DFT Study of Copper(II), Cobalt(II) and Nickel(II)-Selenadiazoloquinolone Complexes Sandra Dorotíková, Peter Herich, Michaela Králóvá, Dana Dvoranová, Lukáš Bučinský</td>
</tr>
<tr>
<td>0030</td>
<td>P-019</td>
<td>Azo-Hydrazone Tautomerism of Some p-Phenyldazo-a-Naphthol Compounds and Their Cyclotriphosphazene Derivatives Günseli Turgut Cın, Mustafa Olbaşoğlu</td>
</tr>
<tr>
<td>0031</td>
<td>P-020</td>
<td>“Molecular Conformational Analysis and Vibrational study of Linoleic Acid” Tugba Göcen, Sevgi Haman Bayan, Mehmet Haluk Güven</td>
</tr>
<tr>
<td>0032</td>
<td>P-021</td>
<td>Structural Characteristics of Wood-polymer Green-composites by FTIR Spectroscopy Elif Hilal Şen, Sevgi Haman Bayan, Erdem Bodur</td>
</tr>
<tr>
<td>Session</td>
<td>Title</td>
<td>Authors</td>
</tr>
<tr>
<td>----------</td>
<td>----------------------------------------------------------------------</td>
<td>--------------------------------------------------------------------------------------------------</td>
</tr>
<tr>
<td>P-022</td>
<td>Two New Nickel (II) Chelidamate Complexes Containing 2, 2'-dipyridylamine Ligand: An Agreement Between Theoretical and Experimental Studies</td>
<td>Hatice Vural, Ibrahim Uçar</td>
</tr>
<tr>
<td>P-023</td>
<td>Analysis of Normal and Rickets Human Skeletal Remains by FT-IR Spectroscopy and SAXS</td>
<td>Sevgi Haman Bayar, Kameray Özdemir, Semra Ide, Yılmaz Selim Erdal, İlghar Orujalipoor</td>
</tr>
<tr>
<td>P-024</td>
<td>Diagenic Alterations in the Anthropological Bone Mineral Structure: FTIR Spectroscopy and SAXS Studies</td>
<td>Sevgi Haman Bayar, Semra Ide, Kameray Özdemir, Yılmaz Selim Erdal, İlghar Orujalipoor, Elif Sen</td>
</tr>
<tr>
<td>P-025</td>
<td>A New Eco-friendly and Rapid Ultrasound Assisted Cloud Point Extraction to Preconcentrate and Determine Sulfitie from Vegetables and Dried Fruit Matrices</td>
<td>Nail Altunay, Ramazan Gürgan, Ulaş Orhan, Emre Yıldırım</td>
</tr>
<tr>
<td>P-026</td>
<td>DFT Computational and Spectroscopic Investigations on (E)-N-((3-fluorophenyl)-1-((5-nitrothiophen-2-yl)methanimine)</td>
<td>Sadıye Karataş, Hasan Tanak, Ayşen Alaman Ağar, Meryem Evence</td>
</tr>
<tr>
<td>P-027</td>
<td>A Combination of Spectroscopic Methods in Determination of a New Cyanogenic Glycoside Compound Structure from Centaurea Microcarpa</td>
<td>Ramdane Seghiri, Baatouche Samia, Cheriet Thamere, Mekkiou Ratiba, Boumaza Ouahiba, Sarri Djamel, Benayache Samir, Benayache Fadila</td>
</tr>
<tr>
<td>P-028</td>
<td>NMR Spectroscopy in the Elucidation of Isolated Flavonoids from Aerial Parts of Astragalus Genus (Fabaceae)</td>
<td>Ratiba Mekkiou, Amina Bougandoura, Brigida D’abroska, Ouahiba Boumaza, Ramdane Seghiri, Antonio Fiorentionio, Djamal Sarri, Samir Benayache, Fadila Benayache</td>
</tr>
<tr>
<td>P-029</td>
<td>Determination of New Flavonoids Using Spectroscopic Methods Isolated from Genista Aspalathoides Ouahiba Boumaza, Rabia Boukaabache, Ratiba Mekkiou, Ramdane Seghiri, Fadila Benayache, Samir Benayache</td>
<td></td>
</tr>
<tr>
<td>P-030</td>
<td>Computational Study on Intermolecular Charge Transfer Complex of 2,2-bipyridine with Picric Acid</td>
<td>Samia Amirat, Abd El Hak Gueid, Amel Zaboub, Rachid Merdes, Fatih Madi</td>
</tr>
<tr>
<td>P-032</td>
<td>Molecular Structure, Vibrational Spectral Investigation and the Confirmation Analysis of 1-(Diphenylmethyl)piperazine</td>
<td>Semran Sağlam, Ahmet Güvenir, Mehmet Tahir Güllüoğlu, Yusuf Erdogdu</td>
</tr>
<tr>
<td>P-033</td>
<td>Nanoscope Analysis of Sugar Beet Seeds</td>
<td>Begüm Çınar, İlghar Orujalipoor, Semra Ide, Dilek Başalma, Aysegül Boyacoğlu</td>
</tr>
<tr>
<td>P-034</td>
<td>On-line Screening and Identification of Antioxidant Phenolic Compounds of Salvia Aegyptica (L.) Benayache Samir, Mohamadi Sabrina, Minjie Zhao, Amrani Amel, Marchioni Eric, Zama Djamila, Benayache Fadila</td>
<td></td>
</tr>
<tr>
<td>P-035</td>
<td>Isostructurality of Single Component Crystals. The Case of 2-amino benzimidazole, 2-amino benzothaloxazole and 2-amino benzoazole Crystals</td>
<td>Tomasz Misiaszek, Jakub Warachim, Katarzyna Pielęga</td>
</tr>
<tr>
<td>P-036</td>
<td>Spectroscopic Characterization of 1-motif Forming Oligonucleotide pH probes containing Fluorescent Cytosine Analog TC</td>
<td>Bernard Juskowiak, Patrycja Rzepecka</td>
</tr>
<tr>
<td>P-037</td>
<td>Optical and Magnetic Properties of Ferromagnetic Co-Ni co-doped TiO2 Thin Films</td>
<td>Rabab Bensaha, Badreddine Touba, Fahrettin Yakuphanoglu</td>
</tr>
<tr>
<td>P-038</td>
<td>Analysis of B Vitamins in Food Matrix by Surface Enhanced Raman Spectroscopy (SERS)</td>
<td>Andreea Radu, Andreea Radu, Maria Thum, Martin Jahn, Martin Jahn, Uwe Huebner, Karina Weber, Karina Weber, Dana Cialla May, Dana Cialla May, Jürgen Popp, Jürgen Popp</td>
</tr>
<tr>
<td>P-039</td>
<td>Designing a Raman Cell For Frequency Shift of Laser Radiation</td>
<td>Ayhan Altun, Karl Kleinermanns, Ayhan Altun, Ayhan Altun</td>
</tr>
<tr>
<td>P-040</td>
<td>Spectroscopic Determination of the Oxygen Reactive Species Photosensitized by the Irradiation of the Antibiotic Ciprofloxacín with UVA Radiation</td>
<td>Jamil Ahmed</td>
</tr>
<tr>
<td>P-041</td>
<td>Rapid Determination of Palladium by a New Spectrofluorimetric Determination in Environmental Samples Using Acriflavine as a Reagent</td>
<td>Sultan Başak Simşek, Serife Saçmacı, Ahmet Ulgen</td>
</tr>
<tr>
<td>P-042</td>
<td>Fluorimetric Determination of Aluminium in Water and Food Samples Using New Fluorescence Reagent</td>
<td>Esra Yıldız, Serife Saçmacı, Mustafa Saçmacı, Ahmet Ulgen</td>
</tr>
</tbody>
</table>
POSTER SESSION 1 / September 15, 2015 - Tuesday

0072 P-043  Raman, Optical Absorption, Thermal and Elastic Characterization of TM Doped 90TeO2-10K2O Glasses
Toufik Mohamed Soltani, Doris Moncke, Ali Erçin Ersundu, Miray Çelikbilek, Lothar Wondraczek

0074 P-044  XRF Spectroscopy and Imaging Investigations on Two Icons with Double painting Layers from R.Macedonia
Svetlana Mamucevska Miljkovikj, Angelina Popovska, Zivko Kokolanski, Saso Cvetkovski, Liliana Kovacevska

0075 P-045  Photo-oxidation of Amoxicillin by αFeOOH/H2O2 Effect of Operating Conditions
Mohamed Mehdi Benacherine, Yazid Mameri, Besma Dekkiche, Nadra Debbache

0081 P-046  Vibrational Spectra, non-linear Optical Properties, NBO Analysis Properties of Acetylcholine by Density Functional Method
Boutasta Amel, Benosman Abdelhakim

0084 P-047  Spectroscopic Investigations and DFT Calculations on 3-(diacetylamino)-2-ethyl-3H-quinazolin-4-one
Yusuf Sert, Fatih Ucan

0085 P-048  Highest-Lowest Occupied Molecular Orbital Analysis of 4-Bromomethyl-6-tert-butyl-2H-chromen-2-one
Yusuf Sert, Fatih Ucan

0086 P-049  Kinetic Calculations of Phase Transformation in Magnetic Cu-based Alloy
Emine Aldırmaz, Nevzat Karakaya, S. Cansel Cüçü, Eren Koyuncuoğlu

0087 P-050  A Comparative Study on Vibrational Spectra of Free Indapamide and its DMSO Solution
Y. Alat, O. Bölükbaş, A. Yilmaz, B. İlhan Ceylan

0088 P-051  Development and Validation of Sensitive Spectrofluorimetric Method for The Determination of Tamsulosin in Spiked Human Urine, in Pure and Pharmaceutical Preparations
Ayva Karasakal, Sevgi Tatarkulu

0089 P-052  Molecular Dynamic Study of A Chiral Schiff Base Derivative Using R1/R2 Ratio Method and Quantum Chemical Investigation for Geometric Properties
Arzu Ekinici, Mehmet Zafer Köylü, Mustafa Büyükat

0090 P-053  Secondary Metabolites and Antioxidant Activity of Limonium Duriusculum (de Girard) Kuntze Extracts
Fatih Ucan, Masoued Kerkatou, Azzedine Salah Redouane, Francisco León, Ignacio Brouard, Ahmed Menad, Djamel Sarri, Samir Benayache

0091 P-054  Molecular Dynamic and Complexation Study of A Chiral Schiff Base Derivative by 400 MHz 1H-NMR
Aliye Aracı, Arzu Ekinici, Mehmet Çolak, Nadir Demirel, Mehmet Zafer Köylü

0093 P-055  The Use of X Fluorescence to Characterize Sludge of Treatment Plants
Wassila Cheurfi, Hassina Bougherara, Brahim Kebabi

0094 P-056  Structural Determination of Secondary Metabolites Using UV and NMR Spectroscopy of Vitex Agnus-castus
Fatih Ucan, Hanane Aliaoui, Samia Mezhoud, Fatih Benayache, Samir Benayache

0095 P-057  Visible Fluorescence from Pr3+ Doped KYF4 Single Crystal
Adel Bitam

0099 P-058  Computational Studies on Structure and Spectroscopic Properties of 1,3′-Dihydrospiro[cyclohexane-1,2′-[2H]imidazo[4,5-b]pyridine]
Hatice Vural, Mehmet Kara

0100 P-059  Experimental and Theoretical Studies of (FTIR, FT-NMR, UV-Visible, X-ray and DFT) 2-(4-Allyl-5-pyridin-4-yl-4H-[1,2,4]triazol-3-ylsulfanyl)-1-(3-methyl-3-phenyl-cyclobutylyl)-ethanone
Cigdem Yuksetepe Ataoğlu, Öner Ekici

0101 P-060  Synthesis, Crystal Structure, Spectroscopic and Electronic Properties of (E)-Trans-2-(2-(Biphenyl-4-ymethylene)Hydrazinyl)-4-(3-Methyl-3-Phenylcyclobutyl)Thiazole
Cigdem Yuksetepe Ataoğlu, Nezihe Caliskan, Ibrahim Yilmaz, Alaadnin Cukurovali

0104 P-061  Spectroscopic Investigation, Structural and Electronic Analysis of 2-(4-ethoxyphenyl)isoindoline-1,3-dione by Experimental and Theoretical Approach
Gülcan Dury, Meryem Eyvenc, Hasan Tanak, Erbil Ağar

0105 P-062  Study on Molecular Structure, Spectroscopic Behavior, HOMO–LUMO and NMR Analysis of 2-(3-o-Tolyl-4-oxo-3,4-dihydroquinazolin-2-ythio)acetohydrazide using theoretical approaches
Meryem Eyvenc, Murat Karabulut

0107 P-063  First Principles Study of Magnetic, charge, and orbital ordering in LuFe2O4
Hayat Si Abdelkader, Houda Imane Farahoun

0106 P-064  Spectroscopic (IR, Raman, NMR), Thermal and Theoretical (DFT, AIM) Study of Alkali Metal Dipicolinates (2,6-pyridinedicarboxylates) and Quinolinates (2,3- pyridinedicarboxylates)
Grzegorz Świderski, Sławomir Wojtulewski, Leszek Siergiejczyk, Agnieszka Zofia Wilczewska, Iwona Misztalewska, Renata Swislocka, Wlodzimierz Lewandowski
<table>
<thead>
<tr>
<th>Poster Number</th>
<th>Title</th>
<th>Authors</th>
</tr>
</thead>
<tbody>
<tr>
<td>P-065</td>
<td>Physico-chemical (spectroscopic: FT-IR, Raman and UV) Studies of Caffeic Acid and Fe(III), Cu(II), Zn(II), Ni(II) Caffeinates</td>
<td>Renata Swislocka, Mariola Samsonowicz, Malgorzata Kowczyk Sadowy, Grzegorz Swiderski,</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Wlodzimierz Lewandowski</td>
</tr>
<tr>
<td>P-066</td>
<td>Determination of Some Metals in Honey Samples with a New Synthesized Resin by Flame Atomic Absorption Spectrometry</td>
<td>Teslima Dasbas, Şerife Saçmaci, Nevin Çankaya, Cengiz Soykan</td>
</tr>
<tr>
<td>P-067</td>
<td>Botanic Origin, Total Phenol-Flavonoid Amount and Antioxidant Activities of Propolis Samples From Trabzon</td>
<td>Ümit Ceylan, Ilgınç Kızılpinar Temizer, Aytaç Güder, Ömür Gencay Çelemli</td>
</tr>
<tr>
<td>P-068</td>
<td>Synthesis, Characterization and Application of a New Chelating Resin For Solid Phase Extraction, Preconcentration and Determination of Trace Metal Ions in Some Dairy Samples by Flame Atomic Absorption Spectrometry</td>
<td>Teslima Dasbas, Şerife Saçmaci, Nevin Çankaya, Cengiz Soykan</td>
</tr>
<tr>
<td>P-069</td>
<td>Spectroscopic (IR, Raman, NMR), Theoretical and Biological Study of Cinnamic, Coumaric, Caffeic and Chlorogenic Acids and Their Complexes with Copper(II)</td>
<td>Wlodzimierz Lewandowski, Renata Swislocka, Grzegorz Swiderski, Monika Kalinowska, Mariola Samsonowicz, Hanna Lewandowska</td>
</tr>
<tr>
<td>Abs-Ref</td>
<td>Pub-Num</td>
<td>Abstract Title</td>
</tr>
<tr>
<td>---------</td>
<td>---------</td>
<td>----------------</td>
</tr>
<tr>
<td>0116</td>
<td>P-070</td>
<td>Electron Paramagnetic Resonance (EPR) study of nano sized emulsions Dilek Killar</td>
</tr>
<tr>
<td>0117</td>
<td>P-071</td>
<td>Structural Properties of Neutral 2D Aun (n=4-13) Clusters: A Comparative Study of MD and DFT Calculations Sertan Kumral, Meral Eryürek</td>
</tr>
<tr>
<td>0118</td>
<td>P-072</td>
<td>The Spectroscopic and Micro-tomographic Analysis of Calcifications in Spinal Ligaments Sylvia Natalia Orzechowska, Andrezj Wrobel, Eugeniusz Rokita</td>
</tr>
<tr>
<td>0119</td>
<td>P-073</td>
<td>Electron Impact Double Ionization of Methane Molecule Aitelhadjali Zakia, Quinto M. A, Champion Christophe, Ouazbazz Dhabia, Kessal Salem</td>
</tr>
<tr>
<td>0120</td>
<td>P-074</td>
<td>Investigation of The Effects of Polymerization Temperature on The Latex Properties Sedef Sismanoglu, Ayfer Sarac</td>
</tr>
<tr>
<td>0121</td>
<td>P-075</td>
<td>The Comparative Vibrational Spectroscopic Study of Diphenylpyraline Hydrochloride and Cyproheptadine Hydrochloride Seda Günesdoğdu Sağdınc, Aybüke Diler, Dilek Erdas</td>
</tr>
<tr>
<td>0122</td>
<td>P-076</td>
<td>Quantum Chemical Investigations of (E)-2-[(4-chlorophenyl)iminomethyl]-4-(trifluoromethoxy)-phenol Ümit Ceylan, Yelda Bingöl Alpaslan, Nuri Öztürk, Gökhan Alpaslan, Halil Göke, Mustafa Macit</td>
</tr>
<tr>
<td>0125</td>
<td>P-077</td>
<td>Synthesis, Experimental Techniques, Spectroscopic Investigations and Quantum Chemical Computational Study of (Z)-N-(2-bromo-3-methylphenyl)-1-(5-nitrothiophen-2-yl) methanimine Gonca Özdemir Tan, Sümayye Gümüş, Erbil Ağar</td>
</tr>
<tr>
<td>0126</td>
<td>P-078</td>
<td>Synthesis, Crystal Structure, Spectroscopic Characterization and Theoretical Calculations of (Z)-N-(naphthalen-2-yl)-1-(5-nitrothiophen-2-yl) methanimine Gonca Özdemir Tan, Sümayye Gümüş, Erbil Ağar</td>
</tr>
<tr>
<td>0127</td>
<td>P-079</td>
<td>Preconcentration of Trace Metals on Amberlite XAD-7 Resin and Determination by X-ray Fluorescence Hassina Bougherara, Soma Zerouel, Braham Kebabi</td>
</tr>
<tr>
<td>0128</td>
<td>P-080</td>
<td>Experimental and Computational Investigations of Indium Doped Gold Clusters: InAu6– Ahmet Guvenir, Kahraman Çetin, Tugce Bahceci, Mustafa Decelioğlu, Ömer Dereli, Mehmet Tahir Gülüoğlu, Yusuf Erdoglu</td>
</tr>
<tr>
<td>0130</td>
<td>P-081</td>
<td>Investigations of Neutral and Singly charged Phosphorus doped Gallium Nanoclusters by DFT Ahmet Guvenir, Kahraman Çetin, Tugce Bahceci, Mustafa Decelioğlu, Ömer Dereli, Mehmet Tahir Gülüoğlu, Yusuf Erdoglu</td>
</tr>
<tr>
<td>0133</td>
<td>P-083</td>
<td>Phytochemical Investigation of the n-Butanol Extract of Linaria tingitana Ramdane Seghiri, Thamere Cheriet, Samia Baatouche, Ines Mancini, Ratiba Mekkiou, Ouahiba Boumaza, Djamel Sarri, Samir Benayache, Fadila Benayache</td>
</tr>
<tr>
<td>0136</td>
<td>P-084</td>
<td>A New Spectrofluorometric Determination of Bismuth in Some Pharmaceutical Samples Nur Öksüz, Şerife Saçmacı, Mustafa Saçmacı, Ahmet Ulgen</td>
</tr>
<tr>
<td>0140</td>
<td>P-086</td>
<td>Investigation of the Interaction between Anti-Cancer Drug and Human Serum Albumin depending on temperature by 400 MHz NMR Spectrometer Sibel Korunur, Bilgin Zengin, Ali Yılmaz</td>
</tr>
<tr>
<td>0141</td>
<td>P-087</td>
<td>Investigation of the Interaction between 5-Fluorouracil (5-FU) and Human Serum Albumin depending on protein concentration by 400 MHz NMR Spectrometer Sibel Korunur, Bilgin Zengin, Ali Yılmaz</td>
</tr>
<tr>
<td>0144</td>
<td>P-088</td>
<td>Synthesis, Crystal Structure, EPR Studies of Doped VO2+ ION in [Co(Him)6] 2Br 4H2O Ilkay Yildirim, Bünyamin Karabulut</td>
</tr>
<tr>
<td>0145</td>
<td>P-089</td>
<td>X-ray Structure and Spectroscopic Characterization of [Cu(1-meim)(H2O)2]•2(sac) COMPLEX Ilkay Yildirim, Bünyamin Karabulut</td>
</tr>
<tr>
<td>Poster Number</td>
<td>Title</td>
<td>Authors</td>
</tr>
<tr>
<td>---------------</td>
<td>----------------------------------------------------------------------</td>
<td>---------------------------------------------------------------------------------------------</td>
</tr>
<tr>
<td>0146</td>
<td>Crystal Water Behavior in MgSO3.6H2O:Co</td>
<td>Petya Nikolaeva Petkova, Youri Tsoukrovsky, Todor Dimov, Ilia Iliev, Ismail Ismailov</td>
</tr>
<tr>
<td>0147</td>
<td>Structural, Spectroscopic and Quantum Chemical Studies of (Z)-N`-(E)-2-(hydroxylimino)-1-phenylethyldene)isonicotinohydrazide</td>
<td>Ayşin Zülfikaroğlu, Çiğdem Yüksektepe Ataol, Hüneyra Bat</td>
</tr>
<tr>
<td>0148</td>
<td>The EPR Study of Cu2+, Mn2+ and VO2+ Ions Doped I-alanine Powder Crystals Produced under High Temperature</td>
<td>Deniz Kurt, Umit Ceylan, Recep Tapramaz</td>
</tr>
<tr>
<td>0149</td>
<td>Theoretical Studies on [(2,4-Dinitrophenyl)hydrazono]1-phenylethylidene)isonicotinohydrazide</td>
<td>Ayşin Zülfikaroğlu, Çiğdem Yüksektepe Ataol, Hüneyra Bat</td>
</tr>
<tr>
<td>0150</td>
<td>The EPR Study of Cu2+ and VO2+ Ion Doped Ca(H2O8PO4)2 H2O Powder Crystals Produced Under High Temperature</td>
<td>Deniz Kurt, Umit Ceylan, Recep Tapramaz</td>
</tr>
<tr>
<td>0151</td>
<td>Label-free Surface-enhanced Raman Spectroscopic Detection of Mycobacterium Smegmatis Using Silver Nanoparticles</td>
<td>Melisew Tadéle Alula, Jonathan Blackburn</td>
</tr>
<tr>
<td>0152</td>
<td>Melting Behaviors of Cu, Pd, Pt and Ti Metal Clusters: Magic Numbers and/or Icosahedral Like Geometries</td>
<td>Meral Eryürek</td>
</tr>
<tr>
<td>0153</td>
<td>A New Dispersive Liquid-Liquid Microextraction Method for Determination of Cobalt in Some Vitamin Tablets</td>
<td>Tuba Ceviz, Serife Sacmac, Ahmet Ulgen</td>
</tr>
<tr>
<td>0154</td>
<td>Anharmonic Behavior in BaTiO3: Investigation by Raman Spectroscopy</td>
<td>Bejaoui Ouni Ines, Fontana Marc, Chapron David, Aroui Hassen</td>
</tr>
<tr>
<td>0155</td>
<td>Raman Spectroscopy of BaCaTiO3</td>
<td>Bejaoui Ouni Ines, Fontana Marc, Chapron David, Aroui Hassen</td>
</tr>
<tr>
<td>0156</td>
<td>Impact of the Sign on the Optical Properties of a Product</td>
<td>Turkta Dimitrova, Petya Nikolaeva Petkova, Darina Bachvarova, Veselina Lalova</td>
</tr>
<tr>
<td>0157</td>
<td>Investigation of Structural, Energetic and Vibrational Properties of 2-Deoxy-2-[(methyl(nitroso)amino)carbonylamino)-β-D-glucopyranose</td>
<td>Mustafa Boyukkutuk, Dilek Pandir, Meryem Evecen, Hatice Ari</td>
</tr>
<tr>
<td>0158</td>
<td>Experimental, Theoretical Investigation and Intramolecular Proton Transfer of Two Tautomers: (E)-4-(((2-methyl-3-nitrophenyl)imino)methyl)benzene-1,2,3-triol and (Z)-2,3-dihydroxy-6-(((2-methyl-3-nitrophenyl)amino)methylene)cyclohexa-2,4-diene</td>
<td>Ersin Temel, Can Alaşalvar, Erbil Ağar</td>
</tr>
<tr>
<td>0160</td>
<td>The Theoretical and Crystallographic Studies on (E)-2-(((4-bromo-2-(trifluoromethoxy)phenyl)imino)methylene)4-nitrophenol</td>
<td>Gunes Demirtas, Ömer Tamer, Necmi Dogu, Davut Arzu, Yusuf Ataly, Mustafa Macit, Songül Şahin</td>
</tr>
<tr>
<td>0161</td>
<td>Structural, Elastic, Electronic and Optical Properties of BeSiN2 from first-principles</td>
<td>Fahiama Arab, Fahiama Arab, Ferhat Ali Sahraoui, Khelifa Haddadi, Layachi Louail</td>
</tr>
<tr>
<td>0162</td>
<td>Application of FTIR Spectroscopy in Microbial Ecology: Studying Different Ecological States of the Rhizobacterium Azospirillum Brasilenses</td>
<td>Anna V. Tagurova, Andrei V. Scheludko, Yulia A. Dyatlova, Alexander A. Kaminer</td>
</tr>
<tr>
<td>0163</td>
<td>Raman Spectroscopy Applied to the Chemical Characterization of mono- and multi- Species Biofilms</td>
<td>Ana María González Amaro, Claudio Frausto Reyes, Adriana Jacome Espadas, Gulce Ogurc İldiz, Rumen Ivanov Tsonchev</td>
</tr>
<tr>
<td>0164</td>
<td>Effect of Intestinal Atom X on Structural, Elastic and Electronic Properties of NbRu3, NbXRu3 (X= B or C)</td>
<td>Ali Benamer, Abd Ekamir Roumili, Youcef Medkour</td>
</tr>
<tr>
<td>0165</td>
<td>Spectroscopic Studies to Clarify the Interactions of Chloroquine Diphosphate and Phenelzine Sulfate Drugs with Human Serum Albumin</td>
<td>Bahar Kancı Bozoğlan, Sibel Tunç, Osman Duman</td>
</tr>
<tr>
<td>0166</td>
<td>Effects of Sodium Dodecyl Sulfate (SDS) on Fluorescence Lifetime Distribution of Bovine Serum Albumin Modified With N-(1-Pyrenyl)maleimide (PM-BSA)</td>
<td>Ibrahim Ethem Özyiğit</td>
</tr>
<tr>
<td>ID</td>
<td>Title</td>
<td>Authors</td>
</tr>
<tr>
<td>------</td>
<td>----------------------------------------------------------------------</td>
<td>---------------------------------------------------------------------------------------------</td>
</tr>
<tr>
<td>P-117</td>
<td>Temperature-Dependent Photoluminescence of Cu, Mn, Co, Zn and Cd Complexes with heptfluorobutanoic Acid and Bipy/Phen</td>
<td>Yalcin Kilic, Ibrahim Kani</td>
</tr>
<tr>
<td>P-112</td>
<td>Temperature-Dependent Photoluminescence of Cu, Mn, Co, Zn and Cd Complexes with heptfluorobutanoic Acid and Bipy/Phen</td>
<td>Yalcin Kilic, Ibrahim Kani</td>
</tr>
<tr>
<td>P-113</td>
<td>XRF Spectrometric Studies on Metallic Decorations from Romanian Heritage Textiles</td>
<td>Angelica Olaru, Maria Geba, Cristina Marta Ursescu, Ana Maria Vlad</td>
</tr>
<tr>
<td>P-114</td>
<td>Theoretical Study of Phosphazenes: Cation −π (Li+, Na+, K+, Be+, Mg+, and Ca2+) Interaction</td>
<td>Fatmagül Tunç, Ahmet Tokatl</td>
</tr>
<tr>
<td>P-115</td>
<td>Investigation of Energetics, Structural Stability and Metalic Impurities of Water Clusters: HF and DFT Study of H2O and (H2O)n for n=3-7 and (H2O)12</td>
<td>Salih Cinal, Mustafa Boyyükata, Yılmaz Dağdemir</td>
</tr>
<tr>
<td>P-117</td>
<td>A Calorimetric Comparison of the Effects of Cholesterol, Desmosterol and 7-Dehydrocholesterol on Zwitterionic DPPC Model Membranes</td>
<td>Cisem Altmayan, Ipek Sahin, Nadide Kazanci</td>
</tr>
<tr>
<td>P-118</td>
<td>Waste Liquid Embryo Samples’ Measurements and Analysis with Raman Spectroscopy</td>
<td>Tuğçe ÖzTÜRK</td>
</tr>
<tr>
<td>P-119</td>
<td>Spectroscopic studies on Cu(II) coordination compound of Sudan Red G [1-(2-methoxyphenylazo)-2-naphthol]</td>
<td>Aslı Eme, Seda Günsedoğdu Sağdıç, Salih Zeki Yıldız</td>
</tr>
<tr>
<td>P-120</td>
<td>FT-IR Spectroscopic and Thermal Study of M(Fumaric Acid)Ni(CN)4.2(1,4-dioxane) Clathrate (M = Mn, Ni and Cd)</td>
<td>Zeki Kartal, Adülkerim Yavuz</td>
</tr>
<tr>
<td>P-121</td>
<td>Photophysical Properties of Octatoxyamido-Substituted Metal-free and Ni(II) Phthalocyanins: A Density Functional Theory Study</td>
<td>Elif Türker Acar, Hatice Can, Ayşe Gül Gürek</td>
</tr>
<tr>
<td>P-123</td>
<td>FT-IR Spectroscopic Study of M(Adipic Acid)Ni(CN)4.1(4,4-dioxane) Clathrate (M = Co and Cu)</td>
<td>Abdülkerim Yavuz, Zeki Kartal</td>
</tr>
<tr>
<td>P-124</td>
<td>Low Temperature Magnetic Properties of “Space Stones”</td>
<td>Gizem Kaban, Atif Siddiki</td>
</tr>
<tr>
<td>P-125</td>
<td>The Cyanide-Bridged Heteronuclear Polymeric Complexes: Syntheses, Spectroscopic and Thermal Properties of [Zn(hmpH)2]M(µ-CN)2(CN)2]n (hmpH = 2-pyrindinemethanol, M = Pd(II) or Pt(II))</td>
<td>Günsel Süheyla Kürkçüoğlu, Elvan Sayın</td>
</tr>
<tr>
<td>P-126</td>
<td>Vibrational Spectra and Electronic Transition Energies from MP2 and DFT Calculations of 1-Ethylimidazole and 2-Ethylimidazole</td>
<td>Ilkan Kavakl, Günsel Süheyla Kürkçüoğlu</td>
</tr>
<tr>
<td>P-127</td>
<td>Synthesis and Characterization of ethyl-4-anilino-1-carbamoyl-2-hydroxy-5-oxo-2-phenyl-2,5-dihydro-1H-yrrole-3-carboxylate</td>
<td>Ibrahim Evren Kıbrıs, Mustafa Şaşmacı, Ismail Yıldırım, Ertan Şahin</td>
</tr>
<tr>
<td>P-128</td>
<td>Sensitive and Selective Determination of Trace Amounts of Azin Dyes in Multi – Component Systems Using First-Order Derivative Spectrophotometric Technique</td>
<td>Elif Türker Acar, Gülten Atun</td>
</tr>
<tr>
<td>P-129</td>
<td>Spectroscopic and Calculated Thermodynamic Properties of 3-Phenyl-4-(3-Cinnamoyloxylbenzylidnamino)-4,5-Dihydro-1H-1,2,4-Triazol-5-one Molecule</td>
<td>Murat Beytur, Haydar Yüksel</td>
</tr>
<tr>
<td>P-130</td>
<td>Gaussian Calculations of New 3-(P-Methylbenzyl)-4-[3-(3-Methoxybenzoxyl)-Benzylidnamino]-4,5-Dihydro-1H-1,2,4-Triazol-5-One</td>
<td>Hilal Medetalibeyoğlu, Haydar Yüksel</td>
</tr>
<tr>
<td>P-131</td>
<td>A Computational Study on the Electronic and Nonlinear Optical Properties of h-BN-Graphyne Subunit</td>
<td>Büşra Aydın, Mehmet Bahat</td>
</tr>
<tr>
<td>P-132</td>
<td>An Investigation of Keto-enol Tautomerism in 2,4-di tert-butyl-6-(Z)-[2- or 4-fluorophenyl] imino</td>
<td>Erol Eroğlu, Murat Kılıç, İlşan Burak Çam, Timur Tongur</td>
</tr>
<tr>
<td>Session</td>
<td>Number</td>
<td>Title</td>
</tr>
<tr>
<td>---------</td>
<td>--------</td>
<td>----------------------------------------------------------------------</td>
</tr>
<tr>
<td>0208</td>
<td>P-133</td>
<td>Effect of Fluoro- and Chloro- substitution of the Phenyl Ring on Enol-keto Tautomeric equilibriums of 2,4-di-tert-butyl-6-(Z)-[(2,5-fluorophenyl or 2,5-Chlorophenyl)imino]Methyphenol: A Spectroscopic and DFT Study</td>
</tr>
<tr>
<td>0209</td>
<td>P-134</td>
<td>Vibrational Spectroscopic Analyses of Pollutants in Soil Samples Collected from Historical Libraries’ Environments.</td>
</tr>
<tr>
<td>0210</td>
<td>P-135</td>
<td>Raman Spectroscopic Investigations on Rare Books’ Covers and Pages from Historical Libraries. Case Study: Recai Mehmet Efendi Library</td>
</tr>
<tr>
<td>0212</td>
<td>P-136</td>
<td>Micro-Raman, Mid-IR and DFT studies on 2-[4-(4-Ethylbenzamido)phenyl]benzothiazole</td>
</tr>
<tr>
<td>0214</td>
<td>P-138</td>
<td>Crystal Structure of 4-fluoro-N-(2-hydroxy-4-nitrophenyl)benzamide</td>
</tr>
</tbody>
</table>
The on-site Analysis of Cultural Heritage Materials and Artefacts

Philippe Colomban1,2

1Sorbonne Universités, UPMC Univ Paris 06, UMR 8233, MONARIS, c49, 4 Place Jussieu, F-75005, Paris, France
2CNRS, IP2CT, UMR 8233, MONARIS, 4 Place Jussieu, F-75005, Paris, France

The reduction in size of instruments enables their use outside the laboratory. Nevertheless, since performances of portable devices are lower than those of fixed ones, appropriate procedures and models must be developed. Here we present the results of nearly 15 years of non-destructive analysis using Raman/Infrared (micro)spectroscopy and X-ray fluorescence on a wide variety of objects and materials. The non-destructive on-site analysis was used to study artefacts never tested before due to their high value and/or weakness (many of them were Advanced Materials at their time of production). It allowed significant contributions to be made to the history of art and techniques: e.g. to distinguish between original productions and non-documented restorations, to identify false or copies or erroneous attributions, but also to better understand the manufacturing techniques and state of conservation. It can be anticipated that the use of portable instruments should rapidly extend to many other fields.

Ph. COLOMBAN, D. MANCINI, Lacquerware pigments identification with fixed and mobile Raman microspectrometer: a potential technique to differentiate original/fake artworks, Arts 2013, 2, 111-123 http://www.mdpi.com/2076-0752/2/3/111/
The Molecular Universe
Spectroscopy as a Tool to Unravel Interstellar Chemistry

Harold Linnartz

Sackler Laboratory for Astrophysics, Leiden Observatory, University of Leiden, PO Box 9513, NL 2300 RA Leiden, the Netherlands
www.laboratory-astrophysics.eu

The conditions in the inter- and circumstellar medium, the space in between and around stars, are extreme; particle densities are exceptionally low, radiation fields intense and temperatures range from 10 to 100 K. Nevertheless, dedicated astronomical observations have proven the existence of more than 180 different molecules, ranging from simple diatomics to large complex molecules, covering both stable and highly reactive species. The identification of these molecules is only possible through accurate high resolution spectroscopic studies in the laboratory and the first part of this talk will show how ultra-sensitive detection techniques can be used to identify ions and radicals in space [1]. Given the low molecular abundances in space, these species play a dominant role in gas phase reactions. However, many of the observed species, in space, particularly abundant species like water, methanol or more complex organics like ethylene glycol or glycol aldehyde cannot be explained through gas phase reactions only. Here other processes may be at work. The second part of the talk discusses the photo-dissociation of GRAND-PAHs, large polycyclic aromatic hydrocarbons that are formed in the outflows of dying stars [2]. The third part switches to surface enhanced processes on cold (15 K) interstellar ice analogues, triggered by vacuum UV irradiation or atom impacts [3-5]. It is shown how water forms through the hydrogenation of oxygen, how photo-desorption determines planet formation and how the formation of COMs (complex organic matter) may be related to the formation of the building blocks of life.

References
Surface-enhanced Raman Scattering from Protein Detection to Cancer Diagnosis

Mustafa Culha

Ginetics and Bioengineering Dept, Yeditepe University, Atasheir, Istanbul, Turkey

Surface-enhanced Raman scattering is investigated not only for detection, identification a variety of analytes with or without biological origins but also disease diagnosis. In this presentation, our effort to use the technique from protein detection to microorganism identification, from cancer diagnosis to nanotoxicity determination is discussed. The pros and cons of the technique for such applications are also discussed to give a better picture of the technique.

Keywords: SERS, detection, diagnosis, proteins, microorganisms and cancer
An Excursion on Molecular Conformational Landscapes: Discovering Rare Species in the Highlands

Rui Fausto

Department of Chemistry, University of Coimbra, Portugal

For many molecules, besides the low-energy conformers that are easily accessible to experiment, high-energy forms exist whose population is negligible (or are not populated at all) in most of the usual experimental conditions. Till very recently, the identification and characterization of these high-energy conformers was done only theoretically. Using a simple analogy, the exploration of the molecular conformational landscapes was confined to the Lowlands, while the Highlands were terra incognita, whose inhabitants were never seen. The recent development of experimental techniques based on the selective in situ generation of high-energy conformers, by selective vibrational excitation (using near-infrared light) of the easily accessible lower-energy conformers, opened a way for journeying to the molecular conformational Highlands. These expeditions have allowed observation of a plethora of novel molecular structures, some of them exhibiting rather unusual properties. Also, narrowband UV-excitation of a matrix-isolated precursor has evolved as a powerful technique to generate high-energy isomeric forms, otherwise not accessible to experimental characterization. Some of these species are pivotal intermediates in the thermally- or/and photochemically-induced reactivity of important chemical systems. In this talk, the attendees will be invited to make an excursion on molecular landscapes, learn how the expedition can be prepared, enjoy the contact with the “highlanders” and see how they behave. Several molecular systems will be addressed, ranging from simple molecules exhibiting only two conformers to complex multi-dimensional systems that embrace not only different conformers, but also other types of isomers.

Acknowledgements: Present and past members of the Laboratory for Molecular Cryospectroscopy and Biospectroscopy, Coimbra, Portugal, who have contributed to the studies addressed in this talk, are acknowledged. I thank also the Portuguese Science Foundation (FCT) for financial support.

Keywords: Molecular landscapes, high-energy species, near-IR vibrational excitation, narrowband UV excitation, quantum chemical calculations
Raman spectroscopy is an approach that during the last years gained a lot of interest in archaeometry [1,2]. Typically, several favourable features are cited, such as the ability to obtain a molecular spectrum from micrometer-sized particles (compatible with the dimensions of a pigment grain), the speed of analysis and the relatively straightforward interpretation (at least as far as comparison with reference spectra is possible). Raman spectroscopy can also often provide information on the inorganic as well as on the organic fraction. Moreover, the technique is non-destructive and thus the microsamples remain available for future investigations. Finally, By using fibre- optics, the approach can perfectly be deployed for in situ studies.

In archaeometry, we often try to minimise the risk on damage, while maximising the obtained information. This approach can be reached by using mobile instrumentation to perform in situ investigations. Other approaches consist of performing several non-destructive investigations on the same micro samples. Combining techniques that provide complimentary information, maximises the information content that is obtained. Typically, the combination of Raman spectroscopy with X-ray fluorescence has proven to be successful. As different approaches all have their pros and cons, it is impossible to say that in situ investigations are always better, or that laboratory experiments always should be preferred. Depending on the research question and the circumstances, the most appropriate approach should be selected.

In this presentation, we will provide plenty of examples to illustrate this approach. We’ll discuss in situ campaigns as well as laboratory experiments that were performed to investigate a broad range of art objects, including panel paintings, wall paintings, rock art, etc.

References.
Based on the above flowchart and among other results we can highlight the analysis of our improvement of the force field previously studied in Ref. [1] for describing nucleosides of RNA with particular attention to glycosidic energies.

In particular, we have recently used Amber and Tinker applied to study a reparametrization of also a recent study proposed to tackle nuclei acids [1]. The latter proposed an efficient parametrization considering glicosidic energies as a case study. The work was carried out at a high level of quantum mechanical methods based on DFT approach. For the parametrization processes the total energy for all interactions was assumed as

\[ E_T = E_{bond} + E_{angle} + E_{dih} + E_{elst} + E_{vdW} \]

where the several energy contributions are namely the bond stretching (E_{bond}), angle bending (E_{angle}), dihedral (E_{dih}), nonbonded electrostatic (E_{elst}) and van der Waals (E_{vdW}). In the present study a Genetic Algorithm (GA) was used to optimize the torsional energies of the RNA (ribonucleosides). Our proposed methodology is given by [2]

Molecular dynamics simulations have been widely used in the literature. CHARM is one of the most popular programs to carry out such simulations. Similarly, Amber and Tinker are also codes widely applied in order to describe inter and intra molecular forces. Apart of each particularity of these programs and their focus on several types of simulations such as torsional or conformational analyses, all of them need efficient functional parametrizations to define their force fields.

In particular, we have recently used Amber and Tinker applied to study a reparametrization of also a recent study proposed to tackle nuclei acids [1]. The latter proposed an efficient parametrization considering glicosidic energies as a case study. The work was carried out at a high level of quantum mechanical methods based on DFT approach. For the parametrization processes the total energy for all interactions was assumed as

\[ E_T = E_{bond} + E_{angle} + E_{dih} + E_{elst} + E_{vdW} \]

where the several energy contributions are namely the bond stretching (E_{bond}), angle bending (E_{angle}), dihedral (E_{dih}), nonbonded electrostatic (E_{elst}) and van der Waals (E_{vdW}). In the present study a Genetic Algorithm (GA) was used to optimize the torsional energies of the RNA (ribonucleosides). Our proposed methodology is given by [2]

Molecular dynamics simulations have been widely used in the literature. CHARM is one of the most popular programs to carry out such simulations. Similarly, Amber and Tinker are also codes widely applied in order to describe inter and intra molecular forces. Apart of each particularity of these programs and their focus on several types of simulations such as torsional or conformational analyses, all of them need efficient functional parametrizations to define their force fields.

In particular, we have recently used Amber and Tinker applied to study a reparametrization of also a recent study proposed to tackle nuclei acids [1]. The latter proposed an efficient parametrization considering glicosidic energies as a case study. The work was carried out at a high level of quantum mechanical methods based on DFT approach. For the parametrization processes the total energy for all interactions was assumed as

\[ E_T = E_{bond} + E_{angle} + E_{dih} + E_{elst} + E_{vdW} \]

where the several energy contributions are namely the bond stretching (E_{bond}), angle bending (E_{angle}), dihedral (E_{dih}), nonbonded electrostatic (E_{elst}) and van der Waals (E_{vdW}). In the present study a Genetic Algorithm (GA) was used to optimize the torsional energies of the RNA (ribonucleosides). Our proposed methodology is given by [2]

Molecular dynamics simulations have been widely used in the literature. CHARM is one of the most popular programs to carry out such simulations. Similarly, Amber and Tinker are also codes widely applied in order to describe inter and intra molecular forces. Apart of each particularity of these programs and their focus on several types of simulations such as torsional or conformational analyses, all of them need efficient functional parametrizations to define their force fields.

In particular, we have recently used Amber and Tinker applied to study a reparametrization of also a recent study proposed to tackle nuclei acids [1]. The latter proposed an efficient parametrization considering glicosidic energies as a case study. The work was carried out at a high level of quantum mechanical methods based on DFT approach. For the parametrization processes the total energy for all interactions was assumed as

\[ E_T = E_{bond} + E_{angle} + E_{dih} + E_{elst} + E_{vdW} \]

where the several energy contributions are namely the bond stretching (E_{bond}), angle bending (E_{angle}), dihedral (E_{dih}), nonbonded electrostatic (E_{elst}) and van der Waals (E_{vdW}). In the present study a Genetic Algorithm (GA) was used to optimize the torsional energies of the RNA (ribonucleosides). Our proposed methodology is given by [2]
Fractional fractional charges and fractional spins provide a clear analysis of the errors of commonly used functionals. For an effective and universal alleviation of the delocalization error, we develop a local scaling correction scheme by imposing the Perdew-Parr-Levy-Balduz linearity condition to local regions of a system. Our novel scheme is applicable to various mainstream density functional approximations. It substantially reduces the delocalization error, as exemplified by the significantly improved description of dissociating molecules, transition-state species, and charge-transfer systems. The usefulness of our novel scheme affirms that the explicit treatment of fractional electron distributions is essentially important for reducing the intrinsic delocalization error associated with approximate density functionals.

Progress with many-body theory approach will be also be presented. We have formulated the ground-state exchange-correlation energy in terms of pairing matrix linear fluctuations, opening new a channel for density functional approximations. This method has many highly desirable properties. It has minimal delocalization error with a nearly linear energy behavior for systems with fractional charges, describes van der Waals interactions similarly and thermodynamic properties significantly better than the conventional RPA, and eliminates static correlation error for single bond systems. It is the first known functional with closed-form dependence on orbitals, which captures the energy derivative discontinuity in strongly correlated systems. We also adopted pp-RPA to approximate the pairing matrix fluctuation and then determine excitation energies by the differences of two-electron addition/removal energies. This approach captures all types of interesting excitations: single and double excitations are described accurately, Rydberg excitations are in good agreement with experimental data and CT excitations display correct 1/R dependence.

References


Invited Speakers' Texts

PL-08

Application of FTIR spectroscopy in proteomics and metabolomics - potentials and challenges

Parvez HARIS
Recent Advances in ATR-sensor Development Based on Silver Halide Fibers for Infrared Spectrometric Process Analysis and Applications in Microbiology and Medicine

H.M. Heise

Interdisciplinary Center for Life Sciences, South-Westphalia University of Applied Sciences,
Frauenstuhlweg 31, D-58644 Iserlohn, Germany

Infrared spectroscopy is a versatile analytical method much used for qualitative and quantitative analysis. While mid-infrared (MIR) measurement techniques have nowadays most often been used in the laboratories, near-infrared (NIR) spectroscopy has been established for monitoring chemical production processes. Despite this, MIR spectroscopy based on the attenuated total reflection (ATR) technique in combination with silverhalide fiber-optics has newly created many opportunities for replacing NIR-measurement probes. For several years, Process Analytical Technology (PAT) has been in the focus of the chemical industry, for which also industrial biotechnology is playing a greater part for, e.g., the production of biofuels, i.e. primarily biodiesel, bioethanol and biogas. Other approaches include the decomposition of lignocellulose and other biopolymers and the further use in fermentation processes or the production of biopolymers, for which the biodegradability is important, especially in view of the environmental problem with non-decaying plastics. There are multi-purpose assays required for the monitoring of food quality and special examples given are from testing the oxygenation stability of vegetable oils and biodiesel.

Other spectroscopic applications are in medical sciences and microbiology, for which several examples will be presented. As demonstrated for PAT applications, fiber-optic probes allow remote sensing and have been successfully employed, e.g., in margin detection during surgery for removing cancerous tissue and lesions. With regard to hygiene issues, micro-techniques have been used in preparation of dry-films from various bacteria suspensions after a standardized 24 h cultivation, which allow the rapid identification of bacteria on the species level based on standard spectral libraries, for example, from the Robert-Koch Institute in Berlin (Germany). Recent results for the identification of fungal pathogens, equally important in hospital hygiene or agricultural sciences, after cultivation on selective nutrient media will also be presented. Conventional species identification is time-consuming and subjective, since it requires culturing for several days and is based on the subjective assessment of the morphological characters. Due to the characteristic spectral fingerprints of fungal mycelium biomass, infrared spectroscopy in combination with fast micro-techniques will gain greater acceptance also in the microbiology field.
Part I
Ferroelectric materials offer a wide range of special physical properties such as high dielectric constant, spontaneous polarisation, pyroelectric and piezoelectric effects which can be applied in non-volatile memories, actuators, thin film capacitors, thermal sensors and transducers. At the nanometer scale physical and chemical properties are expected to differ from those of the bulk material. In particular, a critical particle size was predicted below which ferroelectricity does no longer occur. Electron paramagnetic resonance (EPR) is exceedingly powerful method for depicting the structural changes which is in causal connection with size effects and size-driven ferroelectric-to-paraelectric phase transitions in perovskite nanocrystals (BaTiO₃ and PbTiO₃ doped with paramagnetic ions). Size and interface effects cooperate in determining the ferroelectric, electronic and structural properties of the nanoparticles. This allowed for the first time to delineate a rather detailed idea of their core-shell structure of ferroelectric nanoparticle and the temperature- and size-driven phase transitions.

Part II
Understanding the role of defect centers (i.e. vacancies, interstitials, and antisites) and the incorporation of stable or meta-stable defects is a key tool toward controlling the electronic properties of ZnO. EPR is well suited for this task since it provides a direct method to monitor different paramagnetic states of vacancies and, thus, complements other experimental techniques such as photoluminescence. In this sense, EPR does not only work very well on the identification of defects but also one may obtain reliable correlation to the luminescence properties of the material. In order to characterize the ZnO defect structure, both light induced X band and high field EPR has been applied. To understand the behavior of defects in ZnO nano-particles under light, we imposed in-situ laser light with wavelengths of 445 nm and 532 nm on the samples during the X-band EPR measurements. This is crucially important since defect structures may show different properties under different wavelength. EPR measurement at 208 and 406 GHz allowed resolve small differences in the g-values.

Keywords: EPR spectroscopy; Ferroelectrics; Semiconductors
ORAL ABSTRACTS
Calculation of Transient Absorption Spectra for the Intramolecular Electron Transfer

Vladislav V. Yudanov¹, Serguei V. Feskov²

¹Laboratory of Photochemistry, Voevodsky Institute of Chemical Kinetics and Combustion, Novosibirsk, Russia
²Department of Information Systems and Computer Modeling, Volgograd State University, Volgograd, Russia

Very effective tool for the study of physical and chemical processes in the donor-acceptor molecular systems are the methods of ultrafast time-resolved spectroscopy. Analysis of transient absorption spectra, as a rule, is challenging. The spectra contain information about the many processes that occur simultaneously in a molecular system. Therefore, the most effective method of analysis of experimental data is computer simulation.

The charge transfer in donor-acceptor molecular systems, placed in a polar solvent, is accompanied by the excitation of a large number of vibrational modes, one of which relates to the reorganization of the environment, the other leads to an intramolecular reorganization of the reactants and products [1]. Solvent modes in these reactions, as a rule, are low-frequency with typical values of reorganization energy of 0.2 ÷ 0.5 eV. This allows use to describe methods of classical mechanics and makes it easy. This approach allows to describe the energetics and kinetics of photochemical reactions in terms of one or more energy reaction coordinate.

Intramolecular vibrations, on the contrary, are characterized by high-frequencies and for their description require the use of the principles of quantum mechanics. In typical cases, the ultrafast charge transfer in donor-acceptor system leads to the excitation 3-10 intramolecular quantum modes to the total energy of the reorganization 0.3 ÷ 0.6 eV. The total number of participating in the chemical reaction of the vibrational sublevels of the electronic state of the reactants and products can reach $10^4$-$10^6$. Computer modeling of such systems requires the use of efficient computational approaches. In this work, we implemented the numerical scheme proposed in [1], to calculate the transient absorption spectra of the donor-acceptor molecular systems, placed in a polar solvent, based on recrossing algorithm Brownian simulation of the kinetics of electron transfer reactions in polar solvent. The results of the program coincided with private analytical solutions.

The financial support of the Russian Scientific Foundation (grant No. 15-13-10012 ) is gratefully acknowledged.

References


Keywords: brownian simulations, spectral dynamics, femtosecond pump-probe spectroscopy
Measurement of Air Quality from Greenhouses Based on Photoacoustic Spectroscopy

Ioana Ruxandra Ivascu¹, Consuela Elena Matei², Mihai Patachia¹, Ana Maria Bratu¹, Dan Constantin Dumitras³, Ovidiu Jerca³

¹Department of Lasers, National Institute for Laser, Plasma and Radiation Physics, 409 Atomistilor St., PO Box MG-36, 077125 Magurele - Bucharest, ROMANIA
²Physics Department, Faculty of Applied Sciences, University “Politehnica” of Bucharest, 313 Splaiul Independentei, Bucharest - 060042, ROMANIA
³Faculty of Land Reclamation and Environmental Engineering, University of Agronomic Sciences and Veterinary Medicine of Bucharest, 59 Blvd. Marasti, Bucharest - 011464, ROMANIA

In the modern society, the greenhouses agriculture represents a solution for the great demand on market of herbs, vegetables and fruits round-year. The greenhouses, characterized by an artificial environment specially designed for an optimal growing of plants, offer the opportunity for large and continuous production of vegetables in any season. But the benefits brought by the very controlled climate from inside, are also accompanied by the problem of keeping of a healthy environment for plants and people working there. In order to improve the productivity, various chemicals like fertilizers, pesticides and insecticides are used for treatments during the plant growing cycle, so that high levels of pollutant concentrations could be accumulated in the air from such enclosed spaces.

In this paper we present a multicomponent analysis of the pollutant trace gases in the air from greenhouses, performed by laser photoacoustic spectroscopy. Based on the selective absorption of laser radiation by specific molecules, this technique offers valuable advantages including high selectivity and sensitivity (being able to measure gas concentrations at sub-ppb levels, large dynamic range, multicomponent capability and locally sampling. The experimental chain included a tunable CO2 laser with wavelengths between 9.2 ÷ 10.8 µm, which covers the molecular absorption spectra of our targeted pollutants: ammonia, ethanol, methanol, ethylene, carbon dioxide and water. The pollutant concentrations are determined based on the absorption characteristics of each individual gas species with respect to the 53 vibrational-rotational lines of the CO₂ laser. The analysis of air quality was performed at key moments of the plant growing from seedling to harvest.

Acknowledgements: This work was supported by a grant of the Romanian Ministry of Education, CNCS – UEFISCDI, project number PN-II-RU-PD-2012-3 - 0207.

Keywords: Photoacoustic spectroscopy, CO₂ laser, air pollutants, multicomponent detection
Theoretical Calculation of the Optical And Spin-Hamiltonian Parameters For The Rhombic Cu$^{2+}$ Center in [Cd(sac)$_2$(HydEt-en)$_2$] Powders

Emel Kalfağlu

Ministry of National Education, Samsun, Turkey

The crystal-field parameters ($D_q$, $D_t$, $D_s$, $D_\zeta$ and $D_\eta$) for Cu$^{2+}$ center in [Cd(sac)$_2$(HydEt-en)$_2$] powders are calculated from perturbation theory method (PTM). The spin-Hamiltonian parameters of the Cu$^{2+}$ center ($g_x$, $g_y$, $g_z$ and $A_x$, $A_y$, $A_z$) are determined for a 3d9 ion in rhombically elongated octahedra. The bonding in the Cu$^{2+}$ center is described in terms of molecular orbitals and the molecular orbital bonding coefficients are obtained rhombic Cu$^{2+}$ centers. The theoretical EPR parameters are in reasonable agreement with the experimental values. The results are discussed.

Keywords: EPR, Crystal-field theory, Molecular orbital bonding coefficients, Cu$^{2+}$ ion
Abstract

This study describes the processing of the 2D seismic survey acquired in the Kufra Basin, Area 201, which is situated in the Southeast of Libya. The terrain in Area 201 falls into four distinct categories, gravel plain, sand dunes, rocky ground/jebels and rolling sand. The sand dunes tend to occur in long ‘fingers’ running from the NE to the SW direction and covering approx 5-10%, which are predominantly in the centre of Area 201.

The main objective of this study is to compare and describe the techniques that were done to solve the static problem within the dune areas. Three static scenario models from three different processing contractors were offered and applied on the data to compare the best solution over the dune area. First contractor applied static model with Up-hole model and Residual refraction statics, second contractor applied only Residual refraction statics, where the third contractor applied a static model comprises of Up-hole model, Residual refraction statics and Horizon base static (HBS) correction. The main objective of this study is to compare and describe the techniques that were done to solve the static problem within the dune areas. Three static scenario models from three different processing contractors were offered and applied on the data to compare the best solution over the dune area. First contractor applied static model with Up-hole model and Residual refraction statics, second contractor applied only Residual refraction statics, whereas a local anomaly in some lines was still affected by statics. These anomalies, resulted from the presence of dunes, were not solved by the up-hole model and residual refraction statics. To correct these, the static was locally updated with a third technique, the horizon base static (HBS) correction was applied. For the lines where the HBS corrections were done, the process gave better result. The new processed test was compared to the other two processing tests and a large improvement was noticed in terms of static issues.

Keywords: Seismic Processing Techniques in dune areas

NOT ATTENDED
O-05

Comparison of Photo Physical Properties of 7-diethylamino-3-Thenoyl Coumarin and 7-Diethylamino Coumarin

Sanjay Kumar

Department of Physics, Rajdhani College, University of Delhi, Delhi, India

The photo physical properties like ground state and first excited singlet state dipole moment etc. of 7-diethylamino-3-thenoyl coumarin and 7-diethylamino coumarin were compared. The effect of substituent at position 3 is also discussed in terms of the photo physical parameters. The study is carried out in various polar and non-polar solvents at room temperature using fluorescence and absorption technique. The solvent effect on photo physical behavior of these compounds showed that stokes shift increases with the polarity of solvents. The first excited singlet state dipole moment and ground state dipole moment were calculated using Bakhshiev, Kawski-Chamma-Viallet and Reichardt-Dimroth equations and were compared for both the coumarin studied. In both the cases the dipole moments were found to be higher in the excited singlet state than in the ground state indicating a substantial redistribution of \( \pi \)-electron density in the excited state. The angle between the first excited singlet state and ground state dipole moment was also calculated. The red shift of the absorption and fluorescence emission bands observed for both the coumarin studied upon increasing the solvent polarity indicating that the electronic transitions were \( \pi \rightarrow \pi^* \) nature. Solvatochromic models such as Kamlet-Taft and Catalans 3P were used to correlate the solvatochromic shift in different polar and non-polar solvents with a linear solvation energy relationship.

Keywords: Coumarin, Solvent effects, Excited singlet state dipole moment, Ground state dipole moment, Solvatochromism, Linear solvation energy.
Interaction of 6-methoxyquinoline with Anionic Sodium Dodecylsulfate Micelles: Photophysics and Rotational Relaxation Dynamics at Different pH

Tej Varma Yenupuri, Debi D Pant

Department of Physics, BITS-Pilani, Rajasthan, INDIA

Interaction of different species of 6-methoxyquinoline (6MQ) with anionic micelles has been studied at different pre-micellar, micellar and post-micellar concentrations using steady state, time resolved fluorescence and fluorescence anisotropy techniques. The sensitivity of fluorescence of 6MQ to change in its local environment was used to probe sodium dodecylsulfate micelles (SDS). At post-micellar concentrations of SDS, the observed blue shift in the fluorescence spectrum and increase in quantum yield are attributed to the incorporation of solute molecule to micelles. 6MQ has been found to bind to the surface of the anionic micelles instead of penetrating inside. The binding constant (Kb) calculated for 6MQ revealed that the electrostatic forces mediate charged probe-micelle association, whereas, hydrophobic interaction allowed neutral 6MQ to associate with SDS micelles. The charged 6MQ is inserted deeper into the micelle surface than its neutral form, the later being less exposed to the aqueous phase. The fluorescence anisotropy decay of 6MQ in SDS studied at different pH allowed determination of restriction of motion of the fluorophore. The location of the probe molecule in micellar systems is justified by a variety of spectral parameters such as refractive index, dielectric constant, ET (30), average fluorescence decay time, radiative and non radiative rate constants, and rotational relaxation time. The micro-environment around the fluorophore reveal that the photophysics of 6MQ is very sensitive to the microenvironment of SDS and 6MQ resides at the water-micelle interface at all pH studied.

Keywords: 6-methoxyquinoline, micelles, sds, fluorescence, pH

Emission spectra of 6MQ in bulk water and different concentrations of (b) pH 7

6MQ is present in neutral form depicts the fluorescence spectra of 6MQ in bulk solution and aqueous SDS micellar solution as a function of surfactant concentration.

Different solvent parameters and spectral data of 6MQ+ and 6MQ in different solvents

<table>
<thead>
<tr>
<th>SDS(pH)</th>
<th>(\varepsilon)</th>
<th>(\eta)</th>
<th>ET (30)</th>
<th>va-vf (cm (^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>33.12</td>
<td>1.37</td>
<td>47.63</td>
<td>6241</td>
</tr>
<tr>
<td>7</td>
<td>65.1</td>
<td>1.29</td>
<td>55.8</td>
<td>3184</td>
</tr>
<tr>
<td>12</td>
<td>62</td>
<td>1.31</td>
<td>54.6</td>
<td>2741</td>
</tr>
</tbody>
</table>
Solar energy conversion is among the most widely studied fields of regenerative energy sources. Photophysical properties such as absorption and excited state relaxation pathways have been extensively investigated both spectroscopically and theoretically for a manifold of organic dyes and transition metal complexes. However, much less is known about intermediates formed upon photoexcitation and the subsequent (multi-) electron transfer pathways. Here we present a joint experimental-theoretical approach to access reaction dynamics beyond 1 µs by investigating such intermediates based on spectro-electro-chemical (SEC) methods and quantum chemical calculations.[1] Several ruthenium(II) polypyridyl complexes with 4H-imidazole bridging ligands have been studied with respect to oxidative and reductive UV-vis-SEC and resonance Raman (RR-)SEC, see Figure 1. The quantum chemical calculations have been performed at the (time-dependent) density level of theory (TD)DFT and are in excellent agreement with the experimental data and, hence, can provide detailed insight into the photophysical and photochemical properties of intermediates in stepwise multi-electron transfer processes. UV-vis and RR-SEC of the oxidized complexes determined their multi-photoelectron donor capacity, while multi-photoelectron storage is probed by reductive SEC. This combined approach allows to model multi-electron transfer by a double oxidation/reduction (first electro-chemically and subsequent photochemically) scheme.

References

Keywords: Resonance Raman spectroscopy, Spectro-Electrochemistry, Ruthenium, TDDFT Calculation, Electron Transfer

Figure 1: Light-triggered multi-electron transfer modeled by oxidative and reductive SEC by describing the (multi-)electron donor and acceptor capacity separately.
Near-Infrared (NIR) absorbing carbocyanine dyes have been increasingly used as they are useful for developing bioanalytical, biomedical methods and in many other applications. While NIR carbocyanines typically have relatively lower fluorescent quantum yield as compared to visible fluorophores, but their much higher molar absorptivities facilitates the detection at very low concentration levels. Carbocyanines are relatively easy to synthesize and can be designed to achieve particular spectroscopic properties. For example using appropriate functional moieties absorption and fluorescence properties change when complexed to metal ions, to detect pH changes, bind to biological molecules, etc. Recently large number of in vivo applications has been reported to utilize these. Carbocyanines exhibit unique spectroscopic properties at higher concentrations, such as aggregation, binding, etc, further expanding their utility. Fluorescence intensity of carbocyanines significantly increases by enclosing several dye molecules in silica nanoparticles. Self quenching may become a problem for carbocyanines at high concentration in the silica nanoparticle or other confined spaces. Large Stokes’ shift dyes can significantly decrease this problem. This can be achieved by substituting meso position halogens in the NIR fluorescent carbocyanines with a linker containing amino moiety which also serves as a linker to covalently attach the dye molecule to the nanoparticle backbone. The primary applications of these particles are for bright fluorescent labels to be used in bioanalytical applications such as immunochemistry, flow cytometry, etc. This presentation also discusses facile synthesis of specific carbocyanines designed for different applications and tailoring their spectral properties to specific applications. One of these applications is the use of NIR carbocyanines as enzyme substrates. The studies presented here also describe the use of different visible and NIR dyes in silica nanoparticles. Fluorescent silica nanoparticles can covalently be attached to the biomolecule of interest by activating the silica surface with amino reactive surface moieties. Carbocyanines often bind to large biomolecules such as serum albumins. This binding can be studied in bulk solution or in reverse micellar nano-reactors. Small reversed micelles can often incorporate only one biomolecule hence controlling the stoichiometry of the interaction. Binding constant and spectral property of confined biomolecule-dye complexes were compared to bulk solution measurements.

**Keywords:** Near-Infrared Fluorescence Carbocyanines Nanoparticles
Oral Abstracts

O-09

Using of Egyptian Greensand in Drinking Water Purification (Removal of Iron and Manganese)

Khaled Abdel Aal Selim, Mohamed Abdel Maguid Yousef, Nagui Aly Abdel Khalek, Samah Saleh Abdallah

Minerals Technology Department, Central Metallurgical Research & Development Institute, CARDI, Egypt

Under guidelines for public water supplies set by the Environmental Protection Agency (EPA), iron and manganese are considered secondary contaminants in drinking water supplies. Secondary standards apply to substances in water that cause offensive taste, odor, color, corrosion, foaming, or staining. The standard Secondary Maximum Contaminant Level (SMCL) for iron is 0.3 ppm and 0.05 ppm for manganese. These standards can be used as guidelines to evaluate the quality of water from wells or springs. Manganese greensand is a unique medium used in conjunction with a filtration system to oxidize, precipitate and remove iron, manganese, arsenic and hydrogen sulfide. Its manufacturing process uses the ion exchange properties of its stabilized glauconite (greensand) substrate to form an active manganese oxide coating. While it is not suitable for every iron and manganese application, manganese greensand, by design and operation, can possess great flexibility as an oxidizing filter media. The objective of this work is to study the efficiency of surface modified phyllosilicate mineral (glauconite) in the removal of iron and manganese from Egyptian water. Different operating conditions were tested as bed type, pH range, flow rate, pressure drop, backwash, bed thickness, head loss and regeneration procedures. It is found that Continuous regeneration (CR) operation is recommended for well waters where iron removal is the main objective with or without the presence of manganese. Where, the Intermittent Regeneration (IR) process is preferred when manganese is the predominant component to be removed. Complete iron and manganese removal was achieved using surface modified greensand from water has concentrations of 10-50 mg/L. Results obtained confirmed that when the total combined iron and manganese concentration is less than 15 mg/L, an oxidizing filter (e.g., natural Manganese Greensand) is recommended. Natural manganese greensand has the advantages of both manganese dioxide coating and regeneration by using potassium permanganate solution. The used oxidizing filter supplies oxygen to convert ferrous iron into a solid form which can be filtered out of the water.

Keywords: Greensand, Glauconite, Surface modification, phyllosilicate mineral, adsorption, cation exchange
A series of new pyrano[2,3-d:6,5-d']dipyrimidine derivatives have been synthesized and evaluated for their in vitro anticancer activity. The structure of all the synthesized compounds was confirmed by 1H NMR, 13C NMR, 15N NMR, HR-MS and FT-IR spectral analysis. These compounds were studied for cytotoxic activity against four human cancer (HeLa, SkBr3, HepG2, and Caco2) cell lines. The synthesized compounds showed high selectivity and four compounds (5e, 5f, 5g and 5i) showed excellent potent cytotoxicity against HeLa, SkBr3, and Hep-G2 cancer cell lines. Furthermore, four compounds (5a, 5c, 5b and 5d) have exhibited significant cytotoxicity activity against SkBr3 and HepG2 cell lines and moderate cytotoxicity against HeLa cell line. Virtual screening was performed via docking to determine the binding modes of synthesized compounds into the binding site of Human Kinesin Eg5.

Keywords: Synthesis, Spectral studies, Pyrimidines, Cytotoxicity activity, Pyranes
Relativistic DFT Study of Highly Selective N-Ligands for Lanthanides(III)/Actinides(III) Separation

Belkhiri Lotfi¹, Ephritikhine Michel², Boucekkine Abdou³

¹Department of Chemistry, Mentouri University of Constantine, Algeria
²IRAMIS, UMR 3299 CEA/CNRS SIS2M, CEA/Saclay, France
³Laboratoire Sciences Chimiques de Rennes, UMR-CNRS 6226, Université de Rennes 1, France

The chemistry of lanthanides (Ln) and actinides (An) species has experienced an extensive growth during the past two decades. However, the use of f-elements, e.g. actinides as a nuclear fuel for energy needs, has resulted in an accumulation of contamination issues, including reprocessing and nuclear waste storage. This originate from the long-lived (>103 years) radioactive elements such as americium (Am) and curium (Cm) present in spent nuclear fuel. The main remediation issue is the removal of these minor actinides (Am, Cm) by their partitioning from lanthanide elements (fission products) using selective reagents. Among them, polyazine have emerged as highly selective ligands towards actinides over lanthanides ions. Considerable efforts have been thus devoted at both experimental and theoretical levels, to the design, synthesis and developing of these soft N-donor ligands in order to carry out the challenging Ln(III)/An(III) separation. Theoretical studies still essential to understandings the molecular basis of the observed separation and the different factors, electronic, steric or energetic which can account in favor of the actinide-polyazine selectivity.

In this context, a relativistic computational study using DFT/ZORA approach was carried out to modeling Ln(III)/An(III) differentiation, with a special emphasis on the coordination modes of polyazine complexes, and on the role of f electrons in metal-ligand bonding. Structural, electronic and energetic analysis, in agreement with experimental finding, reveal that the selectivity of soft N-donor ligands to An(III) over Ln(III) may originate from the slightly greater covalent character in An-L bonds with a significant 5f actinide orbitals contribution. DFT/ZORA approach was also found to properly describe the influence of the steric and orbital effects on the selective polyazine complexation on the Ln(III)/An(III) couple.

References

Keywords: Ln(III)/An(III) differentiation, polyazine, DFT/ZORA, 5f orbitals.
Interaction of Protonated 6-methoxyquinolone with Anionic Micelles: Effect of Hydrophobic Chain Length

Tej Varma Yenupuri, Debi D Pant
Department of Physics, BITS-Pilani, Rajasthan, INDIA

Photophysics and rotational relaxation dynamics of protonated 6-methoxyquinoline (6MQ+) have been investigated in anionic sodium n-alkyl sulfate (SNS) micelles using steady state and time-resolved fluorometric techniques. The study reveals modification of its photophysics by the conjugate effect of polarity of the micellar environments with varying alkyl chain lengths of the surfactants. Furthermore, it suggests that the fluorophore resides at the micelle–water interfacial domain. The enhancements in the rotational relaxation time in the micellar media compared to that in pure aqueous solution reflect that the fluorophore resides in a motionally restricted environment introduced by the anionic micelles. The rotational correlation time increases marginally with an increase in the surfactant chain length. The alkyl-chain-length dependence of the solvation dynamics in sodium alkyl sulfate micelles can be attributed to the variation of the micellar surface density of the polar head-group by the change of the alkyl chain length.

Keywords: 6-methoxyquinoline, anionic micelles, chain length, fluorescence, lifetimes

Molecular structure of protonated 6-methoxyquinoline (6MQ+)

Stoke’s shift vs solvent refractive index
Calculation of the EPR and Ground State Wavefunction for VO$^{2+}$ ion in KH$_2$PO$_4$ and KH$_3$C$_4$O$_8$·2H$_2$O Powders by Theoretical Methods

Emel Kalfaoglu

Ministry of National Education, Samsun, Turkey

In this study, the optical spectra and electron paramagnetic resonance parameters of VO$^{2+}$ ion in potassium dihydrous phosphate (KH$_2$PO$_4$) and potassium tetraoxalate (KH$_3$C$_4$O$_8$·2H$_2$O) powders are calculated by using point charge model (PCM). The theoretical spin-Hamiltonian parameters obtained for 3d$^1$ ion in tetragonally distorted octahedra are supported by experimental results. By using these parameters are determined the coefficients of the ground state wavefunctions. These values indicate that the ground is of dxy type with admixtures of dx$^2$-y$^2$ and dyz,xz. The results are discussed.

Keywords: EPR, Crystal-field theory, Ground state wavefunctions, VO$^{2+}$ ion
Use of Fluorescence, Synchronous Fluorescence and Circular Dichroism Spectroscopic Techniques in Protein-Herbicide Interactions: Binding of Dichlorprop and Diquat Dibromide to Human Serum Albumin

Sibel Tunç, Osman Duman, İnanç Soylu, Bahar Kancı Bozoğlan

Department of Chemistry, Akdeniz University, Antalya, Turkey

Herbicides are used for weeds controlling. They maintain until harvest stage and thus contaminate agricultural products. In addition, herbicides can easily reach to surface and ground waters. This situation causes a risk for human health [1]. Dichlorprop (DCP) is a herbicide used in agriculture. It can leach from soil to groundwater due to its high solubility in water and low sorption characteristic [2]. Diquat dibromide (DQ) is commonly used a toxic herbicide for humans. Human serum albumin (HSA) is the most abundant protein in blood plasma, accounting for about 60% of the total protein amount. Therefore, the investigation of interaction mechanisms HSA protein with DCP and DQ herbicides has great importance to understand the possible dangers of these compounds to the human health [3,4].

In this study, interactions of HSA protein with DCP and DQ herbicides were investigated by fluorescence, synchronous fluorescence and circular dichroism (CD) spectroscopic techniques. The formation of HSA-DCP and HSA-DQ complexes were proved by fluorescence spectroscopy. Moreover, for each protein-herbicide system, binding constant (Ka), number of binding site (n), Stern-Volmer quenching constant (Ksv), quenching rate constant (kq) and thermodynamic parameters (ΔH, ΔS and ΔG) were determined at 288, 298, 310 and 318 K.

The results of fluorescence measurements showed that binding affinity of herbicides to HSA displayed a decline with temperature. Also, the HSA-DCP system exhibited smaller binding constants than that of HSA-DQ system at all temperatures. Interactions of herbicides with HSA took place through electrostatic interactions and occurred spontaneously with an exothermic process. The results of synchronous fluorescence and CD analyses explained that the binding of DQ to HSA caused a conformational change in the protein structure, Conversely HSA-DCP system.

References

Keywords: Fluorescence, Circular dichroism, Herbicide, Protein, Binding
O-15

A New Developing Spectroscopy Software and Constructing a Database

Sefa Saylan¹, Murat Gezer², Ozan Unsalan³

¹University of Istanbul, Faculty of Science, Astronomy and Space Sciences Dept., Vezneciler Fatih, Istanbul, Turkey
²University of Istanbul, Dept. of Informatics, Vezneciler Fatih, Istanbul, Turkey
³University of Istanbul, Faculty of Science, Physics Dept., Vezneciler Fatih, Istanbul, Turkey

A new software has been still developing in order to read various spectral formats used in different spectroscopic techniques (IR&Raman spectroscopy and UV-Visible spectroscopy etc.). The language used for developing the software is Python. The aim of this software is to convert the most common spectral output files to other common files i.e. “jdx, spc, sp, jws, gaml” and also convert between them. Another aim of this software is to begin constructing a spectroscopic database of various materials by category. By this way, a new national database will exist compared to other examples of databases which are already in the market.

This project is supported by Research Fund of Istanbul University, Project No: ÖNAP/45582

Keywords: A New Developing Spectroscopy Software And Constructing A Database
Recent improvements in the contemporary quantum chemistry computational tools and computer technology allowed for significant expansion of the molecular sizes attainable by the high-level ab initio calculations. However, precision of the modeling of vibrational spectra of even small flexible molecules in condensed phase remains not satisfactory. Utilization of implicit conductor-like solvent models (e.g., CPCM) provides superior results compared to the vacuum calculations, but the agreement with the experiment is still poor. The main reason for that is omission of effects of explicit solvent, its dynamics, hydrogen bonding as well as conformational dynamics of the solute molecule. We present here a multi-level computational approach, which accounts for these contributions and significantly enhances precision of spectra modeling in condensed phase.

The methodology is based on molecular dynamics (MD) simulations followed by accurate calculations of vibrational spectra for a number of MD snapshots at the density functional theory (DFT) level with their subsequent averaging (MD/DFT approach). As test systems, we used several models of DNA phosphate group (dimethylphosphate (DMP), ethylmethylphosphate (EMP) and ethylmethylthiophosphate (EMSP)), vibrational spectra of which are very sensitive to the environment and extremely difficult to model by the standard approach [1]. The obtained results show that explicit solvent (included at the same level of theory as the solute) and dynamical/conformational averaging of both the solute and the solvent are necessary for correct spectra modeling. Using the developed methodology we could not only correctly reproduce experimentally observed IR and Raman spectra but also rationalize widely used empirical IR marker bands for detecting the B—Z transition in DNA.

References

Acknowledgements
Support from the Grant Agency of the Czech Republic (grant 14-03564S) is gratefully acknowledged. Computational resources were partially provided by the Czech computational network MetaCentrum.

Keywords: vibrational spectroscopy, molecular dynamics, quantum chemistry, DNA, phosphate

MD/DFT modeling of vibrational spectra
Oral Abstracts

O-17

Raman Spectroscopy of Carbonates

Kaabar Wahiba

Department of Chemistry, Freres Mentouri University, Constantine, Algeria

Triple carbonates are specially prepared electronic materials used for efficient thermal electron emission of cathode structures. These carbonates are compounds of barium, strontium and calcium, occurring as homogenous crystallites with an isomorphs crystal structure. Raman spectroscopy is a very useful technique to characterise the carbonate precursor materials. In the present study, Raman microscopy and scanning electron microscopy are used as diagnostic tools for triple carbonate materials produced with different compositions. Raman spectra of the carbonate powder samples prepared are acquired with a Renishaw RM1000 series, using 514.5 nm excitation from an Ar⁺ laser. Spectral manipulation such as base line adjustment, smoothing and normalisation are performed using the software package GRAMS (Galactic Industries Corporation). Analysis of these materials demonstrates the effects of the precipitation parameters on the morphology and Raman signatures of the product, and the relative contributions of the component species are discussed. It has been shown that the Raman spectrum of a sample is exclusively controlled by its composition.

**Keywords:** Raman microscopy, Scanning electron microscopy, Carbonates

Raman spectra for single component carbonate powder samples
According to Ref [1], we study a simple structure of mapping the environment of an open quantum system onto infinite chain representations with nearest neighbour interactions where the system only couples to the first element in the chain. In this paper we explore various properties of exceptional orthogonal polynomials and then use exceptional jacobi polynomials that it can be applied to three types of the bath spectral density sub-Ohmic, Ohmic, and super-Ohmic in open quantum systems.

References:


Keywords: Exceptional Orthogonal Polynomials, spectral density, Open quantum systems.
Bioremoval of Crystal Violet Dye from Egyptian Textile Effluent

Samah Saleh Abdallah, Khaled Abdel Aal Selim, Nagui Aly Abdel Khalek, Samah Mohamed El Sayed

Central Metallurgical Research and Development Institute, CMRDI

World population growth and increasing needs to various industries have led to the accumulation of a wide variety of contaminants in the environment and natural resources. The use of synthetic dyes is increasing in many areas. More than 10,000 chemically different dyes are being manufactured. Synthetic dyes have been widely used in many industries such as textile, tannery, food, pharmaceutical, pulp and paper, paint, plastics, electroplating, and cosmetics industries. The contamination of receiving water bodies by heavy metals constitutes a major environmental concern as these contaminants are extremely toxic, recalcitrant, and exhibit a tendency to bioaccumulate. Although heavy metals can be removed from industrial wastewater by a range of physicochemical treatment technologies such as precipitation, ion exchange, adsorption, electrochemical processes, and membrane processes; however, regulatory standards are not always sufficient.

As an alternative, biological treatments are a relatively inexpensive way to remove dyes from wastewater. Bacteria has been tested for its ability to accumulate heavy metals and dyes. The use of biological methods such as bioaccumulation and biosorption is suitable for the removal of pollutants from wastewaters. These methods have the advantage over such as low operating cost, minimization of the concentration of pollutant and high efficiency in detoxifying very dilute effluents.

In this paper, two types of bacteria were tested in the removal of crystal violet dye from textile effluent. Complete physico-chemical characterization of the effluent as pH, Temp., color, TDS, TSS, COD and BOD have been measured. Bio-Log identification indicated that the two bacterial isolates are Staphylococcus gallinarum and Micrococcus luteus. Removal efficiency was 89.47 % and 88.4% respectively. Complete characterization of such type of bacteria, isolated from Egyptian kaolin ore surface, including gram stain, growth curve, Biolog microbial identification, Zeta potential measurements, FTIR measurements, Scanning Electron Microscope, SEM as well as protein and polysaccharide analysis have been studied.

Keywords: Biotechnology, bioprocessing, bacterial isolates, FTIR, TDS
In this study, the kinetics of the biogas production was studied by conducting a series of laboratory experiment using secondary sludge of purification station as inoculums and dairy wastewater as substrate. The biodegradability tests were carried out in a series of reactor of 500 mL of volume with four arrangements of the initial pH (pH=4; 5.5; 7; and 9.5) in mesophilic phase (T = 37 °C).

Biogas production kinetic in was studied by developing the equation modified Gompertz equation using a nonlinear regression.

The results of the biogas yields show that: For test pH=4 and pH=5 the pH does not have any effect on the productions cumulated out of biogas finale but the kinetics was higher for the pH=5.5 and For test pH=7 and pH=9.5 the pH indeed does not have any effect on the production cumulated out of biogas finale nor in its speed of its obtaining the end values are of the same order of magnitude.

**Keywords:** Anaerobic Digestion, Biogas, Dairy effluents, Production Rate.
Comparative Study of Liver and Spleen Tissues from Healthy Human and Patients with some Hematological Malignancies Using Magnetization Measurements and Mössbauer Spectroscopy

Irina V Alenkina¹, Michael I Oshtrakh¹, Israel Felner², Alexander V Vinogradov³, Tatyana S Konstantinova³, Vladimir A Semionkin¹

¹Institute of Physics and Technology, Ural Federal University, Ekaterinburg, 620002, Russian Federation
²Racah Institute of Physics, The Hebrew University, Jerusalem, Israel
³Ural State Medical University, Repin str., 3, Ekaterinburg, 620028, Russian Federation

Iron in the living systems is accumulated in iron storage protein ferritin in the form of nanosized ferrihydrite cores surrounded with protein shell. Liver and spleen tissues contain a large amount of iron storage proteins. However, the content of these proteins in liver and spleen as well as amount of iron in the core may vary in some diseases, for instant in case of the iron overload diseases. Moreover, the nanosized iron core structure in ferritins may also vary in case of some molecular diseases. The presence of iron in liver and spleen tissues enables to apply magnetization measurements and Mössbauer spectroscopy for studying any variations in the ferritin iron cores from healthy and patients’ tissues. We used magnetization measurements and Mössbauer spectroscopy with a high velocity resolution for comparative study of human liver and spleen tissues obtained from healthy persons and patients with some hematological malignancies. Spleen tissues were obtained from healthy person and from three patients with mantle cell lymphoma stage IVB, acute myeloid leukemia subtype M4 and primary myelofibrosis. Liver tissues were obtained from healthy person and from two patients with mantle cell lymphoma stage IVB and acute myeloid leukemia subtype M4. These samples were lyophilized and powdered. Magnetization measurements carried out using the SQUID magnetometer demonstrated the differences between studied samples. These differences may be a result of different content of iron compounds in the ferritin cores (for instance, admixture of small amount of magnetite in addition to ferrihydrite) as well as of different total iron content in the tissues. Mössbauer spectra of these samples were measured at room temperature using precision Mössbauer spectrometric system with a high velocity resolution. Mössbauer spectra were fitted using two approaches: i) with one quadrupole doublet within the homogeneous iron core model and ii) with two quadrupole doublets within the heterogeneous iron core model. In both approaches a comparison of Mössbauer parameters for healthy and patients’ tissues demonstrated variations in the iron content and possibly some differences in the iron core structure in ferritin.

Keywords: Liver and spleen tissues; Hematological malignancies; Magnetization measurements; Mössbauer spectroscopy; Ferritin iron core structure
Oral Abstracts

O-22

Variation of the Iron-bearing Mineral Content and the $^{57}\text{Fe}$ Hyperfine Parameters in Chelyabinsk LL5 Meteorite Fragments Revealed Using the High Velocity Resolution Mössbauer Spectroscopy

Alevtina A Maksimova¹, Michael I Oshtrakh¹, Zoltan Klencsár², Andrey V Chukin¹, Evgeniya V Petrova¹, Victor I Grokhovsky¹, Erno Kuzmann³, Zoltan Homonnay³, Vladimir A Semionkin¹

¹Institute of Physics and Technology, Ural Federal University, Ekaterinburg, 620002, Russian Federation
²Institute of Materials and Environmental Chemistry, Research Centre for Natural Sciences, Hungarian Academy of Sciences, Magyar tudósok körútja 2, Budapest, 1117, Hungary
³Institute of Chemistry, Eötvös Loránd University, 1117 Budapest, Pázmány sétány1/A., Hungary

Chelyabinsk meteorite fallen in 2013 was classified as ordinary chondrite LL5. The main iron-bearing phases in ordinary chondrites are olivine (Fe, Mg)$_2$SiO$_4$, pyroxene (Fe, Mg, Ca)SiO$_3$, troilite FeS, chromite FeCr$_2$O$_4$, Fe-Ni-Co grains, etc. Different fragments of Chelyabinsk LL5 meteorite with light, mixed light and dark, and black lithology as well as black and grey zones of blackened fragment were chosen for investigation. Comparison of these samples using optical and scanning electron microscopy, X-ray diffraction and Mössbauer spectroscopy with a high velocity resolution was carried out. Metallography and scanning electron microscopy demonstrated the presence of metallic iron grains, troilite and chromite inclusions in olivine and pyroxene matrix in all fragments studied. X-ray diffraction study, however, showed the same iron bearing minerals (olivine, pyroxene and troilite) in all fragments, but with slightly varying ratio. Differences in the unit cell parameters for pyroxene were also revealed. The room temperature $^{57}\text{Fe}$ Mössbauer spectra of various Chelyabinsk LL5 meteorite fragments demonstrated different number of spectral components and some variations in the $^{57}\text{Fe}$ hyperfine parameters and relative areas of spectral components. Revealed spectral components were related to two crystallographically non-equivalent positions M1 and M2 for Fe$^{2+}$ and Mg$^{2+}$ in both olivine and pyroxene, to α-, α₂- and γ-Fe(Ni, Co) phases, to troilite and to chromite. The differences in the hyperfine parameters for M1 and M2 sites in olivine and especially in pyroxene can be associated with small variations in the local microenvironment of $^{57}\text{Fe}$ ions in these silicate crystals. The magnitude of the hyperfine field for troilite appeared to be different for re-melted fragments that may be a result of Fe deficiency in Fe$_{1-x}$S microcrystals. The results obtained demonstrated some differences in iron-bearing phase content and microstructural peculiarities of minerals in Chelyabinsk LL5 meteorite fragments with different lithology. This fact may be related to the features of shock and thermal history of meteorite minerals/fragments that can be a result in meteorite breccia structure formation.

This work was supported in part by the Ministry of Education and Science of Russian Federation and the Russian Foundation for Basic Research (grant No 15-35-21164).

Keywords: Chelyabinsk LL5 meteorite; iron-bearing phases; local microenvironment; the $^{57}\text{Fe}$ hyperfine parameters; Mössbauer spectroscopy
Calculation of The Soft-Mode Frequency For The α-β Transition In Quartz

Hamit Yurtseven¹, Ozlem Tari²

¹Middle East Technical University
²Istanbul Arel University

The α-β structural transition occurs in quartz at TC=846K. The frequency of the soft mode associated with the volume increase, decreases with increasing temperature as the transition temperature is approached.

In this study, we calculate the soft-mode frequency as a function of temperature using the volume data by means of the mode Grüneisen parameter for the α-β transition in quartz.

Our calculated frequencies of the soft-mode agree with the observed data from the literature. This shows that the method of calculating the soft mode frequency from the crystal volume is adequate, which can explain the soft mode behavior associated with the α-β transition in quartz.

Keywords: Soft Mode. alpha-beta transition. Quartz
The Effect of Ni$^{2+}$ in the Fe$^{3+}$ Local Microenvironment in Both Tetrahedral and Octahedral Sites on the $^{57}$Fe Hyperfine Field in NiFe$_2$O$_4$ Nanoparticles

Mikhail V Ushakov$^1$, Baskar Senthilkumar$^2$, R. Kalai Selvan$^2$, Michael I Oshtrakh$^1$

1Institute of Physics and Technology, Ural Federal University, Ekaterinburg, 620002, Russian Federation
2Solid State Ionics and Energy Devices Laboratory, Department of Physics, Bharathiar University, Coimbatore – 641 046, India

Nickel ferrite NiFe$_2$O$_4$ is inverse spinel with 8 tetrahedral (A) and 16 octahedral (B) sites for metal cations. Fe$^{3+}$ ions occupy 8 tetrahedral sites and 8 octahedral sites while Ni$^{2+}$ ions occupy 8 octahedral sites only in the stoichiometric nickel ferrite. Two samples of nickel ferrite nanoparticles were synthesized by solution combustion synthesis technique using EDTA (C$_{10}$H$_{16}$N$_2$O$_8$) and urea (CH$_4$N$_2$O) as fuels and denoted as NA and NB, respectively. The obtained nanoparticles were characterized using X-ray diffraction, scanning electron microscopy with energy dispersive spectroscopy and transmission electron microscopy. The average size of NA nanoparticles was ~20 nm while that of NB nanoparticles was ~30 nm. Mössbauer spectra of these samples were measured at room temperature using high precision and sensitive Mössbauer spectrometric system with a high velocity resolution. In contrast to all previously measured Mössbauer spectra of nickel ferrite samples using conventional spectrometers (with a low velocity resolution) which were fitted using two magnetic sextets related to the $^{57}$Fe in the A and B sites, the high velocity resolution Mössbauer spectra of NiFe$_2$O$_4$ nanoparticles were better fitted using ten magnetic sextets, five of them were related to the $^{57}$Fe in the A sites and five sextets were related to the $^{57}$Fe in the B sites. Evaluation of probabilities of the different numbers of Ni$^{2+}$ ions in the local microenvironment of Fe$^{3+}$ in both A and B sites demonstrated that there is a distribution of various numbers of Ni$^{2+}$ cations for both sites (the meaningful variation was from 2 to 6 in the local microenvironment of Fe$^{3+}$ in the A sites and from 1 to 5 in the local microenvironment of Fe$^{3+}$ in the B sites). These results were compared with the results of Mössbauer spectra fits and spectral components were related to the number of Ni$^{2+}$ cations in the local microenvironment of Fe$^{3+}$ in both sites. It was shown that adding of Ni$^{2+}$ ion in the local microenvironment of Fe$^{3+}$ lead to decrease in the $^{57}$Fe hyperfine field.

Keywords: Nickel ferrite nanoparticles; Ni$^{2+}$ distribution; Fe$^{3+}$ local microenvironment; the $^{57}$Fe hyperfine field; Mössbauer spectroscopy
Structural Investigations of Some Sb$_2$O$_3$- Na$_2$O- ZnO Glasses by Mean of FTIR, Raman and Er$^{3+}$ probe

Toufik Mohamed Soltani$^1$, Majda Hamzaoui$^1$, Ronan Lebullenger$^2$, Alain Moreac$^2$, Marcel Poulain$^2$

$^1$Laboratoire de Physique photonique et nanomatériaux multifonctionnels, Université de Biskra, Algérie
$^2$UMR CNRS 6226 - Institut des Sciences Chimiques de Rennes, Equipe Verres et Céramiques, Rennes, France

Sb$_2$O$_3$ glasses emerges as one major family of Heavy metal oxide glasses and appear promising for potential applications in non linear devices like ultra-fast optical switches and power limiters, broad band optical amplifiers operating around 1.5 µm using antimony–silicate glass fiber. In this paper we investigate new glasses in ternary systems: (90-x-y)Sb$_2$O$_3$-yNa$_2$O-xZnO-0.25Er$_2$O$_3$ in witch antimony oxide is the mean glass former and to investigate their structural properties by using Raman, FTIR and the spectroscopic properties of erbium ions used as structural probe in these glasses. The influence of the glass composition on the structural organization of these glasses is discussed in the light of the role of Na$_2$O and ZnO in these no-conventional glasses.

Keywords: antimony oxide glasses, Raman, FTIR, Er$^{3+}$
Pressure Dependence of The Raman Frequency of An Optical Mode In Cubic Gauche Nitrogen

Hamit Yurtseven, Ozgecan Tiryaki
Middle East Technical University

Solid nitrogen exhibits various phases under different temperatures and pressures. At very high pressures up to about 100 GPa, the most stable structure in nitrogen is the cubic gauche structure and the polymeric crystalline phase is obtained from this structure.

In this study, we calculate the Raman frequency of an optical mode (600 cm⁻¹ at P=0) as a function of pressure for cubic gauche nitrogen using some thermodynamic data from the literature. The calculated Raman frequency of this optical mode increases with the pressure in the cubic gauche nitrogen as expected, which can be compared with the observed data when it is available in the literature. This can explain the thermodynamic properties of the cubic gauche nitrogen at high pressures.

Keywords: Raman frequency, Optical mode, Cubic Gauche Nitrogen
Phonon Spectral Density of the FMO Light-harvesting Complex with Associated and Generalized Jacobi Polynomials

Mahmoud Mahdian

Faculty of Physics, Theoretical and astrophysics department, University of Tabriz, 51665-163 Tabriz, Iran

Energy transfer systems like Fenna-Matthews-Olson (FMO) complex shows quantum coherence between sites of Bacteriophylla molecules in protein environment. In this paper we consider phonon spectral density (PSD) of protein environment in FMO complex and provide a assessment of PSD using associated jacobi polynomials.

References:

Keywords: Jacobi polynomials, protein environment, Energy transfer systems.
Spectroscopic Study of Zinc(II) Tributylphosphine Chalcogenides Complexes

Salima Boughdiri¹, Zied Gouid¹, Ridha Ben Said¹, Mohamed Abderrahmane Khouna Sanhoury²

¹Unité de Recherche: Physico-Chimie des Matériaux à l’état Condensé, Faculty of Sciences of Tunis, University Tunis El Manar, Tunis, Tunisia.
²Laboratory of Structural Organic Chemistry: Synthesis and Physico-chemical Study Department of Chemistry, Faculty of Sciences of Tunis, Campus Universitaire Tunis El Manar Tunis, Tunisia.

Nowadays, certain metal complexes of phosphine chalcogenides have shown to be suitable single-source precursors for the production of thin semiconducting films of metal chalcogenides, for example ME (M = Cd, Zn or Hg; E = O, S or Se) [1,2]. In this work, zinc(II) complexes of the type ZnL₄(ClO₄)₂ and ZnL₂Cl₂ (L =Bu₃P(E) with E=O, S or Se)) have been synthesized and characterized by multinuclear (1H, 13C and 31P) NMR, conductivity and IR techniques. The complex formation was confirmed by a coordination chemical shift of the 31P NMR signals towards lower field compared to those of the free ligands. The results show that the ligand is coordinated to the zinc center through the chalcogenide atom of the group P=E. In addition, a DFT/B3LYP, with def2-svp basis set, theoretical study through geometry optimization, Infra Red frequencies and NMR chemical shift calculations were carried out to more understand the ligand-metal coordination type. A good agreement has been shown between the experimental and theoretical results.

Keywords: Phosphine chalcogenide, zinc complexes, NMR, IR, DFT/B3LYP

NMR spectrums of the complex in CDCl₃ of [ZnCl₂(Bu₃PSe)₂] and the free ligand, IR spectrum of the complex [ZnCl₂(Bu₃PSe)₂] in CDCl₃
Electronic Properties of the Transition Metal (1-phenylazo-2-naphthol) complexes: A TD-DFT Electronic Spectra Study

Bachir Zouchoune¹, Lakhdar Mansouri²

¹Laboratoire de Chimie appliquée et Technologie des Matériaux, Université Larbi Ben M’Hidi-Oum el Bouaghi, (04000) Oum el Bouaghi, Algeria
²Unité de Recherche de Chimie de l’Environnement et Moléculaire Structurale, Université- Constantine, (25000) Constantine, Algeria

The 1-phenylazo-2-naphtol (PhN) as azo dye molecule has been the subject of wide experimental and theoretical investigations [1]. The phenylazo-naphtolate derivative group can provide the N,O-bidentate chelation to stabilize the transition metal complexes [2]. In the current study, we are interested in the electronic structure, the bonding analysis and UV-Vis spectra by means of DFT and TD-DFT methods [3]. The full geometry optimizations show that an ML₄ geometry is adopted for the studied complexes, in which the M(II) cation is surrounded by two N and two O atoms of (PhN) ligands. The geometry around the metal cation is tetra-coordinated with a slight distorted square planar environment and the two nitrogen atoms and the two oxygen atoms are almost coplanar around the metal center.

The electronic spectra of the various compounds investigated in this study were calculated by the TD-DFT method using B3LYP functional [3]. Moreover, the including of solvation model into the calculations generally improved the results when compared with the experimental values [4].

Our theoretical calculations allowed us to clearly identify the spectral shape and position of such transitions affected by the metallic complexation. For this aim, a thoroughly study has been provided in order to give a deeper insight concerning different type of electronic transitions, where a red shift is highlighted for PhN-M(II) complexes.

References

Keywords: TD-DFT, Electronic spectra, Azo dye metal complexation, geometry optimizations
How Does Hyperforin (HYP) Interact with DPPC Membranes?: EPR Spin Labeling and DSC Study

Dilek Yonar¹, Maral M. Sünnetçioğlu²

¹Department of Biological Sciences, Middle East Technical University, Ankara, Turkey
²Department of Physics Engineering, Hacettepe University, Beytepe, Ankara, Turkey

Hyperforin, major antidepressant component in the extract of St. John’s Wort, has known to indirectly inhibit neuronal uptake of serotonin, norepinephrine, dopamine. Since the molecular mechanism of action of hyperforin is not clear yet, the main objective of the present study is to provide a detailed evaluation of the interactions between hyperforin (HYP) and phospholipid membranes at the molecular level. Moreover, it has been known that membrane lipids participate in cellular signaling. Drug–phospholipid interaction will be effective on the pharmaceutical efficacy of the drug. Therefore, hyperforin-dipalmitoyl phosphatidylcholine (DPPC) membrane interactions in presence and absence of cholesterol (CHO) were investigated by Electron Paramagnetic Resonance (EPR) spin labeling and differential scanning calorimetry (DSC) techniques.

EPR spin labeling spectroscopy provides site specific information on ordering, mobility and polarity of membranes. Moreover, more precise description of the membrane characteristics is obtained by computer simulation of EPR spectra. In the EPR spin labeling studies, 5- and 16- doxyl stearic acid (5- and 16-DS) spin labels were used to monitor the head group and alkyl chain region of phospholipids respectively. DSC technique has been widely used to obtain the phase behaviour of hydrated phospholipid membranes and the thermal changes caused by drug incorporation into bilayers. EPR, its computer simulation, and DSC results indicated a shift in the main phase transition of DPPC towards lower temperature side in the presence of HYP. DSC results also demonstrated the pre-transition disappearance, broadened phase transition profile, and two heat flow peaks at higher concentration 10 mol % of HYP, suggesting the occurrence of a new HYP rich phase. According to EPR and simulation results, HYP is an effective drug in the alkyl chain region of DPPC membranes. In this region, the addition of HYP increased the dynamic of the nitroxide especially in the gel phase for pure DPPC and at almost any temperature for CHO incorporated DPPC.

As the changes in the central part of the membrane were more pronounced than in the upper part of the membrane and HYP has lipophilic character, it could be concluded that HYP incorporates into DPPC membranes parallel to the phospholipid chains.

Keywords: phospholipid membrane, hyperforin, EPR spin labeling, DSC
POSTER ABSTRACTS
P-001

TD-DFT Calculations of Visible Spectra and Structural Studies of Ibuprofen Inclusion Complex With β-Cyclodextrin

Madi Fatiha

Laboratory of computational chemistry and nanostructures

The binding of the ibuprofen with β-Cyclodextrin (β-CD) was investigated theoretically using HF/6-31G and B3LYP/6-31G methods. Two modes of complexation were considered for studying such complex. Energetic analysis indicates that the formed complexes are stable and both host and guest were little deformed after complexation. Electronic properties given by TD-DFT calculation clearly demonstrate that a charge transfer was occurred between ibuprofen and β-CD molecules.

Keywords: B3LYP/6-31G, HF/6-31G, TD-DFT, ibuprofen and β-CD
The Redox Behavior of Uranium Complexes. A Relativistic DFT/ZORA Study

Belkhir Lotfi¹, Khireche Moncef¹, Zaiter Abdellah¹, Ephritikhine Michel², Boucekkine Abdou³

¹Department of Chemistry, Mentouri University of Constantine, Algeria
²IRAMIS, UMR 3299 CEA/CNRS SIS2M, CEA/Saclay, France
³Laboratoire Sciences Chimiques de Rennes, UMR-CNRS 6226, Université de Rennes 1, France

Electron affinities (EAs) of a series of metallocene uranium(IV) complexes Cp*₂ULL'₂ (LL' sigma or pi donor; Cp* = C₅Me₅) [1] related to the U(III)/U(IV) and U(V)/U(IV) redox systems were calculated using relativistic Density Functional Theory (DFT) based methods coupled with COSMO-RS (Conductor-like Screening Model - Real Solvents) approach and spin-orbit coupling [2-4].

Experimental measurements of half-wave potentials E₁/₂ (V) in solution (THF) were carried out for all these compounds under the same rigorous conditions. A good correlation (R²= 0.98) is obtained between the calculated EA values, at the ZORA/BP86 level and the redox potentials. Our study brings to light the importance of spin-orbit coupling and solvent effect in order to achieve such a good agreement between theory and experiment.

The electron sigma or pi donating ability of the co-ligand LL', on EA was studied. The role of the involved SOMO (Singled Occupied Molecular Orbital) in anionic species or the LUMO (Lowest Unoccupied Molecular Orbital) in neutral species) in the redox process was discussed.

References:

Keywords: Uranium complexes, DFT/ZORA, Redox properties, Electron affinities, COSMO, Spin-orbit.
Electronic Affinity - Redox potential correlation

The figure shows the good correlation between the computed electronic affinity $EA(eV)$ and the measured redox potential $E1/2(V)$. 
A conventional residual gas analyzer (RGA) has been utilized for the measurement of gaseous subs-
tances of molecular weight $\gg 1,000$ g/mol. The novel method, termed CPC (“crack-product calibrati-
on”), is based on the evaluation of just one or few selected crack products within the range of the RGA. Thus, the method can be applied even if the molecular weight of the substance is far beyond the range of the instrument. Calibration of the RGA is achieved by guiding a quartz-microbalance-controlled molecular beam of the substance under consideration through the RGAs ion source and, at the same time, admitting a noble gas with density defined by a Bayard-Alpert gauge (BAG) – thus anchoring the calibration of the RGA to the readings of the more stable total pressure gauge. In this way, the RGA’s sensitivity can to a large extent be characterized and corrected for. By means of a twin-gas standard, even effects due to drift of the RGA’s field axis potential can be zeroed out. The CPC method is characterized by an accuracy that is essentially limited just by the reproducibility of the BAG readings. The basics of the method and the apparatus are described with special attention to the measurement of Baysilone M 100,000 (a silicone oil with a mean molecular weight of 103,000 00 to 139,000 g/mol), and to the discussion of accuracy concerns.

**Keywords:** Residual gas analysis, vapor, crack-product, calibration
P-004

Theoretical and Experimental Vibrational Spectroscopic Studies of Sulphur Containing Diketopiperazines

Ahsan Ali Khan¹, Babur Zahurridin Chowdhry¹, Andrew Paul Mendham¹, Trevor John Dines², Perry Devo¹

¹Faculty of Engineering and Science, University of Greenwich, Chatham Maritime, Kent, ME4 4TB, UK
²Division of Electronic Engineering and Physics, University of Dundee, Ewing Building, Ground Floor, Nethergate, Dundee DD1 4HN, UK

Research into naturally occurring and synthetic diketopiperazine (DKP) derivatives is an exciting area of significant contemporary scientific interest due, in part, to their potential pharmacological applications. For example, a range of epidithiodiketopiperazines have been investigated for both antimicrobial and anticancer activities.[1]

In this study both cyclo (L-homocysteine-L-homocysteine) and its polymer cyclo(L-homocystine-L-homocystine) (Figure 1) have been synthesised using literature methods[2] and characterised using experimental techniques (Raman and infra-red spectroscopies) in order to understand structural and conformational relationships with theoretically calculated data. Theoretical gas phase structures have been calculated using DFT calculations (Gaussian09, molecular modeling package), utilizing the B3-LYP/ AUG-ccpVTZ basis set. The minimum energy gas phase structure predicts that the cyclo(L-homocysteine-L-homocystine) molecule displays C₂ symmetry and the diketopiperazine ring deviates from planarity towards a boat conformation.

The solid state Raman spectra of cyclo(L-homocysteine-L-homocystine) and its polymer are shown in Figure 2. The band at 2560 cm⁻¹ (a) corresponds to the thiol (S-H) stretching vibration. The cis amide I vibrational mode appears at 1663 cm⁻¹ (b). This band is in good agreement with cis amide I modes observed in other diketopiperazines.[3,4] The cis amide II mode located at 1506 cm⁻¹ (c) occurs at a significantly higher wavenumber than that of other diketopiperazines where the ring is essentially adopting a boat conformation.[5] The polymeric cyclo(L-homocystine-L-homocystine) does not show a S-H signal in the Raman spectrum due to the formation of a disulphide bond. The strong band at 509 cm⁻¹ (d) showcases the S-S stretching vibration in the polymer.

Keywords: Raman, infrared, diketopiperazine, Gaussian09, cis amide

References
2. V. du Vigneaud, W. I. Patterson, and M. Hunt., J. Biol. Chem, 126, 217,1938
The structure of (a) cyclo(L-homocysteine-L-homocysteine) \((R=CH2CH2SH)\) and (b) its polymer cyclo(L-homocystine-L-homocystine).

The solid state Raman spectra of polymeric cyclo(L-homocystine-L-homocystine) (top) and cyclo(L-homocysteine-L-homocysteine) (bottom).
Impact of Iron-complex (Fe(III)-Malonate) on Photoinduced Degradation of Ibuprofen in Aqueous Solution

Debbache Nadra, Dekiche Besma, Ghoul Imene, Ars Khadidja, Adala Amina

Laboratoire Des Sciences Et Technologies De L'environnement, Département De Chimie, Faculté Des Sciences Exactes, Université Frères Mentouri, Constantine, Algérie.

Pharmaceuticals are considered as an emerging environmental problem even at low concentrations. Advanced oxidation processes are technologies based on the intermediacy of hydroxyl and other radicals to oxidize recalcitrant, toxic and non-biodegradable compounds.

The aim of the present work is to investigate the photodegradation of Ibuprofen (IBP), an active substance of many drugs, with an organic complex (Fe (III) malonate) in aqueous solution.

The Fe(III)-malonate was synthesized in the laboratory and was characterized by UV-Visible spectrophotometry and characteristic parameters have been deduced (stoichiometry and stability constant)

The evolution of mixture Fe (III) malonate - IBP is followed by UV-Visible spectroscopy; the concentration of IBP was also measured by HPLC analysis.

UV-Visible spectral changes of IB in the mixture prove weak interaction in the absence of light and at room temperature.

Upon irradiation at 365 nm of the mixture of IBP-Fe (III)-Mal in aqueous solution, ibuprofen disappears from the solution in acidic medium were pH is optimized at 2.8.

The influence of some parameters such as substrate concentration and that of the complex on the kinetics of the reaction was also studied.

The involvement of OH. was not implied in the mechanism; this fact is confirmed by isopropanol used as hydroxyl radical’s scavenger.

Keywords: Fe(III)-malonate complex, Ibuprofen, photo degradation, UV-Visible Spectroscopy.
Total Cross Sections for the Double Ionization of Water Molecule

Dahbia Oubaziz\(^1\), Christophe Champion\(^2\), Michele Arcongelo Quinto\(^2\), Zakia Aitelhadjali\(^3\)

\(^1\)Laboratoire de Mécanique, Structures et Energétique, Université Mouloud Mammeri de Tizi-Ouzou, BP 17, Tizi-Ouzou 15000, Algérie
\(^2\)Centre d'Études Nucléaires de Bordeaux Gradignan, Université de Bordeaux, CNRS/IN2P3, BP 120, 33175, Gradignan, France.
\(^3\)Laboratoire de Sciences Nucléaires et Interaction rayonnement- Matière, Faculté de Physique, USTHB, Alger 16000, Algérie

Double ionization of water molecules remains, still today, rarely investigated on both the experimental and the theoretical side. In this context, the present work reports on a quantum mechanical approach providing a quantitative description of the electron-induced double ionization process on isolated water molecules for impact energies ranging from the target ionization threshold up to about 10 keV. The cross section calculations are here performed within the first Born approximation framework in which the initial state of the system includes a molecular ground-state wave function expressed as a single-center linear combination of atomic orbitals while the final state of the system is characterized by two independent Coulomb wave functions used for describing the two ejected electrons coupled by a Gamov factor used for modeling the electron-electron repulsion. In comparison with the rare available experiments, the double vs single ionization cross section ratio shows an overall good agreement. Besides, in absence of measurement of absolute total cross sections in water vapor, the current theoretical predictions are compared with isoelectronic neon data. A very good agreement is observed over the whole incident energy range investigated. Finally, we report an average energy transfer of the double ionization process and clearly demonstrate the absolute necessity of considering the double ionization process in particular in a radiobiological context.

**Keywords:** Double ionization, Cross section, energy transfer
Computational Investigation of Trans-Pt(II) Oxime Complexes

Koray Sayin, Duran Karakaş

Department of Chemistry, Faculty of Science, Cumhuriyet University, Sivas, Turkey

Trans-platinum(II) oxime complexes, which are represented in Scheme 1, have been synthesized by Keppler et al. in 2012 [1]. As experimentally, some structural parameters and stretching frequencies of selected complexes have been reported in their paper [1]. In this study, eleven methods and six different basis sets are used in calculations. Firstly, best level for studied complexes is investigated and founded as HF/CEP31G level in vacuum [2, 3]. After that IR and UV-VIS spectrum are examined in detail. Platinum complexes are known as anticancer drug and there are a lot of study about this topic. Experimental IC50 values of complex (1-9) have been reported toward CH1, SW480 and A549 cells [1] but there is not any information about complex (10). In this study, a new formula are derivated for each cancer cell by using some quantum chemical descriptors. Computational IC50 ranking are calculated as follow:

(7) > (5) > (8) > (6) > (9) > (2) > (4) > (10) > (3) > (1) [for CH1 cell]
(7) > (5) > (10) > (8) > (6) > (9) > (4) > (2) > (1) > (3) [for SW480 cell]
(10) > (7) > (8) > (9) > (5) > (6) > (2) > (4) > (1) > (3) [for A549 cell]

Keywords: Pt(II) oxime complexes, anticancer drug, computational investigations

Scheme 1. Shematic representation of investigated trans-Pt(II) oxime complexes.
**P-008**

**Spectroscopic Characterization of Carburized Surface of Fe$_{20}$MnCr$_5$ Steel**

*Fatima Zohra Benlahreche$^1$, El Amine Nouicer$^2$, Lazhar Yahia$^3$*

$^1$Pharmaceutical Processes Engineering Faculty, Constantine3 University, Constantine 25000, Algeria  
$^2$Physics Department, Exact Sciences Faculty, Constantine1 University, Constantine 25000, Algeria  
$^3$Department of Technical Sciences, Batna university, Batna, Algeria

The objective of this work is the study the effect of carburizing treatment on physicochemical properties of Fe$_{20}$MnCr$_5$ steel using spectroscopic techniques. The micrographs show that the carburizing specimens followed by tempering and quenching treatment causes significant structural changes in treated steels, it provides a very carburized surface layer through diffusion of carbon cement to the inner part. The heart of the piece, not change and the structure consisting of ferrite and perlite raman spectroscopy and X-ray diffraction shows that's the formed cementation layer consists essentially Of carburized complex layer, iron carbides and martensite. Microhardness testing shows that the surface hardness reaches the value of 3 times of the heart, so this treatment led to a surface hardening.

**Keywords:** Surface treatment, Fe$_{20}$MnCr$_5$, Raman, XRD, hardness
Corrosion Behaviour of Titanium Alloy in Alkaline Solution Using Spectroscopic Techniques

El Amine Nouicer¹, Fatima Zohra Benlahreche², Lazhar Yahia³

¹Physics Department, Exact Sciences Faculty, Constantine1 University, Constantine 25000, Algeria
²Pharmaceutical Processes Engineering Faculty, Constantine3 University, Constantine 25000, Algeria
³Department of Technical Sciences, Batna University, Batna 05, Algeria

The present work study the effect of polarization on the growth of the oxide film on the Ti₆Al₄V alloy surface in alkaline solution. Polarization curves, plotted at different scan rates show a large range of passivation. This observation confirms the formation of TiO₂ passive film on the surface of this alloy. Raman spectroscopy shows that titanium dioxide formed consists of Rutile phase. Electrochemical impedance spectroscopy results show that the system behaviour is purely capacitive. The increasing trend in Rt, θmax and the exponent n with the imposed potential is due to the growth of a passive and compact oxide film.

Keywords: Ti6Al4, Electrochemical impedance spectroscopy, Raman, TiO₂
P-010

A New Preconcentration Procedure to Quantify Total Acid Hydrolyzed Fluoride in Selected Beverages and Foods by Spectrophotometry

Nail Altunay, Ramazan Gürkan, Ulaş Orhan, Emre Yıldırım, Sema Korkmaz

Department of Chemistry, Cumhuriyet University, Sivas, Turkey

A new micellar mediated cloud point extraction (CPE) method has been developed for the quantification of trace levels of fluoride by means of spectrophotometry. The method is based on the selective ion-association of stable anionic complexes, Sn(OH)F\(_2^-\) or Sn(OH)F\(_3^-\) of fluoride with Sn(II) in presence of cationic dye (Nile blue A) at pH 5.0, and its extraction to micellar rich phase of nonionic surfactant polyoxyethylene (7.5) nonylphenyl ether (PONPE 7.5) as extracting agent. Afterwards, the ternary complex formed was spectrophotometrically detected at 638 nm after preconcentration with CPE. Under optimized conditions, the calibration curves were rectilinear in the ranges of 5-25 and 25-360 µg L\(^{-1}\) in linear region with changing sensitivity. The limits of detection and quantification (LOD and LOQ) (3σblank/m and 10σblank/m) was 1.45 and 4.83 µg L\(^{-1}\) respectively, and the precision (as RSD) for determination of 15, 75 and 150 µg L\(^{-1}\) of fluoride was in range of 2.35-4.65 %. The validity of the method has been checked through the recovery experiments, independent analysis by potentiometry and analysis of the standard reference material, SRM 2695. The developed method was successfully applied to the accurate, sensitive and reliable quantification of total acid hydrolyzed fluoride present in selected beverage and food samples.

Keywords: Fluoride, Nile Blue A, Cloud Point Extraction, Beverage/Food Samples, Spectrophotometry
Optimization studies

Figures comprise optimization parameters.

*Figure 1* Effect of range on CPE efficiency. Optimal conditions: 25 μg L⁻¹ F⁻, 1.2×10⁻³ mol L⁻¹ citrate buffer at pH 5.0, 2.4×10⁻³ mol L⁻¹ NaBH₄, 1.2 mg L⁻¹ Sn(II), 1.6×10⁻⁷ mol L⁻¹ KNO₃, and 0.08 % (v/v) PONPE 7.5, with thermostatic water bath at 40 °C for 15 min and centrifugation time of 5 min at 4000 rpm.
Double Ionization of the Hydrogen Sulfide Molecule by Electron Impact: Influence of the Target Orientation on the Fivefold Differential Cross Sections

Noura Imadouchene¹, Hocine Aouchiche¹, Christophe Champion²

¹Laboratoire de Mécanique Structure et Énergétique, Université Mouloud Mammeri, B.P.17, Tizi Ouzou 15000, Algérie
²Centre d’Études Nucléaires de Bordeaux Gradignan (CENBG), BP120, 33175 Gradignan, Université Bordeaux 1, CNRS/IN2P3, France

A fivefold differential cross section (5 DCS) for electron-impact double ionization of hydrogen sulfide molecule is calculated for high incident energy (1 keV) and for three particular target orientations. The theoretical procedure is based on the first Born approximation (FBA) model using a partial wave functions development. In this approach, the incident and the scattered electrons are described by a plane waves and the two ejected electrons are described by a Coulomb wave functions taking into account the repulsion between them by the Gamow factor. Furthermore, we identify clearly the signature of the usual mechanisms involved in the (e, 3e) reaction, namely, the shake-off and the two-step 1.

Keywords: Double ionization, hydrogen sulfide molecule, electron impact cross section
Modeling of Photocataytic Removal of Cresol Red Using Box-Behnken Experimental Design

Razika Zouaghi, Roumayssa Zerti, Narimène Hadj Brahim

Department of Chemistry, University of Constantine 1, Constantine, Algeria

Organic dyes constitute one of the larger groups of pollutants in wastewater released from textile and other industries. The treatment of textile effluents is of interest due to their toxic and esthetic impacts on receiving waters. In recent years, heterogeneous photocatalytic reactions are recognized as a new emerging "advanced oxidation process" (AOP) for the treatment of recalcitrant chemicals present in the wastewater. The rate of photocatalytic degradation of a pollutant is dependent on a number of parameters like photocatalyst loading and its properties, pH of the solution, type and photon flux of the source.

Photocatalytic degradation of Cresol Red was carried out in an aqueous suspension of TiO₂ irradiated by ultraviolet light at 365 nm. Box-Behnken experimental design based on response surface methodology was applied to estimate the individual and interaction factors including pH, TiO₂ loading and initial CR concentration. This novel approach has allowed to modeling the percentage removal of CR by photocatalysis in term of these parameters according to a second-order polynomial equation. The Box-Behnken design for three variables needs 12 experiments arranged in the middle of a cub edges and three central points were added in order to evaluate the experimental error. The percentage of CR removal at 30 minutes of contact time by photocatalysis (Y) was chosen as the response factor. A polynomial expressions was obtained from the data analysis. This model represents well the experiment results where the correlation coefficient was: $R^2 = 0.97$. From the polynomial model, it can be readily seen that the main effect of the three parameters studied is in the following order: pH > [MeO] > [TiO₂] on the dye removal efficiency. However the pH and CR concentration have a negative effect which explains that photocatalysis efficiency is obtained at a very acidic pH medium. Analysis of correlation coefficients between the different parameters studied shows that there is a correlation between TiO₂ concentration and pH only. This correlation is directly related to the surface charge of the photocatalyst which depend on the pH medium.

Keywords: Photocatalysis, Cresol Red, Experimental design, modeling
Photochemical Degradation of the Phenol Red Induced by Goethite in the Aqueous Solution

Debbache Nadra, Belattar Sara, Ghoul Imene, Seraghni Nassira

Laboratory of Science and Technology of Environment, Department of Chemistry, Faculty of Science, University Mentouri Constantine, 25000 Constantine, Algeria.

The Phototransformation of phenol red was studied under irradiation at 365 nm and under sunlight in the presence of Goethite (Fe (III) oxyhydroxyde) in aqueous solution. The thermal study of the mixture Goethite-dye (in dark and at ambient temperature) followed by UV-Visible spectrophotometry does not show a reaction between the dye and Goethite. The evolution of the UV-Visible spectrum of the mixture of phenol red and the Goethite (1g.L⁻¹, 10⁻⁴ M) under irradiation at 365 nm is characterized by a minimal decrease in the principal band of the phenol red. Under solar light an improvement in the performance of discoloration is observed.

The introduction of an activator in the Goethite-phenol red system improves the efficiency of the degradation, where the additions of the hydrogen peroxide (H₂O₂) (5.10⁻³ mol L⁻¹) in the Goethite suspension accelerate the degradation rate of the solution. This fact is due to the •OH radicals contribution generated by the Fenton and Photo-Fenton reactions. The influence of H₂O₂ concentration generates a significant increase in the degradation rate until a limit concentration of H₂O₂ (5.10⁻³ mol.L⁻¹). Moreover, the evolution of the optical density of the mixture (Goethite dye) at different pH values shows that the acidity improves the photochemical reaction.

Keywords: Phenol red, Goethite, photochemistry, UV-Visible spectrophotometry, hydrogen peroxide (H₂O₂).
Crystal Structure, Spectroscopic (FT-IR and UV-Vis) and DFT Studies on (E)-N-[4-bromo-2-(trifluromethoxy)phenyl]-1-(5-nitrothiophen-2-yl)methanimine

Hasan Tanak¹, Figen Koçak¹, Erbil Ağar²

¹Department of Physics, Amasya University, Amasya, Turkey
²Department of Chemistry, Ondokuz Mayıs University, Samsun, Turkey

Schiff bases are an important class of organic compounds. Schiff bases have been playing an important role in the development of coordination chemistry related to catalysis and enzymatic reactions, magnetism and molecular architectures [1]. Moreover, Schiff bases have biological activities such as antimicrobial, antifungal, antitumor activities and herbicidal properties [2].

The title Schiff base compound (Fig. 1) has been synthesized and characterized by FT-IR, UV-Vis, and X-ray single-crystal determination. The molecular geometry from X-ray experiment in the ground state has been compared using the density functional theory (B3LYP) method using the 6-311++G(d,p) basis set. The TD-DFT calculations were carried out using the B3LYP and CAM-B3LYP functionals with the 6-311++G(d,p) basis set to determine the maximum absorbtion wavelength of the UV-Vis spectra for the title compound. The chemical reactivity behavior of the title compound in solvent media has been examined using B3LYP method with the 6-311++G(d,p) basis set by applying the IEF-PCM model. The nonlinear optical properties are also addressed theoretically.

Keywords: X-ray, DFT, FT-IR, UV-Vis, Schiff Base

Figure 1

Structure of investigated molecule
Photodegradation of Paracetamol (PC) Induced by Goethite (α-FeOOH) In Aqueous Solution Up On Irradiation at 365 nm and by Solar Light

Yazid Mameri, Nadra Debbache, Sarah Belattar, Tahar Sehili
Département de chimie, Faculté des sciences exactes, Université des frères Mentouri Constantine, Algérie

Pharmaceuticals in the aquatic environment have received great attentions from the general and scientific community due to their potential impacts on ecological and human health. Iron (III) (hydr) oxides absorb light up to 600 nm. Most of them have semiconductor properties and then can behave as photocatalysts. Many studies have shown that the combination of light UV-Visible and iron oxide can degrade organic pollutants.

In this work, we are interested in studying the heterogeneous photodegradation of Paracetamol (PC) in the α-FeOOH (Goethite) system in aqueous suspension up on irradiation at 365 nm and by solar light.

Monitoring the reaction was carried out by UV-visible spectrometer for spectral evolution, and by HPLC for quantification of the substrate. The mechanism involvement in the PC-Goethite system operate electron–hole pairs. The rate of photocatalytic degradation of PC is slow and follows pseudo-first order kinetics.

The addition of H₂O₂ in the previous solution lead to the formation of HO• radicals via the Fenton system. The influence of reaction parameters such as iron amount, initial concentration of PC, pH value, and hydrogen peroxide dosage was also investigated. The optimal initial concentration of hydrogen peroxide for the PC degradation with Goethite under the experimental conditions is found to be 5×10⁻³ M.

The photodegradation of PC in the mixtures PC-Goethite and PC-Goethite-H₂O₂ under solar light was significantly accelerated in comparison with artificial irradiation at 365 nm.

Keywords: Photodegradation, Paracetamol, Goethite, UV-visible spectrometer, hydrogen peroxide
In study, by applying UV-Visible spectroscopy, enzyme activity of the 6-phosphogluconate dehydrogenase (6PGD; EC 1.1.1.44) enzyme was determined experimentally. After purification of 6PGD from erythrocytes of Van Cat which is an endemic one in Van region of Turkey. The purification of 6PGD was accomplished with the use of affinity chromatography on 2′,5′-ADP Sepharose 4B[1]. The enzyme activity measurements were performed according to Beutler method at 340 nm[2]. The 6PGD protein determination was measured spectrophotometrically at 595 nm according to Bradford’s method[3]. Then, the optimal pH and optimal temperature of enzyme was determined. The optimal pH and optimal temperature of enzyme were measured 8.0 and 50 OC, respectively. The enzyme purity was controlled by using sodium dodecylsulfate-polyacrylamide gel electrophoresis (SDS-PAGE)[4]. The molecular weight was calculated as 52.602 Da.

Kaynaklar


Keywords: UV-Visible spectroscopy, 6PGD, erythrocytes, purification, Van Cat.
P-017

Investigation of Solvent Effect on Biological Reactivity, UV-VIS and NMR Analyses of Zn(II) Complexes with Pentaaza Macrocyclic Schiff-base Ligand

Koray Sayin, Duran Karakaş, Nihat Karakuş, Sultan Erkan Kariper, Tuba Alagöz Sayin

Cumhuriyet University, Faculty of Science, Department of Chemistry, 58140 Sivas, Turkey

Zn(II) complexes, which are represented in Fig. 1, have been synthesized by Keypour et al. in 2009 [1]. As experimentally, some structural parameters and stretching frequencies of selected complexes have been reported in their paper [1]. However, their UV-VIS and NMR spectra have not been investigated up to the present. In this study, B3LYP/6-31G(d,p)(LANL2DZ) and B3LYP/6-31++G(d,p)(LANL2TZ+) levels are used in calculations. The best level is determined as B3LYP/6-31G(d,p)(LANL2DZ) for studied complexes. This level is taken into account for other calculations. UV-VIS and NMR spectrum are calculated and examined in detail. Biological reactivity of these complexes are investigated different solvent which are gas phase, water and chloroform. Some quantum chemical descriptors are used for this analysis. As a result, biological reactivity of [ZnL1Br]+ are more reactive than [ZnL2]2+.


This study was supported by CUBAP (Project No: F-426)

Keywords: Z(II) complexes, Computational investigations, Spectral studies, Biological reactivity

Optimized Structures of Zn(II) complexes at B3LYP/6-31G(d,p)(LANL2DZ) level in vacuo.
Copper(II), cobalt(II) and nickel(II) complexes with selenadiazoloquinolone (SeQ) in the presence of a nitrogen donor heterocyclic ligand 1,10-phenanthroline (phen) have been synthesized and characterized. The presence of biological metal and phen increase the biological activity [1] of studied selenadiazoloquinolone complexes. The crystal structures of copper(II), cobalt(II) and nickel(II) complexes have been determined with X-ray crystallography. According to the quantum chemical calculations and X-ray data, the copper atom is five-coordinated with the slightly distorted square pyramid which is built of a bidentate coordination of SeQ and phen and a monodentate chlorine ligand. In the case of cobalt(II) and nickel(II) complexes, the metal is six-coordinated with a distorted octahedral geometry. The selenadiazoloquinolones ligands behave as bidentate deprotonated ligands being coordinated to cobalt ion via the pyridone and carboxylate oxygen. The coordination of SeQ to the Cu(II), Co(II) and Ni(II) ions via pyridone (O1) and carboxylate oxygen (O2) atoms was confirmed using X-ray (see Fig. 1) and IR spectroscopy [2–4]. The strong band at 1719 cm\(^{-1}\) in the IR spectra of SeQ was assigned to the C=O stretching vibration of carboxyl group. After complex formation with metal ions, this vibration has been replaced with two very strong characteristic bands in the range of 1622–1618 cm\(^{-1}\) and 1363–1338 cm\(^{-1}\) attributed to asymmetric and symmetric (O–C–O) stretching vibrations, respectively. The UV-vis spectra of the complexes have been recorded in aqueous and dimethylsulphoxide solutions.

Acknowledgement: This work was financially supported by the Scientific Grant Agency (VEGA Project 1/0041/15) and Slovak University of Technology in Bratislava (Young Researcher Grant, S. Dorotíková). The calculations were performed at HPC center, SUT Bratislava (SIVVP project, ITMS code 26230120002, funded by the European region development funds) and Computing Centre SAS, code 26210120002 (Slovak infrastructure for high-performance computing) supported by the Research & Development Operational Programme funded by the ERDF. Kristína Plevová, Maroš Bella and Viktor Milata are gratefully acknowledged for synthesis of investigated derivatives.

Keywords: selenadiazoloquinolone, crystal structure, UV-Vis, IR spectroscopy, DFT

Structure of [Ni(SeQ)2(phen)] SeQ=9-ethyl-6-oxo-6,9-dihydro[1,2,5] selenadiazolo[3,4-h]quinoline
Azo compounds have been the most widely used class of organic dyes, due to their versatile application in various fields, such as the dyeing of textiles, and fibers, the coloring of different materials, and high-technology areas, such as laser, electro-optical devices, liquid crystalline displays, and ink-jet printers [1]. Azo dyes containing hydroxy substituent ortho or para to the azo group can in principle exist as mixtures of azo and hydrazone tautomers. While azo–hydrazone tautomerism is quite interesting from a theoretical viewpoint, it is also important from a practical standpoint because the two tautomers have different technical properties [2]. Though many kinds of azo dyes have been synthesized, cyclotriphosphazene derivatives are relatively rare. Phosphazene-bound dye systems are of interest in photochemical research, in photographic processes, and in a number of biologically related applications [3-4]. We report herein the 1H-NMR, FT-IR, and UV–vis study of the tautomeric behavior of some p-phenylazo-α-naphthol compounds and their cyclotriphosphazene derivatives in different polarity solvents as CHCl₃, absolute EtOH, DMSO. UV-vis spectra of the p-phenylazo-α-naphthols (3) have been determined both tautomeric forms in CHCl₃. In generally investigated tautomeric equilibrium of the p-phenylazo-α-naphthols (3) have been shifted from hydrazone to azo in turn in order CHCl₃ < absolute EtOH < DMSO.

The UV-vis spectra taken in chloroform (CHCl₃) and dimethylsulfoxide (DMSO) showed that hexakis(p-phenylazo-α-naphthoxy)cyclotriphosphazene derivative (5) existed only in the azo form and absorption bands of the cyclotriphosphazene derivatives (5) shifted to blue region of the spectra comparing with the starting azo compound (3). It is shown that, p-phenylazo-α-naphthol compounds (3) were connected to cyclotriphosphazene on azo form. These results are in accordance with the 1H-NMR and FT-IR spectra of the compounds.

Keywords: Tautomerism, Cyclotriphosphazene, UV-Vis, IR, NMR, Azo compounds

Synthesis of p-Phenylazo-α-Naphthol Compounds and Their Cyclotriphosphazene Derivatives
Linoleic acid (cis,cis-9,12-octodecadienoic acid) is a polyunsaturated -omega 6- essential fatty acid due to the presence of two C=C double bonds (Figure 1) at positions 9 and 12 that must be consumed for proper health. Linoleic acid (LA) is the main fatty acid found in vegetable oils such as soybean oil, corn oil and rapeseed oil.

The conformational behavior of monomeric linoleic acid in the gas phase was investigated by means of density functional theory. The structures of conformers of LA were optimized by using the B3LYP/6-311++G(d,p) method. The theory showed that the tttttts´CssCs´tt conformation of LA is the more stable than the other conformations and its structure shows very similar parameters as determined by X-ray crystallography [1].

The DFT calculations at the B3LYP/6-311++G(d,p) level of theory on the molecular structure and vibrational spectra of the dimeric form of LA were also performed. Fourier Transform Infrared (FTIR) and Raman spectra of pure LA in liquid form were recorded in the region 4000–700 and 3500–100 cm⁻¹, respectively. The calculated and scaled vibrational values of monomer and dimer forms of LA were used to make mode assignments of observed bands in the FTIR and Raman spectra.

**Keywords:** Linoleic Acid, FT-IR, FT-Raman, Conformational Analysis, DFT
Structural Characteristics of Wood-Polymer Green-Composites by FTIR Spectroscopy

Elif Hilal Şen, Sevgi Haman Bayar, Erdem Bodur

Department of Physics Eng. Hacettepe University, Ankara, Turkey

Wood-polymer composites (WPC) are eco-friendly and have many potential uses. Wood plastic composites have several advantages compared with natural wood and plastic. The presence of wood in a thermoplastic polymer matrix can result in a stiffer and lower-cost material than if polymer alone was used.

Wood is mainly composed of lignocellulosic fibers which have a three-dimensional structure and are composed mainly of cellulose, hemicelluloses, and lignin. It is well known that the uniformity of lignocellulosic materials dispersed in a polymeric matrix greatly affects the mechanical behavior of composites.

In this study, we report a detailed structural analysis of polyethylene composites reinforced with pine and chestnut flour. The objective of this study was also to evaluate the influence of fillers such as silica and talc on the structural properties of wood-reinforced polyethylene (PE) composites [wood flour (50%)-PE (45%)-silica (5%) and wood flour (50%)-PE (45%)-talc (5%)]. The molecular structures of the composites were investigated by Fourier Transform Infrared Spectroscopy (FTIR).

The crystallinity of wood has an important effect on the physical, mechanical and chemical properties of wood-based materials. The crystalline fraction of wood is given by cellulose, since the other two main wood components, hemicellulose and lignin, are amorphous. The relative crystallinity index (CI) was also determined from FTIR spectra of composites.

**Keywords**: wood, composites, FTIR

---

85
Two new mixed chelidamate complexes, \((\text{dipaH})_2[\text{Ni(chel)}_2]\cdot5\text{H}_2\text{O} \) \((1)\) \([\text{Ni(chel)(dipa)}]\cdot\text{C}_2\text{H}_5\text{OH} \) \((2)\) [chel: chelidamate or 4-hydroxypyridine-2,6-dicarboxylate; dipa: 2,2\text{'}-dipyridylamine], have been prepared and characterized through a combination of X-ray diffraction methods, FT-IR and UV-Vis spectroscopy. The complex \((1)\) consists of one \([\text{Ni(HChel)}_2]^{2-}\) anion, two \([\text{dipaH}]^{+1}\) cations and five uncoordinated water molecules. The central Ni(II) ion in complex \((2)\) is coordinated by the dipa nitrogen atoms, chel nitrogen and oxygen atoms and aqua oxygen atom, forming the distorted octahedral geometry. Also, the fully optimized geometries have been calculated using Hartree Fock (HF) and Density Functional Theory (DFT)-B3LYP with 6-31G (d,p) basis set. The energetic behaviors of the complexes have been examined using by time dependent DFT (TD-DFT) method by applying the Polarizable Continuum Model (PCM). Vibrational frequencies and natural bond orbital analysis (NBO) have been investigated by the DFT method. The calculated structural parameters (bond lengths and bond angels) and vibrational frequencies are compared with experimental values of the investigated complexes.

**Keywords:** Chelidamic acid, X-ray diffraction, FT-IR, UV-Vis, HF, DFT
Analysis of Normal and Rickets Human Skeletal Remains by FT-IR Spectroscopy and SAXS

Sevgi Haman Bayarı¹, Kameray Özdemir², Semra Ide¹, Yılmaz Selim Erdal², Ilghar Orujalipoor³

¹Department of Physics Eng., Hacettepe University, 06800 Beytepe, Ankara, Turkey
²Department of Anthropology, Hacettepe University, 06800 Beytepe, Ankara, Turkey
³Department of Nanotechnology and Nanomedicine, Hacettepe University, 06800 Beytepe, Ankara, Turkey

The structural investigation was performed using Fourier transform infrared spectroscopy (FTIR spectroscopy) and Small Angle X-ray Scattering (SAXS) techniques in the framework of a general study of diagenesis. Rib fragments belong to 0 to 3 years old subadults rickets individuals were analyzed and compared with non-rickets individuals in the same age group in Tasmasor (Erzurum, post-Medieval Period) and Oluz Höyük (Amasya, Medieval Period) from Turkey.

In the bones of both rickets samples, the relative mineral-to-matrix and carbonate-to-amide I and carbonate-to-phosphate ratios decreased compared to the normal group. Moreover the relative carbonate-to-phosphate (C/P) ratios for normal samples of Oluz Höyük site are significantly lower than the values of the normal samples of Tasmasor site.

The FTIR crystallinity index (CI) of rickets is significantly higher than the normal bone. The higher CI values indicate a significant decomposition and structural reordering of the apatite lattice. This value is higher in Tasmasor samples compare to Oluz Höyük indicating the bones of this site showed higher disease effect.

The alteration in the mineral due to diagenesis in nano scale was also determined by Small Angle X-ray Scattering (SAXS) technique.

As a conclusion, this study successfully differentiated normal and rickets bone samples based on FTIR and SAXS.

This study is currently being supported by TUBITAK, under the project number TUBITAK-114K272

Keywords: Bone diagenesis; Medieval Period; rickets; taphonomy
Diagenetic Alterations in the Anthropological Bone Mineral Structure: FTIR Spectroscopy and SAXS Studies

Sevgi Haman Bayar1, Semra Ide1, Kameray Özdemir2, Yılmaz Selim Erdal2, Ilghar Orujalipoor3, Elif Sen1

1Department of Physics Eng., Hacettepe University, 06800 Beytepe, Ankara, Turkey
2Department of Anthropology, Hacettepe University, 06800 Beytepe, Ankara, Turkey
3Department of Nanotechnology and Nanomedicine, Hacettepe University, 06800 Beytepe, Ankara, Turkey

Archaeological bone remains are directly influenced by the burial environment and may undergo a range of different alterations due to physical and chemical processes. Bone is a natural composite of collagen protein and the poorly crystalline calcium-deficient apatite. Bone diagenesis has been associated with a variety of mostly anionic substitutions (e.g. Cl⁻ and F for OH⁻; CO₃-² for PO₄-³ (type B apatite) or OH⁻ (type A apatite) ) as well as with changes in crystallinity of bone mineral.

Fourier Transform Infrared Spectroscopy (FTIR) gives information on the chemical composition at molecular level and the relative mineral and organic content and crystallinity of bone mineral. Small-Angle X-ray scattering (SAXS) is also sensitive to detect and investigate the structural changes related with the mineral nanocrystals embedded in collagen fibrils. We present the results of FTIR and SAXS of archaeological human bone remains of the Medieval period recovered from Hakemi Use in Diyarbakır and Komana in Tokat (Turkey) to assess the preservation of biogenic bone mineral. This study also aimed to understand the influence of environment factors on bone mineral for these archeological sites which are located near river in different geographic and climatic areas.

By using FTIR, relative phosphate-to-amide I (mineral-to-matrix), carbonate-to-phosphate and carbonate-to-amide I ratios and crystallinity index (CI) were quantified. To differentiate of bones of two ancient sites based on the molecular alterations from the vibrational spectra, cluster analysis was also performed.

The bone diagenesis and mineral structure at the nanometric scale were also determined by SAXS using the quantitative parameters such as radius of gyration and fractal dimension.

FTIR and SAXS techniques would provide a more complete picture of the digenetic changes undergone by these bone remains specimens.

This study is currently being supported by TUBITAK, under the project number TUBITAK-114K272

Keywords: Bone diagenesis, Medieval Period, CI, FTIR, SAXS
A new eco-friendly, selective and sensitive method was developed for preconcentration and determination of trace levels of sulfite by ultrasonic-assisted cloud point extraction (UA-CPE). The method is based on the selective ion-association of anionic complex, Cu(SO₃)₂⁻, produced depending on sulfite concentration in presence of excess Cu(II) ions with Toluidine blue (TB+) at pH 7.5, and then extraction of the formed ion-associate complex into surfactant rich phase of Triton X-45 micelles. In the optimized reagent conditions, the calibration curve is linear in range of 2.5–350 µg L⁻¹, and the limits of detection and quantification of the method (LOD and LOQ) (3σblank/m and 10σblank/m) are 1.15 and 3.82 µg L⁻¹ with sensitivity enhancement factor of 95. The results demonstrated that the method achieved acceptable quantitative recoveries of 95.7 to 102.9 % with relative standard deviations (RSDs) of 2.1-4.8 %. The method showed good selectivity, and was successfully applied to the quantification of sulfite species in vegetables and dried fruit samples with satisfactory results. The results were compared with those of the standard 5,5′-dithio-bis(2-nitrobenzoic acid (DTNB) method, and the two paired t-test was used to determine whether the results obtained by the two methods differ significantly.

**Keywords:** Vegetables, Dried Fruits, Sulfite, Food Safety, Toluidine Blue, Ultrasonic-Assisted Cloud Point Extraction, Spectrophotometry
Optimization studies

Figures comprise optimization parameters.

Figure 1. Effect of reagents on UA-CPE efficiency. Optimal conditions: 20 μg L⁻¹ SO₄²⁻, 0.75 mL 0.04 mol L⁻¹ BR buffer at pH 7.5, 1.25 mL of 1.0×10⁻⁴ mol L⁻¹ TIB₃⁺, 0.7 mL of 5.0 mg L⁻¹ Cu(II), 1.25 mL of 5.0% (w/v) KCl, 1.75 mL of 2.5% (w/v) Triton X-100 under ultrasonic power (300 watt, 40 Hz) at 40 oC for 5 min, vortex agitator of 2 min at 3000 rpm and centrifugation time of 5 min at 4000 rpm.
DFT Computational and Spectroscopic Investigations on (E)-N-(3-fluorophenyl)-1-(5-nitrothiophen-2-yl)Methanimine

Şadiye Karataş¹, Hasan Tanak¹, Ayşen Alaman Ağar², Meryem Evcecn¹

¹Department of Physics, Faculty of Arts and Sciences, Amasya University, 05100, Amasya, Turkey
²Department of Chemistry, Faculty of Arts and Sciences, Ondokuz Mayıs University, 55139, Kurupelit, Samsun, Turkey

The Schiff base compound (E)-N-(3-fluorophenyl)-1-(5-nitrothiophen-2-yl)methanimine has been characterized by X-ray diffraction, FT-IR and UV-vis spectroscopy. The molecular geometry and vibrational frequencies of the compound in the ground state have been calculated using the density functional method (B3LYP) with 6-311++G(d,p) basis set. The obtained vibrational wavenumbers and optimized geometric parameters were seen to be in good agreement with the experimental data. Based on the UV-vis spectra and TD–DFT calculations, the electronic structure and the assignments of the absorption bands were carried out. To investigate the NLO properties of the title compound, the electric dipole moment (μ), the polarizability (α) and the first hyperpolarizability (β) were calculated using the density functional B3LYP method with the 6-311++G(d,p) basis set. Besides, DFT calculations of the title compound, molecular electrostatic potential (MEP), frontier orbitals and natural bond orbital (NBO) properties were also performed at B3LYP/6-311++G(d,p) level of theory.

Acknowledgment

This study was supported financially by the Research Centre of Amasya University (Project No: FMB-BAP 15-091).

Keywords: Schiff Base, Thiophene, DFT, FT-IR, UV-Vis.
A Combination of Spectroscopic Methods in Determination of a new Cyanogenic Glycoside Compound Structure from Centaurea Microcarpa

Ramdane Seghiri, Baatouche Samia, Cheriet Thamere, Mekkiou Ratiba, Boumaza Ouahiba, Sarri Djamel, Benayache Samir, Benayache Fadila

Unité De Recherche Valorisation Des Ressources Naturelles, Molécules Bioactives Et Analyse Physicochimiques Et Biologiques, Université Frères Mentouri, Constantine, Algérie

The structural elucidation of organic compound by using a combination of METHODS: NMR, infrared spectroscopy (IR), ultraviolet spectroscopy (UV) and mass spectrometry (MS). Centaurea microcarpa is an endemic plant to Algeria. This is the first reported isolation of a novel Cyanogenic glycoside compound using different chromatographic technics, its structure has been determined by combination of several spectroscopic methods.

Keywords: spectroscopic methods, Cyanogenic glucoside, Centaurea, Asteraceae.
The identification of drug metabolites in plants is an important step in drug discovery and development. The use of spectroscopic methods (UV, IR, NMR and MS) for the investigation of drugs is demonstrated, especially in the natural products field.

Some Astragalus species (Leguminosae), are used as an antiperspirant, a diuretic or a tonic and for the treatment of nephritis, diabetes, leukemia and uterine cancer in Oriental medicines. These traditional uses of plants encourage scientists to search novel substances which possess therapeutic properties. In this aim, the phytochemical study of n-butanol extract of Astragalus gombo (Fabaceae), led to the isolation and identification of two flavonoids: 7-Methylkaempferol 3-O-α-rhamnopyranosyl-(1→2)-β-galactopyranoside (1) and kampferol 3-O-α-rhamnopyranosyl-(1→2)[6-O-(3-hydroxy-3-methylglutaryl) β-galactopyranoside] (2). The structures of these compounds were characterized by the use of 1D and 2D NMR (1H,13C, COSY, TOCSY, HSQC, HMBC) as well as UV spectroscopy.

**Keywords:** NMR spectroscopy, Flavonoids, Fabaceae.
Determination of new Flavonoids Using Spectroscopic Methods Isolated from Genista Aspalathoides

Ouahiba Boumaza, Rabia Boukaabache, Ratiba Mekkiou, Ramdane Seghiri, Fadila Benayache, Samir Benayache

Unité de Recherche Valorisation des Ressources Naturelles, Molécules Bioactives et Analyse Physicochimiques et Biologiques (VARENBIOMOL), Université Frères Mentori, Constantine, Algérie

The search for new natural products with therapeutic properties as one of the main objectives for researchers. In this context we have begun to study phytochemical Algerian plants which belonging to the fabaceae family. Therefore, our work is oriented to the extraction, separation, purification and structural determination of flavonoids compounds of the species of the Genista genus. The structural elucidation of these compounds were determined by modern spectroscopic methods including ultraviolet spectroscopy, the magnetic resonance spectroscopy NMR mono and bidimentional (1H, 13C, Dept., COSY, HSQC, HMBC, NOESY, ROESY) and the high-resolution mass spectrometry HR-MSES.

Keywords: NMR spectroscopy, Flavonoids, Genista genus, Fabaceae.
Charge transfer complex of 2,2'-bipyridine with picric acid was investigated by DFT/B3LYP level of theory. Electronic structures were investigated by TD-DFT method and the descriptions of frontier molecular orbitals and the relocation of the electron density were determined. Besides 1H NMR chemical shifts were computed at B3LYP/6-311+G(2d,p) level of theory by Gauge-invariant atomic orbital (GIAO) in DMSO as a solvent using the polarizable continuum model (PCM). The obtained calculations were compared and discussed with experimental results.

**Keywords:** Charge-transfer; TD-DFT, B3LYP /6-31G (d,p), B3PW91/6-31G (d,p)
Comparative Study of Adsorption and Photocatalytic Degradation of Two Dyes in Aqueous Solution in the Presence of TiO$_2$ P25 and TiO$_2$ PC500

Seyfeddine Bendjabeur$^1$, Razika Zouaghi$^1$, Bachir Zouchoune$^2$, Tahar Sehili$^1$

$^1$Department of Chemistry, University of Constantine 1, Constantine, Algeria
$^2$Laboratoire de Chimie appliquée et Technologie des Matériaux, Université Larbi Ben M’Hidi-Oum el Bouaghi, Algeria

Dyes are widely used in printing, food products, cosmetics and clinics, but especially in the textile and tannery for their chemical stability and facility of their synthesis and variety of colors. However, these dyes are the origin of pollution when discharged into the environment, each year the annual production of dyes increases more and more, in virtually found in all aspects of daily life spheres.

In recent years, heterogeneous photocatalytic reactions on n-type semiconductors are recognized as a new emerging “advanced oxidation process” (AOP) for the treatment of recalcitrant chemicals present in the wastewater. The preferential use of TiO$_2$ for the photocatalytic degradation of organic substrates is based on its low-cost, non-toxic, and photochemical stability.

The photocatalytic decolorization of two triphenylmethane dyes, basic Fuchsine (BF) and acid Fuchsine (AF), was investigated in an aqueous suspension of TiO$_2$ using UV-A light at 365 nm in a static batch reactor. The objective of the study was to compare their adsorption and photocatalytic reactivity in the presence of TiO$_2$ P25 and PC500 at different pH solution.

These two dyes have similar absorption spectra with a maximum absorption band located at 544 nm with an hypochromic effect ($\Delta\varepsilon = 27560$ L mol$^{-1}$ cm$^{-1}$) for acid Fuchsin, which is due to the presence of sulfonate groups (SO$_3^-$) on the aromatic ring of AF. The DFT (density functional theory) results of the two dyes show that the theoretical UV-visible spectra of them are similar to the experimental UV-visible spectra and confirm the hypochrom effect.

The adsorption of BF and AF on both photocatalysts was found favorable by the Langmuir approach. The photocatalyst, Degussa P25 was found to be more efficient for the photocatalytic degradation of both dyes; and there is no apparent relationship between photocatalytic activity and specific surface area. A Langmuir–Hinshelwood model was found to be accurate for photocatalytic degradation and indicates that adsorption of the dye on the surface of TiO$_2$ particles plays a role in photocatalytic reaction. The decolorization rate of basic Fuchsine in acidic condition is higher than that of acid Fuchsine.

**Keywords:** Photocatalysis, Adsorption, Dyes, Titanium dioxide
Molecular Structure, Vibrational Spectral Investigation and the Confirmation Analysis of 1-(Diphenylmethyl)Piperazine

Semran Sağlam¹, Ahmet Güvenir², Mehmet Tahir Güllüoğlu², Yusuf Erdoğdu²

¹Department of Physics, Gazi University, Ankara, Turkey
²Department of Physics, Ahi Evran University, Kırşehir, Turkey

1-(Diphenylmethyl)piperazine (DPMP, $\text{C}_{17}\text{H}_{20}\text{N}_{2}$), also known as benzhydrilpiperazine, is a chemical compound and piperazine derivative. It features a piperazine ring with a benzhydryl (diphenylmethyl) group bound to one of the nitrogens. Piperazine derivatives are important pharmacophores that can be found in biologically active compounds in a number of different therapeutic areas [1], such as antifungal [2], antibacterial, antimalarial, antipsychotic [3].

The FT-IR spectrum of DPMP molecule is recorded in the region 4000–400 cm$^{-1}$ on Vertex 80 spectrophotometer. The FT-Raman spectrum of DPMP molecule has been recorded using 1064 nm line of Nd: YAG laser as excitation wavelength in the region 50-3500 cm$^{-1}$ on the Thermo scientific DXR Raman Microscope. The 1H and 13C NMR spectra are taken in solutions and all signals are referenced to TMS on a Bruker Ultrashield FT-NMR Spectrometer. All NMR spectra are measured at room temperature. The calculations were performed at DFT levels by using Gaussian 09 program package, invoking gradient geometry optimization [4-5]. In order to establish the stable possible conformations, the conformational space of DPMP molecule was scanned with theoretical methods. The optimized structural parameters were used in the vibrational frequency calculations at the DFT level to characterize all stationary points as minima. Then, vibrationally averaged nuclear positions of DPMP molecule were used for harmonic vibrational frequency calculations resulting in IR and Raman frequencies. In the present work, the vibrational modes were assigned on the basis of TED analysis for 6-311++G(d,p) basis set, using SQM program [6].


Keywords: 1-(Diphenylmethyl)piperazine, DFT, IR, RAMAN and NMR
Nanoscope Analysis of Sugar Beet Seeds

Begüm Çınar1, Ilghar Orujalipoor2, Semra Ide1, Dilek Başalma3, Ayşegül Boyacıoğlu4

1Department of Physics Eng., Hacettepe University, 06800 Beytepe, Ankara, Turkey
2Department of Nanotechnology and Nanomedicine, Hacettepe University, 06800 Beytepe, Ankara, Turkey
3Department of Agriculture, Ankara University, 06120 Ankara, Turkey
4Turkey Sugar Factory A. Ş, 06930 Ankara, Turkey

Sugar beet is known as eco-friendly and biofuel energy source crops as well as being a renewable raw material. In order to raise the efficiency and quality of fabrication techniques, energy requirements - energy based economy, the raw material used, improving the quality of various matter - products and research on product diversification are important and topical issues in sugar technology.

Various methods are used to investigate and understand seed quality and structural content. Macromolecular formation can be examined by using nanoscopic analysis. One of the most effective methods is known as SAXS (Small Angle X-ray Scattering). The size/size distribution, particle configuration, shapes, electron densities and distance distributions of the nanostructured aggregations can be obtained by using this method.

In this study, macromolecular contents of various sugar beet seed which produced by national and international institutes were examined by SAXS method. At end of the nanoscopic analyses, it was obtained that the radius of gyration values are changing in the range of 201-230 Å for the globular aggregates and 121-163 Å for nano-rod formations of ‘Felicita Turkey’ named seed. So, the richest and the best macromolecular content was recorded for this sample. Therefore, the purification step was also started and the best solvent for the proteins was looked for. As a result of the second phase of the research, propanol was determined as the best solution and the solution is including CP4 EPSPS rich nanoaggregations.

**Keywords:** Sugar beet, Nanoscope, Small Angle X-Ray Scattering,
On-line Screening and Identification of Antioxidant Phenolic Compounds of Salvia Aegytiaca (L.)

Benayache Samir¹, Mohamadi Sabrina¹, Minjie Zhao¹, Amrani Amel¹, Marchioni Eric², Zama Djamila¹, Benayache Fadila¹

¹Unité de recherche Valorisation des Ressources Naturelles, Molécules Bioactives et Analyses Physicochimiques et Biologiques. Université frères Mentouri, Constantine, Route de Ain El Bey- 25000, Constantine, Algérie.

²Equipe de Chimie Analytique des Molécules Bioactives, Faculté de Pharmacie, 74, route du Rhin 67401, Illkirch, Cedex, France.

In this study, the chloroform, ethyl acetate and n-butanol extracts of Salvia aegyptiaca were evaluated for their free radical scavenging capacity by analytical METHODS: 2'-azo-di(3-ethyl-benzo thiazoline -6-sulfonic acid (ABTS.+) and 2,2'- diphenyl-1-picrylhydrazyl (DPPH.) free scavenging capacity assays. On-line HPLC-ABTS+ and subsequent fractionation followed by spectroscopic analysis (HRMS, UV, NMR: 1H, 13C, COSY, NOESY, HSQC and HMBC) were applied to screen and identify free radical scavengers in the extracts. Ten compounds were identified: caffeic acid 1, vanilic acid 2, syringic acid 3, Luteolin 7-O glucoside 4, apigenin 7-O-glucoside 5, diosmin 6, rosmarinic acid 7, Luteolin 8, methyl rosmarinate 9 and apigenin 10. These compounds were the dominant free radical scavengers in the species as expressed by their trolox equivalent antioxidant capacity (TEAC). Rosmarinic acid, methyl rosmarinate, luteolin and caffeic acid were the most active components (TEAC: 32.9, 26.2, 11.9 and 31.93 μg/mL respectively), these results were validated by offline antioxidant DPPH assay. Compounds 2,3, 6 and 9 are described for the first time in Salvia aegyptiaca.

Keywords: Saccocalyx satureioides, antioxidant activity, phenolic derivatives, HPLC-A-BTS
Isostructurality [1] in which two or more structurally related molecules have the same or similar crystal packing provides a useful tool to build materials with tuned desired properties because of changing the intermolecular interactions strength.

Because of similar size and shape, the Cl atom and the methyl group form pair of equivalent functional groups, thus creating the possibility of conservation of similar crystal arrangement upon group replacement. This feature is referred to as the chloro-methyl exchange rule [2]. Moreover the structural equivalence of halogen atoms in the crystal packing is observed [3]. Reports on structural mimicry involving intermolecular interactions e.g. C-O-H…O↔C-H…O, N-H…O↔C-H…O are rare. In turn structural equivalence in aromatic rings are only reported in the case of CH↔N and in acceptor group (N-H, S, O) in the halogen bonded co-crystals. Isostructurality more commonly occurs in multicomponent systems such as solvent inclusion compounds, molecular complexes and cocrystals but in the case of the single component crystal it remains rare [4].

In this Letter we analyze the crystal structure of 2-methylbenzimidazole (ABI) and related compounds, i.e. 2-methylbenzoxazole (ABO) and 2-methylbenzothiazole (ABT) crystals with an eye toward their isostructurality. In particular, we investigate intermolecular interactions employing vibrational spectroscopy (FTIR and Raman) and theoretical methods (interaction topology based on Shishkin’s energy-vector model, topological analysis using Atom in Molecules (AIM) theory and Hirshfeld surface analysis).


Keywords: isostructurality, molecular crystals, intermolecular interaction
Spectroscopic Characterization of I-motif Forming Oligonucleotide pH Probes Containing Fluorescent Cytosine Analog tC

Bernard Juskowiak, Patrycja Rzepecka

Faculty of Chemistry, Adam Mickiewicz University, Umultowska 89b, 61-614 Poznan, Poland

Fluorescently labeled oligonucleotides are widely used as recognition elements for developing molecular sensors. Very interesting group of such devices constitute oligonucleotides able to form tetraplex architecture. Guanosine-rich oligonucleotides form G-quadruplexes while the sequences with cytosine tracks assemble into i-motifs. Folding into i-motif architecture must be preceded by the protonation of half of cytosines in the oligonucleotide and semi-protonated base pairs C-C+ are responsible for the intercalative tetraplex structure (Fig. 1) [1,2]. The feature of C-rich sequences to switch from a folded i-motif to a random coil in response to pH changes was exploited to develop pH biosensors for cellular applications. Typically, C-rich sequences were labeled with external tags: a pair of FRET dyes, fluorophore and quenching groups, or with excimer forming moieties (pyrene) [3,4].

Here in this communication, we propose different labeling approach that is based on the replacement of one cytosine group in a oligonucleotide sequence with a fluorescent analog of cytosine [5], 1,3-diaza-2-oxophenothiazine (tC) as shown in Fig. 1. Incorporation of the fluorescent tC base into oncogene RET sequence have minor effect on the folding propensity of oligonucleotide and stability of i-motif. On the contrary, fluorescence intensity of the tC label appeared to be quenched by i-motif formation induced by pH variation. The system was characterized using circular dichroism (CD), UV-Vis absorption and fluorescence techniques. All these results indicated that our sensor exhibits high sensitivity to pH changes between 6.0 and 7.5 and may be potentially suitable for the cellular pH monitoring.

References

Acknowledgements This work was supported by the National Science Centre of Poland (Grant NCN No. 2014/15/N/ST4/03032)

Keywords: fluorescent cytosine analog, i-motif, pH probe
Fig. 1. Structure of the intramolecular i-motif formed by oncogene RET sequence containing the fluorescent cytosine analog IC, incorporated in the 3rd position. Abbreviation IC stands for 1,3-diaza-2-oxophenothiazole.
Optical and Magnetic Properties of Ferromagnetic Co-Ni Co-doped TiO2 Thin Films

Rabah Bensaha¹, Baddreddine Toubal¹, Fahrettin Yakuphanoglu²

¹Ceramic Laboratory, University of Freres Mentouri, Constantine, ALGERIA.  
²Physics Department, Faculty of Science, Firat University, Elazig, TURKEY.

Co-Ni doped and co-doped TiO₂ thin films with various compositions were prepared by the sol-gel dip coating method. The structural, optical and magnetic properties of the films have been investigated by X-ray diffraction (XRD), Raman spectroscopy, Scanning Electron Microscopy (SEM), energy dispersive X-ray spectroscopy (EDX), UV–Vis spectroscopy and Vibrating Sample Magnetometer (VSM) measurements. A mixture between anatase and brookite phases was found at 450°C for un-doped films. Fully anatase phase was obtained by addition of metal ions without any detectable impurity phase or oxide formed. SEM micrographs clearly confirm that the addition of Co-Ni affects the shape of anatase nanoparticles. The refractive index, thickness and optical band gap values of the films were obtained by means of optical transmittance spectra measurements. The band gap of TiO₂ sample is decreased by Co-doping, Ni-doping and 2.5% (Co–Ni) and 3.5% (Co–Ni) co-doping, respectively. Both un-doped and Co-Ni co-doped films were found to be ferromagnetic at room temperature may due to the migration of oxygen vacancies created by co-doping.

Keywords: Co-Ni co-doped, TiO₂ films, Ferromagnetic, Sol gel method
Analysis of B Vitamins in Food Matrix by Surface Enhanced Raman Spectroscopy (SERS)

Andreea Radu¹,², Maria Thum¹, Martin Jahn¹,², Uwe Huebner², Karina Weber¹,², Dana Cialla May¹,², Jürgen Popp¹,²

¹Friedrich Schiller University Jena, Institute of Physical Chemistry and Abbe Center of Photonics, Helmholtzweg 4, 07745 Jena, Germany.
²Leibniz Institute of Photonic Technology Jena, Albert-Einstein-Str. 9, 07745 Jena, Germany.

B vitamins play a key role for the well-being and growth of the body. In particular, vitamin B2 is used for cellular energy production and is important for the antioxidant activity in the body. Vitamin B12 is involved in the cellular metabolism of carbohydrates, proteins and lipids. It is also needed for DNA synthesis and red blood cell formation. Thus, it is important to guarantee a proper B vitamin uptake for each individual. For that purpose it is of high interest to easily obtain information regarding food composition and quality in particular with respect to vitamin analysis.

Within this contribution, we introduce the application of surface enhanced Raman spectroscopy (SERS) for food vitamin analysis. SERS enables the detection of analytes by measuring their Raman molecular spectral fingerprint with a sensitivity required for trace analysis. SERS enhances the Raman signal of molecules by several orders of magnitude utilizing plasmonic nanoparticles. Accordingly, SERS allows for a fast, specific and rather easy detection of analytes embedded in complex matrices. Thus, SERS is a perfect candidate for food analytics.[1,2]

Here we employed silver deposited micro fabricated quartz arrays[3] (produced by electron beam lithography) as SERS active substrate to detect the two vitamins B2 and B12 in complex food-related matrices. In a first step the analyte molecules are spectroscopically characterized employing Raman and UV VIS absorption spectroscopy followed by mixing the analytes with the substances sugar and starch to account for the complexity of a food matrix. By doing so, we achieved detection limits down to the µM range. Finally, we report about the SERS detection of the analytes in real food extracts.

Acknowledgement:

Funding by projects “QuantiSERS” and “Jenaer Biochip Initiative 2.0” within the framework “InnoProfile Transfer – Unternehmen Region” the Federal Ministry of Education and Research, Germany (BMBF) is gratefully acknowledged.

1 Cialla D. et al. (2012), Analytical and bioanalytical chemistry, 403, (1), 27-54.
2 Hidi I.J. et al. (2014), Analytical Methods, 6, (12), 3943-3947.

Keywords: Raman, SERS, plasmonic structures, electron beam lithography, vitamins
Designing a Raman Cell For Frequency Shift of Laser Radiation

Ayhan Altun1,2,3, Karl Kleinermanns1

1Department of Chemistry, Heinrich Heine University, Düsseldorf, Germany
2Department of Chemistry, Akdeniz University, Antalya, Turkey
3Department of Chemistry, Alparslan University, Muş, Turkey

We have examined the utility of a gas-filled, Nd:YAG-laser-pumped Raman shifter as a possible broad-spectrum light source. For this purpose, new Raman Cell have been designed shown in figure 1. Seven new output frequencies with pulse energies above 0.15 mJ are produced when a pure-hydrogen Raman shifter is pumped with 7.56 mJ of first-harmonic, 10.43 mJ of second-harmonic, 7.78 mJ of third-harmonic, or 1.61 mJ of fourth-harmonic pump pulse energy. Optimum output occurs at pressures of approximately 13 bar for the pure hydrogen gas experiments. Depending on pump energy, light path distance, and pressure, about 10 new output lines with pulse energies over 1 μJ have been produced. We discuss the suitability of new output lines for the application of absorption spectroscopy.

Keywords: Raman, Frequency shift, Laser

Schematic Representation of the Raman Cell
P-040

Spectroscopic Determination of the Oxygen Reactive Species Photosensitized by the Irradiation of the Antibiotic Ciprofloxacin with UVA Radiation

Jamil Ahmed

Jordan University of Science and Technology, Irbid, Jordan

Ciprofloxacin (CPX) is a fluoroquinolone antibiotic that is widely used in the treatment of a wide range of infections. Clinical trials showed that the administration of CPX and exposure to the UVA radiation in the sun light can cause phototoxic reactions manifested as severe skin sun burns in patients. These phototoxic reactions are usually attributed to the ability of ciprofloxacin to photosensitize the formation of oxygen reactive species (ROS) such as singlet oxygen ($^{1}O_2$) and superoxide ion ($O_2^-$).

We found that the photosensitized ROX species generated by the exposure of CPX to UVA radiation can bleach the blue color of the organic dye indigo carmine. The kinetics of the photosensitized bleaching of indigo carmine by ciprofloxacin can be followed very easily by UV-visible spectroscopy. The effect of the singlet oxygen and superoxide ion scavengers, methionine, superoxide dismutase (SOD), sodium azide, and 1,4-diazabicyclo[2,2,2]octane (DABCO) on the rate of bleaching of indigo carmine was used to determine the ROS responsible for the CPX Phototoxicity.

Sodium azide which is known to be a specific singlet oxygen quencher strongly inhibits the photochemical bleaching of indigo carmine by CPX at pH 7. The addition of 10 mM sodium azide decrease the reaction rate to 40 % compared to the sodium azide free solution which implicates singlet oxygen in the phototoxic mechanism of ciprofloxacin. However, it was found that DABCO, superoxide dismutase and methionine increase the rate of bleaching of indigo carmine. Therefore, the photosensitized formation of superoxide ion by irradiation of ciprofloxacin with UVA cannot be confirmed or ruled out.

References:

Keywords: Ciprofloxacin, Indigo carmine, Reactive Oxygen species
Rapid Determination of Palladium by a New Spectrofluorimetric Determination in Environmental Samples Using Acriflavine as a Reagent

Sultan Başak Şimşek, Serifa Saçmacı, Ahmet Ülgen

Erciyes University, Department of Chemistry, Faculty of Science, TR-38039, Kayseri, TURKEY

Noble metals have low crustal abundance (approximately 1 ng g^{-1}), yet they are components of different geological samples such as rocks, ores, concentrates, minerals, soils, and sediments. In the earth's crust, Pd usually occurs in its native form associated with one or more of the other platinum group elements (PGEs) along with gold, iron, copper, nickel, and chromium. Palladium is an element of increasing importance in today’s industries. The annual production of palladium is estimated to be 195 t; the majority of this is used in autocatalysts (55%), with other uses including electronics (16%), jewelry (11%), dental medicine (8%), investment (5%), the chemical industry (4%) and in the purification of hydrogen gas. The low concentration of Pd, together with the high concentration of interfering matrix components, often requires a preconcentration step combined with a matrix separation; this allows an accurate and precise determination of Pd in samples with very low analyte content, such as airborne particulate matter and water. Furthermore, it enables the distinguishing of contaminated from background levels [1].

A new, sensitive, and accurate spectrofluorimetric method for the determination of palladium was developed. The method is based on the reaction between Pd(II) and acriflavine in hydrochloric acid medium. The absorbance of the complex is spectrofluorimetrically measured at 550 nm with a violet laser. Several factors that influence the analytical performance of the method such as acidity of sample, amount of the reagent and sample solutions, concentration of the reagent, and effect of interfering ions were investigated. The calibration curve was obtained in the range of 0–1000 µg L^{-1} Pd(II). The detection limit was 0.1 µg L^{-1} while the relative standard deviation of the method was found to be 1.2% (n = 15) at 4.0 µg L^{-1} Pd(II) level. The method was successfully applied to the determination of palladium in catalytic converter, anodic slime, road sediment, ore, and water samples.
Poster Abstracts

Figure 1. The structure of the acriflavine as fluorescence reagent

References


Keywords: palladium, new spectrofluorimetric, acriflavine, environmental samples
Aluminum (Al) is the third most abundant element in the lithosphere, insoluble, and in most neutral natural waters its concentration is very low. Al is a nonessential element to which humans are frequently exposed by the wide use of aluminum containing foods, drinking waters, pharmaceuticals and cooking utensils. Biological effect of Al has not received much attention in the past. In recent years, a large amount of Al has been released into the environment and its solubility is significantly increasing because human activities have resulted in a serious problem of acidification [1]. In this study, we have synthesized a new fluorescence reagent (see Fig. 1), and characterized. 3',6'-bis(-diethylamino)-2-[(1E)-(4-ethoxyphenyl)methylene]aminospiro[isoindole-1,9'-xanthen]-3(2H)-one (DEMAX) was for the selective and sensitive for Al(III). The reagent was firstly used for the determination of Al(III) in real samples with high salt content such as dialysis concentrates and some food samples using the fluorometry system which a new home-made in our instrumental laboratory. The fluorescence of the complex is monitored at an emission wavelength of 569 nm. Optimum complex formation occurred in HCl/KCl buffer at pH 1.0. Under the optimum conditions, linear calibration curves were obtained from 0 to 1000 µg L−1. The detection limit was 3.02 µg L−1 and the maximum relative standard deviation of the method for 1 µg L−1 was 0.1. The accuracy of the method was verified by analysis of a certified reference material (3101a Aluminum) and recovery measurements made with spiked natural water and food samples. The results showed good agreement with the certified value and the recoveries were sufficiently high. The results in this work demonstrate the feasibility of new fluorimetry system determination of µg L−1 levels of Al(III) in samples with high salt content. The new system minimizes the analysis time and manpower needed in laboratories compared to off-line systems.
Acknowledgment: The author is grateful for the financial support provided by the Unit of Scientific Research Projects of Erciyes University (Project no. FYL-2014-5541).

References


Keywords: Fluorimetric determination, aluminium, fluorescence reagent, Water and food samples
Raman, Optical Absorption, Thermal and Elastic Characterization of TM Doped 90TeO₂-10K₂O Glasses

Toufik Mohamed Soltani¹, Doris Moncke², Ali Erçin Ersundu³, Miray Çelikbilek³, Lothar Wondraczek²

¹Laboratoire de Physique photonique et nanomatériaux multifonctionnels, Université de Biskra, Algérie
²Otto Schott Institute of Materials Research, University of Jena, Fraunhoferstrasse 6, 07743 Jena, Germany
³Yıldız Technical University · Department of Metallurgical and Materials Engineering Turkey · İstanbul

By using conventional melt-quenching technique 0.90TeO₂-0.10K₂O glasses doped with different amount of TiO₂, Fe₂O₃ and CuO are prepared. Several technics have been used to characterize these glasses. The glass transition onset (Tg), first crystallization onset, peak (Tc1/Tp1) temperatures and the glass stability (∆T = Tc − Tg) value, were determined from the DSC curves. The structural organization of these glasses has been investigated by using Raman spectroscopy and optical absorption in the UV-Vis-NIR. Ultrasonic’s echography was used to determine the elastics parameters (E, G, K, L) and other related parameters (Poisson’s ration, acoustic impedance, Debye temperature). These glasses can have potential application in laser device and thermochromics applications.

Keywords: Tellurite glasses, Raman, UV-Vis-NIR, Ultrasonic, TM elements
P-044

XRF Spectroscopy and Imaging Investigations on Two Icons with Double painting Layers from R. Macedonia

Svetlana Mamucevska Miljkovikj¹, Angelina Popovska¹, Zivko Kokolanski², Saso Cvetkovski³, Liljana Kovacevska⁴

¹National Conservation Centre-Skopje, Macedonia
²Faculty of Electrical Engineering and Information Technologies-Skopje, Macedonia
³Macedonian Academy of Sciences and Arts, Center for researches of Cultural Heritage, Skopje, Macedonia
⁴Museum of Macedonia-Skopje, Macedonia

Fifty years ago, the church, St. Elijah from 15th century located in v. Globochica, on the western Macedonia, was sunken by the construction of the hydropower, Globochica, The icons of the church were dislocated in the church St. George, Struga.

Two of the icons, which recorded double iconography, are the object in this present study. The imaging diagnostics methods, non-destructive and sampling micro analytical methods of analyses were used for better understanding manufacture, technology and history of these icons. The focus was the investigation of the two polychrome paint layers, the first layers from the date of origin in the 16th century, and the overpainting of the 20th century signed with the date of 1905.

Imaging diagnostics methods, such as X-radiography and X-ray tomographic provide information about the representation of the lower iconography. Examination of the painting surface was done by using UV fluorescence reflectography. X-Ray Fluorescence Spectrometry and micro chemical analyses were used to obtain information about the composition of paintings material. The wooden supports were analyzed with the identification of the type of the wood.

The results from the researches discover the original form represented as an entity with the scene of the Assumption of the Virgin, to further that the same wooden support was cut in half and repainted with two new scenes in the opposite direction. The upper icon painting represented in Three Holy fathers of the Orthodox church- St. Basil the Great, St. John “Chrysostom” and St. Athanasius the Great and the three saints-monks St. Anthony, St. Ephtimius and St. Theodosius are attributed to the zoograph Seraphim. This author, from Ohrid, in the last two decades of the XIX century, since moving from the village Tresonche, to Ohrid, accomplishes intensive production painting hundreds of icons at the area around Struga, Ohrid and Kichevo up to the areas of Demir Hisar.

The aim of this research is evaluation of the present condition that will form the basis for future conservation and determination of the conservation procedure. Appropriate method for the separation of two polychrome painting layers will be proposed as well as the final presentation of both icons.

Keywords: double painting icons, X-ray and tomographic imaging, UV image, XRF analyses, micro-chemical analyses
Photo-oxidation of Amoxicillin by αFeOOH/H₂O₂ Effect of Operating Conditions

Mohamed Mehdi Benacherine, Yazid Mameri, Besma Dekkiche, Nadra Debbache

Département de chimie, Faculté des sciences exactes, Université des frères Mentouri Constantine, Algerie

The occurrence of pharmaceuticals in aquatic environment is considered as an emerging issue. Antibiotics deserve special attention because they are biologically active molecules leading to emergence of the phenomenon of microorganism's resistance towards the potential pathogens. Amoxicillin is one of the most important commercial antibiotics due to its large spectrum against a wide variety of microorganisms. Removal of amoxicillin residue from the environment is therefore considered important and serves as an attractive case study.

The heterogeneous Fenton-like using goethite as a catalyst is a developing advanced oxidation technology for the treatment of toxic contaminants wastewater, it is based on the activation of H₂O₂ by \( \equiv \text{Fe(II)}/\equiv \text{Fe(III)} \) to produce strong oxidizing hydroxyl radical (OH) radicals.

The aim of this study was to evaluate the effect of some parameters such as pH, initial concentration of H₂O₂ on the photo-oxidative degradation of amoxicillin in aqueous solutions by goethite/H₂O₂. Monitoring the reaction was carried out by UV-visible spectrometer for spectral evolution, and by HPLC for quantification of the substrate.

The results indicated that the degradation of AMX was significantly influenced by the pH of the solution. The optimum solution pH was achieved at pH 3 and the pseudo-first order kinetics rate constants \( k \) were 5,01.10⁻³, 6,87.10⁻³ and 7,96.10⁻³ min⁻¹ at pH 6, 4 and 3 respectively. Although the effect of increasing initial concentration of H₂O₂ from 1 to 50 mM was positive for the degradation.

The photodegradation of AMX in the mixtures AMX-Goethite and AMX -Goethite-H₂O₂ under solar light was significantly accelerated in comparison with artificial irradiation at 365 nm.

Keywords: Amoxicillin, goethite, photofenton, photochemistry, UV-Visible spectrophotometry
P-046

Vibrational Spectra, Non-linear Pptical Properties, NBO Analysis Properties of Acetylcholine by Density Functional Method

Boutasta Amel, Benosman Abdelhakim

Department of Physics, Abou Bekr Belkaid University, Tlemcen, Algeria

The Fourier transform infrared (FT-IR) and FT-Raman of acetylcholine have been recorded in the regions 4000-400 cm⁻¹. A complete assignment and analysis of the fundamental vibrational modes of the molecule were carried out. The observed fundamental modes have been compared with the harmonic vibrational frequencies computed using DFT (B3LYP) method by employing 6-31G(-d,p) basis sets. The vibrational studies were interpreted in terms of potential energy distribution. Natural bond orbital analysis has been carried out for various intramolecular interactions that are responsible for the stabilization of the molecule. HOMO–LUMO energy gap has been computed with the help of density functional theory. The polarizability, first hyperpolarizability, anisotropy polarizability invariant has been computed using quantum chemical calculations.

The infrared and Raman spectra were also predicted from the calculated intensities. Comparison of the experimental and theoretical spectra values provides important information about the ability of the computational method to describe the vibrational modes.

Keywords: DFT calculations, Vibrational analysis, HOMO-LUMO, Hyperpolarizability and NBO analysis.
Spectroscopic Investigations and DFT Calculations on 3-(Diacetylamino)-2-Ethyl-3H-Quinazolin-4-One

Yusuf Sert¹, Fatih Ucun³

¹Department of Physics, Faculty of Art & Sciences, Bozok Univ., Yozgat 66100, Turkey
²Sorgun Vocational School, Bozok Univ., Yozgat 66100, Turkey
³Department of Physics, Faculty of Art & Sciences, Süleyman Demirel Univ., Isparta 32100, Turkey

The theoretical and experimental vibrational frequencies of 3-(diacetylamino)-2-ethyl-3H-quinazolin-4-one were investigated (Optimized structure was given in Fig. 1). The experimental Laser-Raman spectrum (100-4000 cm⁻¹) and FT-IR spectrum (400-4000 cm⁻¹) of the newly synthesized compound were recorded in the solid phase. Both the theoretical vibrational frequencies and the optimized geometric parameters such as bond lengths and bond angles have for the first time been calculated using density functional theory (DFT/B3LYP and DFT/M06-2X) quantum chemical methods with the 6-311++G(d,p) basis set using Gaussian 03 software [1]. The vibrational frequencies were assigned with the help of potential energy distribution (PED) analysis using VEDA 4 software [2]. The calculated vibrational frequencies and the optimized geometric parameters were found to be in good agreement with the corresponding reported experimental data. Also, the energies of the lowest unoccupied molecular orbital (LUMO), highest occupied molecular orbital (HOMO), and other related molecular energies for 3-(diacetylamino)-2-ethyl-3H-quinazolin-4-one have been investigated using the same computational methods.


Keywords: Spectroscopic investigations and DFT calculations on 3-(diacetylamino)-2-ethyl-3H-quinazolin-4-one

Figure 1. The optimized molecular structure of the 3-(diacetylamino)-2-ethyl-3H-quinazolin-4-one.
In this study, theoretical highest occupied molecular orbital (HOMO) and lowest occupied molecular orbital (LUMO) analysis of a newly synthesized bacteriostatic and anti-tumor molecule namely, 4-bromomethyl-6-tert-butyl-2H-chromen-2-one have been investigated by using Gaussian 03 software. The HOMO represents the ability to donate an electron, LUMO as an electron acceptor represents the ability to obtain an electron. The lowering of the energy gap describes that the eventual charge transfer takes place within the compound. The calculated HOMO-LUMO energy gap reflects the chemical activity of the compound, and explains the eventual charge transfer interaction within the compound, which influences its biological activity. The positive phase is represented in red color, and the negative phase in green color. The HOMO-LUMO plots are shown in Fig. 1. As seen from the figure, the HOMO is located on bromomethy and partially over the C8 atoms; the LUMO is more focused on the ring 1 and ring 2 and bromomethyl group.

Keywords: Highest-Lowest Occupied Molecular Orbital Analysis of 4-Bromomethyl-6-tert-butyl-2H-chromen-2-one

Figure 1. Calculated HOMO-LUMO plots of the title compound.
Kinetic Calculations of Phase Transformation in Magnetic Cu-based Alloy

Emine Aldırımaz, Nevzat Karakaya, S. Cansel Cüccü, Eren Koyuncuoğlu

Department of Physics, Science and Arts Faculty, Amasya University, Amasya, TURKEY.

The chemical composition of the alloy, Cu-%24.2Mn (wt%) was obtained by using energy dispersive X-ray analysis (EDAX) technique. In this study was investigated properties of morphological and thermodynamic with scanning electron microscope and differential scanning calorimetry (DSC). From electron microscope observations were found that the austenite phase structure of alloy. Thermogravimetric and differential thermal analysis measurements were investigated phase transformations and kinetic parameters such as enthalpy. The activation energies of the alloy was calculated according to the Kissinger and Augis-Bennett. The activation energy values determined from two different methods were found to be 66.007 kJ mol⁻¹ for Kissinger and 55.805 kJ mol⁻¹ for Augis-Bennet. The phase transformation temperatures and kinetic parameters changed with different heat treatments.

Keywords: Austenite, Activation Energy, Scanning Electron Microscopy (SEM).
A Comparative Study on Vibrational Spectra of Free Indapamide and its DMSO Solution

Y. Alat¹, O. Bölükbaşı¹, A. Yılmaz¹, B. İlhan Ceylan²

¹Department of Physics, Faculty of Science, Istanbul University, Vezneciler-Fatih, 34134, Istanbul, Turkey
²Department of Chemistry, Engineering Faculty, Istanbul University, 34320 Avcılar, Istanbul, Turkey

Indapamide, which is known as a potent diuretic, is currently uses hypertensive and edema. The purpose of this study was to examine the molecular structure of indapamide both in free form and its DMSO solution via vibrational spectra. FT-IR spectra of the title compound were recorded for the solid phase and the solvation of DMSO. Optimized molecular geometry and vibrational wavenumbers of the title molecule were calculated by DFT/B3LYP functional with 6-31G++(d,p) basis set. The assignment of the vibrational modes were performed based on total energy distribution (TED). The same calculations were performed for the molecule in DMSO solution using the polarizable conductor continuum model (CPCM) method. Finally, probable donor-acceptor interactions of the molecule were examined with NBO analysis in two media. In solvation of the molecule, some significant changes were observed in the geometric parameters and the vibrational frequencies.

Keywords: A comparative study on vibrational spectra of free indapamide and its DMSO solution
A novel, sensitive and selective spectrofluorimetric method was developed for the determination of tamsulosin in spiked human urine and pharmaceutical preparations. The proposed method is based on the reaction of tamsulosin with 1-dimethylaminonaphthalene-5-sulfonyl chloride in carbonate buffer of pH 10.5 highly fluorescent derivative this is measured at 397 nm using an excitation wave-length of 514 nm. The described method was validated and the analytical parameters of linearity, limit of detection, limit of quantification, accuracy, precision, recovery and robustness were evaluated. The proposed method showed a linear dependence of the fluorescence intensity on drug concentration over the range $1.22 \times 10^{-7}$ to $7.35 \times 10^{-6}$ M. The proposed method was successfully applied for the determination of tamsulosin in pharmaceutical preparations and the obtained results were in good agreement with those obtained using the reference method.

**Keywords:** derivatization; human urine; method validation; dansyl chloride
Molecular dynamic studies give information about the motion and internal interactions of chemical molecules [1]. The relaxation studies give useful information about molecular dynamics of Chiral Schiff base in free states [2]. Both the spin-lattice (T1) and spin-spin (T2) relaxation times in a solution are dependent on the correlation time $\tau$, which is a characteristic time for the random motions of molecules in solution [2]. In this study, the spin-lattice and spin-spin relaxation times of seven peaks at the proton spectrum of a chiral Schiff base [3] derivative in DMSO-d$_6$ (Fig. 1) were studied at 298 K with a Bruker Avance 400 MHz $^1$H-NMR spectrometer. From R1/R2 ($R_1=1/T_1$, $R_2=1/T_2$) ratio, which is pertaining to dipolar interactions, following equation was obtained [4].

This equation was used to find correlation time $\tau$. The estimated $\tau$ values were ranged from 0.4 ns to 1 ns. It suggested that molecular tumbling is a dominant mechanism for the relaxation. Moreover, the selected title molecule, C$_{24}$H$_{26}$N$_2$O$_5$, was investigated via Density Functional Theory (B3LYP/6-311++G**) [5] to determine its structural and energetic properties.

**Keywords:** Kiral Schiff base, T1 and T2 relaxation times, correlation time.
Secondary Metabolites and Antioxidant Activity of \{Limonium duriusculum\} (de Girard) Kuntze Extracts

Fadila Benayache\(^1\), Messaoud Kerkatou\(^1\), Azzedine Salah Redouane\(^2\), Francisco León\(^3\), Ignacio Brouard\(^3\), Ahmed Menad\(^2\), Djamel Sarri\(^4\), Souad Ameddah\(^2\), Samir Benayache\(^1\)

\(^1\)Unité de Recherche: VARENBIOMOL, Université Frères Mentouri, Constantine 1, Algeria
\(^2\)Laboratoire de Biologie et Environnement, Université Frères Mentouri Constantine 1, Algeria
\(^3\)Instituto de Productos Naturales y Agrobiología, CSIC, Av. Astrofísico Fco. Sánchez, 3, 38206 La Laguna, Tenerife, Spain.
\(^4\)Département de Biologie, Faculté des Sciences, Université Mohammed Boudiaf, 28000, M’Sila, Algeria.

Introduction: Many species of the genus *Limonium* are used in folk and modern medicine and are rich sources of flavonoids [1]. We report in this study, the chemical composition of the chloroform, ethyl acetate and n-butanol soluble parts of the H\(_2\)O-MeOH extract of the aerial parts of *Limonium duriusculum* (de Girard) Kuntze [2], collected from the area of Mila in the North-East Algeria and the antioxidant properties of n-BuOH extract using different assay systems.

Materials and Methods: Air-dried aerial parts of *Limonium duriusculum* (5 kg) collected during the flowering stage were macerated at room temperature with MeOH–H\(_2\)O (70:30, v/v) for 24 h, three times. After filtration, the filtrate was concentrated and dissolved in H\(_2\)O (2 L). The resulting solution was extracted successively with CHCl\(_3\), EtOAc and n-BuOH. The organic phases were dried with Na\(_2\)SO\(_4\), filtered and concentrated in vacuum (up to 35°C) to obtain the extracts: CHCl\(_3\) (5.47 g), EtOAc (50.06 g) and n-BuOH (63.64 g). The three extracts were fractionated by CC (silica gel). The obtained fractions were purified on TLC silica gel plates giving 8 pure compounds. The antioxidant activity of the n-BuOH extract was evaluated by 1,1-diphenyl-2-picrylhydrazyl (DPPH°) free radical scavenging assay, ferrous chelating effect and inhibition of lipid peroxide (LPO) formation induced by Fe\(^2+\)/ascorbic acid system.

Results and Discussion: The structures of the isolated compounds which were identified as: β-sitosterol 1, methyl gallate 4-methyl ether 2, gallic acid 4-methyl ether 3, methyl gallate 4, vanillic acid 5, gallic acid 6, apigenin 5, apigenin 7-O-β-D- (6″-methylglucuronide) 6, pinoresinol 7 and 3β,5,6,7,8,3′,4′-heptahydroxyflavanone 8, were established by spectral analysis, mainly ESIMS, UV and 2D-NMR experiments (COSY, HSQC, HMBC and ROESY). Compound 8 was new, we named it duriusculine while, apigenin 5, was the major constituent of the three extracts (more than 3 g in 22 g of the EtOAc extract). The n-BuOH extract exhibited significant antioxidant activity.

References

Keywords: Flavonoids; Phenolic compounds; \{Limonium duriusculum\}; Plumbaginaceae; Antioxidant activity.
Molecular Dynamic and Complexation Study of A Chiral Schiff Base Derivative by 400 MHz $^1$H-NMR

Aliye Araç¹, Arzu Ekinci², Mehmet Çolak³, Nadir Demirel⁴, Mehmet Zafer Köylü⁵

¹Department of Physics, Faculty of Sciences, Dicle University, Diyarbakır, TR21280 Turkey
²Department of health school, Siirt University, Siirt, TR56100 Turkey
³Department Chemistry, Faculty of Sciences, Dicle University, Diyarbakır, TR21280 Turkey
⁴Department Chemistry, Faculty of Sciences, Ahi Evran University, Kırşehir, TR40100 Turkey
⁵Department of Physics, Faculty of Sciences, Dicle University, Diyarbakır, TR21280 Turkey

In this study, Molecular dynamic properties and complexation of a Chiral Schiff Base Derivative (S,E)-4-((2-hydroxy-1,2,2-triphenylethylimino)methyl)phenol with D, L-phenylalanine methyl ester hydrochloride salts were investigated. Proton spectrum of S3 ligand was taken for molecular study, relaxation times were measured at room temperature (25 °C) for each peak with 400 MHz Avance Bruker NMR spectrometer. correlation time values were found 10⁻⁹ s for all peaks. This value indicates that molecule is acting as a whole and is making molecular tumbling. For complexation (host-guest) study, Ligand solution was kept constant and taking D, L-phenylalanine methyl ester hydrochloride salt solution at different concentrations titration measurements were made. 1/[Go] versus 1/∆δ graphic was plotted from the chemical shift values and binding constants (Ka), enantioselectivity rates (KaL/KaD) and free energy changes (-∆Go) were found. D-enantiomer against to L-enantiomer shows 1.8 times better enantioselectivity (2-3).

Keywords: Kiral Schiff-base, T1 and T2 relaxation times, correlation time, titration
P-055

The use of X Fluorescence to Characterize Sludge of Treatment Plants

Wassila Cheurfi, Hassina Bougherara, Brahim Kebabi

Department of chemistry, Constantine Mentouri University, Constantine, Algeria

The objective of this study is use of X-ray fluorescence as an alternative to atomic absorption for determination of pollution’s degree of sludge treatment plants for its recovery. In contrast to other analysis techniques which allow for analysis only after selective extraction step by appropriate reagents, X-ray fluorescence allows to study directly the solid sample. In addition, atomic absorption can do quantitative analysis of only one item at a time, while the X-ray fluorescence allows in a single experiment a qualitative and quantitative analysis for all elements of the periodic table except hydrogen, lithium and beryllium, the analysis of light elements (boron, carbon, nitrogen and oxygen) is sensitive. In this study we analyzed sewage treatment plant’s sludge Ibn Ziad Constantine by spectrophotometer of X-ray fluorescence Panalytical Epsilon 3. This analysis allowed us to identify the following elements in our sludge: Mg, Al, Si, P, S, Cl, K, Ca, Ti, V, Cr, Mn Fe, Ni, Cu, Zn, Ga, As, Se, Br, Rb, Sr, Y, Zr, Ba, Pb. Present elements which the limit content is regulated are: chromium, copper, nickel, lead and zinc. They are respectively present with the following concentrations: 0.45 mg/g, 0.48 mg/g, 0.11 mg/g, 0.35 mg/g and 2.7 mg/g. None of these concentrations exceeds the limit authorized by the regulations. However, the sludge produced by treatment plant Ibn Ziad Constantine can be spread only with a quantity less than 16.6 tons in ten years (1.66 tones/year) because the flow limit allowed on ten years of chromium, copper, nickel, lead and zinc are respectively: de 15 kg/ha, 15 kg/ha, 3 kg/ha, 15 kg/ha, 45 kg/ha.

Keywords: X-ray fluorescence, treatment plants, sludge, trace element
Secondary metabolites are sought-after because they are well-known for their numerous biological activities that promote health effects. These activities include antibacterial, anticancer, antifungal and antioxidant used in industrial sectors of agriculture, food and pharmaceuticals.

In this perspective, we are interested to the phytochemical study of Vitex agnus-castus which appears to the Vitex genus and Verbenaceae family. This species is widely found in the Algerian Sahara where aerial parts are used in traditional medicine. For that reason, the objective of this work was motivated to study the secondary metabolites of Vitex agnus-castus species. After maceration of the aerial parts in a hydro-alcoholic system EtOH / H₂O (7/3), concentration of the solution followed by a liquid-liquid extraction with solvents of increasing polarity namely CHCl₃, EtOAc and n-butanol successively, we have submitted the ethyl acetate extract to the chromatographic battery to separate and purify the existing products.

The structural elucidation of the isolated products was carried out by combining different spectral methods as UV visible spectrophotometry, ¹H NMR and ¹³C NMR spectroscopy as well as mass spectrometry.

**Keywords:** Vitex agnus-castus, phytochemistry, spectroscopic methods.
Visible fluorescence from Pr\textsuperscript{3+} doped KYF4 single crystal

Adel Bitam

Serssouf Tamanrasset, Algeria

The present work reported a Judd-Ofelt analysis of spectroscopic and lasers parameters of Pr\textsuperscript{3+} ions in crystal hosts. Rare earth-doped fluoride single crystals are considered to be an important class of optical device materials due, mainly, to their low phonon energies. They play a very significant role in the development of laser amplifiers for optical communications. Among the rare earth, trivalent praseodymium ions (Pr\textsuperscript{3+}) have potential for laser applications due to a large number of available energy levels in the visible and near infrared domains.

We have studied the optical properties of Pr\textsuperscript{3+} doped KYF\textsubscript{4} single crystal from the KF – YF\textsubscript{3} pseudo-binary system. Room temperature absorption spectra were recorded in order to investigate optical properties by using the Judd-Ofelt (JO) analysis. The emission spectra, associated to 3P\textsubscript{0} to 3H\textsubscript{6} and 3F\textsubscript{2} levels, have been registered between 560 and 700 nm. They have been calibrated in emission cross-sections using the usual Fuchtbauer-Ladenburg formula. We have also determined the 3P\textsubscript{0} fluorescence lifetime to be compared to the radiative lifetime given par the JO calculation.

Keywords: absorption spectra, rare earth trivalent ion (Pr\textsuperscript{3+}), Judd-Offelt Analysis, emission spectra, fluorescence lifetime.
Computational Studies on Structure and Spectroscopic Properties of 1′,3′-Dihydrospiro[cyclohexane-1,2′-[2H]imidazo[4,5-b]pyridine]

Hatice Vural¹, Mehmet Kara²

¹Department of Electrical and Electronics Engineering, Faculty of Technology, Amasya University, Amasya, Turkey
²Department of Mechanical Engineering, Faculty of Technology, Amasya University, Amasya, Turkey

The optimized molecular geometry and vibrational frequencies of 1′,3′-Dihydrospiro[cyclohexane-1,2′-[2H]imidazo[4,5-b]pyridine] were calculated using Hartree Fock (HF) and Density Functional Theory (DFT) methods. Gauge-independent atomic orbital (GIAO) 1H and 13C nuclear magnetic resonance (NMR) chemical shift values of the 1′,3′-Dihydrospiro[cyclohexane-1,2′-[2H]imidazo[4,5-b]pyridine] were calculated using DFT/B3LYP/6-31G + (d, p). The electronic properties such as HOMO-LUMO energies, absorption wavelengths and excitation energy were investigated by time dependent DFT (TD-DFT) method with integral equation formalism-polarized continuum model (IEF-PCM). The mulliken charges on the atoms and second-order interaction energies were derived from NBO analysis. The electric dipole moment, the mean polarizability and the mean first hyperpolarizability values were also computed by using the DFT method.

Keywords: HF; DFT; IR; UV-Vis; NMR; NLO
Experimental and Theoretical Studies of (FTIR, FT-NMR, UV–Visible, X-ray and DFT) 2-(4-Allyl-5-pyridin-4-yl-4H-[1,2,4]triazol-3-ylsulfanyl)-1-(3-methyl-3-phenyl-cyclobutyl)-ethanone

Cigdem Yuksektepe Ataol¹, Öner Ekici²

¹Department of Physics, Cankiri Karatekin University, Cankiri, Turkey
²Department of Chemistry, Firat University, Elazig, Turkey

The single crystal structure, 2-(4-Allyl-5-pyridin-4-yl-4H-[1,2,4]triazol-3-ylsulfanyl)-1-(3-methyl-3-phenyl-cyclobutyl)-ethanone, has been synthesized and characterized by IR, NMR, UV spectra and X-ray diffraction methods. In addition, the optimized structure, the vibrational assignments, the chemical shifts, the molecular orbital energies, molecular electrostatic potential maps and thermodynamic properties, ionization potential, electron affinity, electronegativity, global chemical hardness and chemical softness of the molecule have been investigated by using Density Functional Theory with B3LYP/6-31G(d) and B3LYP/6-311G(d, p) basis sets. UV–Visible spectrum of the compound was recorded and the electronic properties HOMO and LUMO energies were measured by time-dependent TD-DFT approach. The observed results of the compound have been compared with theoretical results and it is found that the experimental data show good agreement with calculated values. The single crystal structure of the compound crystallizes in the monoclinic system with space group C 2/c.

Keywords: Pyridin Triazole Single crystal Density Functional Theory Vibrational assignment

The contour map of electrostatic potential of the total density of the title compound by B3LYP/6-311G(d, p).
Synthesis, Crystal Structure, Spectroscopic and Electronic Properties of (E)-Trans-2-(2-(Biphenyl-4-ylmethylene)Hydrazinyl)-4-(3-Methyl-3-Phenylcyclobutyl)Thiazole

Cigdem Yuksektepe Ataol¹, Nezihe Caliskan², Ibrahim Yılmaz³, Alaaddin Cukurovali⁴

¹Department of Physics, Cankiri Karatekin University, Cankiri, Turkey
²Department of Physics, Gazi University, Ankara, Turkey
³Department of Chemistry, Karamanoglu Mehmetbey University, Karaman, Turkey
⁴Department of Chemistry, Firat University, Elazig, Turkey

A new compound of (C²⁷H₂₅N₃S) has been synthesized and characterized by ¹H NMR, ¹³C NMR, IR, UV-Visible spectroscopy, and single crystal X-ray diffraction.

The compound crystallizes in the monoclinic space group P2₁/c and crystals of (I) were found approximately 0.5:0.5 ratio to be twinned. The crystal structure is stabilized by N–H...N intermolecular hydrogen bonding. In addition to the molecular geometry and dimeric structure from X-ray experiment, the optimized molecular geometry for monomer and dimer, vibrational frequencies, atomic charges distribution, and total energies of the title compound in the ground state have been calculated using ab initio method. Density Functional Theory (B3LYP) and Hartree-Fock (HF) methods with basis sets 6-31G(d, p) and 3-21G were used in the calculations. Calculated frequencies are in good agreement with the corresponding experimental data. UV-Vis absorption spectra of the compound have been ascribed to their corresponding molecular structure and electrons orbital transitions.

Keywords: Hydrazine Single crystal ab initio calculations

a) ORTEP drawing of the basic crystallographic unit, showing the atom-numbering scheme, b) Gaussian03View drawing of the title compound with monomer, c) with dimer
P-061

Spectroscopic Investigation, Structural and Electronical Analysis of 2-(4-ethoxyphenyl)Isoindoline-1,3-dione by Experimental and Theoretical approach

Gülcan Duru¹, Meryem Evecen¹, Hasan Tanak¹, Erbil Ağar²

¹Physics Department, Faculty of Arts and Sciences, Amasya University, 05100 Amasya, Turkey
²Department of Chemistry, Faculty of Arts and Sciences, Ondokuz Mayıs University, 55139 Kurupelit, Samsun, Turkey

2-(4-ethoxyphenyl)isoindoline-1,3-dione has been synthesized and characterized by IR, UV–Vis, and X-ray single-crystal determination. FT-IR spectra of title molecule has been recorded in the region 4000–400 cm⁻¹. The molecular structural parameters and vibrational frequencies of the fundamental modes have been calculated by density functional theory (DFT) technique in the B3LYP approximation with 6-311G(d,p) basis set. The computed values of frequencies are scaled using multiple scaling factors to yield good coherence with the observed values. By using TD-DFT method, electronic absorption spectra of the title compound have been predicted and a good agreement with the TD-DFT method and the experimental one is determined. Also, molecular electrostatic potential (MEP) and Mulliken's charges analysis have calculated and reported.

Keywords: DFT, FT-IR, HOMO, LUMO

Figure 1
Study on Molecular Structure, Spectroscopic Behavior, HOMO–LUMO and NMR Analysis of 2-(3-o-Tolyl-4-oxo-3,4-dihydroquinazolin-2-ylthio) Acetohydrazide Using Theoretical Approaches

Meryem Evecen, Murat Karabulut

Physics Department, Faculty of Arts and Sciences, Amasya University, 05100 Amasya, Turkey

Quinazolinone derivatives display a wide range of biological and pharmacological activities. In this work, 2-(3-o-Tolyl-4-oxo-3,4-dihydroquinazolin-2-ylthio)acetohydrazide has been characterized by IR, UV–Vis, and X-ray single-crystal determination. The molecular structural parameters and vibrational frequencies performed by density functional theory (DFT) technique in the B3LYP/6-311++G(d,p) and Hartree Fock (HF)/6-311++G(d,p) level of theory. The computed values of frequencies are scaled using multiple scaling factors to yield good coherence with the observed values. The chemical shift values of the title molecules are calculated using GIAO method and compared experimental results. In addition, the electronic properties, absorption wavelengths, excitation energy, dipole moment, molecular electrostatic potential (MEP) and frontier molecular orbital energies are performed. Besides, thermodynamic properties (heat capacity, entropy and enthalpy) of the title compound at different temperatures are calculated.

Acknowledgment

This study was supported financially by the Research Centre of Amasya University (Project No: FMB-BAP 15-092).

Keywords: DFT, FT-IR, HOMO, LUMO, NMR.
P-063

First Principles Study of Magnetic, Charge, and Orbital Ordering in LuFe$_2$O$_4$

Hayet Si Abdelkader, Houda Imane Faraoun

Laboratory of Materials Discovery, Unit of Research Materials and Renewable Energies, LEPM-UR-MER, Abou Bekr Belkaid University - Tlemcen, Algeria

We present a computational study to investigate the magnetic, charge, and orbital ordering of LuFe$_2$O$_4$. The calculations are performed with first-principles density functional theory as implemented in the pseudopotential and the full-potential linearized-augmented plane-wave approaches. We have carried out calculations for paramagnetic, ferromagnetic, ferrimagnetic and antiferromagnetic configurations. The calculations give ferrimagnetic ordering as the most favored one, in agreement with experiments.

Keywords: First-principles calculations, LuFe$_2$O$_4$, Charge–orbital ordering, Magnetic ordering
**Poster Abstracts**

**P-064**

**Spectroscopic (IR, Raman, NMR), Thermal and Theoretical (DFT, AIM) Study of Alkali Metal Dipicolinates (2,6-pyridinedicarboxylates) and Quinolinates (2,3- Pyridinedicarboxylates)**

Grzegorz Swiderski¹, Sławomir Wojtulewski², Leszek Siergiejczyk², Agnieszka Zofia Wilczewska², Iwona Miształewska², Renata Swislocka¹, Włodzimierz Lewandowski¹

¹Division of Chemistry, Białystok University of Technology, Wiejska Street, 45E, 15-351 Białystok, Poland
²Institute of Chemistry, University of Białystok, Ciolkowskiego Street 1K, 15-245 Białystok, Poland

Quinolinic acid (2,3-pyridinedicarboxylic, QA) and dipicolinic acid (2,6-pyridinedicarboxylic, DPA) these are two of the six isomeric pyridinedicarboxylic acids. They are important ligands with high biological importance. Quinolinic acid is one of the final products of tryptophan transformation in the kynurenine pathway. In pathological conditions, the elevated concentration of this acid causes strong neurotoxicity [1]. QA neurotoxicity is suspected to be caused partly by the over-excitation of the N-methyl-D-aspartate (NMDA) receptor and partly by elevated levels of cytotoxic reactive oxygen species (ROS) in the brain tissue [2].

Dipicolinic acid and its salts are a major component of the bacterial spores. These substances increase the resistance of the spores to UV radiation [3], and are also improve the stability of disputes and improve germination.

In this work the thermal, theoretical (DFT) and spectroscopic (IR, Raman, NMR) properties of alkali metal complexes with quinolinic acid (2,3-pyridinedicarboxylic acid) and dipicolinic acid (2,6-pyridinedicarboxylic acid) were studied. The IR and Raman spectra were registered and analyzed in the range of 400–4000 cm⁻¹.¹H NMR and ¹³C NMR spectra of analyzed compounds have been registered and assigned. The electronic charge distribution for the studied acids and their salts with lithium, sodium and potassium was calculated. All the calculations were done in the frame of density functional theory (DFT) using 6–311++G(d,p) basis set. The thermal decomposition of the analyzed compounds was done.

This work was supported by the S/WBiS/1/2012

References


**Keywords:** quinolinic acid, dipicolinic acid, pyridinedicarboxylic acid,
Physico-chemical (Spectroscopic: FT-IR, Raman and UV) Studies of Caffeic Acid and Fe(III), Cu(II), Zn(II), Ni(II) Caffeinates

Renata Swislocka, Mariola Samsonowicz, Małgorzata Kowczyk Sadowy, Grzegorz Swiderski, Włodzimierz Lewandowski

Division of Chemistry, Faculty of Civil and Environmental Engineering, Bialystok University of Technology, Wiejska 45E, 15-531 Bialystok, Poland

Caffeic acid, one of the most widespread in the plant world hydroxycinnamic acid derivatives, has numerous bioactive and health-improving properties. Caffeic acid is known for its antioxidant properties [1-3].

The aim of this study was to investigate the physicochemical properties of caffeic acid (3,4-dihydroxycinnamic acid) and its complexes with transition metals. Metals selected for the study, i.e.: the iron(III), copper(II) and zinc(II) play an important role in biological systems. The spectroscopic properties of caffeic acid complexes were studied using infrared spectroscopy (FT-IR), Raman spectroscopy (FT-Raman) and electronic absorption spectroscopy (UV / Vis).

Studies of differences in the number and position of bands from experimental and theoretical IR, Raman, UV/VIS spectra lead to conclusions concerning the distribution of electron charge in molecule, the delocalization energy of π electrons and the reactivity of ligands in metal complexes [4]. In the last few years there has been a growing interest in the understanding of the mechanisms associated to the biochemical role of phenolic compounds, which, in turn, was found to be strongly dependent on their structural characteristics.

This work was supported by the National Science Centre, Poland (grant no. 2014/13/B/NZ7/02352).

References

Keywords: Caffeic acid, spectroscopic, caffeinates
Determination of Some Metals in Honey Samples with a new Synthesized Resin by Flame Atomic Absorption Spectrometry

Teslima Daşbaşı¹, Şerife Saçmacı², Nevin Çankaya³, Cengiz Soykan³

¹Department of Food Technology, Gemerek Vocational School, Cumhuriyet University, Sivas, Turkey
²Department of Chemistry, Faculty of Sciences, Erciyes University, Kayseri, Turkey
³Department of Material Science and Nanotechnology, Faculty of Engineering, Uşak University, Uşak, Turkey

Trace metals are permanent in the environment, and thus readily accumulate to toxic levels [1]. In recent years, trace metals of interest include those that are naturally incorporated in the food matrix in addition to contributions from atmospheric deposition, agricultural chemicals, processing and environmental contamination [3]. Excessive accumulation of trace metals in the human body such as liver and kidney may result in serious systemic health problems [4]. Therefore, amounts of trace metals in food samples may be determined successfully for human health [5]. On the other hand, the direct determination of trace metals is limited for their low concentrations and matrices. Because of this, determination of trace elements in food samples needs the separation/preconcentration procedures [4, 5].

In this study, we report a simple and rapid solid phase extraction (SPE) method for the separation/preconcentration and determination of some metals by FAAS. A new chelating resin, poly[2-(4-methoxyphenylamino)-2-oxoethyl methacrylate-co-divinylbenzene-co-2-acrylamido-2-methyl-1-propanesulfonic acid] (MPAEMA-co-DVB-co-AMPS) (MDAP) was synthesized for SPE and, characterised by elemental analysis, infrared spectra. The MDAP resin was used as packing for the column on a SPE method for Cd(II), Co(II), Cr(III), Cu(II), Fe(III), Mn(II), Pb(II), and Zn(II) ions determination. The parameters influential on the determination of analyte ions were studied. Under the optimum conditions, the limits of detection of the method for analyte ions were found (3σ) in the range 0.9−2.2 μg L⁻¹ (n = 21), preconcentration factor of 200, and the relative standard deviation of ≤ 2% were achieved (n = 11). The developed method was performed for the determination of analyte ions in some honey samples and standard reference materials.

References

Keywords: Trace Elements, Solid Phase Extraction, Chelating Resin, FAAS, Honey Samples
Propolis is a natural substance collected by honey bees (Apis mellifera) in various plant species. The chemical content of propolis is very complex. Some factors, such as the botanical origin of propolis and its collection time may influence the chemical feature of this resinous material. The aim of this study is to determine the total phenol-flavonoid and antioxidant activities of two propolis samples from Trabzon region. Analyses of samples were performed according to the procedure described in the literature [1-5]. The botanic origins of propolis samples are evaluated as Castanea sativa and mixed. Both propolis samples showed significant antioxidant activities. Free radical scavenging activities were given as SC50 values (µg/mL). According to the obtained results, mixed sample has the highest free radical scavenging activity (21.65 ± 0.43). Others: RUT (17.86 ± 0.08)>C. sativa (17.02 ± 0.20) >TOC (11.63 ± 0.94)>BHA8.33 ± 0.18. Hydrogen peroxide scavenging activities of mixed, C. sativa, BHA, TOC, RUT were found to be 27.86 ± 1.09, 37.45 ± 0.96, 196.08 ± 1.77, 222.22 ± 1.40, 125 ± 0.29 respectively. The metal-chelating activities (%) were in the following order: Mixed (88.08 ± 0.10) > C. sativa (87.60 ± 0.14) > TOC(86.07 ± 0.17) > RUT (85.10 ± 0.85)BHA (76.36 ± 1.39). In addition, mixed and C. sativa total phenol amount 2.55 ± 0.04, 2.49 ± 0.01mg GAE/100 g; total flavonoid amount 0.622 ± 0.01, 0.642 ± 0.11, respectively.

References


Keywords: Botanic origin, Propolis, Antioxidant activity, Phenol, Flavonoid, Trabzon.
Essential trace metals such as Fe, Zn, Cu, Cr, Co and Mn play an important role in human metabolism. Some other metals such as Pb and Cd are toxic even at low levels and have a direct and adverse influence on various biological processes [1, 2]. A gradual increase in total and/or plant available trace metal concentrations of agricultural soils in recent years has been reported in industrialized countries. The results of analyses in various studies are showed that atmospheric deposition, fertilizers, manures (feed additives), industrial by-product wastes and sewage sludges all to be significant contributors to the annual additions to soils of heavy metals [3]. Hence, amounts of trace and essential metals in food samples may be determined successfully for human health [4].

In this study, a simple and rapid solid phase extraction/preconcentration procedure was developed for the determination of Cd(II), Co(II), Cr(III), Cu(II), Fe(III), Mn(II), Pb(II), and Zn(II) ions by FAAS. A new chelating resin, poly (N-cyclohexylacrylamide-co-divinylbenzene-co-2-acrylamido-2-methyl-1-propanesulfonic acid (NCA-co-DVB-co-AMPS) (CDAP name more suit all the manuscript because its short) was synthesized and characterized. The analytical parameters such as pH of the sample solution, type and concentration of eluent, flow rates of the eluent and sample, volume of the eluent, and interference ions were examined. The limit of detection (LOD) of analytes were found (3s) in the range 0.65 and 1.9 µg L⁻¹, preconcentration factor of 200, and the relative standard deviation of ≤ 2% were achieved (n = 11). The developed method was performed for the determination of analyte ions in some dairy samples and certified reference materials.

References


Keywords: Solid phase extraction, Metal ions, Chelating resin, FAAS, Dairy samples
Spectroscopic (IR, Raman, NMR), Theoretical and Biological Study of Cinnamic, Coumaric, Caffeic and Chlorogenic Acids and Their Complexes with Copper(II)

Wlodzimierz Lewandowski¹, Renata Swislocka¹, Grzegorz Swiderski¹, Monika Kalinowska¹, Mariola Samsonowicz², Hanna Lewandowska²

¹Division of Chemistry, Faculty of Civil and Environmental Engineering, Białystok University of Technology, Wiejska 45E, 15-531 Białystok, Poland
²Institute of Nuclear Chemistry and Technology, Dept. of Radiobiology and Health Protection, Dorodna 16, 03-195 Warsaw, Poland

In our previous papers we investigated the influence of the chosen metals on the electronic system of biologically important ligands, such as benzoic, salicylic and nicotinic acids [1-3]. We also investigated the correlation between the molecular structure and biological activity of ligands and their metal complexes. Our present work is a part of a broader project undertaken in order to improve the selectivity and activity of the chosen drugs and natural antioxidants and nature-derived anticancer agents via their complexing with metals. In this work we selected the logical series of ligands: cinnamic, coumaric, caffeic and chlorogenic acids that characterise with the extended conjugated bond system with systematically increasing number of hydroxyl groups and other substituents and their mutual positions. All the mentioned ligands are biologically important in view of their antioxidative and anticancer properties. We addressed a question, how the additional donor groups and the changes of the electronic charge distribution influence the biological activity. Additionally we examined the influence of the complexation with copper on the molecular structure changes and biological activity of ligands. The experimental methods applied included the IR, Raman spectroscopies, ¹H, ¹³C NMR, UV/VIS, theoretical methods and as well the methods for biological activity determination.

This work was supported by the National Science Centre, Poland (grant no. 2014/13/B/NZ7/02352).

References:

Keywords: cinnamic acid, coumaric acid, caffeic acid, chlorogenic acid
Electron Paramagnetic Resonance (EPR) Study of Nano Sized Emulsions

Dilek Kılár, Maral Sunnetcioglu

Department of Physics Engineering, Hacettepe University, 06800 Beytepe, Ankara, Turkey

In our previous studies we investigated drug–phospholipid interactions using liposomes and various drugs. These studies are important to understand drug behaviour until it reaches its target point. The effects of size on these interactions were investigated at room temperature using nano-sized emulsions of dipalmitoyl phosphatidylcholine (DPPC) in presence and absence of cholesterol (CHO), tween 80 and clomipramine (CLO). Studies were performed using Electron Paramagnetic Resonance (EPR) spin labeling technique. 4-amino-2,2,6,6-tetramethyl-1-piperidinyloxy (TEMPAMINE) spin probe and 5- and 16- doxyl stearic acid (5-DS and 16-DS) spin labels were used to follow the changes in the head group and alkyl chain. The EPR parameters of the studied samples were determined both directly from the spectra and also using a simulation programme. The size of the prepared emulsions was determined using photon-correlation spectroscopy. As expected the size of the emulsions were decreased and their stability increased in presence of tween 80. In presence of tween 80 the hyperfine splitting constants were decreased and correlation times increased. CLO caused some changes in the head grup region for the samples without tween 80.

Keywords: emulsion, clomipramine, EPR spin labeling.
Structural Properties of Neutral 2D Aun (n=4-13) Clusters: A Comparative Study of MD and DFT Calculations

Sertan Kurnalı, Meral Eryürek

Department of Physics, Bülent Ecevit University, Zonguldak, Turkey

Gold clusters have contemporary important roles as they have been started to be used in nanoelectronic devices, medicine, chemical catalysts and also used for lithography. As a result, in some recent works the planar geometries of Au clusters have been obtained theoretically and experimentally. In this work, the 2D neutral Aun (n=4-13) cluster geometries with the minimum energies are obtained and 2D global and first three isomers of Aun (n=4-13) clusters have been investigated by steepest descend, basin hopping and simulated annealing methods in MD by using Gupta potential. These obtained structures have been also calculated with DFT using B3LYP functional with LANL2DZ core potential basis set. Some of 2D MD geometries have yielded to same isomers in DFT calculations at the same point of local minima. The electronic energies, bond lengths, and vibrational spectrum of the clusters are calculated by the DFT calculations. The spectroscopic changes in the isomers have been observed and modes with the output of highest intensity have been visualized. The HOMO-LUMO energy gaps for the isomers have been also calculated and visualized.

Keywords: 2D Aun clusters, MD calculations, DFT calculations.
The Spectroscopic and Micro-tomographic Analysis of Calcifications in Spinal Ligaments

Sylwia Natalia Orzechowska¹, Andrzej Wróbel¹, Eugeniusz Rokita²

¹Institute of Physics, Jagiellonian University, Łojasiewicza 11, Kraków, Poland
²Department of Biophysics, Jagiellonian University Medical College, św. Łazarza 16, Kraków, Poland

The mineralization of spinal ligaments is observed as a complication of certain diseases like myelopathy and radiculopathy. Calcification of the ligamentum flavum (LF) is a rarely reported alteration. The aim of our study was the physico-chemical and morphological analysis of the calcium deposits in LF. The structural analysis of deposits may be used to explain the possible connection between crystal formation and spine ailments and to find the factors affecting the mineralization process.

The studies were carried out on 24 surgically removed LF samples. The samples were obtained from 15 patients who underwent surgeries because of the spinal canal stenosis and 9 patients who sustained spinal traumata (control). The ligament samples were examined using the micro-computed tomography technique, X-ray fluorescence, X-ray diffraction and Fourier transform infrared spectroscopy methods.

The mineral deposits were present in 14 of 24 LF samples, both in stenosis and in control groups. The mineral grain has the heterogeneous structure and consists of a calcified phase and an organic material. The volumes of minerals per 100 mm³ of the samples equal to 0.0002-0.5 % for the stenosis group and range 0.0001-0.2 % for controls. The percentage of the inorganic phase in LF minerals ranged from 10% to 80%. The average grain density is identical in both groups and equaled to (2.0 ± 0.2) g/cm³. The elemental concentrations were almost indentical in all samples. The crystallographic results showed that hydroxyapatite is the predominant crystalline phase. In two samples (stenosis group) the calcium pyrophosphate dihydrate was identified. The infrared spectra were in good agreement with crystallographic data. The presence of characteristic bands ν3PO4 (1050-1100 cm⁻¹), ν4PO4 (550-600 cm⁻¹), δCO3 (860 cm⁻¹) and ν3CO3 (1400-1450 cm⁻¹) confirms the B-type carbonate-containing hydroxyapatite structure.

The two different chemical structures suggest two independent processes of mineralization. The occurrence of mineral deposits in both groups indicates that this pathology may be independent on the spine diseases. The presence of hydroxyapatite grains in both groups shows that it could be physiological process of soft tissue degeneration that begins at early age. The calcium pyrophosphate deposits are present as a pathological condition accompanying other diseases.

Keywords: calcification, spinal ligaments, micro-CT, physicochemical characterization
Poster Abstracts

Fourier transform infrared absorption spectra for two LF minerals

Rendering of the LF sample from the stenosis group employing two thresholds. A higher value (grey) for the soft tissue and a lower value for the minerals (black). A voxel size of 13.5 micrometers was applied. Black circle marks the region measured with a voxel size of 2 micrometers. Two dimensional cross section of the region is shown in the insert using the above described thresholds.
Electron Impact Double Ionization of Methane Molecule

Aitelhadjali Zakia¹, Quinto M. A², Champion Christophe², Oubaziz Dahbia³, Kessal Salem¹

¹Laboratoire de Sciences Nucléaires et Interaction rayonnement- Matière, Faculté de Physique/ USTHB (Algérie)
²Centre d’études nucléaires de Bordeaux Gradignan / IN2P3/CNRS/ Université de Bordeaux 1 (France).
³Laboratoire de Mécanique Structure et Energétique/ Université Mouloud Mammeri de Tizi-Ouzou (Algérie)

The process of electron impact double ionization of atoms and molecules is of considerable interest in many branches of physics, such as astrophysics or plasma physics. It is also fundamental in life sciences where it is of prime importance to understand the various mechanisms leading to the double ionization in order to be able to fully master energy deposition by radiation in matter.

In the present theoretical study, we provide an accurate description of the electron impact double ionization of methane molecule. This theoretical treatment has been carried out within the plane wave first Born approximation, where the description of the bound states of the impacted molecular target is performed via the one center molecular wave functions reported by Moccia. Two plane wave functions are associated to the incident and scattered electrons while the two ejected electrons are described in terms of two Coulomb wave functions, together with a Gamow factor to take into account the repulsion effect between them.

We report then the fivefold differential cross sections (FDCSs) corresponding to the double ionization of an oriented methane molecule, the two electrons being ejected from the same molecular orbital. We considered three particular molecular orientations given by the Euler angles triplets: \((\alpha, \beta, \gamma) = (0^\circ, 0^\circ, 0^\circ), (0^\circ, 90^\circ, 0^\circ)\) and \((0^\circ, 90^\circ, 90^\circ)\). In a second step, we have calculated the (FDCSs) averaged over all possible orientations of the molecular target. Thus, a strong dependence of the (FDCSs) versus the molecular orientation is reported when considering the case of each molecular orbital. We also pointed out the signature of the main process involved in the double ionization process, namely the shake-off (SO) and the two step1 (TS1) mechanisms.

Keywords: Methane molecule, ionization, molecular orientation
P-074

Investigation of The Effects of Polymerization Temperature on The Latex Properties

**Sedef Sismanoglu**¹, **Ayfer Sarac**²

¹Department of Metallurgical and Material Engineering, Karabuk University, Karabuk, Turkey
²Department of Chemistry, Yıldız Technical University, Istanbul, Turkey

There are four methods to produce industrial polymers such as bulk, solution, suspension, and emulsion. Emulsion polymerization has a lot of advantages than other polymerization techniques [1]. This polymerization contains mainly four ingredients: initiator, monomer, emulsifier and reaction medium [2]. In the emulsion polymerization products, poly(vinyl acetate) emulsion homopolymer and vinyl acetate based emulsion copolymers have a great importance in industrial aspect as well as scientific aspect [3].

In this study, poly(vinyl acetate-co-butyl acrylate) latexes were synthesized by applying semicontinuous emulsion polymerization method. Copolymerizations were carried out keeping constant monomer ratio of vinyl acetate:butyl acrylate as 85:15 at four different temperatures (55°C, 60°C, 65°C and 70°C) and constant stirring rate (350 rpm) with the using of N-methylol acrylamide as protective colloid, ammonium persulfate as thermal initiator, and 30 mole ethoxylated nonyl phenol as nonionic emulsifier. The characterization of synthesized latexes were done by determining solid content, conversion, Brookfield viscosity, particle size, the particle size distribution, surface tension and surface charges of latexes.

**Keywords:** Emulsion polymerization, latex, vinyl acetate-co-butyl acrylate, polymerization temperature
The Comparative Vibrational Spectroscopic Study of Diphenylpyraline Hydrochloride and Cyproheptadine Hydrochloride

Seda Güneşdoğan Sağdinc, Aybüke Diler, Dilek Erdaş

Department of Physics, Kocaeli University, Kocaeli, Turkey

Diphenylpyraline hydrochloride (Di-HCl), (4-(5H-dibenzo [a,d]cyclohepten-5-ylidene)-1-methylpiperidine hydrochloride) is reported as an H1-receptor antagonist, and it is a very important anti-histamine drug, which is used in combination with other active ingredients, for the common cold. Cyproheptadine hydrochloride, (CYP.HCl) 4-(5H-dibenzo[a,d]-cyclohepten-5-ylidene)-1-methylpiperidine hydrochloride, is an antihistaminic, antiserotonergic agent, known to have inhibitory activities for L-type calcium channels.

In this study, the FT-IR and FT-Raman spectra of diphenylpyraline HCl and cyproheptadine HCl have been recorded in 4000-400 cm⁻¹ and 3500-50 cm⁻¹, respectively. The optimized geometry, energies, nonlinear optical properties and vibrational frequencies of these compounds have been determined using the density functional theory (DFT/B3LYP) method with 6-311G**(d,p) basis set.

The comparison of the experimental and theoretical results of diphenylpyraline HCl and cyproheptadine HCl indicate that the density-functional B3LYP method is able to provide satisfactory results for predicting vibrational properties. The experimental and calculated results for diphenylpyraline HCl have also been compared with cyproheptadine HCl.

**Keywords:** Diphenylpyraline HCl, Cyproheptadine HCl, Vibrational spectra
P-076

Quantum Chemical Investigations of (E)-2-[(4-chlorophenyl)iminomethyl]-4-(trifluoromethoxy)-Phenol

Ümit Ceylan1, Yelda Bingöl Alpaslan2, Nuri Öztürk3, Gökhan Alpaslan1, Halil Gökce1, Mustafa Macit4

1Department of Medical Services and Techniques, Vocational High School of Health Services, Giresun University, 28200, Giresun, Turkey
2Department of Biophysics, Faculty of Medicine, Giresun University, 28100, Giresun, Turkey
3Department of Property Protection and Safety, Dereli Vocational High School, Giresun University, 28200, Giresun, Turkey
4Department of Chemistry, Faculty of Arts & Science, Ondokuz Mayis University, 55139, Samsun, Turkey

The crystal structure of the title compound, C14H9ClF3NO2, has been determined by X-ray single crystal diffraction technique (Fig.1.) [1]. Molecular geometry, vibrational wavenumbers, carbon-13 and proton NMR isotropic chemical shifts and UV-Vis. parameters of the compound in the ground state have been calculated using the density functional method (DFT) with 6-311++G(d,p) basis set. The calculated results show that the optimized geometry can well reproduce the crystal structure. In addition, DFT calculations of the compound, total energy, frontier molecular orbital analyses, molecular electrostatic potential (MEP), naturel bonding orbital (NBO) analysis and non-linear optical (NLO) properties were theoretically performed at B3LYP/6-311++G(d,p) level.

Reference:


Keywords: Schiff base ∙ Spectroscopy ∙ DFT ∙ Non-linear optic

Figure 1. The molecular structure of the compound, showing the atom numbering scheme and 40% probability displacement ellipsoids
Synthesis, Experimental Techniques, Spectroscopic Investigations and Quantum Chemical Computational Study of (Z)-N-(2-bromo-3-methylphenyl)-1-(5-nitrothiophen-2-yl) methanimine

Gonca Özdemir Tatı¹, Sümayye Gümüş², Erbil Ağar²

¹Vezirköprü Vocational School, Ondokuz Mayis University, Samsun, Turkey
²Department of Chemistry, Faculty of Arts & Science, Ondokuz Mayis University, Samsun, Turkey

Schiff bases compounds have been widely used due to their potential applications in many fields, such as photochromic and thermochromic properties [2], proton transfer tautomeric equilibria [3], biological and pharmacological activities [4].

The new Schiff base compound, (Z)-N-(2-bromo-3-methylphenyl)-1-(5-nitrothiophen-2-yl) methanimine, C12H9N2O2SBr, was synthesized and characterized by IR, UV-Vis and X-ray diffraction technique. The compound crystallizes in the monoclinic, space group P 21/c with unit cell dimensions a=11.4938(7), b=7.4128(4), c=14.9302(9), V=1268.7(13), Z=4, and wR2=0.089. The molecular geometry was also calculated using the Gaussian 03 software and structure was optimized using the HF and DFT/B3LYP methods with the 6-311++G(d,p) basis set in ground state. Also, using the TD-DFT method, the electronic absorption spectra of the title compound computed in both the gas phase and ethanol solvent. The harmonic vibrational frequencies of the title compound were calculated using the HF and DFT/B3LYP methods with the 6-311G++(d,p) basis set. The calculated results were compared the experimental determination results of the compound. Besides, the molecular electrostatic potential map (MEP), frontier molecular orbitals (FMO) analysis and thermodynamic properties for the title compound were obtained with the same levels of theory. To investigate second order nonlinear optical properties of the title compound, the dipole moment (μ), linear polarizability (α) and first-order hyperpolarizability (β) were computed using the HF and DFT/B3LYP methods with the 6-311++G(d,p) basis set.


Keywords: Schiff Base, X-ray Diffraction (XRD), Non-linear optical properties (NLO), Hartree Fock (HF), Density Functional Theory (DFT).
Synthesis, Crystal Structure, Spectroscopic Characterization and Theoretical Calculations of (Z)-N-(Naphthalen-2-yl)−1-(5-Nitrothiophen-2-yl)Methanimine

Gonca Özdemir Tari¹, Sümeyye Gümüş², Erbil Ağar²

¹Vezirköprü Vocational School, Ondokuz Mayıs University, 55200, Samsun, Turkey
²Department of Chemistry, Faculty of Arts & Science, Ondokuz Mayıs University, 55139, Samsun, Turkey

Schiff bases are used as starting materials in the synthesis of important drugs, such as antibiotics and antiallergic, antiphlogistic, and antitumor substances [1-3]. The newly synthesized Schiff base compound, (Z)-N-(naphthalen-2-yl)-1-(5-nitrothiophen-2-yl)methanimine, C₁₅H₁₀N₂O₂S, was characterized by IR, UV-Vis and X-ray diffraction technique. All of the theoretical calculations have been calculated by the B3LYP level of the density functional method (DFT) with the 6-31G(d) and 6-311++G(d,p) basis set by Gaussian software. The optimized geometric parameters obtained by different methods show best agreement with the experimental values. UV-Visible absorption spectra of the title compound dissolved in ethanol were recorded and computed using the time dependent density functional theory (TD-DFT). The harmonic vibrational frequencies of the title compound were calculated using the same method with the 6-31G(d) and 6-311++G(d,p) basis sets. Finally the calculated results were compared to simulated IR and UV-Vis spectra of the title compound which show good agreement with recorded spectra. The stability of the title compound, related to hyper-conjugative interactions and charge delocalization were evaluated using natural bond orbital (NBO) analysis. The thermodynamic properties at different temperatures are also calculated using the same methods with the 6-31G(d) and 6-311++G(d,p) basis sets. The results reveals the standart heat capacity, enthalpy and entropy increases with rise in temperature. The Mulliken population method and natural population analysis (NPA) have been calculated. The other molecular properties like frontier molecular orbital (FMOs) analysis, the molecular electrostatic potential (MEP) map and the nonlinear optical properties (NLO) for the title compound were obtained by using same basis sets.


Keywords: Schiff Base, X-ray Diffraction, FT-IR and UV-Vis Spectroscopy, Thermodynamic properties
Preconcentration of trace metals on Amberlite XAD-7 resin and determination by X-ray fluorescence

Hassina Bougherara, Somia Zerouel, Brahim Kebabi

Department of chemistry, Constantine Mentouri University, Constantine, Algeria

The aim of this study is the use of X-ray fluorescence for dosing chemical elements which have too small concentrations to be detected by conventional techniques. In a first step, elements to analyze are concentrated on resin. The analysis of this resin before and after adsorption of micropollutants allows to identify them. This technique can be used for analysis an isolated element or set of chemical elements. Ion preconcentration Cr\textsuperscript{3+} in column of 5 cm containing Amberlite XAD-7 and the use of fluorescence spectrophotometer X Panalytical Epsilon 3 has allowed us to dose solutions of Cr\textsuperscript{3+} with initial concentration of 1. 10-09 M. Direct analysis per X-ray fluorescence of tap water From Constantine city (Algeria) allowed to detect following elements: Mg, Si, P, S, Cl, K, Ca and Pb. In a second phase, we identify by X-ray fluorescence the present elements in drinking water of Constantine city after preconcentration in column of 10 cm XAD-7 amberlite. The results show the presence of following elements: Mg, Si, P, S, Cl, K, Ca, Mn, Fe, Cu, Zn, As, Br, Re, and Pb.

Keywords: X-ray fluorescence, drinking water, chromium, Trace elements
Clusters play an important role in understanding the transition from microscopic to macroscopic structures of matter [1]. Thus, by studying the properties of clusters as a function of size, the evolution of bulk properties can be revealed. In addition, atomic clusters have unique size specific properties that differ from their bulk systems. Clusters of atoms can adopt different atomic arrangements from bulk materials. Consequently, materials synthesized by assembling clusters are technologically important [2].

To determine the global minimum structure of InAu6− we carried out ab initio calculations at different levels of theory. We first performed an unbiased global minimum search for the InAu6− cluster using the CK method [3] at the PBEPBE/3-21G level of theory. Isomers were reoptimized using the PBEPBE, BP86, MP2, TPSS and M06-L functionals and SDD basis sets. All the geometry structures were fully optimized under given symmetry and the nature of the stationary points was checked by vibrational frequency calculations by using Gaussian 09 [4].

The experiment was carried out using a magnetic-bottle PES apparatus equipped with a laser vaporization cluster source, details of which were published elsewhere [5]. Briefly, the InAu6− cluster was produced by laser vaporization of a composite disk target made of Au and In. Clusters formed in the source were entrained by a He carrier gas and underwent a supersonic expansion to from a collimated cluster beam. The He carrier gas was seeded with 5% Ar to achieve better supersonic cooling [6]. The cluster anions were extracted from the cluster beam and analyzed using a time-of-flight mass spectrometer. The InAu6− cluster was mass-selected and decelerated before being photodetached.

References

Keywords: Gold nanoclusters, Photoelectron spectra, DFT, Gaussian 09.
P-081

Investigations of Neutral and Singly charged Phosphorus doped Gallium Nanoclusters by DFT

Ahmet Guvenir¹, Kahraman Çetin¹, Tugce Bahceci¹, Mustafa Develioğlu¹, Ömer Dereli², Mehmet Tahir Güllüoğlu¹, Yusuf Erdoğdu¹

¹Physics, Ahi Evran University, Kirsehir, Turkey
²Physics, Necmettin Erbakan University, Konya, Turkey

There has been much interest in metallic clusters in recent years, particularly in clusters of the group IIIA element aluminum and gallium. Gallium clusters with up to more than ten atoms have been detected following laser vaporization of gallium arsenide and transitions between states of Ga- and Gan have been observed for n=1,16 [1]. Gallium clusters are of interest in intermetallic compounds with alkali metals, where clusters with 8, 12 and 15 atom have been found [2].

In this work, B3LYP, BP86, PW91 and PBEPBE functionals with 3-21 G, SDD basis sets are employed via the Gaussian 09 program [3] to optimize the structures of the neutral and singly charged GanP (n ≤ 7) nanoclusters. The analysis of the energetic and structural stability of these nanoclusters will be determined by various existing isomers. The total and binding energies of the nanoclusters will then be calculated. As a result, their harmonic frequencies, HOMO–LUMO energy gaps, ionization potentials and electron affinities will be determined. The results are evaluated with respect to previous similar works.

The lowest-energy geometries of charged phosphorous doped Gallium nanoclusters in the range of 1-7 derived from CK search program [4]. Computationally, we searched for the global minimum of neutral and singly charged GanP (n ≤ 7) nanoclusters using the B3LYP/3-21 G level of theory firstly. Calculations were carried out without any symmetry restrictions for different starting geometries. Starting with the spin singlet configurations of even electron system and the spin doublet configuration of odd-electron system, the calculation procedures were repeated for various spin multiplicities for the given cluster size.

References

Keywords: Gallium, Nanoclusters, DFT
P-082

A spectroscopic study of the degradation of the antibacterial drug Cycloserine

Andrew Paul Mendham¹, Ahsan Ali Khan¹, Babur Zahruriddin Chowdhry¹, Trevor John Dines², Dominic Kariuki¹, Daniel Jordan¹

¹Faculty of Engineering and Science, University of Greenwich, Chatham Maritime, Kent, ME4 4TB, UK
²Division of Electronic Engineering and Physics, University of Dundee, Ewing Building, Ground Floor, Nethergate, Dundee DD1 4HN, UK

Cycloserine (4-amino-3-isoxazolidinone) is an antibiotic commonly used to combat multi-drug resistant tuberculosis[1]. It has been established that cycloserine (Figure 1a) is unstable in both acidic and neutral solutions, whereby it reacts to form a cycloserine dimer (Figure 1b). This dimer is a diketopiperazine derivative which consists of aminoxy groups that form part of both Cα side-chains. In addition, it has been reported that under basic conditions the diaminoxy diketopiperazine undergoes a further reaction to produce the dimethylene diketopiperazine (Figure 1c).[2]

We have undertaken a ¹H-NMR spectroscopic study that investigates the reaction pathway of cycloserine in an acidic environment. In addition a theoretical (Gaussian 09) and experimental vibrational spectroscopic (Raman and infra-red) study of the structure and conformation of the diketopiperazine degradation products has also been undertaken.

The ¹H-NMR spectra (Figure 2) illustrates the reaction progress of cycloserine. The degradation reaction was monitored in a NMR tube containing 120 µL of glacial acetic acid, 20 mg cycloserine, 1 ml D₂O and 0.75 ml DMSO-d₆. ¹H-NMR spectra were recorded using a JEOL ECA 500 MHz FT NMR spectrometer, at t= 30 min, 2 hr, 8 hr, 14 hr, 24 hr and 48 hr time intervals. The reaction mixture was maintained at 50 °C throughout the acquisition period.

In Figure 2 the reduction in concentration of cycloserine can be observed by the diminishing signals found within region (a).

Indeed, almost complete degradation is observed within 48 hr. The degradation product diaminoxy diketopiperazine is starting to be produced within 30 min (signals within region (b)). Finally, after 8 hr we can witness the production of the final degradation product, dimethylene diketopiperazine (region (c)). This study highlights the ability of ¹H-NMR spectroscopy to monitor the kinetics of degradation reactions of cycloserine.

References

Keywords: Diketopiperazine, Gaussian, Raman, Infra red, NMR, cycloserine
Poster Abstracts

Figure 1.

Schematic molecular structures of (a) cycloserine, (b) diaminoxy diketopiperazine and (c) dimethylene diketopiperazine

Figure 2.

1H-NMR spectra (part) highlighting the acidic degradation of cycloserine over a 48 hr period.
Phytochemical Investigation of the n-Butanol Extract of Linaria Tingitana

Ramdane Seghiri¹, Thamere Cheriet¹, Samia Baatouche¹, Ines Mancini³, Ratiba Mekkiou¹, Ouahiba Boumaza¹, Djamel Sarri², Samir Benayache¹, Fadila Benayache¹

¹VARENBIOMOL, Campus de Chaabet Ersas Université des Frères Mentouri, Constantine, Algérie
²Département de Biologie, Université de M’Sila, Algérie
³Laboratorio di ChimicaBioorganica, Università di Trento, via Sommarive, Povo-Trento, Italy

Plants produce a large number of secondary metabolites, which are classified into several groups according to their biosynthetic routes and structural features. The most known groups using by plants in defense are iridoids and flavonoids. These two classes known as chemotaxonomic markers of the genus Linaria which belongs to the Scrophularioideae- Antirrhineae tribe of the Scrophulariaceae family, this genus comprises about 200 species, widely distributed throughout the northern hemisphere with its center of distribution in the Mediterranean basin and eastern Asia. The utilization of several Linaria species in folk medicine as tonics, anti-scorbutics, laxatives, anti-diabetics, and diuretics, as well as for the treatment of wounds, hemorrhoids, and vascular disorders, has attracted the attention of a number of researchers, as a result of their biological and physiological importance. This genus is presented by 39 species and subspecies in Algeria, one of these species is Linaria tingitana, an endemic spice for Algeria and Morocco. The phytochemical investigation permitted the isolation and the structural elucidation of three iridoids and the detection of another one by LC-MS. These four compounds are described for the first time from this spice. The structures of these compounds were established by spectral analysis mainly 1D NMR (1H, 13C), 2D NMR (COSY, HMBC and HSQC) and mass spectra (ESI/MS, ESI/MSMS).

Keywords: iridoids, LC-MS, Linaria tingitana, Scrophulariaceae
A new Spectrofluorometric Determination of Bismuth in Some Pharmaceutical Samples

Nur Öksüz¹, Şerife Saçmacı¹, Mustafa Saçmacı¹, Ahmet Ülgen²

¹Bozok University, Department of Chemistry, Faculty of Arts and Sciences, TR-66200, Yozgat, TURKEY
²Erciyes University, Department of Chemistry, Faculty of Science, TR-38039, Kayseri, TURKEY

Determination of bismuth is important in environmental chemistry, cosmetic industry, medicine, semi conductors, alloys, metallurgical additives, recycling of uranium nuclear fuel sand fabrication of catalysts. Since the use of bismuth and its compounds in different areas of life increased and this element started to be considered toxic for humans, animal sand plants. As the use of bismuth in medicine increases, it has spread in the environment and the chance of exposure of organisms to bismuth has increased. A number of toxic effects in humans have been attributed to bismuth compounds. Therefore, new methods are required for the low cost and rapid determination of Bi(III) in the pharmaceutical manufacture and quality control process [1].

A new sensitive and selective spectrofluorometric method has been developed for the rapid, simple and cheap determination of bismuth. This method is based on the formation of a complex between bismuth and 2-[(1E)-(4,5-dimethyl-2-furyl)methylene]amino-3',6'-bis(ethylamino)-2',7'-dimethyl spiro[isoindole-1,9'-xanthen]-3(2H)-one (DMBD) (Figure 1). The fluorescence of the complex is monitored at 594 nm. Complex formation occurred at 3 mol L⁻¹ of HNO₃. Under the optimum conditions, linear calibration curve were obtained from 0 to 800 µgL⁻¹. The detection limit was 0.1 µgL⁻¹. The effects of amount of reagent and interference from other ions were studied. The proposed method was applied for the analysis of bismuth ions in pharmaceutical and water sample sand was found to exhibit a low detection limit. The robustness of this method was checked by analysing a certified bismuth standard material.

Acknowledgment: The authors are grateful for the financial support provided by the Unit of Scientific Research Projects of Bozok University (Project no: 2015 FBE/T 169)

Figure 1. The structure of the new fluorescence reagent

References:

Keywords: Rhodamine, Fluorescense, Bismuth
A New Fluorescence Reagent: Synthesis, Characterization and Application for Speciation of Chromium Ions Using Fluorimetry System

Esra Özyol¹, Mustafa Saçmacı¹, Serife Saçmacı², Ahmet Ülgen²

¹Bozok University, Department of Chemistry, Faculty of Arts and Sciences, TR-66200, Yozgat, TURKEY
²Erciyes University, Department of Chemistry, Faculty of Science, TR-38039, Kayseri, TURKEY

Chromium is extensively used either as alloy or as trivalent or hexavalent salt in a variety of industrial processes such as metallurgical, chemical industries, electroplating, refractories, pigments, tanning industries, oxidative dying and cooling water towers. The importance of chromium speciation is governed by the fact that the toxicity and reactivity depend on the chemical form or oxidation state of chromium. Cr(III) is relatively non-toxic and an essential nutrient for humans, and trace amounts of Cr(III) are considered as essential to mammals for the maintenance of normal glucose tolerance factor, lipid and protein metabolism, and are there for essential for human health. These facts show that speciation analysis of Cr, as well as its determination, is very important for its biological and environmental evaluations [1].

A new method for speciation, and separation of Cr(III) and Cr(VI) in different matrices was developed using a new fluorescence reagent and fluorimetry spectrometry. 3',6'-bis(diethylamino)-2-[(1E)-(2,4-dimethoxy phenyl)methylene]amino spiro[isoindole-1,9'-xanthen]-3(2H)-one (BDAS), was synthesized and characterized as a new fluorescence reagent for the speciation and determination of Cr(III)/Cr(VI) species. Cr(III) was quantitatively recovered the BDAS at acidity of 0.1 molL⁻¹ HNO₃, while Cr(VI) was not quantitatively recovered in all the pH's. The optimum conditions for the speciation of Cr(III)/Cr(VI) species were investigated on several commonly tested experimental parameters such as acidity of the sample solution, amount of the reagent, sample volume, and interfering ions. The limit of detection for Cr(III) corresponding to three times the standard deviation of the blank (3s/b) was found 16.7 μgL⁻¹. The method was validated by analysing certified reference materials. The proposed method was applied to the determination and speciation of chromium species in various water and food samples with satisfactory results.

Acknowledgment: The authors are grateful for the financial support provided by the Unit of Scientific Research Projects of Bozok University (Project no: 2015 FBE/T 168).

Figure 1. The structure of the new fluorescence reagent

References

Keywords: Chromium, Fluorescence, Rhodamine
Investigation of the Interaction between Anti-Cancer Drug and Human Serum Albumin depending on temperature by 400 MHz NMR Spectrometer

Sibel Korunur¹, Bilgin Zengin², Ali Yılmaz³

¹Tunceli Vocational School, Electricity and Energy Department, Tunceli University, Tunceli, Turkey
²Faculty of Engineering, Electrical and Electronics Engineering, Tunceli University, Tunceli, Turkey
³Faculty of Art and Sciences, Department of Physics, Batman University, Batman, Turkey

Protein-drug interaction is an important issue that emerged in recent years. Investigation of the interaction between protein and drug is very important in medicinal chemistry. Human serum albumin (HSA) is often selected as a subject of study because albumin is the most abundant protein in human blood plasma. Drug is transported usually as a complex with serum albumins in a circulatory system. In determining of therapeutic dosage of the drugs the binding affinity of drugs with proteins plays an important role. NMR, is recognized as a valuable method for determining the structure of proteins and protein-ligand complexes. In this study, drug-albumin interactions were investigated versus increasing temperature from 298K to 318K by 400 MHz NMR spectrometer for 5-Fluorouracil (5-FU). In this work, using ¹H-NMR spectrums (peaks), chemical shifts and data related to relaxation times of peaks, some data have been obtained depending on temperature. The results obtained from these data gave us useful information about molecular dynamics of drug-albumin interactions.

Keywords: Human serum albumin, 5-Fluorouracil, NMR, relaxation rates
Investigation of the Interaction between 5-Fluorouracil (5-FU) and Human Serum Albumin Depending on Protein Concentration by 400 MHz NMR Spectrometer

Sibel Korunur¹, Bilgin Zengin², Ali Yılmaz³

¹Tunceli Vocational School, Electricity and Energy Department, Tunceli University, Tunceli, Turkey
²Faculty of Engineering, Electrical and Electronics Engineering, Tunceli University, Tunceli, Turkey
³Faculty of Art and Sciences, Department of Physics, Batman University, Batman, Turkey

Investigation of the interaction between protein and drug is very important in medicinal chemistry. Human serum albumin (HSA) is often selected as a subject of study because albumin is the most abundant protein in human blood plasma. Drug is transported usually as a complex with serum albumins in a circulatory system. NMR, is recognized as a valuable method for determining the structure of proteins and protein-ligand complexes. In this study, drug-albumin interactions were investigated versus increasing albumin concentration by 400 MHz NMR spectrometer for 5-Fluorouracil (5-FU). In this work, 'H-NMR spectrums (peaks), chemical shifts and data related to relaxation times of peaks were used. The results obtained from these data gave us useful information about molecular dynamics of drug-albumin interactions.

Keywords: Human serum albumin, 5-Fluorouracil, NMR, relaxation rates
P-088

Synthesis, Crystal Structure, EPR Studies of Doped VO$^{2+}$ Ion in [Co(Him)$_6$]$\cdot$2Br$\cdot$4H$_2$O

Ilkay Yildirim$^1$, Bünyamin Karabulut$^2$

$^1$Department of Radiotherapy, Vocational School of Health Services, Biruni University, Istanbul, Turkey
$^2$Department of Computer Engineering, Faculty of Engineering, Ondokuz Mayis University, Samsun, Turkey

In this study, [Co(Him)$_6$]$\cdot$2Br$\cdot$4H$_2$O (Him: imidazole) complex has been synthesized and its crystal structure has been determined by XRD technique. The magnetic environments of VO$^{2+}$ doped [Co(Him)$_6$]$\cdot$2Br$\cdot$4H$_2$O complex have been identified by EPR technique. The [Co(Him)$_6$]$\cdot$2Br$\cdot$4H$_2$O complex crystallizes in triclinic system with space group P1. The unit cell dimensions of the crystal are $a=8.8660(8)$Å, $b=9.2117(9)$Å, $c=10.7641(10)$Å, $\alpha=76.356(8)^{\circ}$, $\beta=83.275(8)^{\circ}$ and $\gamma=61.527(7)^{\circ}$, with $Z=1$. EPR spectrum of VO$^{2+}$ doped [Co(Him)$_6$]$\cdot$2Br$\cdot$4H$_2$O powder has been studied at room temperature. The spin Hamiltonian parameters were measured and the molecular orbital coefficients were calculated for the central vanadyl ion.

**Keywords:** EPR, VO2+ ion, X-ray, Imidazole
Crystal structure of \([\text{Cu}(1\text{-meim})_4(\text{H}_2\text{O})_2]\)•2(sac) (1-meim: 1-methylimidazole and sac: saccharinate) complex has been determined by XRD analysis and its magnetic environments have been identified by EPR technique. The single crystal is in monoclinic system with the space group P21/c. The unit cell dimensions of the crystal are \(a=8.5156(5)\) Å, \(b=19.4090(9)\) Å, \(c=12.6487(7)\) Å and \(\beta=123.920(4)^\circ\) with \(Z=2\). \([\text{Cu}(1\text{-meim})_4(\text{H}_2\text{O})_2]\)•2(sac) single crystals and powders have been studied at room temperature. EPR analysis indicates the presence of two \(\text{Cu}^{2+}\) sites. The spin Hamiltonian parameters have been calculated. The results show that the symmetry of paramagnetic center is nearly axial. The ground state wave function of \(\text{Cu}^{2+}\) ion has been constructed. The unpaired electrons' life time is spent over \(dx^2-y^2\) orbital.

**Keywords:** EPR, \(\text{Cu}^{2+}\) ion, X-ray, 1-methylimidazole
P-090

Crystal Water Behavior in MgSO₃.6H₂O:Co

Petya Nikolaeva Petkova¹, Youri Tzoukrovsky², Todor Dimov¹, Ilia Iliev¹, Ismail Ismailov¹

¹Faculty of Natural Sciences, Shumen University “Konstantin Preslavsky”
²Department of Radiophysics and Electronics, Faculty of Physics, Sofia University “St. Kliment Ohridski”

Spectral structure in the absorption spectra of magnesium sulfite hexahydrate (MgSO₃.6H₂O) single crystal can be observed in the IR spectral region 1200 – 1800 nm. The water molecules in the crystal lattice stipulated this structure. The investigations show that the structure anisotropy of the crystal causes the appearing of optical anisotropy of the crystal water spectra. The anisotropy manifests itself by the differences of the absorption coefficients measured with linear polarized light E parallel to c, E perpendicular to c (c is the crystal optical axis). The induced anisotropy can be presented by the spectra of the linear dichroism. The influence of Co impurity on the spectra of the crystal water in the crystals of MgSO₃.6H₂O:Co has been proved experimentally.

Figure 1. Absorption spectra of pure and Co doped MgSO3.6H2O in the spectral region 1200 – 1800 nm as follow: 1 - E is perpendicular to c and 2 - E is parallel to c.

Figure 2. The linear dichroism of absorption coefficient of pure and Co doped MgSO3.6H2O in the spectral region 1200 – 1800 nm.

Keywords: IR vibrations, absorption spectra, crystal lattice, cobalt dopant, water molecules, linear dichroism, optical anisotropy
Oximes and hydrazones are interesting subjects because of their wide application in medicine, industry and analytical chemistry [1, 2]. Hydrazones and oximes exhibit biological activity. So, these compounds have been synthesized in order to investigate the relationship between structure and biological activity [3-5].

In recent years, much attention has been given to theoretical studies on hydrazones and oximes. The X-ray crystal structure of (Z)-N’-((E)-2-(hydroxyimino)-1-phenylethylidene)isonicotinohydrazide has been previously reported by our working group [6]. On the other hand, theoretical calculation on this compound hasn’t yet been published.

In this study, the molecular geometry, vibrational frequencies, gauge including atomic orbital (GIAO) 1H and 13C chemical shift values of (Z)-N’-((E)-2-(hydroxyimino)-1-phenylethylidene)isonicotinohydrazide in the ground state have been calculated by using the density functional method (B3LYP) with 6-311++G(d,p) basis set. The calculated results show that the theoretical vibrational frequencies and chemical shift values show good agreement with experimental values. In addition, molecular electrostatic potential (MEP), frontier molecular orbitals (FMO) analysis and thermodynamic properties of the title compound were investigated by theoretical calculations.

Reference:

Keywords: Oxime; Hydrazone; Density Functional Theory; Vibrational Frequencies; GIAO; MEP.
The EPR study of Cu$^{2+}$, Mn$^{2+}$ and VO$^{2+}$ Ions Doped L-alanine Powder Crystals Produced under High Temperature

Deniz Kurt$^1$, Ümit Ceylan$^2$, Recep Tapramaz$^1$

$^1$Department of Physics, Faculty of Arts and Sciences, Ondokuz Mayis University, 55139, Samsun, Turkey
$^2$Department of Medical Services and Techniques, Vocational High School of Health Services, Giresun University, 28200, Giresun, Turkey

In this work, EPR and UV-Vis studies of Cu$^{2+}$, Mn$^{2+}$ and VO$^{2+}$ ions doped l-alanine (C$_3$H$_7$NO$_2$) in autoclave under atmosphere pressure and 210 $^\circ$C temperature in argon atmosphere were made [1,2]. The EPR spectra of powder crystals were recorded at room, high and low temperatures. Zero field splitting (ZFS) parameters D and E due to the spin-spin interactions were found by the simulation techniques. g and hyperfine splitting values were measured from experimental spectra.


Keywords: EPR, UV-Vis, argon atmosphere
Theoretical Studies on [(2,4-Dinitrophenyl)Hydrazono](Phenyl) Acetaldehyde Oxime Monohydrate

Aysin Zulfikaroğlu¹, Çiğdem Yüksektepe Ataol², Hümeysa Bati³

¹Department of Chemistry, Amasya University, Amasya, Turkey
²Department of Physics, Çankırı Karatekin University, Çankırı, Turkey
³Department of Chemistry, Ondokuz Mayıs University, Samsun, Turkey

The compounds containing hydrazone and oxime moieties are widely studied due to their versatile applications in the field of analytical and medicinal chemistry, industry [1].

In our previous publication, the X-ray crystallography of [(2,4-Dinitro-phen-yl)hydrazono] (phen-yl)acetaldehyde oxime monohydrate was studied by our working group [2], but neither spectroscopic properties nor theoretical calculations of the title compound have been investigated so far.

In this study, we focus on the structural and spectroscopic properties of [(2,4-Dinitro-phen-yl)hydrazono] (phen-yl)acetaldehyde oxime monohydrate. The molecular geometry, vibrational frequencies, gauge including atomic orbital (GIAO) ¹H chemical shift values and several thermodynamic parameters of title compound in the ground state have been calculated by using density functional methods (B3LYP) with 6-311++G(d,p) basis set. The results of the optimised molecular structure are compared with the experimental X-ray diffraction. The calculated results show that the optimised geometries can well reproduce the crystal structural parameters and the theoretical vibrational frequencies and ¹H-¹³C-NMR chemical shift values show good agreement with experimental data. Besides, molecular electrostatic potential (MEP) and frontier molecular orbitals (FMO) were performed at DFT level of theory.

Reference:

Keywords: Oxime; Hydrazone; Density Functional Theory; Vibrational Frequencies; GIAO; MEP
**Poster Abstracts**

**P-094**

**The EPR Study of Cu$^{2+}$ and VO$^{2+}$ Ion Doped Ca(H$_2$O$_8$PO$_4$)$_2$$\cdot$H$_2$O Powder Crystals Produced under High Temperature**

**Deniz Kurt**, Ümit Ceylan, Recep Tapramaz

$^1$Department of Physics, Faculty of Arts and Sciences, Ondokuz Mayis University, 55139, Samsun, Turkey

$^2$Department of Medical Services and Techniques, Vocational High School of Health Services, Giresun University, 28200, Giresun, Turkey

EPR study of Cu$^{2+}$ and VO$^{2+}$ ions doped Calcium bis(dihydrogen phosphate) monohydrate [Ca(H$_2$O$_8$PO$_4$)$_2$$\cdot$H$_2$O] powder crystals respectively in autoclave under atmosphere pressure, 250 °C and 50 °C temperatures in argon atmosphere were made [1,2]. The EPR spectra of powder crystals were recorded at different temperatures. g and hyperfine values were measured from experimental spectra. The electronic transitions were determined by the optical absorption spectrum.


**Keywords:** Autoclave, EPR, Calcium bis(dihydrogen phosphate) monohydrate.
Poster Abstracts

P-095

Label-free Surface-enhanced Raman Spectroscopic Detection of Mycobacterium Smegmatis Using Silver Nanoparticles

Melisew Tadele Alula, Jonathan Blackburn

Institute of Infectious Diseases and Molecular Medicine, University of Cape Town, Cape Town, South Africa

The development of surface-enhanced Raman scattering method for the detection of bacteria in different samples has received much attention in recent times. In this work, we present the development of simple, fast, and sensitive surface-enhanced Raman spectroscopy (SERS) for the detection of *Mycobacterium smegmatis* using silver nanoparticles (AgNPs) that are coated on the surface of the bacteria. The silver mirror reaction was used for coating silver nanoparticles on the cell envelope of the bacteria. The bacteria were initially mixed with AgNO₃ and treated with NaOH after which of ammonium hydroxide was added until the Ag₂O was completely dissolved. Treatment of the reaction mixture with glucose at 55 °C resulted in the formation of AgNPs on the surface of the bacteria. The detection of M.smegmatis is simple and straightforward; 4 μL of M.smegmatis coated AgNPs (smegmatis@AgNPs) were pipetted on the hydrophobic plane surface and SERS spectra are collected. Quantitative evaluation of the bacteria was done with the distinguishable strong vibrational band around 735 cm⁻¹.

**Keywords:** M.smegmatis; silver nanoparticles; surface-enhanced Raman scattering
Melting Behaviors of Cu, Pd, Pt and Ti Metal Clusters: Magic Numbers and/or Icosahedral Like Geometries

Meral Eryürek

Physics Department, Bülent Ecevit University, Zonguldak, Turkey

The melting properties of Cu, Pd, Pt and Ti Metal clusters magic numbers and/or icosahedral like geometries were simulated by a microcanonical molecular dynamics method using Gupta many body potential, and their thermodynamic quantities were calculated by using multiple histogram method. The caloric curves and, relative root-mean square (rms) bond length fluctuation, configurational entropy, heat capacity and potential energy distributions graphs were evaluated. The dependence of these quantities on the size of the clusters was examined and it is found that potential energy distribution is the key quantity to determine the melting type.

Keywords: Metal Cluster, Melting, Multiple Histogram Method, Magic Numbers
A New Dispersive Liquid-Liquid Microextraction Method for Determination of Cobalt in Some Vitamin Tablets

Tuba Ceviz, Şerife Saçmacı, Ahmet Ülgen

Department of Chemistry Sciences, Erciyes University, TURKEY

Cobalt is considered an essential ultratrace element to the man because it is a fundamental component of vitamin B12 (Cyanocobalamine), a co-enzyme which takes part on several biological process. Traces of Co are required for utilisation of Fe in the haemoglobin formation and DNA synthesis and its absence can cause anemia. Problems associated to heart, thyroid and lung can be observed if doses higher than 500 mg were ingested [1].

DLLME is a miniaturized sample pretreatment technique based on a ternary component solvent system where the dispersion of fine droplets of the extraction solvent is accomplished within the aqueous phase [2].

In this study, a new dispersive liquid-liquid microextraction (DLLME) preconcentration method was developed for the determination of cobalt. In the proposed approach, 2-(5-Bromo-2-pyridylazo)-5-(diethylamino) phenol was used as chelating agent, while chloroform and methanol were used as extraction and dispersive solvents, respectively. Optimum complex formation occurred in CH₃COOH/NaCH₃COO buffer at pH 4.0. Several factors that influence the microextraction efficiency, such as type and amount of extraction and dispersive solvents, concentration of the chelating agent, and centrifugation time were investigated and the optimized microextraction conditions were established. Under the optimum conditions, the preconcentration factor of this method for cobalt was reached at 250. The limit of detection for palladium was 0.04 μg L⁻¹ (3s), and the relative standard deviation (RSD) was 1.5% (n = 8) at 4 μg L⁻¹ level. The accuracy of the method was performed by analysis of the certified standard reference material. The developed method was applied successfully to the determination of cobalt in the some vitamin tablet samples.

References

Keywords: Cobalt, Microextraction Method, Vitamin Tablets, FAAS
Anharmonic behavior in BaTiO$_3$: Investigation by Raman Spectroscopy

Bejaoui Ouni Ines$^1$, Fontana Marc$^2$, Chapron David$^2$, Aroui Hassen$^1$

$^1$Laboratoire de Dynamique Moléculaire et Matériaux Photoniques, Université de Tunis, TUNISIE
$^2$Laboratoire de Matériaux Optiques, Photonique et Systèmes, Université de Lorraine, FRANCE

BaTiO$_3$ (BT) is a well known ferroelectric material which has been thoroughly studied during several decades since it undergoes successive cubic-tetragonal-orthorhombic-rhombohedral phase transitions on cooling [1]. It has several ferroelectric properties that allow it to be a good material for electronic applications such as the design of ferroelectric memories and pyroelectric elements [2].

In the present work, we report the analysis of temperature dependence of Raman frequency and damping of the A1 modes polarized along the FE c axis as well as the optical phonons E corresponding to the ionic motions in the plane normal to c.

Measurements were carried out at different temperatures ranging from 298 to 408 K (tetragonal phase) within different scattering configurations. Spectroscopic parameters of BT have determined using a high resolution Raman spectrometer and a fitting program.

All the first order frequency modes exhibit a quasi linear decrease as function of the temperature, except for the A1[TO1], E[TO2] and E[TO4] lines which reveal a parabolic dependence illustrating an anharmonic process.

The phonon frequency downshifts and damping evolutions are interpreted in terms of normal volume expansion and third- and fourth-order anharmonic potentials.

REFERENCES

Keywords: BaTiO$_3$, Raman Spectroscopy, Frequency, damping, anharmonic potential.
Due to its excellent ferroelectric properties and the very high stability of its perovskite structure, barium titanate BaTiO₃ (BT) remains the preferred material for many electronic applications. [1] The substitution of Ba by Ca in the BaTiO₃ perovskite permits an improvement of the stability of the piezoelectric properties. For these reasons, the barium calcium titanate BaₓCa_{1-x}TiO₃ (BCT) has attracted great attention for use in the laser systems, electro-optic material for various photorefractive and holographic applications [2].

In this work, we report Raman Spectroscopy investigation carried out in the spectral region between 100 and 1000 cm⁻¹ as a function of temperature in order to detect the effect of the Ca²⁺ ion in the crystal structure of BT.

The Raman Spectra of different samples BCT with the compositions x= 0.03; x=0.24 and x=0.31 were recorded at different temperatures ranging from the ambient (298 K) to Tc using XYYX configuration of the backscattering geometry. These spectra illustrate apparition of A₁[LO₁] and A₁[LO₂] centered respectively around 730 and 490 cm⁻¹. The intensities of these modes increase with the Ca composition.

The transition temperature decreases from 409 K for x=0 to 380 K for x=0.03. This temperature becomes 381 K and 382 K respectively for x=0.24 and 0.31.

After the fitting procedure, the results show an decreasing of line shift and increasing of line width with the temperature for A₁[TO], B₁ and A₁[LO] modes.

On the other hand, the Raman spectra of the BCT show a shift towards the low frequency. This redshift increases with the Ca ion composition, and especially affects A₁[TO₁] and A₁[TO₂] modes which describe respectively the Ti/O and Ba/O movements.

References

Keywords: BaCaTiO₃ (BCT), Raman spectroscopy, Ca composition effect, shift, width.
Impact of the Sign on the Optical Properties of a Product

Trufka Dimitrova, Petya Nikolaeva Petkova, Darina Bachvarova, Veselina Lalova

Shumen University “Konstantin Preslavsky”

The design of a company logo or sign is one of the crucial steps in the initial phase of the development of every company. It can contribute to the establishment of a professional image of the organisation, which can distinguish it from the competitors, it can attract and keep the attention, it can influence the audience and the whole environment. There are basic functions of the sign and rules for its design. In this research we look at the sign as a sacred, holy symbol. The holy symbols of a family, a state or spiritual practice date thousands of years back and they are written on walls, plates, bread, flags, stamps. They have a relation to the spiritual plan of the Universe and they are timeless perfection and reality. The sacred geometry simultaneously consists all the aspects of the language as a basic tool for communication: 1. Sound /vibration, consonance/; 2. Numbers and sequence of numbers; 3. Archetype of the sacred geometry /circle, triangle, square, etc. Therefore the sacred geometry is pure communication because the body reacts to the vibration, the rationality and the messages of the different forms which provoke particular feelings /sensual knowledge/. That is why some authors define the sacred geometry as the mind of the Universe, universal language, omnipresent unity which is a harmonising factor in the exchange. The goal of this research is to find objective evidence and indicators for the impact of “the language of the sign” on a particular product and consequently on the consumer. This will shed a light on the role of the sign, it will increase the responsibility in the usage, the enlightenment and the professionalism in the creation process. We have studied the change in the absorption coefficient of two groups of objects - water and clay solution which have been in touch with different signs. We have investigated normal and unnormal anisotropy of these solutions and we have determined the frequency value of one Lorentz oscillator.

Keywords: optical properties, water and clay solution, normal and unnormal anisotropy, Lorentz oscillator, vibration frequency, company logo or sign, product, consumer
Figure 1

(a) The absorption spectrum of water solution after the touch with sign in the spectral region 300 – 400 nm; (b) The experimental Lorentz profiles of water solution after the touch with sign in the same spectral region.

Figure 2

(a) The absorption spectrum of clay solution after the touch with sign in the spectral region 300 – 400 nm; (b) The experimental Lorentz profiles of clay solution after the touch with sign in the same spectral region.
P-101

Investigation of Structural, Energetic and Vibrational Properties of 2-Deoxy-2-((methyl(nitroso)amino)carbonyl)amino)-β-D-Glucopyranose

Mustafa Böyükata1, Dilek Pandır2, Meryem Evecen3, Hatice Art4

1Department of Physics, Bozok University, 66200 Yozgat, Turkey
2Department of Biology, Bozok University, 66200 Yozgat, Turkey
3Department of Physics, Amasya University, 05000 Amasya, Turkey
4Department of Chemistry, Bozok University, 66200 Yozgat, Turkey

Streptozotocin, 2-Deoxy-2-((methyl(nitroso)amino)carbonyl)amino)-β-D-glucopyranose, is a naturally occurring toxic chemical to the insulin-producing beta cells of the pancreas in mammals [1]. To clarify its geometric properties may help to understand its effects on the human health. In this work, the structural and energetic properties of the title molecule, C8H15N3O7 (Fig. 1), have been determined with ab initio Hartree–Fock and density functional theory (DFT/B3LYP) calculations, considering 6-311++G and 6-311++G(d,p) basis sets [2]. Predicted energy values, bond lengths and angles of the optimized geometries will be compared with available findings in the literature. Experimentally, Raman and IR spectra have been also investigated for the title molecule to clarify the structural properties, in detail.

References

Keywords: Streptozotocin, Hartree–Fock, DFT, Raman, IR
Experimental, Theoretical Investigation and Intramolecular Proton Transfer of Two Tautomers: (E)-4-((2-methyl-3-nitrophenyl)imino)methylbenzene-1,2,3-triol and (Z)-2,3-dihydroxy-6-(((2-methyl-3-nitrophenyl)amino)methylene)cyclohexa-2,4-dienone

Ersin Temel¹, Can Alaşalvar¹, Erbil Ağar²

¹Department of Electric and Energy, Technical Sciences High School, Giresun University, Giresun, Turkey
²Department of Chemistry, Faculty of Arts and Sciences, Ondokuz Mayıs University, Samsun, Turkey

o-hydroxy Schiff bases exhibit two tautomeric forms known as the phenol-imine (OH) and keto-a-amine (NH) forms. In the present study, the tautomerism in the title cocrystal was investigated by experimental (XRD and FT-IR) and theoretical (DFT) methods. Crystal structure was determined by single crystal X-ray diffraction method and reveals that it belongs to the monoclinic system with two molecules in the unit cell (space group P2₁/n). As is seen in the Figure 1, two molecules in the asymmetric unit show different tautomeric behavior. While one of the molecules exhibits NH form, OH and NH forms are together in the other molecule. In addition to the experimental studies, optimized geometry of the molecule, vibrational pattern were derived from density functional theory (DFT) calculations at B3LYP/6-311G(d,p) level and the results are compared with experimental one. The molecular stability were studied by the natural bond analysis (NBO). Molecular electrostatic potential (MEP) was drawn for visualization the charge density distribution and site of chemical reactivity of the molecule. Highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) energy gaps were calculated. Hirshfeld surface was used as an assisting tool for analysis of the inter-molecular interactions (Figure 2).

Keywords: Single crystal X-ray diffraction; FT-IR; Density Functional Method (DFT)
The molecular structure of the title compound, showing the atom numbering scheme and 30% probability displacement ellipsoids.

Hirshfeld surfaces mapped with dnorm for the title compound.
Self-healing Mechanism of Metallopolymers Investigated by QM/MM Simulations and Raman Spectroscopy

Stephan Kupfer\textsuperscript{1}, Linda Zedler\textsuperscript{1}, Julien Guthmuller\textsuperscript{2}, Stefan Bode\textsuperscript{3}, Martin D. Hager\textsuperscript{3}, Ulrich S. Schubert\textsuperscript{3}, Jürgen Popp\textsuperscript{4}, Stefanie Gräfe\textsuperscript{1}, Benjamin Dietzek\textsuperscript{1}

\textsuperscript{1}Institute for Physical Chemistry, Friedrich Schiller University Jena, Helmholtzweg 4, 07743, Jena, Germany
\textsuperscript{2}Faculty of Applied Physics and Mathematics, Gdansk University of Technology, Narutowicza 11/12, 80233 Gdansk, Poland
\textsuperscript{3}Laboratory for Organic and Macromolecular Chemistry, Friedrich Schiller University Jena, Humboldstr. 10, 07743, Jena, Germany
\textsuperscript{4}Institute for Photonic Technology (IPHT) Jena, Albert-Einstein-Str. 9, 07745, Jena, Germany

Self-healing materials feature the ability to heal mechanical damage suffered by chemical or physical stress and to (partially) recover their mechanical properties autonomously or upon application of an external stimulus. Manifold applications for self-healing materials are conceivable ranging from coatings, over asphalts and to steel alloys. One possibility to obtain self-healing is the utilization of (weak) reversible interactions between specific molecular structures embedded, e.g., in a polymer. A promising approach is to utilize metal-ligand interactions.

Recently, a variety of self-healing terpyridine metallopolymers cross-linked by different metal salts have been synthesised based on a lauryl methacrylat polymer backbone and exhibiting pronounced healing properties upon thermal activation at moderate temperatures of approximately 100 °C\textsuperscript{1,2}

In order to improve on the self-healing properties of such materials it is of uttermost importance to unravel the underlying healing mechanism at a molecular scale. One suited tool to investigate structural alterations during the thermally induced healing process is temperature-dependent Raman spectroscopy. To investigate self-healing on a molecular level theoretical simulations aiming to describe the interactions responsible for the healing process in metallopolymers are of great interest.

This work presents a joint theoretical-spectroscopic guided investigation to study the healing process of selected representative metallopolymers cross-linked by metal salts, namely iron(II) sulfate and cadmium(II) bromide. Proposed healing mechanisms are based on a thermal decomplexation of the cross-linking complexes as well as on the formation of ionic clusters, see Figure 1.

Model systems have been constructed in order to address the possibility of both self-healing schemes by means of computational methods. Due to the enormous size of these systems (up to nearly 1300 atoms) mixed quantum mechanical / molecular mechanical (QM/MM) simulations are required. Structural alternations during the healing process, monitored by temperature-dependent Raman spectroscopy, have been thoroughly investigated by means of calculated (resonance) Raman spectra. In addition, the contribution of ionic-clusters with respect to the healing mechanism have been studied based on the QM/MM simulations.
References

Keywords: Self-Healing Materials, Raman Spectroscopy, QM/MM Calculations

Figure 1: Schematic representation of the reversible cross-linking process in metallopolymers.
The Theoretical and Crystallographic Studies on (E)-2-(((4-bromo-2-(trifluoromethoxy)phenyl)imino)methyl)-4-nitrophenol

Güneş Demirtaş1, Ömer Tamer2, Necmi Dege3, Davut Avci2, Yusuf Atalay2, Mustafa Macit4, Songül Şahin4

1Dr. Sedat-Dr. Melehat Baran Secondary School, 19300 Sungurlu, Çorum, Turkey
2Sakarya University, Faculty of Arts and Sciences, Department of Physics, 54187 Sakarya, Turkey
3Ondokuz Mayıs University, Faculty of Arts and Sciences, Department of Physics, 55139 Samsun, Turkey
4Ondokuz Mayıs University, Faculty of Arts and Sciences, Department of Chemistry, 55139 Samsun, Turkey

Compounds which contain C≡N double bond are expressed as Schiff base compounds. Schiff bases display photochromic and thermochromic properties in solid state [1, 2]. In this study, the crystal structure of (E)-2-(((4-bromo-2-(trifluoromethoxy)phenyl)imino)methyl)-4-nitrophenol which is Schiff base compound was disclosed by XRD technique at room temperature. The molecule which has (E) configuration crystallizes in the triclinic space group P-1 with a=7.674 (4) Å, b=12.584 (6) Å, c=15.921 (6) Å, α=89.62 (4)°, β=84.34 (4)°, γ=73.77 (4)° and Z=4. In the crystal structure, intramolecular O⋯H⋯N and intermolecular C⋯H⋯O hydrogen bonds are present.

In addition to crystal structure, the optimized geometry of the molecule was carried out by DFT method. The theoretical ideal conformation was calculated with the same theory and this process bases on potential energy distribution (PED). Besides, the experimental theoretical IR spectra were also handled [3].


Keywords: Schiff base, DFT, PED
Structural, Elastic, Electronic and Optical Properties of BeSiN$_2$ from First-principles

Fahima Arab$^1$, Fahima Arab$^2$, Ferhat Ali Sahraoui$^1$, Khelifa Haddadi$^3$, Layachi Louail$^3$

1Laboratoire d’Optoélectronique et Composants, Département de Physique, Université Ferhat Abbas, Sétif 19000, Algeria.
2Unité de Recherche en Optique et Photonique (UROP), Université de Sétif1, Centre de Développement des Technologies Avancées (CDTA), Alger, Algérie.
3Laboratoire d’Elaboration de Nouveaux Matériaux et leurs Caractérisations (ENMC), Département de Physique, Université Ferhat Abbas, Sétif 19000, Algeria.

Using the plane wave pseudo potential method (PP-PW) within the generalized gradient approximation GGA-PW91, GGA-PBESol and LDA-CAPZ approach, we report the result of the structural, elastic, electronic and optical properties of BeSiN$_2$ in different structural phases. The calculated equilibrium structural parameters are in excellent agreement with available experimental and theoretical results. We have found that BeSiN$_2$ undergoes two structural phase transition under pressure from the stable structure α-BeSiN$_2$ to β-BeSiN$_2$ to γ-BeSiN$_2$ type structure. Single crystal and polycrystalline elastic constants and related properties namely Vickers hardness, acoustic Grüneisen parameter, minimum thermal conductivity, isotropic sound velocities and Debye temperature were numerically estimated for both orthorhombic and tetragonal polymorphs. Electronic properties and chemical bonding nature have been studied throughout the band structure, density of states and valence charge distribution analyses. It is found that the studied compound has an indirect band gap (Γ-X) of 5.439 eV, direct gap (Γ-Γ) gap of 3.70 eV and indirect gap (Γ-Z) of 3.01 eV with a mixture of covalent-ionic character α-BeSiN$_2$, β-BeSiN$_2$, and γ-BeSiN$_2$ type structures respectively. The dielectric function, extinction coefficient, reflectivity and energy loss function for the two structures, have been calculated for a range of 0-30 eV.

Keywords: Density functional theory, Phase transition, optical properties,
Application of FTIR Spectroscopy in Microbial Ecology: Studying Different Ecological States of the Rhizobacterium {Azospirillum Brasilense}

Anna V. Tugarova¹, Andrei V. Schelud’ko², Yulia A. Dyatlova¹, Alexander A. Kamnev¹

¹Laboratory of Biochemistry, Institute of Biochemistry and Physiology of Plants and Microorganisms, Russian Academy of Sciences, Saratov, Russia
²Laboratory of Microbial Genetics, Institute of Biochemistry and Physiology of Plants and Microorganisms, Russian Academy of Sciences, Saratov, Russia

Bacteria are known to naturally exist predominantly as biofilms which play an important role in biosphere processes. This constitutes an important and yet poorly understood field in microbial ecology.

We used transmission FTIR spectroscopy to characterize 6-day-mature biofilms of worldwide-studied rhizobacterium Azospirillum brasilense. Some differences were observed between FTIR spectra of ‘free’ bacteria (sampled from planktonic suspensions) and those of bacterial biofilms (attached to solid surfaces). The most significant differences were: (i) a shift in the amide I band maxima from 1690 to 1650 cm⁻¹ and (ii) a change in the region 1200–950 cm⁻¹ (C–OH, C–O–C and C–C vibrations of polysaccharides and/or PO²⁻). The former indicates changes in the secondary structure of cellular proteins in going from planktonic biomass to biofilms, while (ii) suggests changes in the composition of polysaccharides and/or interaction between biomacromolecules.

FTIR spectroscopy in the diffuse reflectance mode (DRIFT) was used to study the influence of various stress factors (starvation and heavy metals) on A. brasilense [1–3]. Stresses induced poly-3-hydroxybutyrate (PHB) accumulation, enhancing IR absorption in PHB-specific regions (particularly polyester C=O stretching vibrations near 1730 cm⁻¹) [1–3] and inducing a redistribution of the secondary structure components of cellular proteins [2]. Analysis of structure-sensitive PHB vibration bands revealed changes in the degree of PHB crystallinity at different stages of bacterial growth. As enzymatic hydrolysis of PHB depends on its degree of crystallinity, this provides a means of PHB “digestibility” regulation by cells under unfavourable conditions.

Our results show that FTIR spectroscopy is a useful instrumental non-destructive technique for studying different ecological states of bacteria in their environment, providing important structural information on some major components of bacterial cells (e.g., storage biopolymers and cellular proteins) and their changes in different conditions.

References

Keywords: FTIR spectroscopy, Azospirillum brasilense, biofilms, poly-3-hydroxybutyrate
Raman Spectroscopy Applied to the Chemical Characterization of Mono- and Multi- Species Biofilms

Cuauhtemoc Araujo Andrade1, Ana María González Amaro2, Claudio Frausto Reyes3, Adriana Jacome Espadas2, Gulce Ogruc Ildiz4, Rumen Ivanov Tsonchev5

1Academic Unit of Physics, Autonomous University of Zacatecas. Zacatecas, México.
2Maestría en Endodoncia de la de la Facultad de Estomatología de la Universidad Autónoma de San Luis Potosí, San Luis Potosí, México.
3Research Center in Optics (CIO), Aguascalientes, México.
4Istanbul Kultur University, Faculty of Science and Letters, Department of Physics, Ataköy Campus, Istanbul, Turkey.

Bacterial biofilms developed on teeth, can cause dental caries and, biofilms that grow in the gingival sulcus contribute to the pathogenesis of periodontitis [1]. Current literature has demonstrated that biofilms may continue viable in anatomical areas of the root canal system, remaining untouched by either mechanical or chemical disinfection during the root canal therapy [2]. In this sense, the elucidation of the main components of this type of biofilms represents a valuable contribution for the establishment of new methods and treatments for its disintegration and, consequently, to reduce the root-canal persistent infections rates [3].

In this work, we characterize by means of conventional Raman microspectroscopy, diverse mono- and multi- species biofilms associated with the fail in endodontic procedures. Biofilms studied here were produced in-vivo in the extraradicular portion of teeth. The capability of Raman spectroscopy to elucidate the chemical identity of the major components of biofilms can be used as a simple and reliable screening method to evaluate its presence or absence after an endodontic procedure and, as consequence, avoid future complications associated with persistent infections. In addition, the results obtained from this study attempt to contribute into increase the scarce amount of information related with the chemical composition of this type of biofilms.

Among the main components identified on our biofilm samples, we can point out: cellulose, dextrose, xylose and certain saturated triglycerides.

References

Acknowledgements
The authors thank to Mexican Consul of Science and Technology (CONACyT) for the project grant number 153066 and the PIFI program/2014 for the supplementary financial support.

Keywords: Bacterial Biofilms, Raman spectroscopy, polysaccharides
We report results obtained from first principle calculations of NbRu₃, NbBRu₃ and NbCRu₃ compounds with antiperovskite structure [1]. The estimated equilibrium lattice parameters are in agreement with the experimental ones. Elastic constants Cᵢⱼ for single crystal are calculated, then polycrystalline elastic moduli (bulk, shear and Young moduli, Poisson ration, anisotropy factor) are presented [2]. Based on Debye model, Debye temperature $\Theta_D$ is calculated from the sound velocities $V_l$, $V_t$ and $V_m$. Band structure results show that the compounds under study are electrical conductors and the conduction mechanism is assured by Ru-d electrons. Bonding nature and bonds strength are discussed based on the partial densities of states, population analysis and the electronic charge distribution [3].

**Keywords:** Intermetallic compounds, Ab initio calculations, Elastic properties.
P-109

Spectroscopic Studies to Clarify the Interactions of Chloroquine Diphosphate and Phenelzine Sulfate Drugs with Human Serum Albumin

Bahar Kancı Bozoğlan, Sibel Tunç, Osman Duman

Department of Chemistry, Akdeniz University, Antalya, TURKEY

The investigation of drug-human serum albumin (HSA) interaction has a crucial importance for deeply understanding the conformational changes in the secondary structure of protein molecule and the pharmacodynamics and pharmacokinetics of drugs. HSA has many physiological functions in human body and shows high affinity for many drugs [1,2]. Chloroquine diphosphate (CQP) is a drug used in the treatment of various rheumatic diseases and malaria [3]. Phenelzine sulfate (PS) is a kind of antidepressant drug used for the treatment of some psychiatric disorders such as panic disorder, social anxiety disorder and depression [4].

In this work, the interactions of CQP and PS with HSA were studied by various spectroscopic techniques such as fluorescence and circular dichroism. Protein-drug interaction studies were carried out at 288.15, 298.15, 310.15 and 318.15 K and physiological pH value.

For HSA-drug systems, fluorescence measurements showed that there was an interaction between HSA and CQP, whereas HSA-PS system did not show any interaction. Also, static quenching was found as effective quenching mechanism for HSA-CQP system. Binding constant (Kb) value for HSA-CQP system is in the order of 10^4 M^−1 which indicates the presence of strong binding between HSA and CQP. Moreover, stability of HSA-CQP complex showed a decrease with increasing temperature. The numbers of binding sites on HSA for CQP were approximately equal to one at all temperatures studied. For HSA-CQP system, thermodynamic parameters were obtained as negative ΔH and ΔG and positive ΔS values. These results illustrated that the main binding force in this system was the electrostatic interaction. According to the results of circular dichroism (CD) analysis, α-helix amount of HSA decreased from 48.9% to 46.0% in the presence of CQP. This result indicated that the binding of CQP to HSA caused some structural changes in the secondary structure of HSA.

References

Keywords: Drug, Human serum albumin, Interaction, Spectroscopic techniques
In this study, fluorescence lifetime distribution changes of BSA modified with N-(1-pyrenyl)maleimide with the addition of SDS were examined with the time resolved spectrofluorometer PTI C-71. The fluorescence decays were analysed by using Exponential Series Method (ESM) to obtain the changes of lifetime distributions [1]. The complex PM-BSA showed excimer emission (λmax = 462nm) which is extremely sensitive to the structural and conformational changes [2].

SDS caused shifting of the distribution to shorter lifetimes, that express the denaturation of the complex PM-BSA with the addition of SDS (Fig. 2).


Keywords: Fluorescence lifetime distribution, N-(1-pyrenyl)maleimide, Excimer, Bovine serum albumin, Sodium Dodecyl Sulfate

Fluorescence Lifetime Distribution Changes of PM-BSA

Figure 2. Fluorescence lifetime distribution changes of PM-BSA (3,2x10-6M) with the addition of SDS (7,5x10-5M).
Figure 1. Modification of BSA with PM [3]
Temperature-Dependent Photoouminescence of Cu, Mn, Co, Zn and Cd Complexes with Heptafluorobutanoic Acid and Bipy/Phen

Yalcin Kilic, Ibrahim Kani

Department of Chemistry, Anadolu University, Eskisehir, Turkey

The interest in the synthesis of transition-metal complexes, such as catalysis, gas storage, and luminescence applications has increased significantly in recent years[1]. A better knowledge of the parameters which govern the photophysical properties of transition-metal complexes is fundamental for the progress of photochemistry and essential for the design of new photo sensitizer [2]. Temperature dependence studies of the luminescence behavior can yield important pieces of information concerning the energy ordering of the various excited states and the dynamics of interstate conversion [3]. In this study, seven coordination compounds, namely, [Zn(OOC(CF$_2$)$_2$(CF$_3$)$_2$(H$_2$O)(2,2’-bipy)] (1), [Cu(OOC(CF$_2$)$_2$(CF$_3$)$_2$(H$_2$O)(2,2’-bipy)] (2), [Mn(OOC(CF$_2$)$_2$(CF$_3$)$_2$(H$_2$O)(bipy)](OOC(CF$_2$)$_2$(CF$_3$)$_2$(CF$_3$)$_2$(bipy)] (3), [Co$_2$(OOC(CF$_2$)$_2$(CF$_3$)$_2$(bipy)](OOC(CF$_2$)$_2$(CF$_3$)$_2$(bipy)] (4), [Cd$_2$(OOC(CF$_2$)$_2$(CF$_3$)$_2$(2,2’-bipy)] (5) and [Mn(OOC(CF$_2$)$_2$(CF$_3$)$_2$(4,4’-bipy)]n (6) (phen=1,10-phenantroline) were synthesized and characterized through single-crystal X-ray diffraction technique. The photoluminescent spectra of the complexes measured in the solid state. The complexes were introduced into a closed cycle He cryostat and the corresponding temperature was changed between 10 K and 325K.

References:

Keywords: Complex, luminescence, crystallography

Photoluminescence spectra of [Cd$_2$(OOC(CF$_2$)$_2$(CF$_3$)$_2$(2,2’-bipy)] from 10K to 325K
P-112

Nicolae Grigorescu - Researches on Modern Art Works

Maria Geba, Lacramioara Stratulat, Daniela Salajan, Valentina Drutu, Minola Iutis, Lenuta Chirita

Moldova National Complex of Museums, Iasi, Romania

One of the greatest Romanian painters, Nicolae Grigorescu (1848-1907) was one of the founders of modern Romanian painting.

Young Grigorescu, influenced by the artistic concepts of the Barbizon school, looked for new means of expression and followed the trend of “en plein air” painting, artistic movement which preceded the Impressionism. Among his favorites subjects were country scenes with peasants and animals.

This paper presents an analytical study on two of his paintings: “Little Shepard on the field“ and “Return from the Fair”, dated in the beginning of 20th century.

The works were examined by UV, VIS, IR radiations and the pigments were analyzed by non invasive method X-Rays Fluorescence Spectroscopy (XRF) and with Attenuated Total Reflectance Fourier Transform Infrared Spectroscopy (FTIR-ATR).

The UV fluorescence was used to gain important information regarding the vernis degradation, the retouching and other interventions on the painting surface. IR Reflectography showed no alteration in time and no preliminary drawing.

The pigments identified on the two paintings are generally the same, as well as the manner of support preparation.

Acknowledgement

This research represents the second stage of the project “Innovative interactive artistic mediation system designed for the capitalization of the art patrimony of Romanian museums” (SIMAP), funded by the UEFISCDI, PN-II-PT-PCCA-2013-4-2158.

Keywords: Pigment, XRF, FTIR-ATR, IR Reflectography
XRF Spectrometric Studies on Metallic Decorations from Romanian Heritage Textiles

Angelica Olaru, Maria Geba, Cristina Marta Ursescu, Ana Maria Vlad

“Moldova” National Complex of Museums

Since the third millennium BC, metallic accessories had been used to decorate clothing and household items made from textiles. Within heritage collections, the particular case of the ethnographical objects shows textiles that are embroidered with metallic threads and sequins. The aim of the present study is to provide information about the materials and techniques used for making metallic accessories. XRF analysis was carried out in situ on 19th and 20th century clothing (shirts, skirts and handkerchiefs) that belonged to different geographical regions in Romania.

The selected items were primarily examined by optical microscopy, in order to reveal the manufacturing techniques. All studied threads are made of thin metal strips, wrapped around a core yarn: usually cotton (Fig. 1) and sometimes fine wool.

Table 1 contains the results from XRF analysis that led to the identification of the metals and/or combinations of metals within metallic elements.

Due to high concentration of elements such as Fe, Cu, Zn -from metal accessories- and Cr -due to threads dyeing process- that were detected in the textile coloured spots around the decoration, corrosion products were identified (Fig. 2). These may be leading to oxidative degradation mechanisms on the natural fibres within the objects when stored in an inappropriate museum environment.

The very accessible XRF analysis provides an easy way to identify both the metal-based compounds and the degradation products, in the attempt to gather information on a scarcely studied domain: metal accessories and their influence on the state of conservation of ethnographical textile collections within museums.

Acknowledgement
This work was funded by the UEFISCDI, PN-II-PT-PCCA-2011-3-1742, project TEXLECONS, contr. no. 213/2012

Keywords: XRF analysis, metallic accessories, heritage textiles
Fig. 2. Coloured spot on flax fibers, due to metal corrosion

Fig. 1. Metallic threads with cotton fibers core

Table 1. XRF analysis of metallic accessories

<table>
<thead>
<tr>
<th>Threads</th>
<th>Sparkles</th>
<th>Sequins</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cu or brass (alloy of Cu and Zn) plated with Ag</td>
<td>Cu, Pb and Zn contaminated, silvered or Ni plated</td>
<td>Cu with 1-11% Pb, silvered or brass plated</td>
</tr>
<tr>
<td>Brass, Pb and Fe, plated with Ag or Zn</td>
<td></td>
<td>Fe and Pb</td>
</tr>
<tr>
<td>Cu wire, containing Pb (1-10%), Zn and Fe as impurities, plated with Ag or brass</td>
<td></td>
<td>Fe, Ni, Zn or brass plated</td>
</tr>
</tbody>
</table>
Theoretical Study of Phosphazenes: Cation –π (Li+, Na+, K+, Be^2+, Mg^2+, and Ca^{2+}) Interaction

Fatmagül Tunç¹, Ahmet Tokatlı²

¹Vocational High School of Health Services, Kırklareli University, Kırklareli, Turkey
²Department of Physics, Faculty of Arts and Science, Süleyman Demirel University, Isparta, Turkey

The geometries of the complexes of Li⁺, Na⁺, K⁺, Be^{2+}, Mg^{2+}, and Ca^{2+} metal cations with phosphazenes ((NPX₃₂; X=H, F, Cl and Br) ring were studied. The complexes were optimized at the B3LYP level and the 6-311++G(d,p) basis set. The interaction energies corrected by basis set superposition error were calculated in the same level. The calculations show that interaction energy is strongly dependent on the charge-to-size ratio of the cation. Natural bond orbital analysis was performed to calculate the charge transfer and natural population analysis of the complexes. Quantum theory of atoms in molecules (QTAIM) was also applied to analyze the properties of the bond critical points (electron densities and their Laplacians) in the coordination between phosphazenes ring and the metal cations. Finally, nucleus independent chemical shift (NICS), electric field gradient (EFG), aromatic fluctuation index (FLU), para-delocalization (PDI) and multicenter bond (MCI) aromaticity indices were used for calculation of aromaticity values of phosphazenes ring and its complexes.

Keywords: DFT, QTAIM, aromaticity, phosphazenes
Investigation of Energetics, Structural Stability and Metallic Impurities of Water Clusters: HF and DFT Study of \((H_2O)_n\) for \(n=3-7\) and \((H_2O)_{12}\)

Salih Cınaklı\(^1\), Mustafa Böyükata\(^1\), Yılmaz Dağdemir\(^2\)

\(^1\)Department of Physics, Bozok University, 66200, Yozgat, Turkey.
\(^2\)Department of Physics, Erciyes University, 38039, Kayseri, Turkey.

Studies on water clusters at nano-scale are still active research area [1,2]. In the present work, particularly ring structure of water clusters, \((H_2O)_n\) for \(n=3-7\), have been studied by using Hartree-Fock (HF) and Density Functional Theory (DFT/B3LYP) at 6-311++G(d,p) basis set [3]. Additionally, \((H_2O)_{12}\) clusters consisting of \(n=3, 4\) and 6-molecular rings have been investigated and compared with each other. Energetics and structural stability of these clusters have been analysed. It has been observed that \((H_2O)_6\) is more stable than the neighbors sizes with respect to the second energy differences of the total energies of the clusters for \(n\leq 7\). Moreover, the configuration 12-molecular water cluster containing two 6-molecular rings is relatively more stable than the other isomers due to its lowest potential energy well. Finally, metallic impurities of these water clusters have been examined with Cr, Fe, Co, Ni, Cu and Zn.

References:
3) M. J. Frisch, et. al., Gaussian 03, Revision D.01 (Wallingford, CT: Gaussian Inc.) (2004).

Keywords: Water clusters, HF, DFT, Metallic impurity.
Authentication of Meteorites by Raman Spectroscopy and Multivariate Analysis

Alejandro Gonzalez Sanchez1, A. Magallanes Lujan2, C. Araujo-Andrade3, C. Frausto Reyes3, H. Hernández Cocoletzi3, E. Esparza Ibarra5, D. Valls Gabaud6

2Programa de Licenciatura en Física, Unidad Académica de Física, Universidad Autónoma de Zacatecas. Zacatecas, México.
3Centro de Investigaciones en Óptica, A.C. Unidad Aguascalientes. Aguascalientes, México.
4Facultad de Ingeniería Química, Benemérita Universidad Autónoma del Estado de Puebla. C.P. 72570, Puebla, México
5Unidad Académica de Biología Experimental. Universidad Autónoma de Zacatecas. Zacatecas, México.
6LERMA, CNRS UMR 8112, Observatoire de Paris, 61 Avenue de l’Observatoire, 75014, Paris, France.

We propose a novel, fast, reliable and non-destructive method based on Raman spectroscopy and chemometrics for the analysis and authentication of rocky meteorites. We use the spectral information obtained from rocky samples to discriminate between ordinary terrestrial rocks (with morphology and observable characteristics like meteorites) and authentic meteorites. Applying unsupervised statistical methods, such as Principal Component Analysis, we can discriminate between both groups of samples, being the main discriminating factor, the bands ascribed to hematite, present in all the terrestrial samples. A classification model for the authentication of meteorites was calibrated using supervised methods, such as partial least square regression under the discriminant analysis modality (PLS-DA). The calibrated model was able to correctly classify meteorites and ordinary rocks with sensitivity and specificity values of 78.5% and 85.1%, respectively. The proposed novel methodology is hence a feasible and reliable way for the authentication of meteorites in a non-destructive way allowing analyzing also samples of micrometric size.

Acknowledgements

To CONACYT under the projects CB-2010-01/153066 and UAZ-PIFI 2014.

Keywords: Acknowledgements To CONACYT under the projects CB-2010-01/153066 and UAZ-PIFI 2014.
A Calorimetric Comparison of the Effects of Cholesterol, Desmosterol and 7-Dehydrocholesterol on Zwitterionic DPPC Model Membranes

Cisem Altunayar, Ipek Sahin, Nadide Kazanci

Department of Physics, Faculty of Science, Ege University, 35100 Bornova-Izmir, Turkey

Cholesterol is a main lipid in higher eukaryotic cellular membranes [1]. In between the structurally nearest relatives of cholesterol are its immediate biosynthetic precursors [2]. 7-dehydrocholesterol and desmosterol perform immediate biosynthetic precursors of cholesterol in the Kandutsch-Russell and Bloch pathways, respectively [1]. Zwitterionic dipalmitoyl phosphatidylcholine (DPPC) is the most prevalent phospholipid in native lung surfactant [3]. The studies on the interactions of cholesterol, desmosterol and 7-dehydrocholesterol with membranes at molecular level are very limited [4,5]. In the present study, a calorimetric comparison of the effects of cholesterol, desmosterol and 7-dehydrocholesterol on zwitterionic dipalmitoyl phosphatidylcholine (DPPC) multilamellar vesicles (MLVs) was investigated for the first time by using differential scanning calorimetry (DSC). The result of DSC studies reveals that with the incorporation of 1 mol % concentration of cholesterol, desmosterol and 7-dehydrocholesterol into pure DPPC MLVs, the pretransition starts to shift to lower temperatures. Moreover, the pretransition disappears at \( \sim 10 \) mol % concentration of all the three sterols. With the addition of increasing concentrations of these sterols into pure DPPC MLVs, the main phase transition disappears at \( \sim 40 \) mol % sterol concentration, thus we found that all sterols display the same calorimetric phase behaviour.

References

Keywords: Cholesterol, Desmosterol, 7-dehydrocholesterol, DPPC, DSC
Waste Liquid Embryo Samples’ Measurements and Analysis with Raman Spectroscopy

Tuğçe Öztürk

Department of Physics, Gebze Technical University, Kocaeli, Turkey

Raman spectroscopy is a spectroscopic method which is based on measuring the scattered light from the molecules of samples. A very small portion of the light makes inelastic scattering. This scattering is called Raman scattering. The energy difference between the incident beam and the scattered beam depends on the energy difference between the vibrational energy levels of molecules. It explains why the scattering of Raman bands characterizes the molecules as a fingerprint.

In this study, we measured Raman spectra of embryo culture liquids and compared Raman spectra of embryo liquids in different grades after spectral analysis. Embryo culture liquid samples are prepared for the Raman measurements in IVF clinics of Istanbul University Faculty of Medicine. In Laser Spectroscopy Laboratory of Istanbul Technical University embryo culture liquid waste samples' Raman spectras were measured by using discs. In IVF clinics, embryo culture liquid samples are classified as Grade1 (G1) and Grade2 (G2). G1 has a high potential to give birth more than G2.

Components in the samples are compared with the value of measured Raman spectrums and statistical procedures as principal component analysis (PCA) and linear discriminant analysis (LDA) have been performed. Measurements were taken for each patient with different measuring discs. Embryos waste follicles were tested for reliability of the results of IVF clinic.

The amino acid sequence of bovine serum albumine and histidine aqueous solutions at %50, %10, %2 concentrations were measured as a model for the suspectivity of embryo culture liquid waste samples statistical analysis.

PCA and LDA analysis showed that sensitivity ratio of embryo liquid samples is %75 and susceptivity ratio is %73. As a model of embryo culture liquid waste samples, bovine serum albumine and histidine aqueous solutions at %50, %10 and %2 concentrations; sensitivity and susceptivity ratios for %50, %10 and %2 concentration are measured %100. When histidine component %2 increase, it can be distinguished according to the statistical analysis of the Raman spectroscopic measurements.

Keywords: Raman Spectroscopy In vitro Fertilization
<table>
<thead>
<tr>
<th>Raman Shift</th>
<th>Band Assignment</th>
</tr>
</thead>
<tbody>
<tr>
<td>850</td>
<td>Tyrosine</td>
</tr>
<tr>
<td>897</td>
<td>Glycine, Glutamine</td>
</tr>
<tr>
<td>937</td>
<td>Valine</td>
</tr>
<tr>
<td>1003, 1204</td>
<td>Phenylalanine</td>
</tr>
<tr>
<td>1126</td>
<td>Glucose</td>
</tr>
<tr>
<td>1156</td>
<td>Beta Carotene</td>
</tr>
<tr>
<td>1176</td>
<td>Lysine</td>
</tr>
<tr>
<td>1271, 1341</td>
<td>Phospholipid</td>
</tr>
<tr>
<td>1314</td>
<td>Histidine</td>
</tr>
<tr>
<td>1419, 1449</td>
<td>Some of the amino acid and lipids</td>
</tr>
<tr>
<td>1647</td>
<td>Amide 1 Band</td>
</tr>
</tbody>
</table>
Spectroscopic studies on Cu(II) coordination compound of Sudan Red G [1-(2-methoxyphenylazo)-2-naphthol]

Asli Esme1, Seda Güneşdoğan Sağdınç2, Salih Zeki Yıldız3

1Department of Elementary Science Education, Kocaeli University, Izmit, 41380, Kocaeli, Türkiye.
2Department of Physics, Kocaeli University, Izmit, 41380, Kocaeli, Türkiye.
3Department of Chemistry, Faculty of Arts and Sciences, Sakarya University, 54187, Serdivan, Türkiye.

In this study, we have been report crystal structure determination of the copper (II) coordination compound of Sudan Red G. The selected experimental X-ray data (bond lengths, bond angles and dihedral angles) of the Cu(II) coordination compound of SRG were investigated and compared with the geometrical parameters of SRG using ab initio/Hartree-Fock (HF) and density functional theory (DFT/B3LYP) methods with 6-311++G(d,p) basis set. The vibrational studies in the solid state of the SRG and its Cu(II) coordination compounds were performed by IR spectroscopy. The changes observed between the IR spectra of the ligand and of the complexes allowed us to establish the coordination mode of the metal in the complex. The electronic absorption spectra of the UV–vis area (300–800 nm) of SRG and its Cu(II) coordination compound were measured in a DMSO solution and briefly discussed.

Keywords: Sudan Red G, Cu(II) coordination compound, FT-IR

Fig. 1:

FT-IR spectra of (a) SRG and (b) Cu(II) coordination compound with SRG.
In this study, clathrate of fumaric acid–tetracyanonickel–dioxane, given by the formula M(fumaric acid)Ni(CN)$_4$.2(1,4–dioxane) (M = Mn, Ni and Cd), is obtained for the first time through chemical methods. The FT-IR spectroscopic data in the region of (4000–400) cm$^{-1}$ was recorded and the IR frequencies were given and explained in detail. The thermal behavior of these clathrates was also investigated by thermo-gravimetric analysis (TGA), differential thermal analysis (DTA) and derivative thermal gravimetric analysis (DTG). The spectral and thermal analyses results of the newly synthesized clathrate of fumaric acid–tetracyanonickel–dioxane suggest that these clathrates are new examples of the Hofmann–type dioxane clathrates. In our study, the Hofmann-type dioxane clathrates formed by bounding electrons of oxygen–donor atoms of the carboxyl groups of fumaric acid ligand molecule to transition metal atoms consist of the corrugated $|M$–Ni(CN)$_4|\infty$ polymeric layers which are held in parallel through the chain of ($-$M–FA–M–FA–M–$)$.

**Keywords:** Inclusion Compounds; fumaric acid (FA); Fourier Transform Infrared Spectroscopy (FT-IR); Thermal Analysis; 1,4–dioxane (D); Hofmann–type Clathrate.

The FT-IR spectra of (a), Mn(FA)Ni(CN)$_4$.2D clathrate.
The FT-IR spectra of (b), Ni(FA)Ni(CN)$_2$2D clathrate.

The FT-IR spectra of (c), Cd(FA)Ni(CN)$_2$2D clathrate.
Photophysical Properties of Octatosylamido-Substituted Metal-free and Ni(II) Phthalocyanines: A Density Functional Theory Study

Elif Türker Acar¹, Hatice Can², Ayşe Gül Gürek²

¹Department of Chemistry, Engineering Faculty, Istanbul University, Istanbul, Turkey
²Department of Chemistry, Gebze Technical University, Gebze, Kocaeli, Turkey

Photodynamic therapy (PDT) is currently being studied intensively in the diagnosis, management, and treatment of various neoplasms, based on the selective uptake of a photosensitizer into the malignant tissues followed by local irradiation with either visible or near-infrared light [1]. Metallophthalocyanine complexes have proved to be highly promising as photosensitizers for photodynamic therapy (PDT), due to their intense absorption in the red region of the visible light. High triplet state quantum yields and long triplet lifetimes are required for an efficient sensitization. The photophysical properties of the phthalocyanine dyes are strongly influenced by the presence and nature of the central metal ion.

Reported herein is a DFT/TDDFT theoretical investigations of the ground and excited states of Octatosylamido-substituted metal-free and Ni(II) phthalocyanines. Effect of metal on the photophysical and photochemical parameters of Octatosylamido-substituted phthalocyanine derivatives is studied in DMSO. The detailed atomistic-level excited state DFT calculations of the phthalocyanines bring some valuable directions in the rational designing of new metallo phthalocyanine compounds having photodynamic potential in cancer treatment as well as in the experimental synthesis. The calculated results are in good agreement with the experimental data [2], indicating that the method and the basis set selected are feasible for calculating such a large molecule as Octatosylamido-substituted phthalocyanines.

References:

Keywords: Phthalocyanine, Photophysical Properties, Density Functional Theory

Tülin Gürkan Polat, Osman Duman, Sibel Tunç

Department of Chemistry, Akdeniz University, Antalya, Turkey

Synthetic dyes are broadly used in various industries [1]. The treatment of wastewaters including dyestuffs is quite difficult because of their complex structure. There are various methods to remove dyes from wastewaters. Among of these methods, adsorption is an attractive treatment due to its cheapness, effectiveness and simplicity of process [2]. Clay minerals have excellent adsorption capacity owing to their unique physicochemical properties, high specific surface area and high cation exchange capacity [3].

The aim of this work was to study the adsorption mechanism and adsorption kinetics of a cationic dye, Basic Red 9 (BR9), onto sepiolite from aqueous solution in respect of initial dye concentration, temperature and pH and also to understand the interactions between adsorbent and dye molecule. The surface and textural properties of sepiolite were investigated by zeta potential and SEM measurements, respectively. XRD analysis was carried out to determine the type of clay mineral. The chemical composition of sepiolite was analyzed by XRF spectrometer. FTIR spectra of sepiolite (before and after BR9 adsorption) were recorded by FTIR spectrometer. Adsorption process was followed by UV-vis spectrophotometric method. In conclusion, XRD analysis showed that the clay mineral used in this study is primarily sepiolite. The results of SEM analysis indicated that sepiolite has a fibrous structure. The adsorption amount of BR9 onto sepiolite is higher at low temperatures. The adsorption of BR9 onto sepiolite is an exothermic process. The dye adsorption amount of sepiolite exhibited an increase with increasing initial BR9 concentration due to the presence of greater amount of BR9 molecules in solution. The pH change of dye solution have a minor impact on the adsorption process. Adsorption kinetics of BR9 follows the pseudo second-order kinetic model. The increase in the adsorption amount of BR9 caused a decrease in the zeta potential of sepiolite.

References

Keywords: Adsorption, Spectroscopy, Basic Red 9, Sepiolite.
In this study, clathrate of adipic acid–tetracyanonickel–dioxane, given by the formula M(adipic acid)Ni(CN)$_4$.(1,4–dioxane) (M = Co and Cu), is obtained for the first time through chemical methods. The FT-IR spectroscopic data in the region of (4000–400) cm$^{-1}$ was recorded and the IR frequencies were given and explained in detail. The spectral analyses results of the newly synthesized clathrate of adipic acid–tetracyanonickel–dioxane suggest that these clathrates are new examples of the Hofmann–type dioxane clathrates. In our study, the Hofmann-type dioxane clathrates formed by bounding electrons of oxygen–donor atoms of the carboxyl groups of adipic acid (AA) ligand molecule to transition metal atoms consist of the corrugated [$\text{M–Ni(CN)}_4$]$\infty$ polymeric layers which are held in parallel through the chain of (–M–AA–M–AA–M–).

**Keywords:** Inclusion Compounds; adipic acid (AA); Fourier Transform Infrared Spectroscopy (FT-IR); 1,4–dioxane (D); Hofmann–type Clathrate.

The FT-IR spectra of (a) Co(AA)Ni(CN)$_4$.D clathrate.

The FT-IR spectra of (a) Cu(AA)Ni(CN)$_4$.D clathrate.
Material composition of Universe is a central question, since the first scientific surway. Answers to this question requires inter-disciplinary reseach, such as astrophysics, solid state physics, atomic physics. An extraordinary method to investigate material composition of Universe on Earth is to study meteroids, which provides outer-space information. Here, we discuss and investigate the magnetic properties of outer-space materials, starting from magneic properties of ordinary materials. We, propose that investigating low temperature magnetization properties of “space stones” would pave the path to understand material composition of the Universe.

**Keywords:** temperature, low, space, stones, magnetic, properties
The cyanide-bridged heteronuclear complexes, $[\text{Zn}(\text{hmpH})_2 \text{M}(\mu-\text{CN})_2(\text{CN})_2]_n$ (M(II) = Pd or Pt, hmpH = 2-pyridinemethanol) have been synthesized and characterized by FT-IR and Raman spectroscopies, thermal and elemental analyses. The FT-IR and Raman spectra of the complexes were reported in the range of 4000-225 cm$^{-1}$ (Figure 1). The M(II) ions are coordinated by four cyanide ligands, while Zn(II) ion is also surrounded by the two hmpH and two cyanide ligands. Thermal stabilities and decomposition products of the complexes were investigated from 30 to 700 °C in air. Spectral, elemental and thermal analyses of the complexes indicate that the complexes are similar to Cu(II) complexes with hmpH; $[\text{Cu}(\text{hmpH})_2\text{M}(\mu-\text{CN})_2(\text{CN})_2]_n$ (Figure 2), $[\text{Cu}(\text{hmpH})_2\text{Pt}(\mu-\text{CN})_2(\text{-CN})_2]_n$ [1].

**Keywords:** Tetracyanometalate(II) complex; 2-pyridinemethanol complex; Vibrational spectroscopy; Cyanide-bridged complex, thermal analysis.
P-126

Vibrational Spectra and Electronic Transition Energies from MP2 and DFT Calculations of 1-Ethylimidazole and 2-Ethylimidazole

Ilkan Kavlak, Güneş Süheyla Kürkçüoğlu

Eskişehir Osmangazi University

In this study, the optimized geometry, harmonic vibrational frequencies, infrared intensities and the corresponding vibrational assignments of 1-ethylimidazole and 2-ethylimidazole molecules were calculated by DFT-B3LYP and MP2 methods with 3-21G, 6-31G, 6-311G, CEP-4G, CEP-31G, CEP-121G, SDD, LANL2DZ basis sets using Gaussian09W packet program. The Fourier transform infrared spectra of these molecules were recorded using FT-IR Spectrometer in the range of 4000-250 cm⁻¹. The effects of the methods and the basis sets used on the calculated vibrational frequencies were discussed. Electronic Transition Energies of these molecules have been calculated with TD-B3LYP methods with 3-21G, 6-31G, 6-311G, CEP-4G, CEP-31G, CEP-121G, LANL2DZ, SDD basis sets. The calculated HOMO and LUMO energies show that charge transfer occur in these molecules.

Keywords: 1-ethylimidazole, 2-ethylimidazole, Vibrational spectra, MP2, TD-B3LYP, B3LYP, HOMO, LUMO.
Heterocyclic compounds having 1H-pyrrole-1-carboxamide derivative of its structure is involved actively in the treatment of diabetic diseases [1].

In this study, a new pyrrole compound was synthesized from 2-aminooxazole (1) and aniline (2) by refluxing in methyl alcohol. The product was characterized with molecular spectroscopic techniques (FT-IR, 1H-NMR, 13C-NMR and X-ray) and elemental analysis.

**Keywords:** 2-aminooxazole, Pyrrole, Synthesis and Characterization

ORTEP diagram of compound.
Sensitive and Selective Determination of Trace Amounts of Azin Dyes in Multi-component Systems Using First-Order Derivative Spectrophotometric Technique

Elif Türker Acar, Gülten Atun

Istanbul University, Engineering Faculty, Department of Chemistry, Avcilar 34320, Istanbul, Turkey

Dye effluents are one of the major water pollutants due to the wide variety of sources. Approximately $7 \times 10^4$ tons/year of dyes discharged into waste streams by only textile industry [1]. There is an increasing demand for sensitive and selective methods for dye detection identification and quantification in water at low levels because of their carcinogenic properties. First-order derivative spectrophotometric (FODS) technique is one of sensitive and selective methods for simultaneous analysis of the dyes in multi-component dye systems.

Thionin (TH), methylene blue (MB) and safranine O (SO) are similar types of azine dyes which are widely used in textile industry. All of the dyes were determined sensitively and selectively in their single, binary and ternary dye mixtures using (FODS) method. Concentration of any dye in the TH-MB, TH-SO, MB-SO and TH-MB-SO mixtures was measured using the peaks at the zero-crossing points of other dyes in single solution [2] or where its absorbance is zero [3]. Analytical parameters, molar extinction coefficient ($\varepsilon$), limit of detection (LOD) and root mean square error (RMSE), were determined using the calibration curves. The LOD values obtained by (FODS) method were found at the nanomolar concentration level for azin dyes.

References:

Keywords: First-order derivative spectrophotometric technique, Sensitive Determination, Azin Dyes.
In this study, 3-phenyl-4-(3-cinnamoyloxybenzylideneamino)-4,5-dihydro-1H-1,2,4-triazol-5-one were synthesized by the reaction of 3-phenyl-4-amino-4,5-dihydro-1H-1,2,4-triazol-5-one with 3-sinnamoyloxybenzaldehyde [1].

The molecule was optimized by using the B3LYP/631G (d) and HF/631G (d) basis sets [2,3]. Afterwards, 1H-NMR and 13C-NMR isotropic shift values were calculated by the method of GIAO using the program package Gaussian G09W [2]. Experimental and theoretical values were inserted into the graphic according to equitation of $\delta_{\text{exp}}=a+b$. $\delta_{\text{calc}}$. The standard error values were found via SigmaPlot program with regression coefficient of a and b constants. Furthermore, theoretical bond lengths, bond angles, UV-Vis values, dipole moments, formal charges, HOMO-LUMO energies, total energy of the molecule, ionization potential, electron affinity, electronegativity and calculated thermodynamic properties for both methods were calculated.

This study is supported by a grant (Project Number: 2014-FEF-24) from Scientific Research Projects Coordination Unit of Kafkas University.

Keywords: synthesis, theoretical, gaussian
References


Gaussian Calculations of New 3-(p-Methylbenzyl)-4-[3-(3-Methoxybenzoyl)-Benzylydenamino]-4,5-Dihydro-1H-1,2,4-Triazol-5-one

Hilal Medetalibeyoğlu, Haydar Yüksekg

Department of Chemistry, Kafkas University, Kars, Turkey

3-(p-Methylbenzyl)-4-[3-(3-Methoxybenzoyl)-Benzylydenamino]-4,5-dihydro-1H-1,2,4-triazol-5-one molecule [1] was optimized by using the B3LYP/6-311G (d) and HF/6-311G (d) basis sets [2, 3]. 1H-NMR and 13C-NMR isotropic shift values were calculated by the method of GIAO using the program package Gaussian G09W [3]. Experimental and theoretical values were inserted into the graph according to equation of δ exp=a+b. δ calc. The standard error values were found via SigmaPlot program with regression coefficient of a and b constants. IR absorption frequencies of analysed molecule were calculated by two methods. Then, they were compared with experimental data, which are shown to be accurate. Infrared spectrum were composed by using the data obtained from both methods. The veda4f program, was used in defining IR data, which were calculated theoretically [4]. Additionally, this compound was found bond angles, bond lengths, the HOMO-LUMO energy, ionization potential, electron affinity, electronegativity and Mulliken charges by using the B3LYP/6-311G (d) and HF/6-311G (d) basis sets.

Keywords: Experimental, theoretical, HOMO-LUMO, GIAO

Optimized structure of the molecule
References

1 Bazı Yeni 4-[3-(3-Metoksibenzoksii)-Benziilenamino]-4,5-Dihidro-1H-1,2,4-Triazol-5-On Türevlerinin Sentezi, DeneySEL ve Teorik Özelliklerinin İncelemesi, Doktora Tezi, Kafkas Üniversitesi, Fen Bilimleri Enstitüsü, Kars (2015).


A Computational Study on the Electronic and Nonlinear Optical Properties of h-BN-Graphyne Subunit

Büşra Aydin, Mehmet Bahat

Gazi Üniversitesi, Ankara, TURKEY

After the experimental isolation of graphene, all 2D materials sparked a general interest in both fundamental and practical nanotechnology because of significant potential for applications in molecular electronics, nanomechanics, optics, and sensors. Graphyne is a two-dimensional carbon allotrope as graphene. A recent study indicates that the electronic properties of graphyne is potentially superior to graphene. Boron nitride (BN) chemical doping of graphene and graphyne have recently been achieved in different configuration and concentrations. Structurally, a single layer of hexagonal boron nitride (h-BN) is very similar to a graphene sheet. Recently, hexagonal boron nitride analog structures of graphene, graphyne, and graphyne and their some substructures have been studied computationally. One of substructures of graphyne is tribenzocyclyne (TBC, C₆H₁₂) compound. In this work, we present a computational study of the electronic, and nonlinear optical properties of the h-BN analog of TBC (triborazinecyclyne, B₉N₆C₆H₁₂) and their flor derivatives (replacing hydrogen on the one borazine ring with florine). The calculated properties are the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) energies, polarizability and first hyperpolarizability which important to design materials. The density functional theory (DFT) based method B3LYP/6-31+G(d,p) were carried out.

**Keywords:** h-BN graphyne subunit; polarizability; hyperpolarizability; B3LYP
An Investigation of Keto-enol Tautomerism in 2,4-di-tert-butyl-6-{(Z)-[(2-or 4- fluorophenyl)imino]methy}Phenol by Spectroscopic and Quantum Chemical Calculation Methods

Erol Eroğlu¹, Murat Kılıç², Ihsan Burak Çam², Timur Tongur²

¹Akdeniz University, Faculty of Education, Department of Primary Sciences Education, Kampüs, 07059, Antalya, Turkey
²Akdeniz University, Gıda Güvenliği ve Tarımsal Araştırmalar Merkezi, Kanpüs, 07059, Merkez, Antalya, Turkey

In this study, we investigated the tautomeric equilibrium of the title compound by means of experimental IR and UV-Visible spectroscopy methods and quantum chemical calculations. IR (in solid phase) and UV-Visible (in acetone, methanol and chloroform) spectra of the compound were measured. Energetics, IR and UV-Visible spectra of the two possible tautomeric forms were calculated at the TDDFT/DFT/B3LYP together with 6-311+G (d, p) basis set level of the theory. Results of the calculation indicated that enol form is more stable keto form in vacuum and solvents. The lowest barrier height for the tautomerization reaction was about 3 kcal/mole solvent.

Keywords: keto-enol tautomerism, solvent affect, dft, uv-visable spectroscopy
Effect of Fluoro- and Chloro- Substitution of the Phenyl Ring on Enol-keto Tautomeric Equilibriums of 2,4-di-tert-butyl-6-{(Z)-[(2,5-fluorophenyl or 2,5-Chlorophenyl)imino]methy}phenol: A Spectroscopic and DFT Study

Erol Eroğlu1, Nuri Torulmaz, Zekiye Eda Bıyluğ, Mehmet Murat Yaşar

Akdeniz University, Faculty of Education, Department of Primary Sciences Education, Kampüs, 07059, Antalya, Turkey

In this study, we investigated Fluoro- and Chloro- substitution effect on the tautomeric equilibrium of the 2,4-di-tert-butyl-6-{(Z)-[(2,5-fluorophenyl or 2,5-Chlorophenyl)imino]methy}phenol by means of experimental IR and UV-Visible spectroscopy methods and quantum chemical calculations. IR (in solid phase) and UV-Visible (in acetone, methanol and chloroform) spectra of the compounds were measured. Energetics, IR and UV-Visible spectra of possible tautomeric forms were calculated at the TDDFT/DFT/B3LYP together with 6-311+G (d, p) basis set level of the theory. The polarizable continuum model (PCM) was used to calculate the energetics and spectral properties of the compounds in solvent media. Result of the calculations indicated that enol form is more stable than keto form in vacuum and solvents. The lowest barrier height for the tautomerization reaction from enol to keto form were calculated in methanol is 2.051 kcal/mole for 2,5-Chlorophenyl substituted one.

Keywords: keto-enol tautomerism, dft, molecular spectroscopy
Vibrational Spectroscopic Analyses of Pollutants in Soil Samples Collected from Historical Libraries’ Environments.

Ozan Unsalan¹, Alpaslan Kuzucuoğlu², Ersin Kaygısız¹

¹University of Istanbul, Faculty of Science, Physics Dept., Atomic and Molecular Physics Div. 34134, Vezneciler, Fatih, Istanbul
²İstanbul Yeni Yüzyıl University, Occupational Health and Safety Department, Zeytinburnu, 34010 Istanbul, Turkey

By vibrational spectroscopic techniques, 3 regions of 8 different historical libraries’ (İlim Yayma Vakfı Recâi Mehmed Efendi, Atıf Efendi, Süleymaniye, Millet, Beyazıt Yazma Eser, Nur-u Osmaniye, Köprülülü and Ragıp Paşa Libraries) soil samples were examined in order to understand how various pollutants effected these soil samples. Thus, it will be possible to say how the rare manuscripts could be affected by these pollutants. For this purpose Infrared and Raman spectroscopic methods were used. This study is still being continued and preliminary results were presented here.

Keywords: Raman spectroscopy, preventive conservation, non destructive methods, information and document management

Figure 1.

The points which were soil samples collected from rare books’ libraries for Raman spectroscopic analysis
P-135

Raman Spectroscopic Investigations on Rare Books’ Covers and Pages from Historical Libraries. Case Study: Recai Mehmet Efendi Library

Ozan Unsalan¹, Alpaslan Kuzucuoğlu²

¹University of Istanbul, Faculty of Science, Physics Dept., Atomic and Molecular Physics Div. 34134, Vezneciler, Fatih, İstanbul
²İstanbul Yeni Yüzyıl University, Occupational Health and Safety Department, Zeytinburnu, 34010 Istanbul, Turkey

Raman spectroscopic methods are frequently used in protecting cultural heritage. These techniques give important knowledge when especially combined with other techniques such as XRF and SEM-EDX. For example, Raman spectroscopic techniques play an important role in determining the pigments used in paintings. On the other hand, good information can be extracted from the samples of the rare books’ either inner pages or covers. Aim of this study is, as an interdisciplinary study case, to contribute cultural heritage by investigating the conditions of rare books’ covers by Raman spectroscopic techniques. In this study, some rare books’ inner pages and covers which located at Recai Mehmet Efendi library were investigated by Raman spectroscopy and comments were given on their protection status.

Keywords: Raman spectroscopy, preventive conservation, non destructive methods, information and document management
Micro-Raman, Mid-IR and DFT Studies on 2-[4-(4-Ethylbenzamido)phenyl]benzothiazole

K. Bolelli¹, H. Ari², M. Boyukata³, I. Yalcin¹, O. Unsalan⁴

¹Ankara University, Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Tandoğan, TR-06100, Ankara, Turkey
²Bozok University, Faculty of Science and Letters, Chemistry Department, 66200 Yozgat, Turkey
³Bozok University, Faculty of Science and Letters, Physics Department, 66200 Yozgat, Turkey
⁴University of Istanbul, Faculty of Science, Physics Department, Vezneciler-Fatih, TR-34134 Istanbul, Turkey

Molecular structure of 2-[4-(4-Ethylbenzamido)phenyl]benzothiazole (BSN-009) [1] was identified by Fourier Transform Infrared (with KBr and ATR techniques), Raman spectroscopy and quantum chemical calculations. Mid-IR spectrum was recorded on Perkin–Elmer Spectrum Two FT-IR Spectrometer with 0.5 cm\(^{-1}\) resolution at room temperature in the 4000-400 cm\(^{-1}\) region for the first time. Raman spectrum was recorded on Renishaw inVia Raman Microscope Spectrophotometer with 0.5 cm\(^{-1}\) resolution, in the 4000-100 cm\(^{-1}\) range. Optimized molecular structure, the most stable conformers and vibrational wavenumbers of the compound in its ground state have been calculated by using Density Functional Theory (DFT) using B3LYP functional with 6-311++G(d,p) basis set. All calculations were performed with Gaussian09 software [2]. Vibrational wavenumbers and optimized geometric parameters were seen to be in good agreement with the experimental data. Furthermore, assignments of each vibrational mode were interpreted in terms of potential energy distributions in detail.

References

Keywords: Micro-Raman, Mid-IR and DFT studies on 2-[4-(4-Ethylbenzamido)phenyl]benzothiazole
FT-IR Spectroscopy and Multivariate Analysis as an Auxiliary Tool for Diagnosis of Mental Disorders: Bipolar and Schizophrenia Cases

G. Ogruc Ildiz1, O. Unsalan2, C. Araujo Andrade3, M. Arslan4, H. T. Karatepe4, A. Yilmaz2, O. B. Yalcinkaya2, H. Herken4

1Istanbul Kultur University, Faculty of Science and Letters, Department of Physics, Atakoy Campus, 34156 Bakirkoy, Istanbul, Turkey
2Istanbul, Faculty of Science, Physics Department, Vezneciler-Fatih, 34134 Istanbul, Turkey
3Unidad Académica de Física de la Universidad Autónoma de Zacatecas, Zacatecas, Mexico
4Pamukkale University, Faculty of Medicine, Department of Psychiatry, Bayramyeri, Denizli, Turkey

In this study, a methodology based on Fourier-transform infrared spectroscopy and principal component analysis and partial least square methods is proposed for the analysis of blood plasma samples in order to identify spectral changes correlated with some biomarkers associated with schizophrenia and bipolarity. Our main goal was to use the spectral information for the calibration of statistical models to discriminate and classify blood plasma samples belonging to bipolar and schizophrenic patients. IR spectra of 30 samples of blood plasma obtained from each, bipolar and schizophrenic patients and healthy control group were collected. The results obtained from principal component analysis (PCA) show a clear discrimination between the bipolar (BP), schizophrenic (SZ) and control group (CG) blood samples that also give possibility to identify three main regions that show the major differences correlated with both mental disorders (biomarkers). Furthermore, a model for the classification of the blood samples was calibrated using partial least square discriminant analysis (PLS-DA), allowing the correct classification of BP, SZ and CG samples. The results obtained applying this methodology suggest that it can be used as a complimentary diagnostic tool for the detection and discrimination of these mental diseases.

Keywords: FT-IR spectroscopy and multivariate analysis as an auxiliary tool for diagnosis of mental disorders: Bipolar and schizophrenia cases

Figure.1
Crystal Structure of 4-fluoro-N-(2-hydroxy-4-nitrophenyl)Benzamide

Janina Karolak Wojciechowska¹, Malgorzata Szczesio¹, Tugba Ertan Bolelli², Esin Aki², Ismail Yalcin²

¹Technical University of Sódœ, Institute of General and Ecological Chemistry, Łeromskiego 116, 90-924 Łódzœ, Poland
²Ankara University, Faculty of Pharmacy, Department of Pharmaceutical Chemistry, 06100 Ankara, Turkey

The crystal structure studies of the title compound were conducted with the aim to obtain 3D structure which subsequently can be used as a starting point for molecular modeling of other (2-hydroxyphenyl)benzamides. The dihedral angle between two aromatic rings, describing whole molecule deviation from planarity, is the most important geometrical parameter in the studied structure. The CSD search for (2-hydroxyphenyl)benzamide leading as the basic structure moiety gave three similar structures. Among them one is almost flat (angle close to 0°), while remaining two molecules assume butterfly shape with the higher dihedral angle values exciding 8° and 14°, respectively. In the title crystal structure, the dihedral angle between the aromatic rings is 14.1(2)°. The angles between the plane of the amide group and both aromatic rings are not equal. The 4-fluoro-substituted phenyl (ring A) is inclined at 20.9(2)°, while 2-hydroxy-4-nitrophenyl (ring B) - only at 6.8(2)°. This important flattening of the B ring and amide group is caused by stable five-membered ring constructed by intramolecular hydrogen bond of d(N3–H3•••O36) = 2.573(1) Å. The crystal structure consists of infinite ribbons of 4-fluoro-N-(2-hydroxy-4-nitrophenyl)-benzamide molecules connected by intermolecular hydrogen bonds between the hydroxyl and carbonyl groups of adjacent molecules. The interaction O36–H36•••O2 occurring over a distance of 2.591(1) Å and possessing angle of 174.9°, can be classified as a strong hydrogen bond.

Reference

Keywords: Crystal structure of 4-fluoro-N-(2-hydroxy-4-nitrophenyl)benzamide

Figure.1
<table>
<thead>
<tr>
<th>Author Name</th>
<th>First Page</th>
<th>Last Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>ABDALLAH Samah Saleh</td>
<td>O-09</td>
<td>O-19</td>
</tr>
<tr>
<td>ABDDELHAKİM Benosman</td>
<td>P-046</td>
<td></td>
</tr>
<tr>
<td>ABDELLAH Zaiter</td>
<td>P-002</td>
<td></td>
</tr>
<tr>
<td>ABDOU Boucekkine</td>
<td>O-11</td>
<td>P-002</td>
</tr>
<tr>
<td>AĞAR Ayşen Alaman</td>
<td>P-026</td>
<td>P-025</td>
</tr>
<tr>
<td>AĞAR Erbil</td>
<td>P-014</td>
<td>P-061</td>
</tr>
<tr>
<td>AİOB Ziad Siad</td>
<td>O-04</td>
<td></td>
</tr>
<tr>
<td>AİSSAOUIİ Hanane</td>
<td>P-056</td>
<td></td>
</tr>
<tr>
<td>AİTELHADJALİ Zakia</td>
<td>P-006</td>
<td></td>
</tr>
<tr>
<td>AKİ Esin</td>
<td>P-138</td>
<td></td>
</tr>
<tr>
<td>ALAGÖZ SAYİN Tuba</td>
<td>P-017</td>
<td></td>
</tr>
<tr>
<td>ALAŞALVAR Can</td>
<td>P-102</td>
<td></td>
</tr>
<tr>
<td>ALAT Y.</td>
<td>P-050</td>
<td></td>
</tr>
<tr>
<td>ALDIRMAZ Emine</td>
<td>P-049</td>
<td></td>
</tr>
<tr>
<td>ALENKİNA Irina V</td>
<td>O-21</td>
<td></td>
</tr>
<tr>
<td>ALİ SAHRAOÜİ Ferhat</td>
<td>P-105</td>
<td></td>
</tr>
<tr>
<td>ALPASLAN Gökhan</td>
<td>P-076</td>
<td></td>
</tr>
<tr>
<td>ALTUN Ayhan</td>
<td>P-039</td>
<td></td>
</tr>
<tr>
<td>ALTUNAY Nail</td>
<td>P-010</td>
<td></td>
</tr>
<tr>
<td>ALTUNAYAR Cisem</td>
<td>P-117</td>
<td></td>
</tr>
<tr>
<td>ALULA Melisew Tadele</td>
<td>P-095</td>
<td></td>
</tr>
<tr>
<td>AMARO Ana María</td>
<td>P-107</td>
<td></td>
</tr>
<tr>
<td>AMEDDAH Souad</td>
<td>P-053</td>
<td></td>
</tr>
<tr>
<td>AMEL Amrani</td>
<td>P-034</td>
<td></td>
</tr>
<tr>
<td>AMEL Boutasta</td>
<td>P-046</td>
<td></td>
</tr>
<tr>
<td>AMİNA Adala</td>
<td>P-005</td>
<td></td>
</tr>
<tr>
<td>AMIRAT Samia</td>
<td>P-030</td>
<td></td>
</tr>
<tr>
<td>ANDIRMAZ Emine</td>
<td>P-049</td>
<td></td>
</tr>
<tr>
<td>ANDRADE Cuauhtemoc</td>
<td>P-107</td>
<td></td>
</tr>
<tr>
<td>ANDRUSHCHENKO Valery</td>
<td>O-16</td>
<td></td>
</tr>
<tr>
<td>ANDRUSHCHENKO Valery</td>
<td>O-16</td>
<td></td>
</tr>
<tr>
<td>AOUCHİCHE Hocine</td>
<td>P-011</td>
<td></td>
</tr>
<tr>
<td>ARAB Fahima</td>
<td>P-105</td>
<td>P-105</td>
</tr>
<tr>
<td>ARAÇ Aliye</td>
<td>P-054</td>
<td></td>
</tr>
<tr>
<td>ARAUJO ANDRADE C.</td>
<td>P-137</td>
<td></td>
</tr>
<tr>
<td>AŘİ H.</td>
<td>P-136</td>
<td></td>
</tr>
<tr>
<td>ARSLAN M.</td>
<td>P-137</td>
<td></td>
</tr>
<tr>
<td>ATSİLAN M.</td>
<td>P-137</td>
<td></td>
</tr>
<tr>
<td>ATALAY Yusuf</td>
<td>P-104</td>
<td></td>
</tr>
<tr>
<td>ATUN Gülten</td>
<td>P-128</td>
<td></td>
</tr>
<tr>
<td>AVCI Davut</td>
<td>P-104</td>
<td></td>
</tr>
<tr>
<td>AYDİN Büşra</td>
<td>P-131</td>
<td></td>
</tr>
<tr>
<td>BAATOUCHE Samia</td>
<td>P-083</td>
<td></td>
</tr>
<tr>
<td>BACHVAROVA Darina</td>
<td>P-100</td>
<td></td>
</tr>
<tr>
<td>BAHAT Mehmet</td>
<td>P-131</td>
<td></td>
</tr>
<tr>
<td>BAHCECİ Tugçe</td>
<td>P-081</td>
<td></td>
</tr>
<tr>
<td>BAHCECİ Tugçe</td>
<td>P-080</td>
<td></td>
</tr>
<tr>
<td>BAŞALMA Dilek</td>
<td>P-033</td>
<td></td>
</tr>
<tr>
<td>Author Name</td>
<td>Page Numbers</td>
<td></td>
</tr>
<tr>
<td>-----------------------------------</td>
<td>--------------</td>
<td></td>
</tr>
<tr>
<td>BATI Hümyera</td>
<td>P-091, P-093</td>
<td></td>
</tr>
<tr>
<td>BLACKBURN Jonathan</td>
<td>P-095</td>
<td></td>
</tr>
<tr>
<td>BEN SAİD Ridha</td>
<td>O-28</td>
<td></td>
</tr>
<tr>
<td>BENACHERİNE Mohamed Mehdi</td>
<td>P-045</td>
<td></td>
</tr>
<tr>
<td>BENAMER Ali</td>
<td>P-108</td>
<td></td>
</tr>
<tr>
<td>BENAYACHE Fadila</td>
<td>P-028, P-029, P-053, P-056, P-083</td>
<td></td>
</tr>
<tr>
<td>BENAYACHE Samir</td>
<td>P-028, P-029, P-053, P-056, P-083</td>
<td></td>
</tr>
<tr>
<td>BENDJABEUR Seyfeddine</td>
<td>P-031</td>
<td></td>
</tr>
<tr>
<td>BENLAHRECHE Fatima Zohra</td>
<td>P-008, P-009</td>
<td></td>
</tr>
<tr>
<td>BENSİHA Rabah</td>
<td>P-037</td>
<td></td>
</tr>
<tr>
<td>BESMA Dekiche</td>
<td>P-005</td>
<td></td>
</tr>
<tr>
<td>BEYTUR Murat</td>
<td>P-129</td>
<td></td>
</tr>
<tr>
<td>BİNGÖL ALPASLAN Yelda</td>
<td>P-076</td>
<td></td>
</tr>
<tr>
<td>BİTAM Adel</td>
<td>P-057</td>
<td></td>
</tr>
<tr>
<td>BIYLUĞ Zekiye Eda</td>
<td>P-133</td>
<td></td>
</tr>
<tr>
<td>BODUR Erdem</td>
<td>P-021</td>
<td></td>
</tr>
<tr>
<td>BOUGANDOURA Amina</td>
<td>P-028</td>
<td></td>
</tr>
<tr>
<td>BOUGHERARA Hassina</td>
<td>P-055</td>
<td></td>
</tr>
<tr>
<td>BOUGHERA Bachia</td>
<td>P-029</td>
<td></td>
</tr>
<tr>
<td>BOUMAZA Ouahiba</td>
<td>P-028</td>
<td></td>
</tr>
<tr>
<td>BOURINGHABACHA Rabia</td>
<td>P-029</td>
<td></td>
</tr>
<tr>
<td>Bouabhi</td>
<td>P-029</td>
<td></td>
</tr>
<tr>
<td>BOYACIOĞLU Ayşegül</td>
<td>P-033</td>
<td></td>
</tr>
<tr>
<td>BOYUKAT Mustafa</td>
<td>P-052</td>
<td></td>
</tr>
<tr>
<td>BOYUKATA M.</td>
<td>P-136</td>
<td></td>
</tr>
<tr>
<td>BOYUKATA M.</td>
<td>P-136</td>
<td></td>
</tr>
<tr>
<td>BÖYÜKAT Mustafa</td>
<td>P-101, P-115</td>
<td></td>
</tr>
<tr>
<td>BÖYÜKAT Mustafa</td>
<td>P-101, P-115</td>
<td></td>
</tr>
<tr>
<td>CHEURFİ Wassila</td>
<td>P-055</td>
<td></td>
</tr>
<tr>
<td>CHİRİTA Lenuta</td>
<td>P-112</td>
<td></td>
</tr>
<tr>
<td>CHAMPİON Christophe</td>
<td>P-006, P-011</td>
<td></td>
</tr>
<tr>
<td>CHAPMAN Gala</td>
<td>O-08</td>
<td></td>
</tr>
<tr>
<td>CEVİZ Tuba</td>
<td>P-097</td>
<td></td>
</tr>
<tr>
<td>ÇELENİLİKBEK Miray</td>
<td>P-043</td>
<td></td>
</tr>
<tr>
<td>ÇANKAYA Nevin</td>
<td>P-066, P-068</td>
<td></td>
</tr>
<tr>
<td>ÇAM Ihsan Burak</td>
<td>P-132</td>
<td></td>
</tr>
<tr>
<td>CAN Hatice</td>
<td>P-121</td>
<td></td>
</tr>
<tr>
<td>ÇETİN Kahraman</td>
<td>P-080, P-081</td>
<td></td>
</tr>
<tr>
<td>CHERİET Thamere</td>
<td>P-083</td>
<td></td>
</tr>
<tr>
<td>CHİRİTA Lenuta</td>
<td>P-112</td>
<td></td>
</tr>
<tr>
<td>CRISTIANA Maria</td>
<td>P-087</td>
<td></td>
</tr>
<tr>
<td>ÇALİSKAN Nezihe</td>
<td>P-060</td>
<td></td>
</tr>
<tr>
<td>ÇAM Ihsan Burak</td>
<td>P-132</td>
<td></td>
</tr>
<tr>
<td>BİLGİN Tuba</td>
<td>P-112</td>
<td></td>
</tr>
<tr>
<td>BİLGİN Tuba</td>
<td>P-112</td>
<td></td>
</tr>
<tr>
<td>CALİSKAN Nezihe</td>
<td>P-060</td>
<td></td>
</tr>
<tr>
<td>ÇAM Ihsan Burak</td>
<td>P-132</td>
<td></td>
</tr>
<tr>
<td>CAN Hatice</td>
<td>P-121</td>
<td></td>
</tr>
<tr>
<td>ÇAM Ihsan Burak</td>
<td>P-132</td>
<td></td>
</tr>
<tr>
<td>CAN Hatice</td>
<td>P-121</td>
<td></td>
</tr>
<tr>
<td>ÇAM Ihsan Burak</td>
<td>P-132</td>
<td></td>
</tr>
<tr>
<td>CAN Hatice</td>
<td>P-121</td>
<td></td>
</tr>
<tr>
<td>Author Index</td>
<td></td>
<td></td>
</tr>
<tr>
<td>--------------</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CHOWDHRY Babur Zahurridin</td>
<td>DAŞBAŞI Teslima</td>
<td>DJAMEL Sarri</td>
</tr>
<tr>
<td>P-082</td>
<td>P-066</td>
<td>P-027</td>
</tr>
<tr>
<td>P-068</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CHOWDHRY Babur Zahurridin</td>
<td>DAVID Chapron</td>
<td>DJAMILA Zama</td>
</tr>
<tr>
<td>P-004</td>
<td>P-098</td>
<td>P-034</td>
</tr>
<tr>
<td>P-099</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CHRİSTOPHE Champion</td>
<td>DEBBACHE Nadia</td>
<td>DOBROZEMSKY Rudolf</td>
</tr>
<tr>
<td>P-073</td>
<td>P-015</td>
<td>P-003</td>
</tr>
<tr>
<td>P-045</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CHUKİN Andrey V</td>
<td>DECELİOĞLU Mustafa</td>
<td>DRUTU Valentina</td>
</tr>
<tr>
<td>O-22</td>
<td>P-080</td>
<td>P-112</td>
</tr>
<tr>
<td>CIALLA MAY Dana</td>
<td>DEGE Necmi</td>
<td>DUMAN Osman</td>
</tr>
<tr>
<td>P-038</td>
<td>P-104</td>
<td>O-14</td>
</tr>
<tr>
<td>P-038</td>
<td></td>
<td>P-122</td>
</tr>
<tr>
<td>CİNAKLİ Salah</td>
<td>DEKKİCHE Besma</td>
<td>DUMİTRAS Dan Constantin</td>
</tr>
<tr>
<td>P-115</td>
<td>P-045</td>
<td>P-02</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>ÇİNAR Begüm</td>
<td>DEMİREL Nadir</td>
<td>DURU Gülcan</td>
</tr>
<tr>
<td>P-033</td>
<td>P-104</td>
<td>P-061</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>COCOLETZİ H. Hernández</td>
<td>DEMİRTAŞ Güneş</td>
<td>DVORANOVÁ Dana</td>
</tr>
<tr>
<td>P-116</td>
<td>P-081</td>
<td>P-018</td>
</tr>
<tr>
<td>P-081</td>
<td></td>
<td></td>
</tr>
<tr>
<td>ÇOLAK Mehmet</td>
<td>DERELİ Ömer</td>
<td>DYATLOVA Yulia A.</td>
</tr>
<tr>
<td>P-054</td>
<td>P-080</td>
<td>P-106</td>
</tr>
<tr>
<td></td>
<td>P-081</td>
<td></td>
</tr>
<tr>
<td>CROW Sidney</td>
<td>DEVELİOĞLU Mustafa</td>
<td>EKİCİ Öner</td>
</tr>
<tr>
<td>O-08</td>
<td>P-015</td>
<td>P-059</td>
</tr>
<tr>
<td>DEVO Perry</td>
<td>P-081</td>
<td></td>
</tr>
<tr>
<td>P-004</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CÜCÜ S. Cansel</td>
<td>DIETZEK Benjamin</td>
<td>EKİNCİ Arzu</td>
</tr>
<tr>
<td>P-049</td>
<td>O-07</td>
<td>P-052</td>
</tr>
<tr>
<td></td>
<td>P-103</td>
<td>P-054</td>
</tr>
<tr>
<td>CUKUROVALİ Alaaddin</td>
<td></td>
<td></td>
</tr>
<tr>
<td>P-060</td>
<td></td>
<td>ELSAYED Samah Mohamed</td>
</tr>
<tr>
<td>DEĞER Aybüke</td>
<td>EROĞLU</td>
<td>O-19</td>
</tr>
<tr>
<td>P-075</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CVETKOVSKI Saso</td>
<td>EROĞLU Ayşe</td>
<td>EMER Kyle</td>
</tr>
<tr>
<td>P-044</td>
<td></td>
<td>O-08</td>
</tr>
<tr>
<td>D'ABROSKA Brigida</td>
<td>DIMİTROVA Trufka</td>
<td>ERDAŞ Dilek</td>
</tr>
<tr>
<td>P-028</td>
<td>P-100</td>
<td>P-075</td>
</tr>
<tr>
<td>DİMOV Todor</td>
<td>DİMOV Todor</td>
<td></td>
</tr>
<tr>
<td>P-090</td>
<td></td>
<td></td>
</tr>
<tr>
<td>DAĞDEMİR Yılmaz</td>
<td></td>
<td></td>
</tr>
<tr>
<td>P-115</td>
<td></td>
<td></td>
</tr>
<tr>
<td>DİNES Trevor John</td>
<td></td>
<td></td>
</tr>
<tr>
<td>P-004</td>
<td></td>
<td></td>
</tr>
<tr>
<td>P-082</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Author Index</td>
<td></td>
<td></td>
</tr>
<tr>
<td>--------------</td>
<td>-----------------</td>
<td>-----------------</td>
</tr>
<tr>
<td>ERDEM Emre</td>
<td>FELNER Israel</td>
<td>GÜMÜŞ Sümayye</td>
</tr>
<tr>
<td>0057</td>
<td>O-21</td>
<td>P-077</td>
</tr>
<tr>
<td>P-032</td>
<td>P-080</td>
<td>P-078</td>
</tr>
<tr>
<td>ERDOĞDU Yusuf</td>
<td>FESKOV Serguei V.</td>
<td>GÜNEDOĞDU SAĞDINÇ</td>
</tr>
<tr>
<td>P-081</td>
<td>P-081</td>
<td>Seda</td>
</tr>
<tr>
<td>P-028</td>
<td>P-028</td>
<td>P-075</td>
</tr>
<tr>
<td>ERİC Marchioni</td>
<td>GABAUD D. Valls</td>
<td>GÜREK Ayşe Gül</td>
</tr>
<tr>
<td>P-034</td>
<td>P-116</td>
<td>P-121</td>
</tr>
<tr>
<td>ERKAN KARİPER Sultan</td>
<td>GEBA Maria</td>
<td>GÜRKO POLAT Tülin</td>
</tr>
<tr>
<td>P-017</td>
<td>P-112</td>
<td>P-122</td>
</tr>
<tr>
<td>P-063</td>
<td>P-113</td>
<td>GEFRA FERDINAN</td>
</tr>
<tr>
<td>P-132</td>
<td>P-133</td>
<td>P-029</td>
</tr>
<tr>
<td>EROĞLU Erol</td>
<td>GENCAÇ ÇELEMLİ Özü</td>
<td>GÜVEN Mehmet Haluk</td>
</tr>
<tr>
<td>P-133</td>
<td>P-067</td>
<td>P-020</td>
</tr>
<tr>
<td>ERSUNDU Ali Erçin</td>
<td>GEZER Murat</td>
<td>HADDADİ Khelifa</td>
</tr>
<tr>
<td>P-043</td>
<td>O-15</td>
<td>P-105</td>
</tr>
<tr>
<td>ERTAN BOLELLİ Tugba</td>
<td>GÖCEN Tugba</td>
<td>HADJ BRAHİM Narimène</td>
</tr>
<tr>
<td>P-138</td>
<td>P-020</td>
<td>P-012</td>
</tr>
<tr>
<td>ERYÜREK Meral</td>
<td>GÖKCE Halil</td>
<td>HAGER Martin D.</td>
</tr>
<tr>
<td>P-071</td>
<td>P-076</td>
<td>P-103</td>
</tr>
<tr>
<td>P-096</td>
<td>GORLE Sridevi</td>
<td></td>
</tr>
<tr>
<td>P-119</td>
<td>O-10</td>
<td></td>
</tr>
<tr>
<td>ESME Asli</td>
<td>GOUİD Zied</td>
<td></td>
</tr>
<tr>
<td>P-107</td>
<td>O-28</td>
<td></td>
</tr>
<tr>
<td>ESPADAS Adriana Jacome</td>
<td>GOUİD Zied</td>
<td></td>
</tr>
<tr>
<td>P-107</td>
<td>O-28</td>
<td></td>
</tr>
<tr>
<td>EVECEN Meryem</td>
<td>GRÄFE Stefanie</td>
<td></td>
</tr>
<tr>
<td>P-026</td>
<td>P-103</td>
<td></td>
</tr>
<tr>
<td>P-061</td>
<td>P-062</td>
<td></td>
</tr>
<tr>
<td>P-101</td>
<td>GROKHOVSKY Victor I</td>
<td></td>
</tr>
<tr>
<td>FADİLA Benayache</td>
<td>GÜDER Aytac</td>
<td></td>
</tr>
<tr>
<td>P-027</td>
<td>P-067</td>
<td></td>
</tr>
<tr>
<td>FARAOUN Houda Imane</td>
<td>GUEİD Abd El Hak</td>
<td></td>
</tr>
<tr>
<td>P-063</td>
<td>P-030</td>
<td></td>
</tr>
<tr>
<td>FATİHA Madi</td>
<td>GÜLLÜOĞLU Mehmet Tahir</td>
<td></td>
</tr>
<tr>
<td>P-032</td>
<td>P-032</td>
<td></td>
</tr>
<tr>
<td>FAUSTO Rui</td>
<td>P-080</td>
<td></td>
</tr>
<tr>
<td>0171</td>
<td>P-081</td>
<td></td>
</tr>
</tbody>
</table>

222
<table>
<thead>
<tr>
<th>Author Index</th>
<th>Page Numbers</th>
</tr>
</thead>
<tbody>
<tr>
<td>HENARY Maged</td>
<td>O-08, P-038</td>
</tr>
<tr>
<td>HERİCH Peter</td>
<td>P-018, O-02</td>
</tr>
<tr>
<td>HERKEN H.</td>
<td>P-137, O-10</td>
</tr>
<tr>
<td>HOMEMONAY Zoltan</td>
<td>O-22, P-082</td>
</tr>
<tr>
<td>HUEBNER Uwe</td>
<td>P-038, P-116</td>
</tr>
<tr>
<td>IBARRA E. Esparza</td>
<td>P-036, P-116</td>
</tr>
<tr>
<td>IDE Semra</td>
<td>P-023, P-024</td>
</tr>
<tr>
<td>ILİHAN CEYLAN B.</td>
<td>P-050, P-057</td>
</tr>
<tr>
<td>ILLİEV Ilia</td>
<td>P-090, P-109</td>
</tr>
<tr>
<td>IMADOUCHENE Noura</td>
<td>P-011, P-111</td>
</tr>
<tr>
<td>IMENE Ghoul</td>
<td>P-005, P-013</td>
</tr>
<tr>
<td>INES Bejaoui Ouni</td>
<td>P-098, P-099</td>
</tr>
<tr>
<td>ISMAİLOV Ismail</td>
<td>P-090, P-062</td>
</tr>
<tr>
<td>IUTİS Minola</td>
<td>P-112, P-007</td>
</tr>
<tr>
<td>IVASCU Ioana Ruxandra</td>
<td>O-02, P-049</td>
</tr>
<tr>
<td>JAHN Martin</td>
<td>P-038, P-038</td>
</tr>
<tr>
<td>JERCA Ovidiu</td>
<td>O-02</td>
</tr>
<tr>
<td>JONNALAGADDA Sreekanthbabu</td>
<td>O-10</td>
</tr>
<tr>
<td>JORDAN Daniel</td>
<td>P-082</td>
</tr>
<tr>
<td>JUSKOWİAK Bernard</td>
<td>P-124</td>
</tr>
<tr>
<td>KABAN Gizem</td>
<td>P-124</td>
</tr>
<tr>
<td>KALİNOWSKA Monika</td>
<td>P-069</td>
</tr>
<tr>
<td>KAMNEV Alexander A.</td>
<td>P-106</td>
</tr>
<tr>
<td>KANCI BOZOĞLAN Bahar</td>
<td>O-14, P-109</td>
</tr>
<tr>
<td>KANİ İbrahim</td>
<td>P-111</td>
</tr>
<tr>
<td>KARA Mehmet</td>
<td>P-058</td>
</tr>
<tr>
<td>KARABULUT Bünyamin</td>
<td>P-088, P-089</td>
</tr>
<tr>
<td>KARABULUT Murat</td>
<td>P-062</td>
</tr>
<tr>
<td>KARAKAŞ Duran</td>
<td>P-007, P-017</td>
</tr>
<tr>
<td>KARAKAYA Nevzat</td>
<td>P-049</td>
</tr>
<tr>
<td>KARASAKAL Ayça</td>
<td>P-051</td>
</tr>
<tr>
<td>KARATAŞ Fikret</td>
<td>P-016</td>
</tr>
<tr>
<td>KARATAŞ Şadiye</td>
<td>P-026</td>
</tr>
<tr>
<td>KARATEPE H. T.</td>
<td>P-137</td>
</tr>
<tr>
<td>KARİUKİ Dominic</td>
<td>P-082</td>
</tr>
<tr>
<td>KAROLAK WOJCIECHOWSKA Janina</td>
<td>P-138</td>
</tr>
<tr>
<td>KARTAL Zeki</td>
<td>P-120, P-123</td>
</tr>
<tr>
<td>KAVLAK Ilkan</td>
<td>P-126</td>
</tr>
<tr>
<td>KAYGİSIZ Ersin</td>
<td>P-134</td>
</tr>
<tr>
<td>KEBABİ Brahim</td>
<td>P-055, P-079</td>
</tr>
<tr>
<td>KERKATOU Messaoud</td>
<td>P-053</td>
</tr>
<tr>
<td>KERROUM Derbal</td>
<td>O-20</td>
</tr>
<tr>
<td>KHADİDJA Ars</td>
<td>P-005</td>
</tr>
<tr>
<td>KHAN Ahsan Ali</td>
<td>P-004, P-082</td>
</tr>
<tr>
<td>KHEİREDİNE Bani</td>
<td>O-20</td>
</tr>
</tbody>
</table>
Author Index

KİBRİZ Ibrahim Evren  Koyuncuoğlu Eren  LOTFI Belkhiri
P-127  P-049  O-11  P-002

KİLİÇ Murat  KRáľOVá Michaela  LOUAÎL Layachi
P-132  P-018  P-105

KİLİC Yalcin  KUMAR Sanjay  LUJAN A. Magallanes
P-111  O-05  P-116

KİLİÇ Serpil  KUPFER Stephan  M. A Quinto
P-016  O-07  P-073

KILLAR Dilek  KÜRKÇÜOĞLU Güneş  MACİT Mustafa
P-070  Süheyyla  P-076  P-104

KIZILPINAR TEMİZER  KURNALI Sertan  MADDİLA Suresh
Ilginç  P-126  O-10

P-067

KLEİNERMANNS Karl  KUZMANN Erno  MADİ Fatiha
KLENCsáR Zoltan  KOÇAK Figen  P-039
O-22  P-014  P-092  P-094

KOKOLANSKÎ Zivko  KUZUCUOĞLU Alpaslan  MAKŞİMOVA Alevtina A
P-044  P-134  P-135  O-22

KONSTANTİNOVA Tatyana  LALOVA Veselina  MAMERİ Yazid
S  P-010  O-21  O-100  P-015  P-045

KORKMAZ Sema  LEBULLENGER Ronan  MAMUCEVSKA
P-010  O-25  MILJJKOVÍKJ Svetlana

KORUNUR Sibel  LEóN Francisco  MANCİNİ Ines
P-086  P-087  P-053  P-083

KOVACEVSKA Liljana  LEWANDOWSKA Hanna  MANSOURLAKhdar
P-044  P-069  O-29

KOWCZYK SADOWY  LEWANDOWSKÝ  MARC Fontana
Małgorzata  Wlodzimierz  P-098  P-099
P-065  P-064  P-065  P-069

KÖYLÜ Mehmet Zafer  LEWİS Erica  MATEİ Consuela Elena
P-052  P-054  O-02  O-08  O-130

MEDETALİBEYOĞLU Hilal
<table>
<thead>
<tr>
<th>Author Index</th>
<th>Author Index</th>
<th>Author Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>MEDKOUR Youcef</td>
<td>NOUİÇER El Amine</td>
<td>ÖZYOL Esra</td>
</tr>
<tr>
<td>P-108</td>
<td>P-008</td>
<td>P-085</td>
</tr>
<tr>
<td>P-109</td>
<td></td>
<td></td>
</tr>
<tr>
<td>MEKKİOU Ratiba</td>
<td>ODABAŞOĞLU Mustafa</td>
<td>PANDIR Dilek</td>
</tr>
<tr>
<td>P-028</td>
<td>P-019</td>
<td>P-101</td>
</tr>
<tr>
<td>P-029</td>
<td></td>
<td></td>
</tr>
<tr>
<td>P-056</td>
<td></td>
<td></td>
</tr>
<tr>
<td>P-083</td>
<td>ÖKSÜZ Nur</td>
<td>PANT Debi D</td>
</tr>
<tr>
<td></td>
<td>P-084</td>
<td>O-06</td>
</tr>
<tr>
<td></td>
<td></td>
<td>O-12</td>
</tr>
<tr>
<td>MENAD Ahmed</td>
<td>OLARU Angelica</td>
<td>PATAŞHI Mihai</td>
</tr>
<tr>
<td>P-053</td>
<td>P-113</td>
<td>O-02</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>MENDHAM Andrew Paul</td>
<td>ORHAN Ulaş</td>
<td>PATONAY Gabor</td>
</tr>
<tr>
<td>P-004</td>
<td>P-010</td>
<td>O-08</td>
</tr>
<tr>
<td>P-082</td>
<td>P-025</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>MERDES Rachid</td>
<td>ORUJALİPOOR Ilghar</td>
<td>PETKOVA Petya Nikolaev</td>
</tr>
<tr>
<td>P-030</td>
<td>P-023</td>
<td>P-090</td>
</tr>
<tr>
<td></td>
<td>P-024</td>
<td>P-100</td>
</tr>
<tr>
<td></td>
<td>P-033</td>
<td></td>
</tr>
<tr>
<td>MEZHOUD Samia</td>
<td></td>
<td>PETROVA Evgeniya V</td>
</tr>
<tr>
<td>P-056</td>
<td></td>
<td>O-22</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>MİCHEL Ephritikhine</td>
<td>ORZECHOWSKA Sylwia</td>
<td>PİELA Katarzyna</td>
</tr>
<tr>
<td>O-11</td>
<td>Natalia</td>
<td>P-035</td>
</tr>
<tr>
<td>P-002</td>
<td>P-072</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>MİSİASZEK Tomasz</td>
<td>OSHTRAKH Michael I</td>
<td>POPOVSQA Angelina</td>
</tr>
<tr>
<td>P-035</td>
<td>O-21</td>
<td>P-044</td>
</tr>
<tr>
<td></td>
<td>O-22</td>
<td></td>
</tr>
<tr>
<td>MİSZTALEWSKA Iwona</td>
<td>OUAHİBA Boumaza</td>
<td>POPP Jürgen</td>
</tr>
<tr>
<td>P-064</td>
<td>P-027</td>
<td>P-038</td>
</tr>
<tr>
<td></td>
<td></td>
<td>P-038</td>
</tr>
<tr>
<td></td>
<td></td>
<td>P-103</td>
</tr>
<tr>
<td>MOGANEVERLİ Singh</td>
<td>OUBAZÍZ Dahbia</td>
<td>POULAIN Marcel</td>
</tr>
<tr>
<td>O-10</td>
<td></td>
<td>O-25</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>MONCEF Khireche</td>
<td>ÖZDEMİR Kameray</td>
<td>QUİNTO Michele Arcongelo</td>
</tr>
<tr>
<td>P-002</td>
<td></td>
<td>P-006</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>MONCKE Doris</td>
<td>ÖZDEMİR TARI Gonca</td>
<td>RADU Andreea</td>
</tr>
<tr>
<td>P-043</td>
<td>P-023</td>
<td>P-038</td>
</tr>
<tr>
<td></td>
<td>P-024</td>
<td>P-038</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>MOREAC Alain</td>
<td>ÖZTÜRK Nuri</td>
<td>REYES C. Frausto</td>
</tr>
<tr>
<td>O-25</td>
<td>P-076</td>
<td>P-116</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>MOSAAB Benchikhloucine</td>
<td>ÖZTÜRK Tuğçe</td>
<td>REYES Claudio Frausto</td>
</tr>
<tr>
<td>O-20</td>
<td>P-078</td>
<td>P-107</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>NADRA Debbache</td>
<td>NASSİRA Seraghi</td>
<td></td>
</tr>
<tr>
<td>Author Index</td>
<td>Author Index</td>
<td>Author Index</td>
</tr>
<tr>
<td>----------------------------------------------------------------------------</td>
<td>----------------------------------------------------------------------------</td>
<td>----------------------------------------------------------------------------</td>
</tr>
<tr>
<td>ROKİTA Eugeniusz</td>
<td>SAMİR Benayache</td>
<td>SELİM Khaled Abdel Aal</td>
</tr>
<tr>
<td>P-072</td>
<td>P-027</td>
<td>O-09</td>
</tr>
<tr>
<td></td>
<td>P-034</td>
<td>O-19</td>
</tr>
<tr>
<td>ROUMİLİ Abd Ekarim</td>
<td>SAMSONOWİCZ Mariola</td>
<td>SELİM ERDAL Yılmaz</td>
</tr>
<tr>
<td>P-108</td>
<td>P-065</td>
<td>P-023</td>
</tr>
<tr>
<td></td>
<td>P-069</td>
<td>P-024</td>
</tr>
<tr>
<td>RZEPECKA Patrycja</td>
<td>SANCHEZ Alejandro</td>
<td>SELVAN R. Kalai</td>
</tr>
<tr>
<td>P-036</td>
<td>Gonzalez</td>
<td>O-24</td>
</tr>
<tr>
<td>SABRİNA Mohamadi</td>
<td></td>
<td></td>
</tr>
<tr>
<td>P-034</td>
<td></td>
<td></td>
</tr>
<tr>
<td>SAÇMACI Mustafa</td>
<td>SANHOURY Mohamed</td>
<td>SEMİONKİN Vladimir A</td>
</tr>
<tr>
<td>P-042</td>
<td>Abderrahmane Khouna</td>
<td></td>
</tr>
<tr>
<td>P-084</td>
<td>O-28</td>
<td></td>
</tr>
<tr>
<td>P-085</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>SAÇMACI Şerife</td>
<td>SARA Belattar</td>
<td>SEN Elif</td>
</tr>
<tr>
<td>P-041</td>
<td></td>
<td>P-024</td>
</tr>
<tr>
<td>P-042</td>
<td>SARAC Ayfer</td>
<td></td>
</tr>
<tr>
<td>P-066</td>
<td></td>
<td></td>
</tr>
<tr>
<td>P-068</td>
<td></td>
<td></td>
</tr>
<tr>
<td>P-084</td>
<td></td>
<td></td>
</tr>
<tr>
<td>P-085</td>
<td></td>
<td></td>
</tr>
<tr>
<td>P-097</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>SAÇMACİ Mustafa</td>
<td>SAYIN Elvan</td>
<td></td>
</tr>
<tr>
<td>P-127</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>SAĞDINÇ Seda Güneşdoğan</td>
<td>SAYIN Koray</td>
<td>SI ABDELKADER Hayet</td>
</tr>
<tr>
<td>P-119</td>
<td></td>
<td>P-063</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>SAĞLAM Semran</td>
<td>SAYLAN Sefa</td>
<td>SIĐĐİKİ Afif</td>
</tr>
<tr>
<td>P-032</td>
<td></td>
<td>P-124</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>ŞAHİN Ertan</td>
<td></td>
<td></td>
</tr>
<tr>
<td>P-127</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>ŞAHİN Songül</td>
<td>SCHELUD’KO Andrei V.</td>
<td>ŞİMŞEK Sultan Başak</td>
</tr>
<tr>
<td>P-104</td>
<td></td>
<td>P-041</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>SALAH REDOUANE</td>
<td>SCHUBERT Ulrich S.</td>
<td></td>
</tr>
<tr>
<td>Azizedine</td>
<td></td>
<td></td>
</tr>
<tr>
<td>P-053</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>SEGHIRİ Ramdane</td>
<td>SİSMANOGLU Sedef</td>
</tr>
<tr>
<td></td>
<td>P-027</td>
<td>P-074</td>
</tr>
<tr>
<td>SALAJAN Daniela</td>
<td></td>
<td></td>
</tr>
<tr>
<td>P-112</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>SOLTAN MOHAMMADI</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Jamshid</td>
</tr>
<tr>
<td></td>
<td></td>
<td>P-003</td>
</tr>
<tr>
<td>SALEM Kessal</td>
<td></td>
<td></td>
</tr>
<tr>
<td>P-073</td>
<td>SEHİLİ Tahar</td>
<td>SOLTANİ Toufik Mohamed</td>
</tr>
<tr>
<td></td>
<td></td>
<td>O-25</td>
</tr>
<tr>
<td></td>
<td></td>
<td>P-043</td>
</tr>
<tr>
<td>SAMİA Baatouche</td>
<td></td>
<td></td>
</tr>
<tr>
<td>P-027</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Author Index

SOYKAN Cengiz
P-066
P-068

SOYLU İnanç
O-14

STRATULAT Lacramioara
P-112

SÜNNETÇİOĞLU Maral M.
O-30

SWİDERSKİ Grzegorz
P-064
P-065
P-069

SWİSLOCKA Renata
P-064
P-065
P-069

SZCZESİO Malgorzata
P-138

TAMER Ömer
P-104

TANAK Hasan
P-014
P-026
P-061

TAPRAMAZ Recep
P-092
P-094

TARİ Özlem
O-23

TATAR ULU Sevgi
P-051

TEMEL Ersin
P-102

THAMERE Cheriet
P-027

THUM Maria
P-038

TİRYAKİ Ozgcan
O-26

TOKATLI Ahmet
P-114

TONGUR Timur
P-132

TORULMAZ Nuri
P-133

TOUBAL Baddreddine
P-037

TSOVCHEV Rumen Ivanov
P-107

TUNÇ Fatmagül
P-114

TUNÇ Sibel
O-14
P-122
P-109

TÜRKER ACAR Elif
P-121
P-128

TZOUKROVSKY Youri
P-090

ÜÇAR İbrahim
P-022

UCUN Fatih
P-047
P-048

ÜLGEN Ahmet

WAHİBA Kaabar
O-17

WARACHİM Jakub
P-035

WEBER Karina
P-038
P-038

VİNOGRADOV Alexander V
O-21

VLAD Ana Maria
P-113

VURAL Hatice
P-022
P-058

WAHİBA Kaabar
O-17

WARACHİM Jakub
P-035

WEBER Karina
P-038
P-038

VİNOGRADOV Alexander V
O-21

VLAD Ana Maria
P-113

VURAL Hatice
P-022
P-058

WILCZEWSKA Agnieszka
Zofia
P-064

WOJTELEWSKI Ławomir
P-064

WONDRAČZEK Lothar
P-043

WRoBEL Andrzei
P-072

YAHİA Lazhar
P-008
P-009

YAKUPHANOĞLU Fahrettin
P-037
Author Index

YALCİN I. P-136
YOUSSEF Mohamed Abdel Maguid P-012 O-09 P-031

YALCİN Ismail P-138
YUDANO V Vladislav V. O-01

YALCÎNKAYA O. B. P-137
YÜKSEK Haydar P-129 P-130

YAŞAR Mehmet Murat P-133
YUKSEKTEPE ATAOL P-091 P-093

YAVUZ Abdülkerim P-123
YUKSEKTEPE ATAOL Çiğdem P-059 P-060

YAVUZ Adülkerim P-120

YENUPURİ Tej Varma O-06 O-12

YİLDİRİM Emre P-010 P-025
YÜRTSEVEN Hamit O-23 O-26

YİLDİRİM İlkay P-088 P-089
ZABOUB Amel P-030

YİLDİRİM Ismail P-127
ZAKİA Aitelhadjali P-073

YILDIZ Esra P-042
ZEDLER Linda O-07

YILDIZ Salih Zeki P-119 P-086 P-087

YILMAZ Ibrahim P-060
ZEROUEL Somia P-079

YILMAZ A. P-050 P-137
ZERTİ Roumayssa P-012

YİLMAZ Ali P-086 P-087
ZHANG Ying O-07

YONAR Dilek O-30
ZHAO Minjie P-034
SPONSORS and CONTRIBUTORS

The organisation of the International Turkish Congress on Molecular Spectroscopy (TURCMOS 2015) would not possible without the generous support of our sponsors and supporting organisations. Therefore, our particular thanks go to the following organisations and companies:

- American Elements
  THE MATERIALS SCIENCE COMPANY®
- CompecT™
  IT Consulting & Integration Services
- Turkish Airlines
  A STAR ALLIANCE MEMBER
- CREON
  Creativity on Engineering
- EserDoktor
- “Istanbul Physics Calendar”
  (M.Cem Guclu)
- International Light Year 2015
- Chemistry and Industry
  published by Turkish Chemical Society
- ELSEVIER-GLOBAL EVENTS LIST
LOCAL CONGRESS ORGANISER

Assoc. Prof. Dr. Ozan ÜNSALAN (İstanbul University, TURKEY), President
unsalan@istanbul.edu.tr

Asst. Prof. Dr. Gülce ÖĞRÜÇ ILDIZ (İstanbul Kültür University, TURKEY), Vice President
g.ogruc@iku.edu.tr

CONGRESS SECRETARIAT

BROS CONGRESS

Osmanbey - Sisli - Istanbul / Turkey
Phn.: +90 (212) 296 66 70
Fax: +90 (212) 296 66 71
E-mail: alen.demirel@brosgroup.net