



III. International Turkish Congress on Molecular Spectroscopy



**AUGUST 26-29**

**Bodrum | Turkey**

**BOOK OF ABSTRACTS**



III. International Turkish Congress on Molecular Spectroscopy

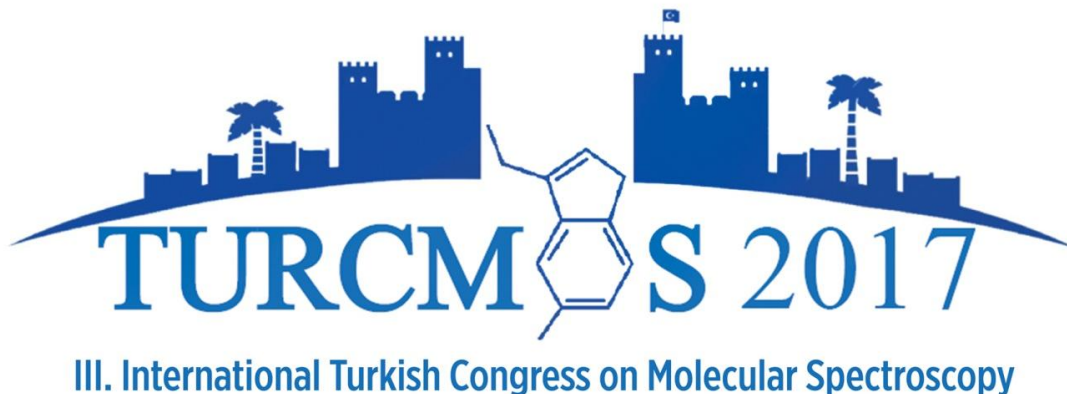
**B O D R U M**  
**T U R K E Y**

AUGUST 26-29

2017

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### **WELCOME TO TURCMOS 2017,**

On behalf of the Scientific and Organizing Committee, we would like to welcome you all to the “**International Turkish Congress on Molecular Spectroscopy (TURCMOS2017)**”. 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 would like to express our acknowledgements to Muğla Sıtkı Koçman University Rectorateship, Faculty of Fine Arts Deanship and Turkish Physics Foundation for their support.

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

**Ozan ÜNSALAN**

*President*

**Gülce ÖĞRÜÇ İLDİZ**

*Vice President*

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*\*Alphabetically ordered by surname*

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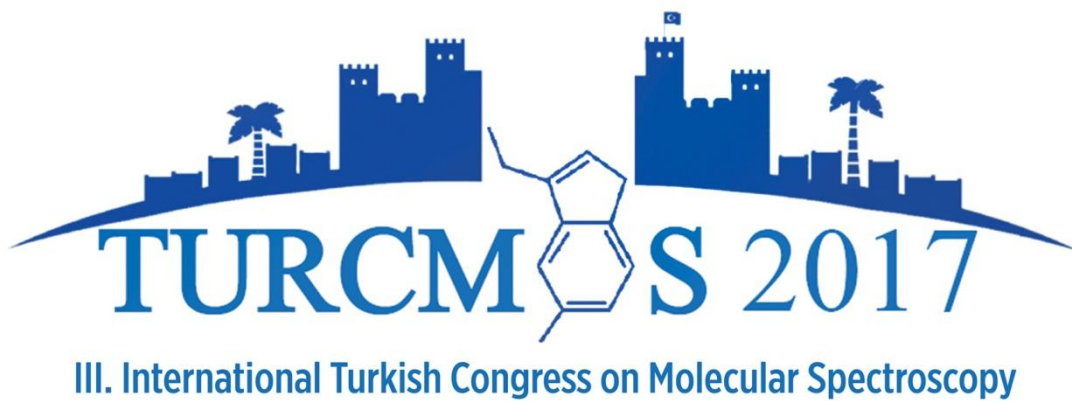
(Ankara University, Ankara, Turkey)

Weitao YANG

(Duke Uni., Trinity College of Arts & Science, Durham, USA)

Hamit YURTSEVEN

(Middle East Technical University, Ankara, Turkey)



## Scientific Program

27 August 2017 Sunday	
08:00-09:00	Registration at Congress Venue
09:00-09:20	<b>OPENING CEREMONY</b>
09:20-10:00	<b>PL-1- Rui Fausto</b> Probing Radical and Nitrene Intermediates in Narrowband UV-Induced Photoreactions in Cryogenic Inert Matrices
10:00-10:20	<b>O-01-Laurence Nafie</b> Structural Characterization Of Amyloid Fibrils Using Vibrational Circular Dichroism
10:20-10:40	<b>O-02- Selçuk Topal</b> Line Ratio Diagnostics in Early-Type Galaxies: NGC4710 and NGC5866
10:40-11:00	<b>COFFEE BREAK</b>
11:00-11:40	<b>PL-2- Philippe Colombar</b> Low wavenumber Raman and IR spectra: a very informative but poorly studied domain to understand ion dynamics, phase transitions, mechanics and (nano)structure of solids
11:40-12:00	<b>O-03-Emre Erdem</b> Point defects in semiconductor nanocrystals: EPR spectroscopy
12:00-12:20	<b>O-04-Şeyma Gözde Bakış</b> Fourier Transform Infrared Spectroscopy (FT-IR) Coupled with Chemometric Analysis Approach Enables to Determine Temperature and Time Dependent Alterations in The Content of Blood Stain on Cotton Fabric
12:20-13:20	<b>LUNCH BREAK</b>
	<b>HALL- A</b>
	<b>HALL- B</b>
13:20-13:40	<b>O-05- Hamit Yurtseven</b> Calculation of the Raman and IR Frequencies from the volume data at high pressures in N <sub>2</sub>
13:40-14:00	<b>O-06-Necati Kaya</b> Photo-fragmentation of H <sup>2+</sup> with femtosecond laser pulses by employing a time-sliced 3D imaging technique
14:00-14:20	<b>O-07-Zeki Kartal</b> Crystal Structure and Spectroscopic Properties of Redetermination Poly-bis[diaminozinc(II)]fumarato(tetracyanonickelate)dihydrate
14:20-14:40	<b>O-08- Hamdi Tekin</b> Use of spectroscopic methods in construction sector in Turkey
14:40-15:00	<b>O-09-Gökhan Alpaslan</b> X-ray and quantum chemical investigations of (E)-4-nitro-2-[(5,6,7,8-tetrahydronaphthalen-1-ylimino)methyl]phenol
15:00-15:20	<b>Coffee Break</b>
15:20-15:40	<b>O-10- Mehmet Pişkin</b> The Novel 2,6-Dimethoxyphenoxy Substituted Zinc(II) Phthalocyanine Dyes Having High Singlet Oxygen Quantum Yields
15:40-16:00	<b>O-11- Sedef Şişmanoğlu</b> Investigation by UV Spectrophotometry of Removal Para-Nitrophenol on Raney Alloy
16:00-16:20	<b>O-12- Beşir Dağ</b> {Synthesis, Characterization and Determination of Sorption Properties of Silica Gel-Immobilized Schiff Base Derivative For Removal of Co(II) Ions From Aqueous
16:20-16:40	<b>Coffee Break</b>
16:40-17:00	<b>O-13-Ömer Faruk Öztürk</b> Synthesis, characterization and spectroscopic properties of novel quite soluble tetrakis -substituted phthalocyaninato lead
17:00-17:20	<b>O-14-Fehmi Bardak</b> Experimental and ab initio DFT analysis of structural and spectroscopic features of Nitroterephthalic acid, and computational insights into its molecular interactions with estrogen receptor alpha
17:20-17:40	<b>O-15- Wusiman Muersha</b> Effect of Metal Oxide Semiconductors on the Photocatalytic Degradation of 4-Nitrophenol
17:40-19:20	<b>POSTER PRESENTATIONS (1)</b>
19:20-20:00	
20:00-22:00	<b>WELCOME PARTY</b>



28 August 2017 Monday	
08:00-09:00	Registration at Congress Venue
09:00-09:40	<b>PL-2-Herbert M. Heise</b> Reliable blood monitoring by microdialysis and infrared spectrometry for diabetic and critically ill patients: Fourier-transform spectrometry or quantum cascade laser technology - quo vadis?
09:40-10:00	<b>O-27-Fatma Küçük Baloğlu</b> Investigation of Obesity Induced Type 2 Diabetes Dependent Molecular Alterations and Therapeutic Effect of Palmitoleic Acid on These Alterations in Adipose
10:00-10:20	<b>O-28-Fatma Alazzam</b> Protein Therapeutics Structural Attributes Are Critical For Developing Effective Biopharmaceutical Product
10:20-10:40	<b>O-29-Rina Dukor</b> Advanced Vibrational Spectroscopy For Structure Elucidation Of Chiral and Biological Molecules
10:40-11:00	<b>COFFEE BREAK</b>
11:00-11:40	<b>PL-4- Mehmet Yeşiltaş</b> Three-dimensional Infrared and Raman Tomography of Extraterrestrial Materials
11:40-12:00	<b>O-30-Gülce Öğrücü İldiz</b> A Multi-Technique Approach to the Study of Hydrantoin
12:00-13:00	<b>LUNCH BREAK</b>
	<b>HALL- A</b>
13:00-13:20	<b>O-31- Halit Muğlu</b> Synthesis of some new 1,3,4-thiadiazole compounds derived from 3,4-(methylenedioxy) cinnamic acid and Characterization of structures by spectroscopic methods
13:20-13:40	<b>O-32-Gül Yakalı</b> The Analysis of Crystal Structure and Spectroscopic datas of the (2E,6E)-2,6 bis((E)-3 phenylallylidene)cyclohexanone with XRD and Gama Irradiated Effect
13:40-14:00	<b>O-33-Burcu Özkardaş</b> Spectroscopic Applications To W UMa Type Eclipsing Binary BO Ari
14:00-14:20	<b>O-34-İlyas Gül</b> Deformation effect on magnetic properties of ferromagnetic Fe-27%Ni-4%Mn-1%Zn Alloy
14:20-14:40	<b>O-35-Yahya Nural</b> An ICP-MS Study for Determination of the Effects of Anti-TNF Therapy on Bone Quality in Mice with Chronic Allergic Asthma
14:40-15:00	<b>Coffee Break</b>
15:00-15:20	<b>O-36-Umut Güzel</b> Crystal Structure of Yb(III)-MOFs Produced via Hydrothermal Synthesis
15:20-15:40	<b>O-37-Tolga Göktürk</b> Determination of Sun Protection Factor by Using UV-Visible Spectrophotometer and Fatty Acid Composition by Using Gas Chromatography-Mass Spectrometry of {Sesamum indicum} Oil
15:40-16:00	<b>O-38-Sevil Sener</b> Synthesis and Characterization of Metal Carbonyls [ M(CO) <sub>6</sub> (M=Cr, Mo, W), Mn(CO) <sub>5</sub> Cp] with 3[4-ethyl(phenyl)imino][1H-indol-2-one] (ISE) and 3[4-butyl(phenyl)imino][1H-indol-2-one] (ISB)
16:00-16:00	
16:20-16:40	
16:40-17:00	
17:00-17:20	
17:20-17:40	
17:40-18:00	
18:00-18:20	
18:20-18:40	
18:40-19:00	
19:00-19:20	
19:20-20:00	
20:00-22:00	<b>GALA DINNER</b>

EXCURSION (Boat Trip to Bodrum's bays)

NOT ATTENDED

NOT ATTENDED



29 August 2017 Tuesday		
08:00-09:00	Registration at Congress Venue	
09:00-09:40	<b>PL-5- Stefan Weber</b> Unraveling the mechanisms of light-active proteins using time-resolved electron paramagnetic resonance	
09:40-10:00	<b>O-47-Michael I. Oshtrakh</b> A study of metallic Fe-Ni-Co alloy and stony part isolated from Seymchan meteorite using X-ray diffraction, magnetization measurement and Mössbauer spectroscopy	
10:00-10:20	<b>O-48-Çiğdem Dönmez Güngüneş</b> Mössbauer Spectroscopy of Magnetite Nanoparticles for Applications in Biotechnology and Biomedicine	
10:20-10:40	<b>O-49-Serap Gül</b> Magnetic properties of thermally induced martensite in a Fe-27%Ni-4%Mn-1%Zn (wt.%) alloy	
10:40-11:00	<b>COFFEE BREAK</b>	
11:00-11:40	<b>PL-6- Parvez HARIS</b> PSD (Protein Spectra Database): A platform for analysis and sharing of protein spectroscopic data	
11:40-12:00	<b>O-50-Ozan Ünsalan</b> Spectroscopic and structural investigations on Bursa L6 meteorite	
12:00-12:20	<b>O-51-Üftade Muşkara</b> The Analysis of Colored Plasters of Saraylı Rural Architecture by UV-VIS SpectrophotometerT	
12:20-13:20	<b>LUNCH BREAK</b>	
13:20-13:40	<b>POSTER PRESENTATIONS(2)</b>	
13:40-14:00		
14:00-14:20		
14:20-14:40		
	<b>HALL- A</b>	<b>HALL- B</b>
14:40-15:00	<b>O-52-Begüm Çınar Bam</b> Grazing Incidence Small Angle X- ray Scattering (GISAXS) Analysis on Nanostructured Thin Films Synthesized for Optoelectronic Applications	<b>O-66-Etem Köse</b> The spectroscopic and quantum chemical studies on structural, vibrational, electronic and chemical properties of 2,2'-bipyridine by using density functional theory (DFT)
15:00-15:20	<b>O-53-Cisem Altunayar Unsalan</b> Concentration and temperature dependent studies of interaction of provitamin D3 with zwitterionic DPPC model membranes	<b>O-67-Yelda Bingöl Alpaslan</b> Spectroscopic Characterization and Density Functional Studies of New Thiadiazole 1,1-dioxide Compounds
15:20-15:40	<b>O-54-Gülen Atiye Organ</b> {Synthesis, Characterization and Spectroscopic Properties: Schiff Base Derivative Bearing Zinc(II) Phthalocyanine	<b>O-68-Sibel Bilgili</b> The exploring of the anion effect on the structure, spectroscopic and electronic features of some imidazolium based ionic liquids
15:40-16:00	<b>O-55-Elif Özdemir</b> Development and Validation of Sensitive Spectrophotometric Method for the Determination of Rilmenidine in Pure and Pharmaceutical Preparations	<b>O-69-Sibel Çelik</b> Investigation of geometrical, electronic and spectroscopic properties of Fluorene-9-phenol molecule
16:00-16:20	<b>O-56- Melisew Tadele Alula</b> Induction of aggregation of silver nanoparticles via pH variation for sensitive spectrophotometric determination of creatinine in urine	<b>O-70-Talat Özpozan</b> Heteroatom Effect on the Band Gap of Five-Membered Fused Bicyclic Polymers
16:20-16:40	<b>COFFEE BREAK</b>	
16:40-17:00	<b>O-57-İbrahim Dolak</b> Preparation of a New Lanthanide-Chelate Cross-Linked, Myoglobin (Mb) Imprinted Affinity Cryogel for Selective Recognition of Myoglobin (Mb) in Blood Serums and Determination of Myoglobin (Mb) by UV-VIS-Near Infrared Spectroscopy (UV-VIS-NIR'S)	<b>O-71-Zeki Büyükmumcu</b> Isotopic Effect on Vibrational Spectra of $TcX_3^+$ and $TcX_3OH$ (X: O, S and Se): A DFT Study
17:00-17:20	<b>O-58-Rahmani Abdelali</b> Identification of multilayer graphene films: X-Ray and Raman studies	<b>O-72-Rachid Atmani</b> Numerical study and simulation of the vibrational modes in a long cylindrical packaging material in one-dimensional
17:20-17:40	<b>O-59-Ali Arslantaş</b> A comparative study on DNA binding properties of 2,10,16, 24  -tetrakis 4-(4-hydroxyphenyl)-1-phenylethyl) phenoxy substituted cobalt (II) and Mg (II) phthalocyanine compounds	<b>O-73-Hatice Ari</b> Systematic Vibrational Study of Saturated Chain Alcohols by DFT
17:40-18:00	<b>O-60-Fazıl Fazıl Kulucan</b> The martensite transformation characteristics on the magnetic properties of Fe-27%Ni-4%Mn-2%Zn Alloy	<b>O-74- Abdelatif Messaoudi</b> Electronic Underpinnings of the Fascinating Class of Phosphido-Bridged Trinuclear Platinum Clusters
18:00-18:20	<b>O-61- Suat Ekin</b> Antioxidant and Antiradical Properties of Ruscus hypoglossum L. and Trace elements, Minerals and Vitamin C Levels	<b>O-75- Oğuz Çakır</b> Development of Quartz Crystal Microbalance Sensor by Molecularly Imprinted for Sensitive and Selective Detection of Pesticide in Apple

18:20-18:40	<b>COFFEE BREAK</b>	
18:40-19:00	<b>O-62-Esvet Akbas</b> Multicomponent cyclocondensation reaction of $\beta$ -diketone, arylaldehyde and urea	<b>O-76-Abdullah Akkaya</b> Structural and spectroscopic analysis of (E)-2-((2,3-dihydroxybenzylidene)amino)-3a,7a-dihydro-1H-isoindole-1,3(2H)-dione
19:00-19:20	<b>O-63-Fatih Doğan</b> Synthesis and Spectroscopic Properties Of Newly Peripheral Tetra Substituted Zinc(II) Phthalocyanine Bearing Benzene Sulfonamide Derivative Containing 1,3,4-Thiadiazol, Schiff Base and Bromine	<b>O-77-Levent Semiz</b> Analysis on molecular, spectroscopic and electronic behavior of $C_{30}N_{12}O_2H_{32}Cl_2$ molecule: A theoretical approach
19:20-19:40	<b>O-64-Burcu Aydinler</b> A coumarin-thiophene based fluorescent chemosensors bearing mono and disulfonamide receptoric part for selective determination of fluoride via reaction based mechanism	<b>O-78-Yunus Kaya</b> Experimental and Theoretical studies on Conformational, Molecular Docking, FT-IR, NMR and UV-vis spectroscopy of 1-Phenyl-ethanone O-propyl-oxime and 1-(4-Bromo-phenyl)-ethanone O-propyl-oxime
19:40-20:00	<b>O-65-Hasan Yakan</b> Synthesis of some novel 3-acetoxy-2-methyl and 2,3-dimethoxy benzamides	<b>O-79-Rada Simona</b> Ferric oxide and yttria-stabilized zirconia for dental applications
20:00-20:15	<b>CLOSING CEREMONY</b>	



# Poster List

**POSTER SESSION 1 (P-001 / P-112) | August 27, 2017 - Sunday**

Number	Abstract title   Authors
P-001	Theoretical and experimental vibrational spectroscopic study of 3X-thiophene-2-carbaldehyde [X=F, Cl or Br] <u>Mustafa Senyel</u> , Esmâ Güneş, Özge Bağcıyan, Özgür Aıvel, Cemal Parlak <b>NOT ATTENDED</b>
P-002	Experimental Studies On Infrared Spectra And Molecular Structure Of The C <sub>20</sub> H <sub>18</sub> N <sub>40</sub> Molecule <u>Serap Yücesan</u> , Erol Taşal <b>NOT ATTENDED</b>
P-003	Vibrational Spectra and Molecular Structure of The 1-(o-tolyl)-3-(o-hydroxyphenyl)-5-phenylformazans Molecule Experimental Study <u>Seren Sağlam</u> , Erol Taşal <b>NOT ATTENDED</b>
P-004	FT-IR Spectroscopic Study of M(Terephthalic Acid) Ni(CN) <sub>4</sub> Complexes (M = Mn, Co, Ni, Cd and Hg) <u>Abdülkerim Yavuz</u> , Zeki Kartal
P-005	Crystal Structure and Infrared Spectroscopic Properties of Redetermination poly-[cobalt (II)(tetraaqua)(fumarato)] <u>Abdülkerim Yavuz</u> , Zeki Kartal, Onur Şahin
P-006	Removal of Lead(II) by biosorption of Bacillus subtilis ATCC 6051(B1) and two wild strain Bacillus licheniformis (Fl and Fs) with a comparative study from aqueous solutionsö <u>Mehmet Fırat Baran</u> , Husamettin Aygun, Fikret Uyar, Mehmet Duzgun, Ersin Kilinc, Mehmet Zahir Duz
P-007	Determination of Paraben Preservatives in Cream Samples Using Matrix Solid-Phase Dispersion Coupled with Supramolecular Solvent-Based Microextraction and HPLC-UV <u>Elif Yıldız</u> , Hasan Çabuk
P-008	Hf and Dft Study of Prism Structure of Water Clusters Salih Cinakli, <u>Mustafa Büyükkata</u> , Yılmaz Dağdemir
P-009	Synthesis, characterization, spectroscopic properties, DFT calculations and antimicrobial activities of p-toluenesulfonamide,N,N'-1,3-propanediylbis(ptspr) and [Cu(II)(phenanthroline) <sub>2</sub> ]ptspr <u>Fatih Akyıldız</u> , Hamit Alyar, Saliha Alyar
P-010	Synthesis, Characterization, DFT Calculations and Antimicrobial Studies of Heteroaromatic Diimines and Their Copper(II) Complexes <u>Fatih Akyıldız</u> , Ayla Balaban Gündüzalp, Hamit Alyar, İffet Özsen, Neslihan Özbek, Saliha Alyar
P-011	Estimation of Bloodstain Age on Linen Fabric by Fourier Transform Infrared Spectroscopy <u>Şeyma Gözde Bakış</u> , Özkan Aksakal, Nihal Şimşek Özek
P-012	Synthesis and Characterization of Noscapine Loaded Hydroxyapatite Nanoparticles İbrahim Bulduk, <u>Süleyman Gökce</u> , Yavuz Ergün
P-013	Determination of Progress in Acrylic Acid Modification on Polyvinylidene Fluoride Membrane by Infrared Spectroscopy <u>Hüseyin Gümüş</u> , Erdal Eren
P-014	Investigation of the molecular structure of 3-formylphenylboronic acid molecule by density functional approach <u>Mustafa Kurt</u> , Emine Tanış, Emine Babur Şaş
P-015	Structural and vibrational spectroscopy investigation of the 4-formylphenylboronic acid molecule <u>Mustafa Kurt</u> , Emine Babur Şaş, Emine Tanış
P-016	Characterization of TiO <sub>2</sub> Blended Polyvinylidene Fluoride Composite Materials for the Removal of Organic Substance from Water by Spectroscopic Techniques <u>Hüseyin Gümüş</u> , Erdal Eren
P-017	Density Fuctional Theory and Spectroscopic Studies of 5-Nitro-2-Oxindole <u>Banu Kevser Yıldırımgeç</u> , Seda Sağdıç

P-018	Theoretical and vibrational studies of a tricyclic antidepressant, Imipramine hydrochloride <u>Seda Sagdinc</u> , Caner Azkeskin
P-019	Determination of the Effect of Polymeric Nanoparticle in Biological Samples with ATR-FTIR Spectroscopy <u>Buket Bakan</u> , Gunnur Guler, Sinan Akgol, N. Ulku Karabay Yavasoglu
P-020	The Effects of Combined Treatment of Extremely Low Frequency Magnetic Field (50 Hz, 1 mT) and Pterostilbene on Renal Ischemic Injury Ozlem Bozkurt Girit, <u>Hatice Keser</u> , Feride Severcan, Mehmet Dincer Bilgin
P-021	"Raman spectra of C <sub>60</sub> confined inside a single-wall boron nitride nanotubes" <u>Fakrach Brahim</u> , Rahmani Abdelhai, Boutahar Mourad, Fatima Fergani, Chadli Hassan, Rahmani Abdelali <b>NOT ATTENDED</b>
P-022	Semiclassical line broadening calculations with exact trajectory of NH <sub>3</sub> in collision with He <u>Chaima Avari</u> , Mohamed Dhib, Hassen Arodi <b>NOT ATTENDED</b>
P-023	Uniaxial Tensile and Structural Properties of Poly(vinyl alcohol) and Graphene Oxide Composite Films with Different Weight ratios: The Influence of Heating <u>Altan Bozdoğan</u> , Baki Aksakal, Utkan Şahintürk, Önder Yargı, Murat Çalışkan
P-024	Structural and Tensile Characteristics of rGO/PVA Composite Films: Influence of UV Irradiation <u>Altan Bozdoğan</u> , Baki Aksakal, Utkan Şahintürk, Önder Yargı
P-025	Conformational analysis and h-DFT study of N,N'- phenylene-diylbis[3-(1-aminoethyl)-6-methyl-2H-pyran-2,4(3H)-dione] <u>Muhammet Okur</u> , Arslan Ünal, Yusuf Atalay
P-026	Density functional theory calculations on spectroscopic and electrical properties of N,N'- propylene-diylbis[3-(1-aminoethyl)-6-methyl-2H-pyran-2,4(3H)-dione]: a potential nonlinear optical material <u>Muhammet Okur</u> , Arslan Ünal, Yusuf Atalay
P-027	Influence of UV Irradiation on the Structural and Mechanical Properties of TiO <sub>2</sub> /GO/PVA Composite Films <u>Baki Aksakal</u> , Altan Bozdoğan, Utkan Şahintürk, Murat Çalışkan, Önder Yargı
P-028	Heating Effect on Spectroscopic and Mechanical Properties of rGO/PVA Composite Films Altan Bozdoğan, <u>Baki Aksakal</u> , Utkan Şahintürk, Önder Yargı, Hasan Samed Gez
P-029	Spectroscopic parameters of NH <sub>3</sub> in the 2v <sub>4</sub> band <u>Maaroufi Nourhene</u> , Kwabia Tchana Fr <b>NOT ATTENDED</b>
P-030	Production of Baicalein Containing Electrospun Scaffolds and Characterization through Raman Spectroscopy Thereof Kamel Bachimam, Ezgi Emul, Ugur Tamer, <u>Necdet Sağlam</u>
P-031	Comparison of Extra Virgin Olive Oil (EVOO) and {Hypericum perforatum} Oil by Using ATR-FTIR Spectroscopy <u>Tolga Göktürk</u> , Şeyda Kıvrak, Ibrahim Kıvrak
P-032	Experimental and theoretical studies of the vibrational and electronic properties of 2-methylimidazole <u>Biray Kinik</u> <b>NOT ATTENDED</b>
P-033	Molecular Geometry, Vibrational Spectra (Ft-Ir And Raman), Vibrational Assignments By Density Functional Theory (DFT) Calculations For Complex $(CN)_2(CN)_2]_n$ <u>Biray Kinik</u> <b>NOT ATTENDED</b>
P-034	Use of EVA Descriptor to Construct Linear QSAR Model for Determining Inhibitory Activity of Sulfonamides against Carbonic Anhydrase and Sweetness Index of Aspartame Derivatives Erol Eroğlu, Nuri Yorulmaz, Oral Oltulu, Mehmet Murat Yaşar, <u>Ihsan Burak Çam</u>
P-035	Inhomogeneity of tooth enamel evaluated by vibrational micro-spectroscopy <u>Dimitar Vasilev</u> , Rositsa Titorenkova, Biserka Titorenkova, Galina Jegova, Maya Rashkova <b>NOT ATTENDED</b>

P-036	<b>Molecular Structure and Vibrational Spectroscopic Study of 2-[4-(4-Nitrobenzamido)phenyl]benzothiazole using DFT Method</b> <u>Kayhan Bolelli</u> , Hatice Ari, Mustafa Boyukata, Ismail Yalcin, Ozan Unsalan
P-037	Nonadiabatic molecular alignment of linear molecules using circularly polarized femtosecond laser pulses <u>Necati Kaya</u> , Gamze Kaya <b>NOT ATTENDED</b>
P-038	Synthesis and Structural Characterization of 1D Coordination Polymer with Co(II)-3,3-Dimethylglutarate Hakan Erer, Samet Karaçam, <u>Okan Zafer Yeşilel</u>
P-039	Effect of plant sterol stigmasterol on the physical properties of DMPC membranes: an FTIR study <u>Cisem Altunayar Unsalan</u> , Ipek Sahin, Nadide Kazanci
P-040	Investigation of physical properties of Betula Pendula (Silver Birch) bark by calorimetric, spectroscopic and microscopic techniques <u>Ozan Unsalan</u> , Cisem Altunayar Unsalan
P-041	Mössbauer analysis and Cation distribution of Zn substituted BaFe <sub>12</sub> O <sub>19</sub> hexaferrites <u>Hakan Güngüneş</u> , Abdulhadi Baykal, Sagar E. Shirstah
P-042	The effect of Ti on Mechanical, Morphological and Magnetic Properties in Fe-Ni-Ti Alloys <u>Hakan Güngüneş</u> , Ozan Önal
P-043	Magnetic properties of deformation induced martensite in a Fe-27%Ni-4%Mn-1%Zn (wt.%) alloy <u>İlyas Gül</u> , Melek Güler, Emine Aldırmaz, Emre Güler
P-044	An analysis of orthopyroxene from Tsarev L5 meteorite using X-ray diffraction and Mössbauer spectroscopy Alevtina A. Maksimova, Robert V. Kamalov, Andrey V. Chukin, <u>Michael I. Oshtrakh</u>
P-045	Investigation by Mössbauer spectroscopy of magnetic properties in Fe-27%Ni-4%Mn Alloy <u>Serap Gül</u> , Hasan Sezgin Yılmaz, Melek Güler, Emine Aldırmaz, Emre Güler
P-046	Mössbauer Spectroscopy of Various Iron Compounds <u>Tuna Alp</u>
P-047	Solid Phase Extraction Using Modified Magnetic Iron Oxide Nanoparticles for Extraction and Spectrofluorimetric Determination of <b>NOT ATTENDED</b> Plasma Samples <u>Ahad Bavili Tabrizi</u> , Ahad Bavili Tabrizi, Mahdi Panahi
P-048	Fluorescence Spectroscopy: applications in immunology <u>Ouadi Ouadi Ibtissem</u> , Gadiri Meriche Sabiha, Meriche Meriche Hacem
P-049	Imidazole/Benzimidazole-Modified Cyclotriphosphazenes as Fluorescent Probes for Cu <sup>2+</sup> <u>Aylin Uslu</u> , Süreyya Oğuz Tümay, Elif Özcan, Serkan Yeşilot
P-050	Three Curcuminoids Upon Inclusion Into (2-Hydroxypropyl)-β-Cyclodextrin: An Absorption and Fluorescence Spectroscopic Study <u>Zeynep Kalaycıoğlu</u> , F. Bedia Erim
P-051	Determination of Aluminum in Water Resources With New Synthesized N,N'-Bis (2,5-dihydroxybenzylidene)-4,4'-diamino Diphenyl Ether by Using Fluorimetric Method <u>S. Beniz Gündüz</u> , Havva Nur Köstekçi, Mustafa Şahin, Nuriye Koçak <b>NOT ATTENDED</b>
P-052	Photophysical and photochemical properties of an unmetalled phthalocyanine obtained at low temperature <u>Mevlude Canlica</u>
P-053	Characterization of some vegetable oils by Fourier transform infrared and Synchronous fluorescence spectroscopy <b>NOT ATTENDED</b> <u>Soraya Nigri</u> , Rabah Oumeddour
P-054	Synthesis, Crystal Structure and Luminescence Properties of 3D Zn(II) Coordination Polymer Constructed from Thiophene-2,5-Dicarboxylate and 1,4-Bis(2-Ethylimidazol-1-yl)Butane Hakan Erer, <u>Okan Zafer Yeşilel</u>

P-055	X-ray Absorption Fine Structure Spectroscopic Study of The Chemical Speciation of Mercury and Selenium in Fish-eating Birds: Complexation by Se as a Possible Detoxification Mechanism <u>Cahit Karanfil</u> , Karyn Bischoff, Grant Bunker
P-056	Analysis of Hydrolytic Differences of Free and "Polyacrylic Acid (PAA)-Conjugated Trypsin and Chymotrypsin" by Using Fluorescence Lifetime Distributions <u>İbrahim Ethem Özyiğit</u> , Emine Karakuş
P-057	A highly selective and sensitive fluorescence probe for Iron(III) ions based on a cyclotriphosphazene scaffold <u>Serkan Yeşilot</u> , Süreyya Oğuz Tümay, Semiha Yıldırım Sarıkaya, Aylin Uslu
P-058	A water-soluble fluorescence sensor based on a phosphazene platform for Iron(III) ions <u>Serkan Yeşilot</u> , Süreyya Oğuz Tümay, Elif Özcan, Aylin Uslu
P-059	Spectroscopic Investigation of Synthesized Water Soluble Metallo Phthalocyanines: Absorbance, Fluorescence, Mass and Voltammetric Studies <u>Bahadır Keskin</u>
P-060	Study of the influence of the electromagnetic field on the state of erythrocytes of patients with acute ischemic stroke by the method of UHF dielectrometry <b>NOT ATTENDED</b> <u>Liliya Batyuk</u> , Yuriy Shkorbatov, Nataliya Kizilova, Nataliya Kizilova, Dmitriy Astapovich, Vladimir Berest
P-061	Magnetic and Microwave Absorption Properties of $Ni_{0.1}Zn_{0.8-x}Mn_{0.1}Cu_{0.1}Fe_2O_4$ Substituted Ni-Zn Nanoparticles <b>NOT ATTENDED</b> <u>Fazilet Genç</u> , Fazilet Genç, İbrahim Ünver, Hüseyin Sözeri
P-062	Line Ratio Diagnostics in Early-Type Galaxies: NGC4710 and NGC5866 <u>Selçuk Topal</u>
P-063	Structural, Spectroscopic and Thermal Characterization of 5-Methylhydantoin: From the Isolated Molecule to Solid State Polymorphism <u>Gulce Ogruc Ildiz</u> , Bernardo A. Nogueira, João Canotilho, Ermelinda S. Eusébio, Marta S. Henriques, José António Paixão, Rui Fausto
P-064	Conformational Landscape and Polymorphism in 5-Acetic Acid Hydantoin <u>Gulce Ogruc Ildiz</u> , Bernardo A. Nogueira, João Canotilho, Ermelinda S. Eusébio, Marta Henriques, José António Paixão, <u>Rui Fausto</u>
P-065	Determination of Ammonia and Nitrite in Exhaled Breath Condensate of Healthy Humans By Using a Sensitive Spectrophotometric Method <b>NOT ATTENDED</b> <u>Ahad Bavili Tabrizi</u> , Benyamin Sepehr, Vahid Jouyban Gharamaleki, Maryam Khoubnasabjafari, Abolghasem Jouyban
P-066	Novel Ideal Soluble And Non-Aggregated Copper(II) Phthalocyanines: Synthesis, Structure, Spectroscopic Properties <u>Ömer Faruk Öztürk</u> , Mehmet Pişkin
P-067	Boron Compounds with Magnetic Properties and Their Catalytic Applications <u>Engin Meydan</u> , Nurettin Şahiner, Ömer Faruk Öztürk
P-068	Nitro compounds reduction reaction with novel synthesized magnetic nanoparticules which are prepared with different metal salts and reducing agents <u>Engin Meydan</u> , Ömer Faruk Öztürk, Nurettin Şahiner
P-069	Periferal Tetrakis-Benzenesulfonamide Derivative Substituted Phthalocyanine:Solid State Synthesis, Structure, Spectroscopy <u>Gülen Atiye Organ</u> , Hakan Şahal, Fatih Mutlu, Mehmet Pişkin, Ömer Faruk Öztürk, Erdal Canpolat
P-070	Development and Validation of a New Spectrophotometric Method for the Determination of Rivastigmine in Pharmaceutical Formulations <u>İbrahim Bulduk</u> , <u>Süleyman Gökce</u> , Yavuz Ergün
P-071	Forced Degradation Study on Rilmenidine by first order derivative spectrophotometric method <u>Elif Ozdemir</u> , Ayça Karasakal



P-072	The Novel Zinc (II) Phthalocyanine Substituted With Benzene Sulfonamide Derivative Compound Containing Pyridine And Nitro Units: Synthesise, Structured Lighting, Spectroscopic Features <u>Fatih Doğan</u>
P-073	Removal of Methylene Blue Dye Using Cerium Based Nano-Photocatalysis <u>Birsen Demirata Ozturk, Dilek Ozyurt</u>
P-074	In Vitro Effects of Fexofenadine on PON1(Q192R) Isoenzymes in Patients with Sleep Apnea Serum <u>Kübra Çıkrıkçı, Nahit Gençer, Nurhan Sarıoğlu</u>
P-075	Identification and Classification of Polymers Using LIBS and Chemometry <u>Belgin Genç Öztoprak, Erhan Akman, Arif Demir</u>
P-076	Vortex assisted microextraction followed by UV-Vis spectrophotometric determination of mercury in fish samples <u>Nail Altunay, Adil Elik, Emre Yıldırım, Ramazan Gürkan</u>
P-077	Fe And Al Removal From The Waste Water Of Hendek Industrial Zone With Adsorption Method Colar And Turbidity Removal By Waste Water Adsorption Method <u>Nilgün Başok</u>
P-078	Colar And Turbidity Removal By Waste Water Adsorption Method <u>Nilgün Başok</u>
P-079	(Chemical Oxygen Demands (Cod) Removal From The Waste Water Of Hendek Industrial Zone With Adsorption Method) <u>Mehtap Karakaş</u>
P-080	(Total Organic CarbonMatter (TOC)Removal from the Waste Water of Hendek Industrial Zone with Adsorption Method) <u>Mehtap Karakaş</u>
P-081	Experimental and computational study on furan-3-methanol <u>Davut Avcı, Ömer Tamer, Sümeyye Altürk, Yusuf Atalay</u>
P-082	A new spectrophotometric method for the determination of nicotinamide (vitamin B3) in real samples after microextraction <b>NOT ATTENDED</b> <u>Emre Yıldırım, Nail Altunay, Ramazan Gürkan</u>
P-083	Synthesis, Structure and Spectroscopic Properties af Novel Zinc(II) Phthalocyanine Using Sonogashira Cross-Coupling Reaction <u>Mehmet Pişkin, Mahmut Durmuş</u>
P-084	Determination of Total Antioxidant Capacity of Shampoos by Spectrophotometric Method <u>Dilek Ozyurt, Birsen Demirata</u>
P-085	Structural and Optical Characterisation of CuInSe <sub>2</sub> Thin Films Maharram Zarbali, Abdullah Göktaş, Ferhat Aslan, <u>Ahmet Tumbul</u> , Nuri Yorulmaz
P-086	Effects of Highly Mg dopant level on the structiural and optical properties of ZnO thin films Abdullah Göktaş, Ferhat Aslan, <u>Ahmet Tumbul</u> , Maharram Zarbali, Ibrahim Boz
P-087	Optical Properties of SiO <sub>2</sub> /MPS-Capped CdS Quantum Dots Mixture Thin Films <u>Kenan Koç</u>
P-088	Thin Films of Fluorescent N-isopropylacrylamide Nanogels: Optical Investigation <u>Kenan Koç, Esra Alveroglu</u>
P-089	Hydrothermal Synthesis and Characterization of New Erbium(III) Complex <u>Gorkem Oylumluoglu, M. Burak Coban, Cagdas Kocak, Muhittin Aygun, Hulya Kara</u>

P-090	Theoretical studies of structural, optic and electronic properties of polypyrrole (PPy) oligomer <u>Yunus Kaya</u> , Asli A. Kaya
P-091	Kinetic Study of Oxidation of Indigo Carmine by Pyridinium Chlorochromate <u>Jamil Ibrahim Saleh Ahmed</u> , Aya Ahmed Alkhrateeb <b>NOT ATTENDED</b>
P-092	Determination of H <sub>2</sub> O <sub>2</sub> and Organic Peroxides by Spectrophotometry Using Nanoceria Particles <u>Reva Bayraktar</u> , Dilek Ozyurt, Gozde Kamer, Resat Apak, Birsen Demirata
P-093	Cyclophosphazene Based-Oligospiranes as New Molecular Rods <u>Serap Beşli</u> , Ceylan Mutlu Balcı, Aylin Uslu
P-094	Cyclotriphosphazene Derivatives Bearing Glycol Groups <u>Aylin Uslu</u> , Orçun Balkaner, Serkan Yeşilot
P-095	Deprotonation Reactions of Fluorodioxo Substituted Cyclophosphazene and Investigation of Thermal Properties <u>Serap Beşli</u> , Ceylan Mutlu Balcı
P-096	Synthesis of Bimetallic Ruthenium Complexes and their Spectroscopic Properties <u>Hatice Dilayla Altıok</u> , Hayati Türkmen
P-097	The gentisic acid salts of the tetrapyrrolidino and tetrapiperidino mono (4-fluorobenzyl)spirocyclotriphosphazenes: spectroscopic and thermal results <u>Aytuğ Okumuş</u> , <u>Hüseyin Akbaş</u> , Ahmet Karadağ, Zeynel Kılıç
P-098	Synthesis Of Mono Metallic Ru(II) Arene Complexes And Spectroscopic Properties <u>S.Batıkan Kavukcu</u> , Hayati Turkmen
P-099	Synthesis of some new 1,3,4-thiadiazole compounds derived from butyric acid and Characterization of structures by spectroscopic methods <u>Halit Muğlu</u> , Nesrin Şener, Hamza Ahmed Mohammad Emsaed, Sevil Özkınalı Özkınalı, Osman Emre Özkan, Mahmut Gür
P-100	The synthesis and investigation of different cobaloximines by spectroscopic methods Ahmet Kılıç, Mustafa Durgun, <u>Nuri Yorulmaz</u> , Rahime Yavuz
P-101	Synthesis and spectroscopic characterization of bulky hemi-salen ligands and their triboron complexes Ahmet Kılıç, Mustafa Durgun, <u>Nuri Yorulmaz</u> , İsmail Özaslan, İbrahim Halil Kaya
P-102	Synthesis of Benzothiazole Derivative Mono Azo Dispers Dyeing, Investigation of Structure Analysis and Absorption Spectrum <u>İzzet Şener</u> , Nesrin Şener, Mahmut Gür
P-103	Synthesis and characterization of 5,6-dihydro-1H-cyclopropa[c]indole-2,7(1aH,3H)-dione by NMR spectroscopy and single crystal x-ray analysis <u>Mehmet Yılmaz</u> , Aslı Ustalar, Sedanur Birincioğlu <b>NOT ATTENDED</b>
P-104	One-pot Synthesis of 3-(Acylamino)-4(3H)-quinazolinones Utilizing N-(2-Aminobenzoyl)benzotriazoles <u>İbilge Merve Şenol</u> , İlhami Çelik
P-105	Amino acid bounded quinazolinones by a one-pot, three-component reaction of N-(2-aminobenzoyl)benzotriazoles, amino acids and aldehydes <u>Büşra Demir</u> , İlker Avan, İlhami Çelik <b>NOT ATTENDED</b>
P-106	Synthesis of novel piperazine derivatives and comparative characterization of their experimental and theoretical NMR spectra <u>Sait Sari</u> , Seda Ünalın, Kübra Çakır, Mehmet Yılmaz <b>NOT ATTENDED</b>

P-107	Synthesis, X-ray Crystal Structure and NMR Study of 3-butyl-4-iodo-6-methoxybenzo[c][1,2]oxaborol-1(3H)-ol via Consecutive Metal-Iodine Exchange <b>NOT ATTENDED</b> Raed M Al Zoubi
P-108	Investigation of Heavy Metal Contents of Some Spices Sold in Market Places Hacer Sibel Karapınar, Fevzi Kılıçel
P-109	Investigation of The Heavy Metal Content of Soil Taken from Field Corn Silage Hacer Sibel Karapınar, Fevzi Kılıçel, Fadimana Ünüvar
P-110	Adsorption of Phenoxyacetic acid on Polymeric Adsorbents Using UV and FTIR spectrophotometer Fatih Bildik, Gizem Akdut, Filiz Şenkal, Tuba Şişmanoğlu
P-111	Adsorption of Dyes with Natural Resin Functionalized Hollow Silica Sphere Bionanocomposite Material Hakan Duran, Tuba Şişmanoğlu
P-112	Synthesis and Characterization of Nano Metal Oxides Prepared by Different Methods for Photocatalytic Degradation of Benzoquinone Gülin Selda Pozan Soylu, Yasar Zengin

**POSTER SESSION 2 (P-113 / P-212) | August 29, 2017 - Tuesday**

Number	Abstract title   Authors
P-113	The Investigation of Physical and Chemical Structure Properties of the (1E,2Z)-1-(4-nitrobenzylidene)-2-[4-(propan-2-yl)benzylidene]hydrazine with Spectroscopic Techniques and Quantum Chemical Computational Methods <u>Ersin Inkaya</u> , Melek Gül, Serpil Eryılmaz
P-114	4-(3-mesityl-3-methylcyclobutyl)-3-(phenylamino)thiazol-2(3H)-thione: Experimental and DFT Studies <u>Ersin Inkaya</u> , Alaaddin Cukurovali, Muharrem Dincer
P-115	Determination of crystal structure of 2-aminopyridine molecule from X-ray powder diffraction data <u>Zeki Kartal</u> , Angela Altomare
P-116	Effects of chemical structures of omega-6 fatty acids on the molecular parameters and quantum chemical descriptors <u>Tugba Göcen</u> , Sevgi Haman Bayarı, Mehmet Haluk Güven
P-117	Synthesis, Characterization and Theoretical Study of N,N'-(oxybis(4,1-phenylene))bis(1-(4-fluorophenyl)methanimine) <b>NOT ATTENDED</b> <u>Dilek Elmalı</u> , Türkay Aytekin, Halil Berber
P-118	Synthesis, spectroscopic studies and calculation of 5-benzoyl-6-phenyl-4-(4-methylthiophenyl)-1,2,3,4-tetrahydro-2-thioxopyrimidine <u>Erdem Ergan</u> , Esvet Akbaş, Metin Çakır
P-119	The solvent effects the C=O stretching vibrations of the 4-formylphenylboronic acid molecule <u>Emine Babur Şaş</u> , Emine Tanis, Zühre Çalışır, Mustafa Kurt
P-120	Synthesis, molecular structure and theoretical calculation of (2-imino-4-(4-(methylthio)phenyl)-6-phenyl-1,2,3,4-tetrahydropyrimidin-5-yl) (phenyl) methanone <u>Esvet Akbas</u> , Erdem Ergan, Metin Cakir
P-121	Optoelectronic Properties of Donor-Acceptor Type Conjugated Polymers <u>Kübra Uludağ</u> , Can Karadeniz, Tolga Ortakçı, Pervin Ünal Cıvır
P-122	Spectroscopic Study of Furan and Benzofuran Derivatives Combined with DFT Calculations <u>Can Karadeniz</u> , Kübra Uludağ, Gülbin Kurtay, Pervin Ünal Cıvır
P-123	Molecular, electronic and spectroscopic, properties of 6-Chloroquinoline by using DFT method <u>Etem Köse</u> , Fehmi Bardak, Ahmet Atac, Çağlar Karaca
P-124	Computational Investigation of Metal Complexes of ISE (3[4-ethyl(phenyl)-imino][1H-indole-2-one]) Sevil Şener, <u>Nursel Acar</u>
P-125	Spectroscopic Analysis and DFT Calculation of poy(epichlorhydrin-b-ε-caprolactone) and poy(ε-caprolactone-b-tetrahydrofuran-b-ε-caprolactone) Block Copolymers <u>Ismail Çakmak</u> , Sevil Savaşkan Yılmaz, Murat Mısır
P-126	Spectroscopic and Computational Investigation of Selected Porphyrins <u>Cenk Selçuki</u> , Hakan Apat, Nursel Acar
P-127	The spectroscopic properties and theoretical calculation of some new disazo dyes derived from 2,4-Dihydroxyquinoline <u>İzzet Şener</u> , Nesrin Şener, Mahmut Gür, Muhammed Serdar Çavuş

P-128	NMR and IR Spectroscopy and DFT Calculation of Polymers Bearing Side Chain Aziridine Group <u>Ismail Çakmak</u> , Sabri Ulukanlı
P-129	Morphological Characteristics of 4-n-octyl-4'-cyanobiphenyl (8CB) at the Air/Water Interface as Studied by Molecular Dynamics Simulation <u>Oğuz Gürbulak</u> , Emine Cebe
P-130	Orientalional Order Properties of 4-n-pentyl-4'-cyanobiphenyl (5CB) Molecules at the Air/Water Interface: A Molecular Dynamics Simulation Study <u>Oğuz Gürbulak</u> , Emine Cebe
P-131	DFT Computational Studies of 2-((E)-{4-(Hydroxymethyl)phenyl}-imino)methyl)phenol Hasan Tanak, <u>Şenol Toprak</u> , Metin Orbay
P-132	A Study on Spectroscopic (FT-IR and NMR) Properties and DFT Computations of N-[[4-(diphenylamino)phenyl]methylene]-2,3,5,6,8,9,11,12-octahydro-1,4,7,10,13-benzopentaoxacyclopentadecin-15-amine <u>Gökhan Alpaslan</u> , Öznur Şener, Gökhan Sevinç, Zeliha Hayvalı, Hüseyin Ünver
P-133	Theoretical Study on the origins of the gap bowing in $\text{Ca}_{1-x}\text{Mg}_x\text{S}$ alloys <u>Boutarfa Bariza</u> <b>NOT ATTENDED</b>
P-134	Investigation of the interactions of Tamoxifen with the estrogen receptor alpha via quantum mechanics methods and molecular docking Fehmi Bardak, <u>Sibel Bilgili</u> , Ahmet Ataç
P-135	Effect of External Electric Field on Intermolecular Halogen Bond of the N-Substituted Imidazoles ••• $\text{X}_2/\text{XY}$ Complexes <u>Fatmagül Tunc</u> , Ahmet Tokatlı, Fatih Uçun
P-136	Salicylaldehyde based a hydrazone compound: Synthesis, crystal structure, a comparison of theoretical and experimental spectroscopic results and the investigation of interaction with Pd(II) and Pt(II) by DFT calculations <u>Ayşin Zülfikaroğlu</u> , Çiğdem Yüksektepe Ataoğ
P-137	Quantum Chemical Computational Study of N'-((E)-2-(hydroxyimino)-1-phenylethylidene)furan-2-carbohydrazide <u>Ayşin Zülfikaroğlu</u> , Hümeysra Batı
P-138	Conformational, Structural, Electronic and Vibrational Investigations on 5-Methyl-4-(2-thiazolylazo)resorcinol by FT-IR, FT-Raman, NMR and DFT <u>Semran Sağlam</u> , Yusuf Erdoğan, Ümran Ceren Başköse, Mehmet Tahir Güllüoğlu
P-139	Investigation of Solvent Effect of Molecular Structures on Molecular Orbital Energies by Density Functional Theory <u>Çiğdem Yüksektepe Ataoğ</u>
P-140	Investigations on the FT-IR, FT-Raman, Conformational analysis, Molecular docking, Fukui function, DFT of 2-Isopropyl-6-methyl-4-pyrimidinol Yusuf Erdoğan, <u>Semran Sağlam</u> , Ümran Ceren Başköse, Mehmet Tahir Güllüoğlu
P-141	Investigation of D-H... A Hydrogen Bond Effect on Vibration Frequencies of Molecular Structures by Density Functional Theory <u>Çiğdem Yüksektepe Ataoğ</u>
P-142	Investigation on spectroscopic and quantum chemical calculation studies of Aloe Emodin molecule Ömer Dereli, <u>Ümran Ceren Başköse</u> , Yusuf Erdoğan, Semran Sağlam
P-143	Supramolecular self-assembly of new benzamide derivatives directed by intermolecular and $\pi$ -stacking interactions: Crystal structures and Hirshfeld surface analyses <u>İlkay Gumus</u> , Hakan Arslan, Ummuhan Solmaz, Ebru Keskin, Gun Binzet, Birdal Arslan, Ali Nail Selcik, Suleyman Bozkurt

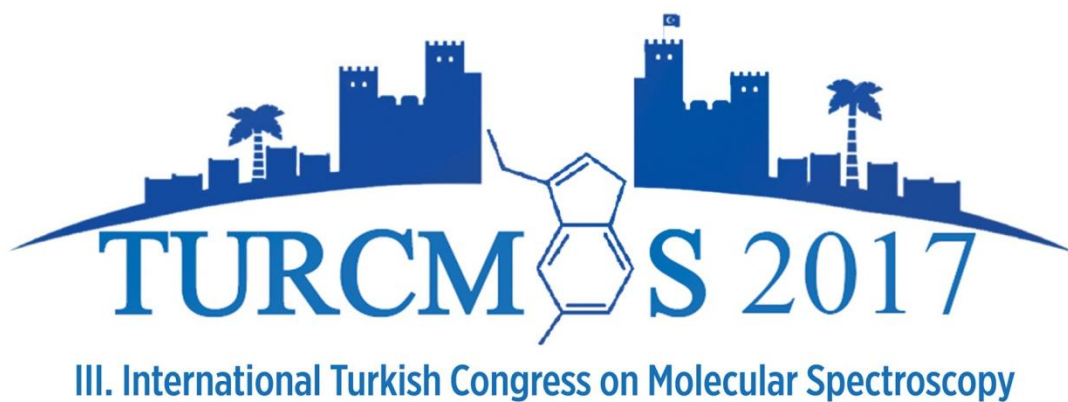
P-144	Experimental and theoretical studies of the molecular structure of 7-Methyl-3-[(3-methyl-3-mesityl-cyclobutyl)-5-phenyl-5H-thiazolo[3,2- $\alpha$ ]pyrimidine-6-carboxylic acid ethyl ester <u>Betül Acar, Nezihe Çalışkan, İbrahim Yılmaz, Alaaddin Çukurovalı</u>
P-145	Synthesis, Spectroscopic (FT-IR, UV-Vis), Experimental (X-Ray) and Theoretical (HF/DFT) study of: ((E))-2-chloro-{N}-((4-nitrocyclopenta-1,3-dienyl)methylene)benzenamine <u>Gonca Özdemir Tari, Ümit Ceylan, Erbil Ağar, Orhan Büyükgüngör</u>
P-146	Crystal Structure Analysis, Spectroscopic Characterization and Theoretical Calculations of: (E)-4-bromo-5-methoxy-2-((p)-tolylimino)methylphenol <u>Gonca Özdemir Tari, Seda Nur Aygün, Necmi Dege, Erbil Ağar</u>
P-147	Spectroscopic (FT-IR / NMR) and quantum chemical study on 3,4-dicyanophenyl 4-methylbenzenesulfonate <u>Yasemin Inkaya, Canan Kazak, Nesuhi Akdemir, Ersin Inkaya</u>
P-148	Experimental and Theoretical Investigation of the Molecular and Electronic Structure of 2,3-dicyanophenyl 4-methylbenzenesulfonate <u>Yasemin Inkaya, Canan Kazak, Nesuhi Akdemir, Ersin Inkaya</u>
P-149	Experimental (x-ray, ft-ir and uv-vis spectra) and theoretical methods (dft study) of n'-(dipyridin-2-ylmethylene)-4-methylbenzenesulfonohydrazide <u>Erbil Murat Aydın, Murat Çınarlı, Hümeysra Batı, Nezihe Çalışkan, Çiğdem Yüksektepe Atal</u>
P-150	A density functional theory study on geometric, spectroscopic and electronic properties of BTPCA <u>Ömer Tamer, Davut Avcı, Yusuf Atalay</u>
P-151	Combined experimental (FT-IR, FT-Raman, NMR) and theoretical studies on the molecular structure, vibrational spectra, reactivity descriptor and molecular docking 4,4'-dimethyl-2-2/dipyridyl <u>Ümran Ceren Başköse, Yusuf Erdoğan, Semran Sağlam, Mehmet Tahir Güllüoğlu</u>
P-152	Optimized geometry, spectroscopic (IR, UV-Vis and NMR) characterization and nonlinear optical properties of 4-(4-methoxy-2-nitrophenylamino)-4-oxobutanoic acid; A DFT study <u>Ömer Tamer, Davut Avcı, Yusuf Atalay</u>
P-153	5-Methyl-2-thiophenecarboxaldehyde: Experimental and TD/DFT study <u>Davut Avcı, Ömer Tamer, Adil Başoğlu, Yusuf Atalay</u>
P-154	A theoretical study of solvent effects on 2-acetoxybenzoic acid molecule <u>Sibel Çelik, Emine Tanış, Selin Özkan Kotiloğlu, Mustafa Kurban</u>
P-155	Theoretical evaluation of triazine derivatives as steel corrosion inhibitors: DFT <u>Burak Tüzün, Gamze Tüzün</u>
P-156	Structural considerations on benzamide derivatives: Synthesis, crystal structure and Hirshfeld surface analysis <u>Hakan Arslan, İlkay Gumus, Ummuhan Solmaz, Ebru Keskin, Gun Binzet, Birdal Arslan, Ali Nail Selcik, Suleyman Bozkurt</u>
P-157	Computational Investigation Of Cadmium(II)-Nickel(II) Imidazole Complex: $[Cd(imidazole)_4Ni(\mu - CN)_4]_n$ <u>Güneş Süheyla Kürkcüoğlu, İlkan Kavlak</u>
P-158	A Copper-Paladium(II) Cyanide Complex Containing N-Methylimidazole Ligand: An Agreement Between Theoretical And Experimental Studies: $[Cu(N - Meim)_2Pd(CN)_4H_2O]_n$ <u>Güneş Süheyla Kürkcüoğlu, İlkan Kavlak</u>
P-159	An Investigation of Substitution and Solvent Effects on Intramolecular Proton Transfer in Fluorophenyl Derivatives of (Z)-2,4-di-tert-butyl-6-(((phenyl)imino)methyl)phenol by Means of Spectroscopic Measurements and Quantum Chemistry Calculations <u>Erol Eroğlu, Bahar Kancı, Nuri Yorulmaz, Abdurrahman Şengül</u>
P-160	Time Dependent DFT Study of UV-Visible Spectrum of Polyselenophene Molecular Segment as a H <sub>2</sub> O Sensor <u>Zeki Büyükmumcu, Fatma Selampınar</u>

P-161	Analytical solutions to the Kratzer potential in the presence of a constant magnetic field: non-relativistic neutral 2-body system Oğuzhan Uzun, Kübra Uzun, Uğur Çevik, Azar Ahmadov
P-162	DFT Calculations of Hybrid Compound Based on Curcumin and Thalidomide for Multiple Myeloma Kübra Uzun, Uğur Çevik, Yusuf Atalay
P-163	Crystal structure, Hirshfeld surfaces and DFT computation of (E)-2-(((5-nitrothiophen-2-yl)methylene)amino)benzonitrile Abdullah Akkaya, Ersin Temel, Seher Meral, Ayşen Alaman Ağar
P-164	Molecular Structure of 4-Amino-3-(thiophen-2-ylmethyl)-1H-1,2,4-triazole-5(4H)one Monohydrate Hasan Tanak, Meryem Evecen, Levent Semiz, Yasemin Ünver
P-165	Chelate Cross-Linked Affinity Ion-Imprinted Cryogel for Selective Recognition of Ce(III) in Environmental Samples and Determination of Ce(III) by ICP-OES Ruken Onat
P-166	An X-Ray Study for Structural Characterization of cis-Bis(methyl 2-(benzoyl carbamothioyl)-3-(4-chlorophenyl)-5-methyl-4,6-dioxo-1-phenyl-octahydropyrrolo[3,4-c] pyrrole-1- carboxylate)platinum(II) Yahya Nural, Müge Gemili, Ertan Şahin
P-167	NMR-QSAR Model of Some Imidazole Derivatives Pervin Ünal Cıvırcı, İrfan Cıvırcı, Gülbin Kurtay
P-168	Quantum mechanical calculated reactivity and molecular docking features of difluoroanilines Fehmi Bardak, Etem Köse, Ahmet Ataç, Çağlar Karaca
P-169	Theoretical evaluation of triazine derivatives as steel corrosion inhibitors: Monte Carlo simulation approach Burak Tüzün, Savaş Kaya, Cemal Kaya
P-170	Synthesis and spectroscopic studies of substituted 5,6,7,8-tetrahydroquinazolin-2-amine compounds via one-pot method F. Tülay Tugcu, Kadir Turhan
P-171	Synthesis and spectroscopic studies of substituted 6,7-dihydrocyclopentapyrimidin-2-amine compounds via one-pot method F. Tülay Tugcu, Kadir Turhan
P-172	Application of Fluorescence Intercalator Displacement (FID) Method for Determination of G-quadruplex DNA Binding Selectivity of Water Soluble PIP and HPIP Analogs Ufuk Yıldız, Buraj Çoban
P-173	EPR Investigation of Heating Process on Carob Müberra Maral Süneciöğlü, Özgür Taylan Akdağ
P-174	ESR dating of fossil mollusc shells from Sarıcalar, Konya Closed Basin (Turkey) Hülya Aydın, Birol Engin, Ülkü Sayın, Gamze Ekici, Mesut Işık, Sevinç Kapan, Arif Delikan, Ahmet Demir, Hükmü Orhan, Recep Bıyık, Recep Tapramaz, Ayhan Özmen
P-175	A new phenolic sulfate ester from the aerial parts of {Tamarix balansae} J. Gay Ahmed Kabouche, Abbas Benmerache, Toufik Boune, Djemaa Berrehal, Zahia Kabouche, Abdulmagid Alabdul Magid, Laurence Voutquenne Nazabadioko
P-176	A new sulfonlated flavonoid and other compounds isolated from the aerial parts of {Cotula anthemoides} L Zahia Kabouche, Wafa Tadrent, Ahmed Benmerache, Toufik Boune, Djemaa Berrehal, Zahia Kabouche, Abdulmagid Alabdul Magid, Laurence Voutquenne Nazabadioko2
P-177	Phenolic Profile and Antiproliferative Activity of Carduncellus helenioides (Asteraceae) Extracts Faiza Meratate, Aissa Lalaoui, Khellef Rebbas, İbrahim Demirtas, Hocine Laouer, Salah Akkal
P-178	Determination of essential and toxic microelements in the bran and wheat flour grown in Southeastern of Turkey by ICP-OES Mehmet Zahir Düz, Mehmet Duzgun, Hüsnü Aktaş, Mehmet Firat Baran, Ersin Kilinc, Mehmet Karaman



P-179	<b>Determination of Multielement in the Grains Grown Around Karacadağ and Tigris River of Southeastern Turkey by ICP-OES</b> <u>Mehmet Zahir Düz</u> , Mehmet Duzgun, Irfan Erdemci, Serif Kahraman, Mehmet Firat Baran, Ersin Kilinc
P-180	<b>Removal of Hg(II) from aqueous solution by Bacillus subtilis ATCC 6051(B1) biomass</b> <u>Mehmet Firat Baran</u> , Serhat Uzan, Fikret Uyar, Kadir Serdar Celik, Ersin Kilinc, Mehmet Zahir Duz
P-181	<b>Preparation and Application of Surface Plasmon Resonance Sensors Based on Molecularly Imprinted for Detection of Pesticide in Green Pepper</b> <u>Oğuz Çakır</u> , Fatma Yılmaz, Zübeyde Baysal, Adil Denizli
P-182	<b>Synthesis, Crystal Structures, Spectral FT-IR, NMR and UV-Vis Investigations and Theoretical Studies of N-phenyl-2-imino-5-methylthiophene and N-(4-chlorophenyl)-2-imino-5-methylthiophene</b> <u>Duygu Barut Celepci</u> , Aydın Aktaş, Gül Yakalı, Yetkin Gök
P-183	<b>Electrochemical Determination of Rivastigmine Hydrogen Tartrate in Pharmaceutical Samples at <math>\beta</math>-Cyclodextrine/Multi-walled Carbon Nanotubes Modified Electrode</b> <u>Kubilay Güçlü</u> , Hayati Filik, Mustafa Özyürek, Buğçe Kılıçyıldır
P-184	<b>High-Resolution Infrared Spectroscopy of Field Red Horizontal Branch Stars</b> <u>Melike Afşar</u> , Christopher Sneden, Zeynep Bozkurt, Gamze Böcek Topcu, Gregory N. Mace, Hwihyun Kim, Daniel T. Jaffe
P-185	<b>Synthesis and Evaluation of Antioxidant Activity of Some Pyrimidine compounds</b> Esvet Akbas, <u>Suat Ekin</u> , Erdem Ergan, Yagmur Karakus, Ertan Sahin
P-186	<b>Synthesis, characterization of polymer-graft-calixarene molecules in different structures and interactions with volatile organic compounds</b> <u>Zeynep Genç</u> , Nilgün Kızılcan, Çağatay Altinkök, Ilke Gürol, Cihat Taşaltın
P-187	<b>Spectroscopic Details of the Synthesized Novel Benzofuran compound with Experimental and Quantum Chemical Studies: F-TIR, <sup>1</sup>HNMR, <sup>13</sup>CNMR and DFT</b> <u>Gül Yakalı</u> , Duygu Barut Celepci, Esra Barım, Mustafa Değirmenci, Cumhur Kırılmış
P-188	<b>SAXS Analyses on Nanostructured Chocolates which have Different Cocoa Ratios</b> <u>Damla Karaarslan</u> , Semra Ide
P-189	<b>Preparation and Characterization of Crosslinked Polymer Hydrogel Microbeads by Copolymerizing Ethylene Glycol Dimethacrylate with n-Vinyl Imidazole</b> <u>Nalan Tekin</u> , İnci Özdemir, Ali Kara
P-190	<b>FTIR Spectroscopic Studies of Spider Dragline Silk of Different Species</b> <u>Sevgi Haman Bayarı</u> , Tuncay Türkes, Wei Tsung Chuang
P-191	<b>Proficiency Testing by Inductively Coupled Plasma Mass Spectrometry Multi-Elemental Analysis in the Chilli Powder</b> <u>Serpil Kiliç</u> , Murat Kiliç
P-192	<b>Adsorption of Arsenic(V) on Adsorbents Produced from Solid Wastes</b> <u>Kubilay Güçlü</u> , Mehmet Mahramanlioğlu, Mustafa Özyürek, Fatih Özbaş, Muhammed Zahoor
P-193	<b>Structural Properties of Fe-27%Ni-4%Mn-2%Zn alloy</b> <u>Fazıl Fazlı Kulucan</u> , Melek Güler, Emine Aldırmaz, Emre Güler
P-194	<b>Development of a fast analytical microextraction method for the determination of Sudan (II) in foodstuffs by spectrophotometry</b> <u>Nail Altunay</u> , Ramazan Gürkan, Ulaş Orhan
P-195	<b>Isotopic and elemental markers for the differentiation of Transylvanian vegetables</b> <u>Dana Alina Magdas</u> , Ioana Feher, Adriana Dehelean, Gabriela Cristea, Cezara Voica, Stelian Radu, Romulus Puscas
P-196	<b>Discrimination markers for geographical and species origin of raw milk produced in three Romanian farms</b> <u>Dana Alina Magdas</u> , Ioana Feher, Adriana Dehelean, Gabriela Cristea, Cezara Voica, Stelian Radu, Romulus Puscas, Sorin Daniel Dan, Darius Cordea

P-197	The Spectroscopy of Environmental Structure Caused The Winds of CW Cep Eclipsing Binary Star Mehmet Tanriver, Ahmet Avcı, <u>Ahmet Keskin</u>
P-198	Development of a robust ultrasonic assisted ionic liquid-based dispersive liquid-liquid microextraction for preconcentration of Pb in vegetable samples <u>Emre Yıldırım</u> , Nail Altunay, Ramazan Gürkan
P-199	Infrared Spectroscopy And Thermostatic Analysis On New Generation Plastic Additives Including Transition Metal(II) Complex With Stearic Acid <u>Ilkan Kavlak</u> , Güneş Süheyla Kürkçüoğlu
P-200	Vibrational Spectral Analysis And Thermostatic Properties Of The Pvc Dry Blends Consisting Of Transition Metal Borax Complex With Stearic Acid <u>Ilkan Kavlak</u> , Güneş Süheyla Kürkçüoğlu
P-201	Synthesis, Spectroscopic and Thermal Investigation of Poly(triethoxyvinylsilane-co-vinyltris(trimethylsiloxy)silane-co-divinylbenzene) <u>Talat Özpozan</u> , Hatice Arı, Mine Dede
P-202	Synthesis of Poly(triacetoxyvinylsilane-co-trimethylvinylsilane-co-divinylbenzene) and Determination of Spectroscopic and Thermal Behaviors <u>Mine Dede</u> , Hatice Arı, Talat Özpozan
P-203	Polyethylene imine/Fe[NiFe]O <sub>4</sub> and Polyethylene imine/Fe <sub>3</sub> O <sub>4</sub> Magnetic Composite nanoparticles: An application for enzyme technology <u>Yasemin Ispirli Doğaç</u> , Mustafa Teke
P-204	Characterization of Chitosan/TiO <sub>2</sub> Composite Beads: An Application for Enzyme Technology Ilyas Deveci, <u>Yasemin Ispirli Doğaç</u> , Bedrettin Mercimek, Mustafa Teke
P-205	Synthesis, Crystal Structure and Spectroscopic Properties of New Co(II/III) Complex <u>Umut Güzel</u> , M. Burak Çoban, Yasemin Acar, Elif Güngör, Görkem Oylumluoğlu, Hülya Kara
P-206	Single Crystal Structure of Holmium(III) Based Porous Coordination Polymer M. Burak Coban, <u>Gorkem Oylumluoğlu</u> , Cagdas Kocak, Muhittin Aygun, Hulya Kara
P-207	Structural Characterization of Electrospun PVA/ZnO Composite Nanofibers Gökmen Arabacı, Yasemin Ispirli Doğaç, Ilyas Deveci, <u>Ceyhun Işık</u> , Mustafa Teke
P-208	Determination of chemical composition of Petroselinum crispum L. seed by GC/MSD <u>Ceyhun Işık</u> , Şeyda Kıvrak, Tolga Göktürk, Ibrahim Kıvrak
P-209	The Determination of Some Trace Elements (As, Be, Cd, Co, Cr, Cu, Li, Mn, Pb, Se, Sr, Ti, V, Zn) and Mineral (Mg) Levels of {Dactylorhiza umbrosa} (Kar. & Kir.) Nevski (Orchiaceae) Plant <u>Hatice Kiziltaş</u> , Suat Ekin, Damla Yıldız, Süleyman Mesut Pinar
P-210	The effect of the sodium oxide in the silicate-yttria-zirconia vitroceramics <u>Marius Rada</u> , Hendea Radu, Simona Rada, Jing Zhang, Zhonghua Wu, Lidia Magerusan



# Invited Speakers Abstracts

## PL-01

### Probing Radical and Nitrene Intermediates in Narrowband UV-Induced Photoreactions in Cryogenic Inert Matrices

Rui Fausto

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Radical and nitrene intermediates play a fundamental role in chemical reactivity. However, their capture and characterization, as well as the precise description of their reactivity, pose always enormous challenges to investigation.

Matrix isolation is a powerful tool to study short-living species, and is nowadays a mature technique suitable to address complex problems of chemical reactivity involving reaction intermediates. In fact, when used together with contemporary computational methods of quantum chemistry and up-to-date narrowband tunable light sources, matrix isolation may be used very successfully for investigation of elusive reaction intermediates, in a very elegant and direct way.

In this talk, I will describe a series of possible strategies for research on the structures and reactivity of radical and nitrene intermediates participating in photochemical processes, based on the conjugated use of theoretical methods and matrix isolation coupled with spectroscopic probing. Recent results on the photochemistry of phenols and thiophenols, in which radicals play a prominent role, and of several types of nitrene precursors, like isoxazoles, azides and tetrazoles, will be presented. In these studies, narrowband tunable light sources were used to selectively excite the different species formed along the targeted reactions, allowing the unequivocal identification of the transient radicals and nitrenes formed along these processes, their structural characterization and the evaluation of their specific reactivity. On the way, the first direct observation of a tunneling reaction involving a nitrene, and the production of several rare high-energy species resulting from photochemical processes where radical and nitrene intermediates play central mechanistic roles will be reported.

*Acknowledgements: Present and past members of the Laboratory for Molecular Cryospectroscopy and Biospectroscopy, Coimbra, Portugal, and research partners from other laboratories, who have contributed to the studies addressed in this talk, are acknowledged. I thank also the Portuguese Science Foundation (FCT) for financial support (Project PTDC/QEQ-QFI/3284/2014 – POCI-01-0145-FEDER-016617, also funded by FEDER/COMPETE 2020-UE). The Coimbra Chemistry Centre (CQC) is supported by FCT, through the project UI0313/QUI/2013, also co-funded by FEDER/COMPETE 2020-EU.*

## PL-02

### Vibration spectroscopies at low and very high wavenumbers: Why & how

Philippe Colomban

*Pierre and Marie Curie University, France*

Most of the spectroscopists, in particular in analytical chemistry, use only a part of the vibration domain, the 200-3200  $\text{cm}^{-1}$  region, the Raman and infrared instruments becoming more expensive – and rare - below 120 and 400  $\text{cm}^{-1}$ , respectively, and their attention to water and protonic species patterns is very limited. With the technological progresses, in particular the replacement of monochromators with Notch filters, the practice is changing. Taking examples chosen in the fields of polymer fibres, solid electrolytes, and nanoparticles we explain how the spectra can be collected and interpreted and how various information regarding the mechanics, ionics/protonics and dynamics can be extracted at low and high wavenumbers. Particular attention is given to the advantage of isotopic substitution and dilution and to operando/in situ measurements.

**Keywords:** Vibration, spectroscopy, polymer fibres, solid electrolytes, and nanoparticles

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## PL-03

### Reliable blood monitoring by microdialysis and infrared spectrometry for diabetic and critically ill patients: Fourier-transform spectrometry or quantum cascade laser technology - quo vadis?

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Andreas Ostendorf<sup>2</sup>

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Nowadays, point-of-care diagnostics is demanding for continuous sensing systems, especially for blood glucose monitoring, although intermittent testing is still practiced even for critically ill patients. In this context, micro-dialysis has often been used in the clinical environment for continuously harvesting body fluids in a minimal invasive manner, but a drawback of this process are variable recovery rates. By using multivariate infrared spectroscopy and its inherent multi-analyte capability for whole blood, interstitial fluid or dialysate measurements, the application of a marker substance containing perfusates has been investigated. The use of an internal standard for reliable recovery assessment allows also a safe lifetime extension of  $\mu$ -dialysis catheters or ex-vivo whole blood  $\mu$ -dialysators [1, 2]. Recently, FTIR-mini-spectrometers have been successfully employed for the development of bed-side monitoring systems. In-vivo applications for intensive care patients can be envisaged, especially as further analytes and parameters are accessible, which are of interest for intensive medicine such as lactate, urea,  $pCO_2$  and pH [3].

However, for implementation in further miniaturized portable systems, quantum cascade lasers (QCL) appear to be most suitable. External cavity (EC) - QCLs promise gapless spectral recording and broad tuning ranges, especially if the infrared fingerprint region has to be covered for quantitative multi-parameter analysis [4, 5]. We present measurements taken with an ultra-broadly tunable EC-QCL system covering a spectral range from 1920 to 780  $cm^{-1}$  and discuss its performance also with regard to trans-mission measurements of aqueous biofluids. A comparison and discussion of weaknesses and advantages versus the performance of FTIR-spectrometers will be presented.

**Keywords:** FTIR-spectroscopy, EC-QCLs, clinical chemistry, patient blood monitoring

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PL-04

**Three-dimensional Infrared and Raman Tomography of Extraterrestrial Materials**

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<sup>2</sup>*Stony Brook University, New York, USA*

<sup>3</sup>*University of Central Florida, Orlando, USA*

We have demonstrated nondestructive three-dimensional microscopic in-situ imaging (infrared and Raman) of extraterrestrial samples. Qualitative and quantitative investigation through these analytical techniques can help us elucidate the origin and evolution of meteoritic compounds as well as parent body alteration and thermal processes without damaging the investigated samples. Using infrared tomography, spatially resolved chemical composition and spatial correlations are investigated within a single ~50  $\mu\text{m}$  grain of the Murchison meteorite, a CM2 carbonaceous chondrite [1]. Using confocal Raman imaging, we studied the unequilibrated ordinary L3 chondrite QUE 97008 and our tomographic results show the presence of organic matter near  $z = 18 \mu\text{m}$  underneath a large olivine grain [2]. These highly novel analytical techniques will help us understand distribution and spatial relations of organic matter with inorganic materials, which will potentially provide clues for the formation and evolution histories of chemical constituents present in meteorites.

**Keywords:** infrared, Raman, tomography, imaging, spectroscopy



PL-05

**Magnetic Resonance Characterization of Short-Lived Paramagnetic States in Photoactive Proteins**

Stefan Weber

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In this contribution, the focus will be on radical pairs generated in the course of photo-induced electron-transfer reactions of blue-light photoreceptors (cryptochromes [1,2], LOV domains of phototropins [3], BLUF domains [4]) and other photo-active proteins (DNA photolyases) harboring flavin cofactors. Representative results from EPR (transient EPR, out-of-phase electron-spin-echo envelope modulation (OOP-ESEEM), ENDOR and HYSCORE) and also NMR will be presented, that helped drawing a clearer picture of flavin-based protein photoreaction mechanisms. It will be furthermore demonstrated that the principles of generation of paramagnetic species, such as triplet states and radical pairs, and their characterization by the above-mentioned methods may also be applied to photo-induced charge separation in energy-conversion devices [5].

*Acknowledgements: Support by the Deutsche Forschungsgemeinschaft (DFG) and the Struktur- und Innovationsfonds Baden-Württemberg (SI-BW) is gratefully acknowledged.*

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**Keywords:** Electron Paramagnetic Resonance; Nuclear Magnetic Resonance; Electron Transfer; Radical Pairs; Electron-Spin Polarization

## PL-06

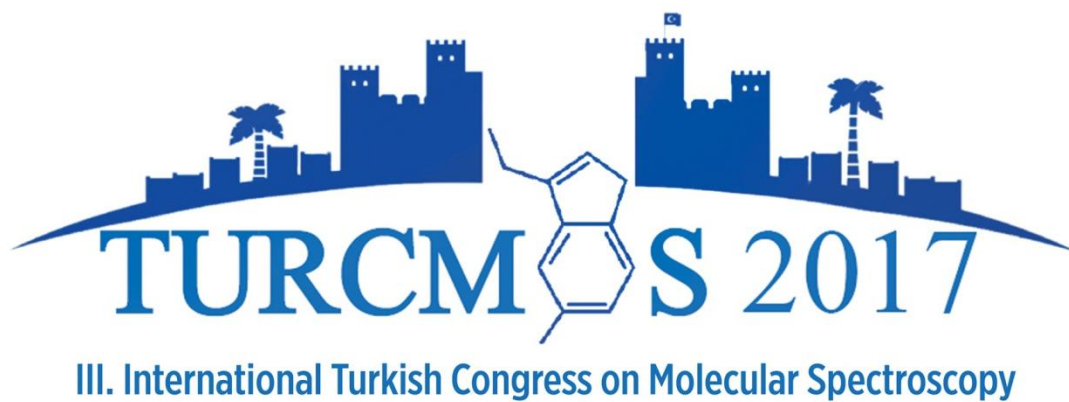
### PSD (Protein Spectra Database): A platform for analysis and sharing of protein spectroscopic data

Parvez Haris

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There are several different spectroscopic techniques that provide valuable information regarding protein secondary structure including NMR, CD, FTIR and Raman spectroscopy. We have been applying FTIR spectroscopy for determining the secondary structure of proteins in aqueous and non-aqueous media. We have also been developing tools for estimating the secondary structure of proteins from FTIR spectra using artificial intelligence techniques. Unfortunately, very little effort has been made to develop a publically available database, for depositing protein spectral data that could be shared by the scientific community to further develop predictive methods and for obtaining a better understanding of protein-spectra relationship. We are developing a database for this purpose that will be freely accessible to the scientific community that will include not only FTIR spectra but data from other complementary techniques such as CD, Raman and NMR spectroscopy. The presentation will discuss the challenges and benefits offered by a protein spectra database

**Keywords:** Protein Spectra Database, NMR, CD, FTIR



## Oral Abstracts

**O-01**

**Structural Characterization Of Amyloid Fibrils Using Vibrational Circular Dichroism**

Laurence Nafie

*Biotools Inc.*

Structural Characterization Of Amyloid Fibrils Using Vibrational Circular Dichroism

**Keywords:** Amyloid Fibrils, Vibrational Circular Dichroism, VCD

O-02

Usage of CO and High Density Tracers to Probe the Physics of Star-Forming Gas in Galaxies

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CO is the second most abundant molecule after H<sub>2</sub> and it provides indirect probe for the physics of molecular gas in galaxies. Line ratio diagnostics of CO and some other high density tracers allow us to probe not only the physics of the gas, i.e density, temperature, opacity, but also the gas kinematics which allows us to study the evolution of galaxies. While disc galaxies, like our own Milky Way, are so rich in molecular gas, the fuel for star formation, its abundance is much less in lenticular galaxies and almost no molecular gas present in elliptical galaxies. Our studies revealed that i) physical conditions of molecular gas is different in the center, arms and inter-arms of spiral galaxies, ii) The conditions in the lenticulars appear intermediate between those of spirals and starburst galaxies, iii) based on our CO Tully-Fisher Relation studies the distant galaxies appear to be more massive and luminous than the local ones.

**Keywords:** galaxy kinematics, galaxy evolution, spiral galaxies, lenticular galaxies, molecular gas

## O-03

### Point defects in semiconductor nanocrystals: EPR spectroscopy

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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.

**Keywords:** EPR spectroscopy, Point defects, Photoluminescence

O-04

**Fourier Transform Infrared Spectroscopy (FT-IR) Coupled with Chemometric Analysis Approach Enables to Determine Temperature and Time Dependent Alterations in The Content of Blood Stain on Cotton Fabric**

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Blood stains, one of the most common body fluids at the crime scene, are often used to determine the identity of the suspect, the event sequence, and the timing of the event. Therefore, the correct age estimation of this stain is really important in forensic cases. Recent studies indicated the potential of Attenuated total reflectance Fourier Transform Infrared Spectroscopy (ATR-FTIR) in the identification and age estimation of bloodstains. However, the effect of temperature on the blood stain age has not been studied yet. The current study was conducted to determine temperature and time-dependent alterations in the blood stain on cotton fabric by ATR-FTIR spectroscopy together with quantitative and multivariate analyses. 200 µl of blood sample was dropped on cotton samples and then were kept at 10°C and 40°C temperature and for 24,48,72 hours and 5,10 days. Their spectra were collected via ATR-FTIR spectroscopy. The spectral analyses were performed in the protein region (1740-1475 cm<sup>-1</sup>). Quantitative spectral analysis indicated the shift in the wavenumber of amide I band and the alterations in the intensity of protein secondary structures (α-helix, aggregated β-sheet and random coil) depending on temperature and time. Unsupervised chemometric analysis demonstrated the successful clustering of the studied groups from each other. These findings prove that ATR-FTIR spectroscopy coupled with chemometric analysis could be efficiently used to determine temperature and time-dependent alterations in the bloodstains.

**Keywords:** ATR-FTIR spectroscopy, Bloodstain, Chemometric analysis, Temperature, Time



## O-05

### Calculation of the Raman and IR Frequencies from the volume data at high pressures in N<sub>2</sub>

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<sup>2</sup>*Faculty of Arts and Science, Physics group, Piri Reis University, 34940, Istanbul-TURKEY*

Raman and IR frequencies of N<sub>2</sub> in the molecular state are calculated as a function of pressure up to 160 GPa by using the volume data from the literature through the mode Grüneisen parameter. By determining the Grüneisen parameters for the lattice modes and vibrons which decrease mostly with increasing pressure from the observed frequency (Raman, IR) and volume data, the Raman and IR frequencies of those modes are calculated at various pressures at room and low temperatures. We find that the Raman and IR frequencies increase as the pressure increases in N<sub>2</sub> as observed experimentally. This method of calculating the Raman and IR frequencies from the volume data can be applied to the some other molecular crystals.

**Keywords:** Raman and IR frequencies, Volume, Mode Grüneisen parameter N<sub>2</sub>

O-06

**Photo-fragmentation of  $H_2^+$  with femtosecond laser pulses by employing a time-sliced 3D imaging technique**

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<sup>5</sup>*Department of Physics, Canakkale Onsekiz Mart University, Canakkale, Turkey*

The photo-fragmentation of  $H_2^+$  was investigated with 800nm, 50fs laser pulses by employing a time slicing 3D imaging technique that enables the simultaneous measurement of all three momentum components, which are linearly related with the pixel position and the slicing time. By experimentally reconstructing the laser-induced photo-fragmentation of  $H_2^+$  with direct measurement of the three-dimensional fragment momentum vector distribution, we show that the employed time-slicing technique allows to register the fragment momentum distribution that reflects the initial molecular states with greater detail, revealing features that were concealed in the full time-integrated distribution on the detector. A series of slices through  $H_2^+$  momentum sphere after photo-dissociation was obtained (Fig.1(a)). The analysis of these slices indicates that the center slice of the time-of-flight distribution (Fig.1(b)) is clearly sharper than the momentum distribution of the full data set, which enables resolving the peaks corresponding to different vibrational states (Fig. 1(c)). Consequently, the full 3D image of the fragment momentum distribution sliced according to the arrival time was obtained (Fig.1(d)). The method is a promising tool for imaging studies of photo-fragmentation of atomic and molecular systems of interest [1].

*This work was supported by the Robert A. Welch Foundation, grant No. A1546 and the Qatar Foundation, grant NPRP 8-735-1-154.*

[1] N. Kaya et. al., Review of Scientific Instruments, 88, 2, 2017, 023104.

**Keywords:** Atomic and molecular physics, ultrafast measurements, molecular photo-fragmentation

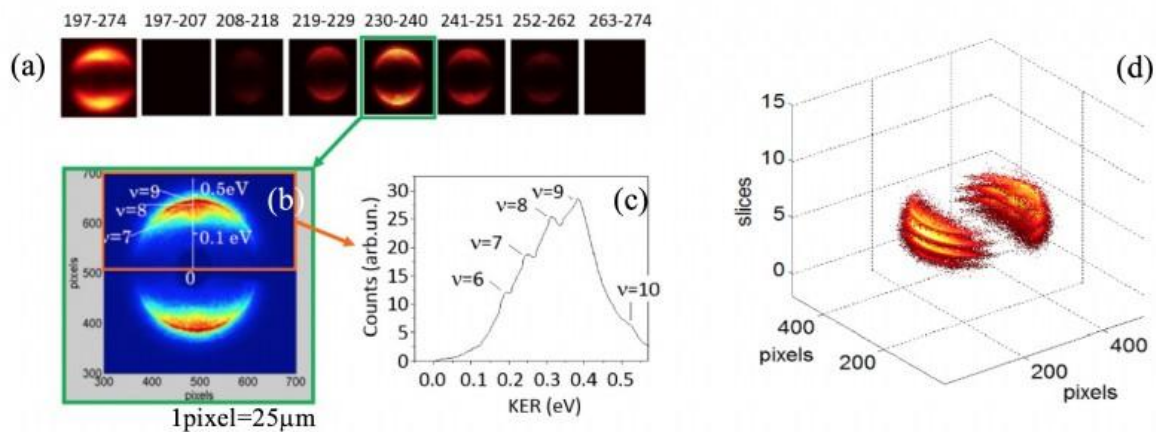


Fig. 1. (a) Series of time slices (10 ns intervals between 197 ns and 274 ns) through the hydrogen molecular ion momentum distribution. (b) The momentum distribution of the center slice (230 ns–240 ns) is clearly sharper than the momentum distribution of the full data set (197 ns–274 ns). (c) KER distribution of H and H<sup>+</sup> fragments, calculated for the apex portion (10 degrees) of the center slice 230–240 ns. The labels  $v = 6 \dots 10$  correspond to peaks due to the most prominent transitions from the vibrational levels of H<sub>2</sub><sup>+</sup>. (d) 3D reconstruction of the fragment momentum distribution consisting of separate slices from photo-dissociation of the hydrogen molecular ions.

O-07

**Crystal Structure and Spectroscopic Properties of Redetermination  
Poly-bis[diaminozinc(II)]fumarato)(tetracyanonickelate)dihydrate**

Zeki Kartal<sup>1</sup>, Cem Cüneyt Ersanlı<sup>2</sup>, Abdülkerim Yavuz<sup>3</sup>

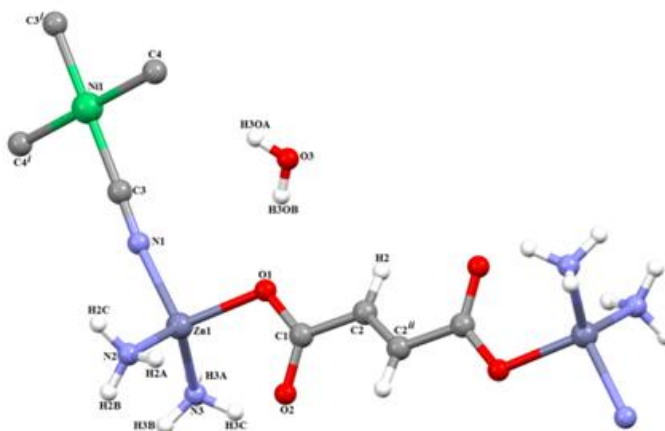
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In the present work; the crystal structure of the title compound,  $C_8H_{18}N_8NiO_6Zn_2$ , has been reinvestigated with improved precision. The title compound was re-synthesized and structurally characterized by vibrational spectral method and single-crystal X-ray diffraction. The structure of the complex consists of a one-dimensional polymeric chain, in which the Zn(II) and Ni(II) ions are linked by CN groups. The Ni(II) ion is four coordinated with four cyanide-carbon atoms in a square planar arrangement and the Zn(II) ions are four coordinated with one cyanide nitrogen atom, two amine nitrogen atoms and one fumarate oxygen atom, in a distorted tetrahedral arrangement. The diffraction data of title compound was collected using MoK $\alpha$  radiation on a Bruker APEX-II CCD diffractometer at 296(2) K. The crystal structure was determined with direct methods and were refined by the full matrix least squares method to  $R = 0.0448$ . The compound crystallizes in the triclinic space group  $P\bar{1}$  with  $a = 6.0575(10)\text{\AA}$ ,  $b = 7.9293(14)\text{\AA}$ ,  $c = 9.5863(16)\text{\AA}$ ,  $\alpha = 85.679(6)^\circ$ ,  $\beta = 81.524(5)^\circ$  and  $\gamma = 85.832(5)^\circ$ . Furthermore, an extensive series of strong N-H...N, N-H...O, O-H...N and O-H...O hydrogen-bonding interactions involving both the complex molecule and water molecule generate a three-dimensional network.

**Keywords:** Cyanide complex, fumarate complex, X-ray; vibrational spectra



**Fig. 1. The molecular structure of poly-bis[diaminozinc(II)]fumarato)(tetracyanonickelate)dihydrate**

## O-08

### Use of spectroscopic methods in construction sector in Turkey

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The history of spectroscopy, defined as the study of the interaction between matter and electromagnetic radiation dates back to older times. With the development of technology, the number of areas in which spectroscopy is used has increased. The construction sector is also one of the sectors benefiting from the spectroscopy. In this study, information was given about the different usage areas of the spectroscopy with many types in the construction area in Turkey, by gathering data from the literature and different sources. Spectroscopy is used in a wide range of fields ranging in construction, such as geology, materials science, archeology, mining and petroleum engineering. Carbon-14 age determination, electrical conductivity and chemical structure of various materials, characterization of composites and reinforcement corrosion can be investigated thanks to spectroscopy.

**Keywords:** Spectroscopy, Spectroscopy in construction, Spectroscopy usage

O-09

**X-ray and quantum chemical investigations of (E)-4-nitro-2-[(5,6,7,8-tetrahydronaphthalen-1-ylimino)methyl]phenol**

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The molecular structure of the title compound, C<sub>17</sub>H<sub>16</sub>N<sub>2</sub>O<sub>3</sub>, was determined by X-ray single crystal diffraction technique. The compound crystallizes in the monoclinic, space group P21/c with unit cell dimensions a=6.0757(4) Å, b= 26.382(2) Å, c= 9.9186(7) Å, β=111.636(5)°, Z=4 and R1=0.053. The molecule is in a phenol-imine form with an intramolecular O–H...N hydrogen bond. Spectroscopic characterization was performed by using experimental FT-IR and UV-Vis. spectroscopic methods. The optimized molecular geometry, vibrational wavenumbers and UV-Vis. absorption wavelengths of the compound have been calculated using the density functional method (DFT) in the ground state and compared with the experimental data. The calculated results show that the optimized geometry can well reproduce the crystal structure. In addition, DFT calculations of the compound, molecular electrostatic potential (MEP), non-linear optical properties (NLO) and frontier molecular orbital calculations were performed at B3LYP/6-311++G(d,p) level of theory.

**Keywords:** X-ray, Spectroscopy, DFT

O-10

The Novel 2,6-Dimethoxyphenoxy Substituted Zinc(II) Phthalocyanine Dyes  
Having High Singlet Oxygen Quantum Yields

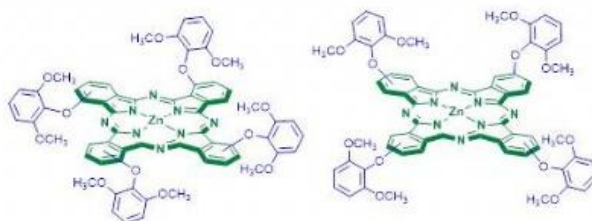
Mehmet Pişkin

*Çanakkale Onsekiz Mart University, Vocational School of Technical Sciences, Department of Food Technology,*

Phthalocyanines (Pcs) show excellent chemical and physical properties. Pcs have found widespread application in various areas including liquid crystals, non-linear optical devices, catalysts, electrochromic and photochromic materials, chemical sensors, data storage systems, organic photovoltaics in solar cells and second generation photosensitizers for photodynamic therapy (PDT)[1]. PDT uses a combination of nontoxic dyes known as photosensitizers (PSs) and harmless visible light leads to the generation of reactive oxygen species. It can damage cellular constituents leading to cell death. Pcs have stronger absorptions in the near-IR region which allows a deeper light penetration into tissues. Pcs fulfil PDT requirements such as high singlet oxygen generation, chemical stability, fast distribution and elimination, activation wavelength ranging from 600 to 800 nm, high photocytotoxicity, and lack of dark toxicity[1]. Especially zinc Pc complexes are often used due to their long triplet lifetimes. The aim of the present research is to produce new, soluble and non-aggregated PDT agents combining two functional materials (phthalocyanines as PSs and 2,6-dimethoxyphenoxy group as a bioactive compound). In this study, the peripherally and non-peripherally 2,6-dimethoxyphenoxy substituted zinc(II) Pcs were synthesized (Fig. 1) and their photophysical and photochemical properties were investigated and in DMF solution.

[1] C.C. Lenzoff, A.B.P. Lever, *Phthalocyanines Properties and Applications*, Vol 3, VCH Publisher, New York 1993.

**Keywords:** Phthalocyanine; 2,6-Dimethoxyphenol; photodynamic therapy, zinc(II).



**Fig. 1. Synthesis of 2,6-dimethoxyphenoxy substituted zinc(II) phthalocyanines**

## O-11

### Investigation by UV Spectrophotometry of Removal Para-Nitrophenol on Raney Alloy

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The adsorption characteristics of several phenolic pollutants on various adsorbents have previously been extensively investigated. In the past years, a number of methods have been devised for degradation, such that pollutant free water can be reused. The methods include biological treatment, chemical oxidation, electrochemical decomposition, photocatalytic and chemical coagulation [1], physical and physico-chemical treatment [2].

In the present work, the sonochemical degradation of p-nitrophenol (p-Nph) has been made. The cavitation technique is the basic phenomenon in sonochemistry. Cavitation is a natural phenomenon based on low ultrasonic waves. Ultrasonic waves create air bubbles that grow in the liquid and explode at a certain magnitude. The energy of the least heat effect and the pressure wave which has the greatest effect are released. In this study, solutions of p-Nph at initial concentrations of 40,50 and 75 ppm have been used. 50%Al–50%Ni raney alloy (100 mg) was suspended in deionized water and sonicated with Bandelin Sonoplus homogenizers HD2070 MS 97% (Fig. 1) for 15 minute.

Then, p-Nph (40,50,75 ppm) has been added to the preactivated alloy. The reaction mixture has been sonicated for 15,30 and 45 minutes at 30°C. The concentration of p-Nph in the solution after adsorption at different times has been determined by Uv-visible spectrophotometer. For 40 ppm, the percentage of removal of para nitrophenol by Ni-Al alloy has been found to be 98% after 45 minutes. Adsorption isotherm type L has been found for Ni-Al alloy.

[1] A.K. Moawad, R. Abdel Wahaab, Enas Abou Taleb, World Applied Sciences Journal, 8,2010,462-469.

[2] Iordache Ioan, Toedor Mircea Nechita, Rosca Ioan, Aelenei Nicolae, Turkish J. Eng. Env. Sci.,28, 2004, 377-380.

**Keywords:** sonochemistry, para nitrophenol, Ni-Al alloy



Fig. 1 Bandelin Sonoplus homogenizers HD2070



O-12

## Synthesis, Characterization, and Determination of Sorption Properties of Silica Gel-Immobilized Schiff Base Derivative For Removal of Co(II) Ions From Aqueous Solution

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The contamination by heavy metal pollutants in water sources is an important environmental concern. Generally, heavy metal ions are toxic, non-biodegradable, and tend to be accumulated in the human vital organs, where they can act progressively over a long period through food chains. In this study, a new alternative sorbent for removal of Co(II) ions from aqueous solution was prepared and then the adsorption capabilities of this prepared sorbent was investigated. The novel sorbent was prepared by chemically immobilizing Schiff base derivative benzaldehyde 5-aminoisophthaloylhydrazine (BAH) onto silica gel surface previously modified with silylant agent 3-chloropropyltrimethoxysilane (CPTS). The present investigation is focused on the thermodynamic investigation and interaction of divalent Co with modified silica gel. The immobilization reaction was confirmed through elemental analysis and Fourier transform infrared spectroscopy. The sorption experiments were performed according to the batch method. The effects of solution pH and temperature on the sorption were obtained by using the batch method. In addition, the sorption characteristics and thermodynamic properties of this novel modified sorbent were separately determined.

**Keywords:** Modified silica gel, Hydrazone derivative, Heavy metal, Adsorption

[1] C.C. Lenzoff, A.B.P. Lever, Phytholocyanides Properties and Applications, Vol 3, VCH Publisher, New York 1993.

O-13

Synthesis, characterization, spectroscopic properties of novel quite soluble tetrakis -substituted phthalocyaninato lead

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Phthalocyanines (Pcs) are composed of 18  $\pi$ -electron conjugated macrocyclic compounds, and their derivatives generally are non-toxic. They have very good structural chemical stability and delocalization of electrons in 18- $\pi$  electron system[1]. Because of these important features. phthalocyanines are used in many areas from medicine to electronics. The electrochemical and spectroscopic properties can be altered by changing the metal center. The other way to tune the properties of phthalocyanines is to introduce different kinds of substituents onto the peripheral and non-peripheral positions of the phthalocyanine ring. Particularly, the optical, electrochemical and spectroscopic properties of phthalocyanines can be significantly altered by incorporating substituents at the non-peripheral positions. They are also the presence of a highly conjugated 18  $\pi$ -electron system, intense absorption in the red/near-IR (Q band) region, capability to exhibit changeable conductivity and photocatalytic effects. The significant aim of the present research was to synthesize (Fig. 1) non-aggregated, highly soluble and capable of long wavelength absorption maximum non-peripheral and peripheral substituted lead(II) (PbPcs) phthalocyanine complexes (3 and 4 in Fig. 1) to investigate the effects of non-peripheral or peripheral substituent on their spectroscopic, photochemical and photophysical properties for the PbPcs.

[1] C.C. Lenzoff, A.B.P. Lever, Phthalocyanides properties and applications, Vol. 3, VCH Publisher, New York 1993.

**Keywords:** Lead(II); phthalocyanine; soluble, photochemical, spectroscopic.

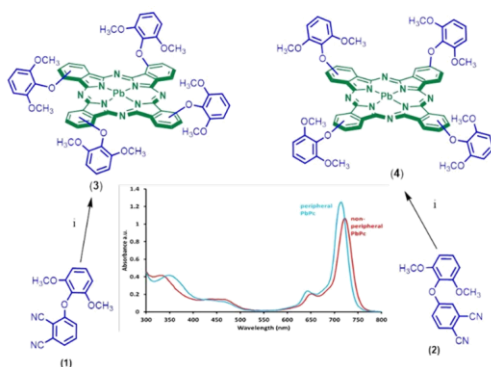


Fig. 1. Synthesis of non-peripherally and peripherally substituted lead(II) phthalocyanines (3 and 4). Reagents and conditions: (i) N<sub>2</sub>, PbO, DMF, DBU, 360° C, 25 min.

O-14

**Experimental and ab initio DFT analysis of structural and spectroscopic features of Nitroterephthalic acid, and computational insights into its molecular interactions with estrogen receptor alpha**

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It has become clear that exposure to the ubiquitous xenoestrogens such as bisphenol A and methyl paraben are the first line causatives for human breast cancer. Terephthalic acid (TPA), which is the major chemical constituent in the synthesis of polyethylene terephthalate (PET), also shown to have carcinogenic effects. Nitroterephthalic acid (NTPA) modified polyethylene glycol (PEG) polymers are also produced, however little known about the reactive nature of NTPA especially in terms of its interactions with estrogen receptors. Therefore, this study focuses on the investigation of structural and spectroscopic behaviors of NTPA through experimental and theoretical methods, and the exploration of interactions with estrogen receptor alpha in comparison with that of benzoic acid, phthalic acid, and TPA by using molecular docking methodology. Essential quantum descriptors obtained for NTPA include electrostatic potential surface, electrophilicity and nucleophilicity from Fukui analysis, aromaticity indexes from nuclear independent chemical shift (NICS) analysis, dipole moment and polarizability tensors, and electronic properties like band gap and ionization potentials from population analysis. Infrared, Raman, and UV spectra are presented both experimentally and via ab initio density functional theory calculations obtained at the B3LYP 6-311++G(d,p) level of theory. Ligand-enzyme interactions were discussed within a dependency on the structural variations in four ligands in docking analysis (Fig. 1). NTPA was found to behave like phthalic acid and highly rich in terms of conformations in monomeric and dimeric structures.

**Keywords:** Nitroterephthalic acid, Vibrational Spectroscopy, UV, DFT, Estrogen receptor alpha, Molecular docking

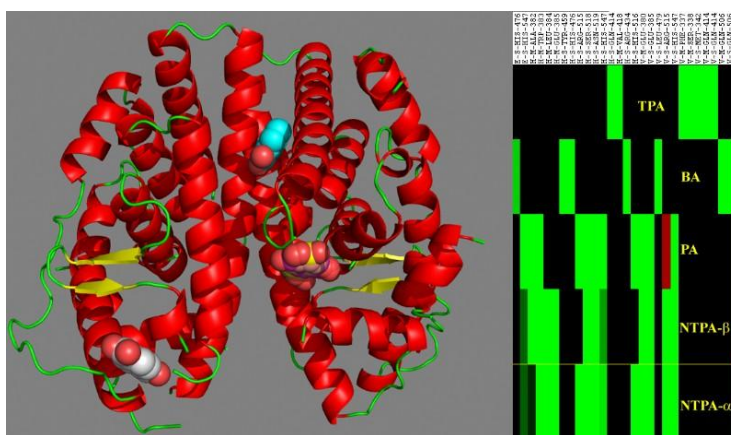


Fig. 1. Molecular docking situations and interaction profiles of BA, PA, TPA, and NTPA in ER(alpha)

O-15

**Effect of Metal Oxide Semiconductors on the Photocatalytic Degradation of  
4-Nitrophenol**

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<sup>2</sup>*Istanbul University, Engineering Faculty, Chemistry Department, Istanbul, Turkey*

During the past decade, various catalytic techniques have been investigated to solve the increasingly serious environmental pollution problems. Heterogeneous photocatalysis [1–3] has shown a high efficiency in the photooxidation of many organic pollutants present in air.

In this study, some oxide (TiO<sub>2</sub>, ZnO, ZrO<sub>2</sub>, Bi<sub>2</sub>O<sub>3</sub>) semiconductors were successfully prepared coprecipitation method. The nanoparticles were analyzed by XRD, DRS, FT-IR, SEM and BET techniques. The concentration of 4-nitrophenol was analysed by UV-Vis Spectrophotometer.

The photocatalytic activities of the catalysts were evaluated for the degradation of 4-nitrophenol under Hg lamp irradiation. Bi<sub>2</sub>O<sub>3</sub> exhibited much higher photocatalytic activity than other metal oxide. It is concluded that the optical and electronic properties of semiconductors remarkably affected the photocatalytic activity.

**Keywords:** 4-nitrophenol, degradation, semiconductor, metal oxide, characterization

O-16

**Analytical evaluation of Holtsmark distribution of energies and its role in plasma microfields**

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The distribution of electric microfields influences many elementary processes in plasma as well as governs a number of its optic properties. It is well known that the Holtsmark distribution was first used for plasma microfields. Because the stars are consisting of plasmas, the Holtsmark distribution may give valuable information to the astrophysicists. With this spirit in mind, we have proposed an analytical expression for the calculation of Holtsmark distribution. The obtained results show that our approximation is in good agreement with literature data. The proposed method can be easily applied in plasma physical and astrophysical studies.

**Keywords:** Holtsmark distribution, plasma microfields, microfield calculations

**NOT ATTENDED**

O-17

**New 1,3,4- Thiadiazoles Derived from Azo Dyes: Synthesis and Characterization of Structures By Several Spectroscopic Methods**

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Among the different five membered heterocyclic compounds, 1,3,4-thiadiazoles and its derivatives have been constituted an important class of heterocyclic compounds because of biological activities. 2,5-disubstitute-1,3,4-thiadiazoles have significantly remarked due to several biological properties such as antibacterial, antienflamatuar, antifungal, anti-tubercular, antiviral, antioxidant, antitumoral, antinflammator and anticonvulsant. Furthermore, recently, they had implementations of hypertension, schizophreria, HIV infection bacterial DNA gyrase B inhibitor as well.

In this study, 1,3,4- thiadiazole derivatives were synthesized from different heterocyclic azo dyes (Fig. 1). The synthesized compounds were characterized by using several spectroscopic methods.

**Keywords:** 1,3,4-thiadiazole, azo dyes, heterocyclic.

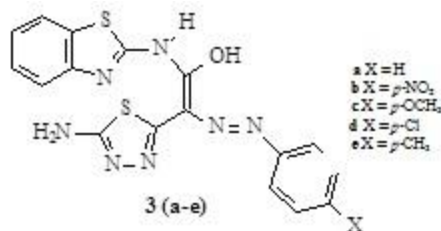


Fig. 1. General structure of synthesized compounds

O-18

**Synthesis of New Disazo Dyes Derived from 2,4-Dihydroxyquinoline and Characterization of structures by spectroscopic methods**

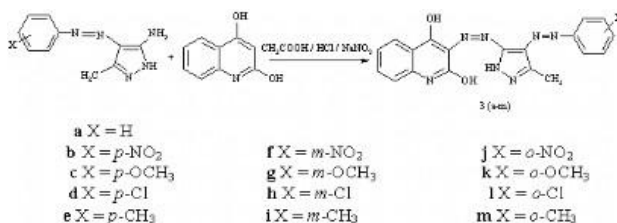
Nesrin Şener, Hassan Jaballah Mohammed

*Kastamonu University, Department of Chemistry, Kastamonu, Turkey*

Azo dyes are important class of organic colorants consists of at least a conjugated chromophore azo (-N=N-) group and the largest and most versatile class of dyes. This chromophoric system is associated with two or more aromatic or heterocyclic rings. Heterocyclic compounds are extensively used in non-linear optical systems, photodynamic therapies and lasers in textiles. Also, azo benzene derivatives are frequently used in inkjet printers, as coloring agents in foods, and in electrooptic devices due to their pharmacological and microbiological properties.

In this study, synthesis of disazo 2,4-quinolindiol derivatives which are not included in the literature were performed (Fig. 1). The synthesized compounds were characterized by using spectroscopic methods such as FT-IR and <sup>1</sup>H-NMR.

**Keywords:** Heterocyclic, disazo dyes, 2,4-dihydroxyquinoline



**Fig. 1. General synthesis of compounds**

O-19

**Experimental and Theoretical Studies of bis1-[[p-phenxyphenylimino]methylenyl]-2-naphthalenolato-N,OCopper Complex**

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<sup>3</sup>Ondokuz Mayıs University, Faculty of Arts and Sciences, Department of Chemistry, 55139 Samsun, Turkey

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Over the past 25 years, extensive research has surrounded the synthesis and use of Schiff base compounds in organic and inorganic chemistry, as they have important medicinal and pharmaceutical applications. These compounds show biological activities including antibacterial, antifungal, anticancer and herbicidal activities. Furthermore, Schiff bases are utilized as starting materials in the synthesis of compounds of industrial and biological interest. Schiff bases are also becoming increasingly important in the dye and plastic industries as well as for liquid-crystal technology and mechanistic investigation of investigation of drugs used in pharmacology and biochemistry. Schiff base ligands consist of a variety of substituents with different electron-donating and electron-withdrawing groups, and therefore may exhibit interesting electron-chemical properties. The Schiff base compounds have been also under investigation during last years because of their potential applicability in optical communications and many of them have nonlinear optical (NLO) behavior.

In this work, we report a combined experimental and theoretical study on molecular structure, vibrational spectra and electronic absorption spectra of the bis1-[[p-phenxyphenylimino]methylenyl]-2-naphthalenolato-N,OCopper. The FT-IR spectra of the compound have been recorded at 4000-400  $\text{cm}^{-1}$  region. The compound crystallizes in the noncentrosymmetric space group of monoclinic system. The optimized structure and vibrational wavenumbers have been calculated by using density functional method (B3LYP) with LANL2DZ basis set. The obtained vibrational wavenumbers and optimized geometric parameters were seen to be in good agreement with the experimental data. In addition, DFT calculations of the title compound, mulliken charges, molecular electrostatic potential, frontier orbitals were also performed at B3LYP/LANL2DZ level of theory.

**Keywords:** Schiff Base, FT-IR, DFT.



O-20

**Experimental and Theoretical Investigation on Tautomeric Rates of  
Quinolone–Hydroxyquinoline in 4-Hydroxyquinoline-2,3-dicarboxylates**

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4-Quinolones that is a tautomeric form of 4-hydroxyquinolines comprise an important class of synthetic antibiotics used in the treatment of various infectious diseases having respiratory tract, urinary tract, gastrointestinal and skin infections, and sexually transmitted disease. In the present study, 4-hydroxyquinoline-2,3-dicarboxylates were first synthesized by the reaction of N-(2-aminobenzoyl)benzotriazole with dimethyl acetylenedicarboxylate in the absent of base catalyst. Then, the tautomeric rates of quinolone-hydroxyquinoline in 4-hydroxyquinoline-2,3-dicarboxylates were investigated by <sup>1</sup>H NMR in CDCl<sub>3</sub>, DMSO-d<sub>6</sub> and CD<sub>3</sub>OD. The stabilization energies, reactivities and spectroscopic properties of possible tautomers were calculated theoretically. The theoretical calculations were carried out in vacuum and mentioned solvents by DFT-B3LYP method 6-31 G (d,p) basis set in Gaussian 09. The experimental and the calculated spectroscopic data were compared. Last, the availability of used theoretical method and the basis set were discussed

**Keywords:** 4-Hydroxyquinoline-2,3-dicarboxylates, quinolone, hydroxyquinoline, tautomerism.

## O-21

### Electron spin resonance identification of gamma irradiated 2,4'-dichlorodiphenyl dichloroethane and 6-mercaptoporine monohydrate in the solid state

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The purpose of this study was to study the effects of ionizing radiation on two anticancer drugs, 2,4'-dichlorodiphenyl dichloroethane and 6-mercaptoporine monohydrate, by using electron spin resonance (ESR) spectroscopy. The intensity of ESR signals of the samples as a function of the microwave power was investigated in the range of 0.01-100 mW at room temperature. While unirradiated samples presented no ESR signal, irradiated samples exhibited significant ESR spectra. ESR measurements were performed at low and high temperatures to study the dosimetric features of free radicals induced by gamma irradiation. In order to obtain the dose-response curves, samples irradiated with gamma at 1,5,10,15, 20 and 25 kGy dose values were used. The g values of the radicals and the hyperfine coupling constants were also determined. Additionally the time dependency of the samples was analysed to study the stability of the radicals.

**Keywords:** EPR, Free radicals,  $\gamma$ -irradiation.

O-22

**Determination of force-free wet adhesion of DOPA-PEG conjugates to spin labeled nanobeads: An ESR study**

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It is well known that synthetic adhesives lose their ability to adhere in aqueous media. Therefore, wet adhesives are desirable for every application where water is present. Marine mussels living in water has become the inspiration for the development of wet adhesives. Adhesive proteins called as mussel foot proteins (Mfps) can stick on versatile surfaces; ships, rocks and even polymeric materials like teflon, etc. All Mfps are containing posttranslationally modified 3,4-dihydroxyphenylalanine (DOPA) amino acids which plays a critical role in the adhesion of Mfps to wet surfaces as well as in the cohesions between Mfps.

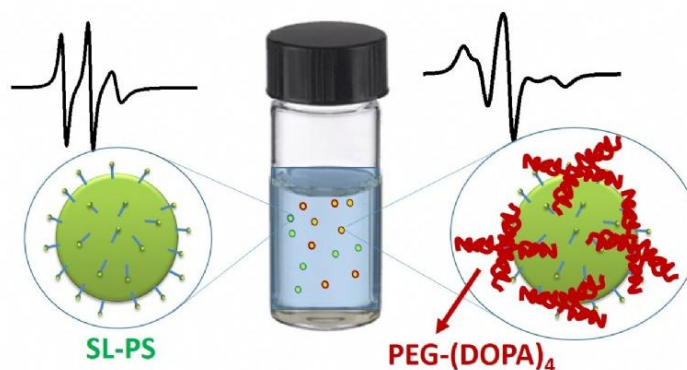
Here, we studied adhesion properties of mussel inspired DOPA containing synthetic polymers by Electron Spin Resonance (ESR) spectroscopy. Therefore, we synthesized 4-armed PEG polymers end functionalized with DOPA groups (PEG-(DOPA)<sub>4</sub>). In addition, we obtained hydrogels from PEG-(DOPA)<sub>4</sub> via crosslinking in the presence of oxidizing agents. As model surfaces, we prepared spin labeled suspended polystyrene and silica nanobeads. Using ESR spectroscopy, we detected spontaneous (without applying any force) adhesion of DOPA containing polymers and gels to suspended spin labeled hydrophobic polystyrene nanobeads at molecular level (Fig. 1). The surface coverage up to 82% is obtained from ESR measurements. However, in the force-free condition, ESR measurements do not show any detectable DOPA based adhesion to hydrophilic silica nanobead [1, 2].

*This work was financially supported by Tübitak via 3501 Program under grant 114Z318.*

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**Keywords:** ESR spectroscopy, adhesion, DOPA, hydration layers.



**Fig. 1. Schematic representations of PEG-(DOPA)<sub>4</sub> adhesion to SL-PS and its characterization by ESR.**

O-23

**Identification of gamma irradiated *Elaeagnus Angustifolia* by electron spin resonance spectroscopy**

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Electron Spin Resonance (ESR) investigation on gamma irradiated *Elaeagnus angustifolia* was carried out in the dose range of 0.5–10 kGy. Skin parts of *elaegnus* were separated from white inner part and skin parts were used for ESR measurements. Unirradiated *elaegnus* samples exhibit one singlet ESR signal centered at 2.0032. Besides this singlet signal, two weak satellite signals situated about 3 mT left and right of it in the spectra which recorded using irradiated samples. This is cellulose-like ESR spectrum typical for irradiated plants. The dose-response curve constructed by using left satellite cellulose signal ( $g=2.0206$ ) and it has been best fitted by a linear function. Variable temperature and fading studies at room temperature showed that the radiation-induced radicals in *elaegnus* samples are very sensitive to temperature. The present work also explores the possibility to identify irradiated *elaegnus* by the relaxation characteristics and thermal behaviour of the radicals. This work reports the first results obtained by the ESR technique on *elaegnus* samples. Results suggest that the analysis of ESR spectrum in *elaegnus* samples can be used to evaluate the gamma treatment of *elaegnus*.

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**Keywords:** Food irradiation, *elaegnus angustifolia*, gamma-irradiation, Electron Spin Resonance.

O-24

**Novel one pot synthesis of thiazolo[3,2-a]pyrimidin and pyrimido [2,1-b][1,3]thiazin compounds**

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The 5-benzoyl-6-phenyl-4-(4-methylthiophenyl)-1,2,3,4-tetrahydro-2-thioxopyrimidine (1) have been prepared via Biginelli cyclocondensation reaction. The starting compound 1 was cyclized with various bromo compounds to the thiazolopyrimidine 2 and pyrimido[2,3-b]thiazine 3 derivatives (Fig. 1), in approximately 55–78% yields. The purpose of synthesizing the thioxopyrimidine derivatives is because of the high biological activities. All of these derivatives have been characterized by analytical and spectroscopic studies and the reaction mechanism is discussed.

**Keywords:** Thiazol, Thiazin, Synthesis

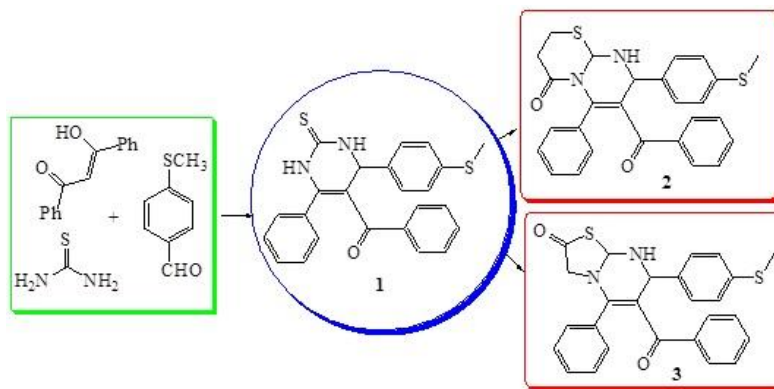


Fig. 1. Synthesis of compound 1-2

O-25

**Computational Studies on The Molecular Structure, Vibrational and Conformational Analysis of 2-Methoxypyridine-3-Boronic Acid and 6-Substituted-2-Methoxypyridine-3-Boronic Acid Derivatives**

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Pyridylboronic acids and their derivatives have aroused growing interest because of their important applications such as; material science, supra-molecular chemistry, analytical chemistry, medicine, biology, catalysis, crystal engineering and organic synthesis. In this study, ab initio Hartree-Fock (HF) and Density Functional Theory (DFT), using B3LYP functional, calculations have been performed to characterize the ground state geometrical energy, vibrational frequencies, the dipole moment ( $\mu$ ), mean polarizability ( $\alpha$ ), the total first static hyperpolarizability ( $\beta$ ) of 2-Methoxypyridine-3-boronic acid (I), 6- Fluoro-2-methoxypyridine-3-boronic acid (II) and 6- Chloro -2-methoxypyridine-3-boronic acid (III) molecules using the 6-311++G (d, p) basis set. <sup>1</sup>H NMR and <sup>13</sup>C NMR chemical shifts calculations have been performed by using the both models, where the various basis sets were employed. Also, EHOMO (the highest occupied molecular orbital energy), ELUMO (the lowest unoccupied molecular orbital energy), HOMO-LUMO energy gap ( $\Delta E_g$ ), the dipole moment ( $\mu$ ), mean polarizability ( $\alpha$ ) and the total first static hyperpolarizability ( $\beta$ ) are investigated as a function of the torsional angle, for each molecule. The dipole moment for I, II, and III molecules are calculated at 1.17, 1.19 and 1.25 with DFT/B3LYP level of the theory 6-311++G (d, p) basis set and at the HF/6-311++ G (d, p) 1.17, 1.16 and 1.29 Debye, respectively. Structure parameters such as bond lengths, bond and dihedral angles of the studied molecules compared data in literature. All computational studies have been performed with the Gaussian 09W program package.

**Keywords:** 2-Methoxypyridine-3-boronic acid, hyperpolarizability, HOMO-LUMO energy gap

O-26

Synthesis, Characterization of Novel Some Schiff Base Ligands Derived From 4-aminoantipyrine

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Schiff bases and their complexes are widely studied because of the increasing recognition of their role in biological systems. In azomethine derivatives, the C=N linkage is essential for biological activity; several azomethines were reported to possess remarkable antibacterial and antifungal, anticancer. With the increasing incidence of deep mycosis, there has been increasing emphasis on the screening of new and more effective antimicrobial drugs with low toxicity. These compounds were recently found to have significant antitumor and biological activity. Antipyrine derivatives are reported to exhibit analgesic and anti-inflammatory effects, antiviral, antibacterial, and herbicidal activities, and have also been used as hair color additives and to potentiate the local anesthetic effect of Lidocaine. Transition metal complexes with ligands derived from 4-aminoantipyrine have significant biological activity. This prompted us to synthesize a new series of heterocyclic Schiff bases containing the antipyrinyl moiety. The present study reports synthesis and characterization of Schiff bases derived from 1-phenyl-2,3-dimethyl-4-(N-2 hydroxybenzylidene)-3-pyrazolin-5-one and 1-phenyl-2,3-dimethyl-4-(N-2 hydroxynaphthylidene)-3-pyrazolin-5-one with 5-aminoisophthalic acid (Fig. 1). These compounds were synthesized in high yield and characterized by SEM, FT-IR, <sup>1</sup>H NMR and <sup>13</sup>C NMR.

**Keywords:** Schiff bases, 4-aminoantipyrine, Azomethine derivatives, Characterization, NMR

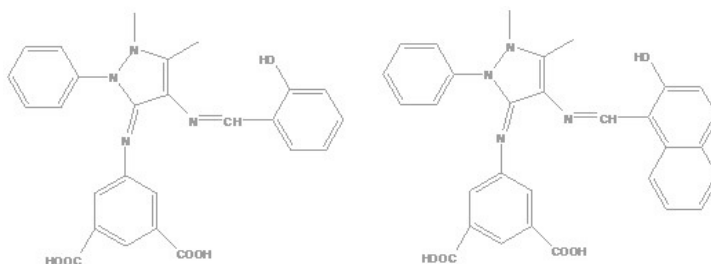


Fig. 1. Chemical structures of Schiff base derivatives

Schiff bases derived from 1-phenyl-2,3-dimethyl-4-(N-2 hydroxybenzylidene)-3-pyrazolin-5-one and 1-phenyl-2,3-dimethyl-4-(N-2 hydroxynaphthylidene)-3-pyrazolin-5-one with 5-aminoisophthalic acid

O-27

**Investigation of Obesity Induced Type 2 Diabetes Dependent Molecular Alterations and Therapeutic Effect of Palmitoleic Acid on These Alterations in Adipose Tissue by Fourier Transform Infrared Microspectroscopy**

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Fundamental investigations on obesity and obesity related type 2 diabetes which are common diseases nowadays are so important for therapeutic studies in future. In the light of this information, it was aimed to investigate the structural and compositional alterations in adipose tissue caused by obesity related type 2 diabetes and also the therapeutic effect of palmitoleic acid (PA) on these alterations was performed by examining its potential of reversing effect.

Obesity is especially characterized by adipocyte hypertrophy, the expansion of visceral (VAT) and subcutaneous (SCAT) adipose tissue mass in the body, and alterations in cellular biology. The increase in the expansion of VAT and SCAT mass is the main reason of obesity and mostly this process results in disturbed glucose and lipid metabolism. Since VAT and SCAT have a critical role in obesity related type 2 diabetes, these two types adipose tissues were used in the present work. The molecular alterations in the concentration and composition of adipose tissue arising from obesity related type 2 diabetes were investigated by Fourier transform infrared (FTIR) microspectroscopy. Afterwards, the current study which reveals the potential of PA as an anti-obesity and anti-diabetic drug is carried out by the same technique.

The results of the current study revealed that obesity and type 2 diabetes caused some alterations in molecular composition in adipose tissue as an increased lipid/protein ratio, an increased carbonyl/lipid ratio and a decreased unsaturated/saturated lipid ratio. However, our results indicated that the PA shows a therapeutic effect on body weight, glucose and insulin levels in diabetic mice. On the other hand, FTIR microspectroscopy confirmed that the PA has a reversing effect on these destructive alterations of obesity and type 2 diabetes in adipose tissue.

**Keywords:** Obesity, Type 2 Diabetes, Adipose Tissue, FTIR Microspectroscopy, Palmitoleic Acid



O-28

## Protein Therapeutics Structural Attributes Are Critical For Developing Effective Biopharmaceutical Product

Fatma Alazzam

*Technopharmasphere*

Proteins are composed of amino acid chains fold into higher order structures called 3-dimensional structures. Amino acids are joined together by specific order into a chain by peptide bond to form the first structural attribute called primary structure. The side chains of amino acids form hydrogen bonds to have 3-dimensional local conformations called secondary structures such as  $\alpha$ -helix,  $\beta$ -sheet, turns, and loops. These structural moieties form various bonds to form tertiary and Quaternary structures [1]. In Biopharm industry the amino acid sequence is referred to as primary protein structures, while other structures are referred to as higher order structures (HOS).

Therapeutic proteins have complex structures, which possess inherent chemical and physical instabilities. The loss of structural integrity can be detrimental on safety and efficacy of biopharmaceutics [2]. Therefore, it is essential to maintain the native structure of protein therapeutics throughout manufacturing, storage, and delivery to patients to ensure safety, potency, and efficacy. One should establish a strategy with cutting edge technologies to monitor the structure of biopharmaceutical products including various mathematical and statistical approaches to quantitatively measure protein primary and higher order structures and characterize particles of various sizes [3, 4].

Molecular mass, net charge, primary structure, higher order structures, carbohydrate moieties are among the protein therapeutics structural attributes that need to be monitored. Criticality of product quality attributes is typically assessed during the product development phases and ultimately critical quality attributes are monitored to characterize or release batches during manufacturing. FTIR, DSC, MS, CD, Raman, ROA, PROFILE NMR, 2-dimensional NMR, and flow imaging technologies are commonly used technologies for characterization and comparability of biopharm products.

In conclusion, understanding of structural attributes of proteins, is critical to design effective pharmaceutical candidate and successfully develop protein therapeutics. In this oral presentation, we will review technologies used in biopharmaceutical product development.

*Acknowledgments: We would like to thank Dr. Rina Dukor and Dr. Laurence A. Nafie (Biotools Inc., USA), Muhammet Demir and Erdinc Demirci (Bentley-MERKIM, MERKIM, Turkey), and all team members involved in this scientific project for their support.*

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**Keywords:** Protein Therapeutics, Structural Attributes, Biopharmaceutical Development

**O-29**

**Advanced Vibrational Spectroscopy For Structure Elucidation Of Chiral and Biological Molecules**

Rina Dukor

*Biotools Inc.*

**Keywords:** Vibrational Spectroscopy, Chiral molecules, Biological Molecules

## O-30

### A Multi-Technique Approach to the Study of Hydantoins

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Hydantoins have remarkable interest from the chemical and biological perspectives, and they have also been shown to receive widespread applications in medicine, agriculture and chemical industry. They have been clinically used as antiepileptic and antibacterial drugs and for cancer and AIDS treatments. They are also used currently as herbicides and fungicides.

In this talk, I will present recent data on a series of simple hydantoins (the parent hydantoin, and its 1-methyl, 5-methyl and 5-acetic acid derivatives), obtained using a multi-technique approach that allowed characterizing the single molecules of these compounds in relation to their structure, vibrational spectra and photochemistry, and also to determine the spectroscopic and thermal properties of their neat condensed phases (with emphasis given to polymorphism).

The main technique used for the structural, vibrational and photochemical characterization of the isolated molecules was matrix isolation infrared spectroscopy, complemented by up-to-date quantum chemical calculations, including the natural bond orbital (NBO) and atoms in molecules (AIM) theories. For the investigation of the condensed phases, differential scanning calorimetry (DSC), polarized-light thermomicroscopy (PLTM), X-ray diffraction (XRD; both for single crystals and powders), and infrared and Raman spectroscopies (in the latter case, including single crystal measurements) were used.

The used multidisciplinary methodology allowed to attain a considerably broad understanding of the structural, vibrational, photochemical and thermal properties of the hydantoin moiety, which may be seen as a gateway for assessing the properties, reactivity and biological activity of this type of compounds.

*Acknowledgements: Project PTDC/QEQ-QFI/3284/2014 – POCI-01-0145-FEDER-016617, funded by FCT (Portugal) and FEDER/COMPETE 2020-EU, and the CQC and CFisUC Research Centres (Projects UI0313/QUI/2013 and UID/FIS/04564/2016, also co-funded by FEDER/COMPETE 2020-EU) are acknowledge for financial support.*

**Keywords:** Hydantoins, Structural, Vibrational, Photochemical and Thermal Properties, Polymorphism.

O-31

**Synthesis of some new 1,3,4-thiadiazole compounds derived from 3,4-(methylenedioxy) cinnamic acid and Characterization of structures by spectroscopic methods**

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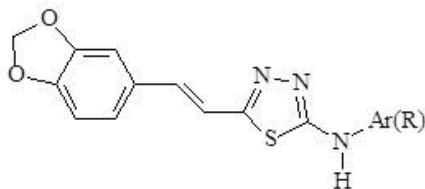
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It was synthesized some new 1,3,4-thiadiazole compounds (Fig. 1) derived from 3,4-(methylenedioxy) cinnamic acid in this study. The structures of synthesized compounds were illuminated by using spectroscopic methods such as UV-Vis, IR, <sup>1</sup>H-NMR and <sup>13</sup>C-NMR spectroscopies. Moreover, antibacterial activities of new 1,3,4-thiadiazole derivatives were tested against gram negative bacteria (*Salmonella enteritidis*, *Salmonella typhimurium*, *Enterobacter aerogenes*, *Salmonella infantis*, *Salmonella kentucky*, *Escherichia coli*) and gram positive bacteria (*Staphylococcus aureus*, *Bacillus subtilis*, *Enterococcus durans*) by using disk diffusion method. Furthermore, antifungal activity experiment was carried out against *Candida albicans* by using disk diffusion method. The synthesized compounds (5, 7, 10, 13 and 14) showed antibacterial activity against *S. aureus*. Also, the synthesized compound (8) showed antibacterial activity against *E. coli* as 8, 9 mm inhibition zone using 50, 80 µL. The compound (9) showed antibacterial activity against *E. aerogenes* as 12 mm inhibition zone using 80 µL. The compound (13) showed antibacterial activity against *S. kentucky* about 9 mm inhibition zone using 80 µL. And also, the compound (7) showed antibacterial activity against *E. durans* as 7, 7 and 8 mm inhibition zone using 30, 50 and 80 µL. Compounds (1-15) did not show antifungal activity against *C. albicans*. The results showed that the some synthesized compounds could be used as a potential source of antibacterial agents.

**Keywords:** 1,3,4-Thiadiazole, antimicrobial activity, IR and NMR spectroscopies



Ar(R): phenyl-, benzyl-, 2-phenylethyl-, 2,4-dichlorophenyl-, 2-ethylphenyl-, 4-nitrophenyl, 2-(methoxycarbonyl)phenyl-, ortho-, meta- and para- chlorophenyl-, ortho-, meta- and para- fluorophenyl-, ortho-, meta- and para- methoxyphenyl-

**Fig. 1. General structure of synthesized 1,3,4-thiadiazole compound**

## O-32

### The Analysis of Crystal Structure and Spectroscopic datas of the (2E,6E)-2,6 bis((E)-3 phenylallylidene)cyclohexanone with XRD and Gama Irradiated Effect

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Chalcones (1,3-diaryl-2-propen-1-ones), have a framework, where two aromatic rings are linked by the a three carbon  $\alpha,\beta$ -unsaturated carbonyl system [1]. Chalcones exhibit numerous physical and biological properties, for instance optical and fluorescence properties, dielectric properties, antioxidant and soybean lipoxygenase inhibitory activity, antimicrobial activity, anti-HIV activity, antibacterial activity, anti-inflammatory and anti-cancer activities [2]. Chalcones also represent one of the largest classes of plant metabolites and are important precursors in the biosynthesis of flavonoids and related compounds that play major role in the plant defense mechanism [3].

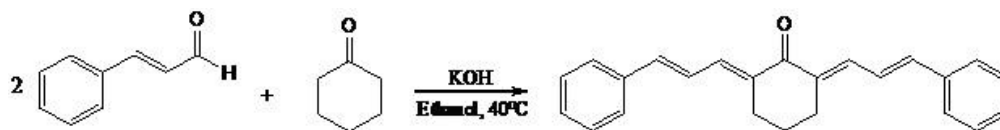
A bis (chalcone) (2E, 6E)-2,6-bis((E)-3phenylallylidene) cyclohexanone (Scheme 1) was characterized by <sup>1</sup>H NMR, <sup>13</sup>C NMR, FT-IR, UV-vis spectroscopy and single crystal X-ray structural analysis. The compound was gama-irradiated using <sup>60</sup>Co gamma-ray source. The crystal structure of the compound was investigated by single crystal X-ray diffraction (Fig. 1). The structure exhibits an weak C-H..O intramolecular and strong bifurcate intermolecular hydrogen bonds. The crystal packing is stabilised by strong intermolecular bifurcate C-H..O hydrogen bonds and  $\pi\cdots\pi$  stacking interactions. The irradiation of the single crystal does not change the geometry of the crystal and changes unit cell parameters, lattice constants, unit cell volume and density due to to a distortion of the crystal structure. Effect of gama irradiation on sample were investigated through FT- IR, UV-vis and NMR spectroscopy. These spectral studies specified structural changes after gama irradiation. No new peaks were observed in the IR spectrum of the irradiated sample, but a decrease in the intensity of most characteristic bands was recorded. In the UV-vis spectrum, irradiation can induce perturbation of energy levels as well as deformity in the molecule.

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**Keywords:** Chalcones, XRD, NMR, F-TIR, gama-ray irradiated



Scheme 1. Ortep drawing of the molecular structure of the bis(chalcone) derivative.

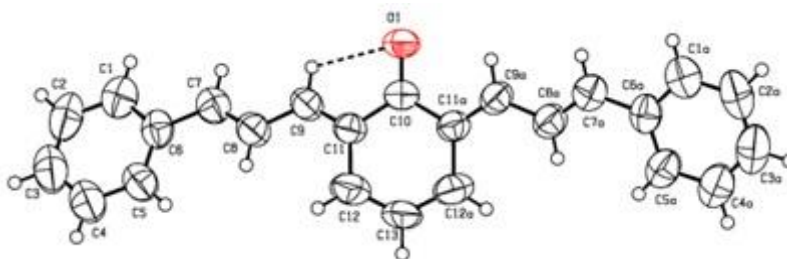


Fig. 1. Synthesis procedure for title compound.

O-33

**Spectroscopic Applications To W UMa Type Eclipsing Binary BO Ari**

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This study represents an analysis of new spectroscopic observations of the eclipsing binary star BO Ari. The medium resolution ( $R \sim 10000$ ) spectroscopic observations of the system were made at Dominion Astrophysical Observatory (DAO) in Victoria, B.C. Canada by using the Cassegrain spectrograph (Fig. 1) attached to the 1.85 m Plaskett Telescope. Radial velocities of the component stars of the system were determined using the broadening function (BF) method developed by Rucinski [1, 2] and described in more detail by Nelson [3]. The radial velocity curve solution yielded the values  $K_1 = 43.9 \pm 2.7$  km/s,  $K_2 = 274.4 \pm 2.6$  km/s and  $V_\gamma = -10.4 \pm 1.6$  km/s, and thus the mass ratio of the system  $q = 0.16 \pm 0.01$ .

*Acknowledgements: R.H.N. wishes to thank the staff members at the DAO (especially Dmitry Monin, David Bohlender, and the late Les Saddlemyer) for their usual splendid help and assistance.*

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**Keywords:** Stars, Binary, Eclipsing, Spectroscopy



**Fig. 1.** The Cassegrain spectrograph (right panel) attached to the 1.85 m Plaskett telescope (left panel)

O-34

Deformation effect on magnetic properties of ferromagnetic

Fe-27%Ni-4%Mn-1%Zn Alloy

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The martensite formation in ferrous alloys leads researchers to a continuous interest for clarifying and understanding the martensite formation under various distinct conditions. This unique microconstituent forms by applying various external driving forces such as thermal affect (cooling), deformation affect, external magnetic field and hydrostatic pressure to the austenite phase of studied ferrous alloys. The alloy used in the present study was Fe-27%Ni-4%Mn-1%Zn (wt %) which was prepared by vacuum induction melting under an argon atmosphere from pure (99.9 %) alloying elements. In this work, some physical and mechanical properties of Fe-27%Ni-4%Mn-1%Zn (wt %) alloy have been investigated Scanning Electron Microscopy (SEM) and compression deformation test. The magnetic properties of the alloy are measured with the PPMS instrument. The alloy exhibit ferromagnetic behaviour with small hysteresis.

**Keywords:** Deformation, Magnetic Field, Magnetic Materials, SEM.



O-35

## An ICP-MS Study for Determination of the Effects of Anti-TNF Therapy on Bone Quality in Mice with Chronic Allergic Asthma

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It is known that there are many studies that have shown a relationship between chronic allergic asthma (CAA) and bone loss in recent years [1,2]. However, the effect of anti-TNF using in asthma treatment on bone quality is not completely known. Therefore, it is important to examine whether anti-TNF therapy has protective effects on asthma-related bone loss and bone damage. In this study, we used a chronic inhalational exposure model of asthma in ovalbumin-sensitized BALB/c male mice (8-10 weeks-old) to generate CAA. Twenty-four mice were assigned randomly into four groups (eight mice per group): control (intact group), CAA (treated with saline), CAA+6.25 mg/kg of anti-TNF groups. After immunization, saline or anti-TNF administrations were performed intraperitoneally in five sessions at 15-days interval. Three-point bending test was used for biomechanical evaluation. Bone mineral composition (Ca, P, Mg, Se, and Ca/P-ratio) was determined by ICP-MS after a microwave assisted digestion method. Our findings showed that the deteriorative effects of CAA on bone quality and strength can be prevented by administering 6.25 mg/kg of anti-TNF. Moreover, we found that the anti-TNF administration has protective effects on mineral loss and bone integrity against CAA-related impairment. It can be suggested that the anti-TNF therapy may inhibit these impairments. The results showed that the use of anti-TNF may have protective effect on bone quality.

*We thanks Advanced Technology Research & Application Center of Mersin University (Turkey)*

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[2] J-W, Jung, H-R, Kang, J-Y, Kim, S-H, Lee, SS, Kim, SH, Cho, Ann Allergy Asthma Immunol, 112, 2014, 426-431.

**Keywords:** Anti-TNF, Asthm, ICP-MS, Microwave assisted digestion

O-36

Crystal Structure of Yb(III)-MOFs Produced via Hydrothermal Synthesis

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Recently, the lanthanide-carboxylate/sulfonate based metal-organic frameworks (Ln-MOF) have attracted much attention in many field because of their fascinating architectures topologies and also special chemical and physical properties arising from the 4f electrons. In this work, a novel lanthanide coordination polymer associated with organic ligand 2-sulfoterephthalate (2-stp): [Yb(2-stp).3(H<sub>2</sub>O)], 1 has been prepared by hydrothermal methods and structurally characterized by single crystal x-ray diffraction. The asymmetrical unit of compound 1 contains one 2-stp ligand, one unique Yb(III) ion and three coordinated water molecules (Fig. 1). Each crystallographic unique Yb(III) ion is eight-coordinated, in which four oxygen atoms from two carboxylate groups from 2-stp ligands, one oxygen atoms from sulfonate group from 2-stp ligands and three oxygen atoms from coordinated water molecules. Two adjacent dimers are further linked up via two carboxylate groups of two different 2-stp ligands in a  $\eta^1: \eta^1: \eta^1: \eta^1: \mu^3$  mode to form an infinite chain with a Yb...Yb distance of 5.710 Å between the adjacent dimers.

*This work was supported by BAP 16/108 (Mugla Sıtkı Kocman University, The Scientific Research Projects Coordination Unit).*

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**Keywords:** Hydrothermal Synthesis, Crystal structure, Yb(III) complex

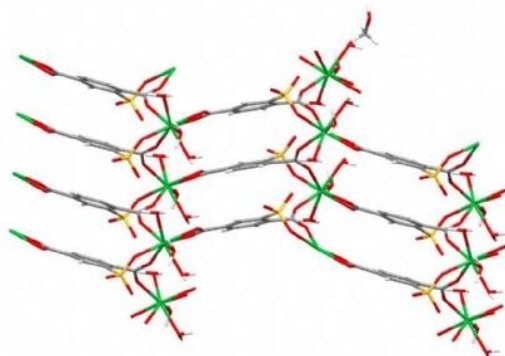


Fig. 1. Crystal Structure

O-37

**Determination of Sun Protection Factor by Using UV-Visible Spectrophotometer and Fatty Acid Composition by Using Gas Chromatography-Mass Spectrometry of Sesamum indicum Oil**

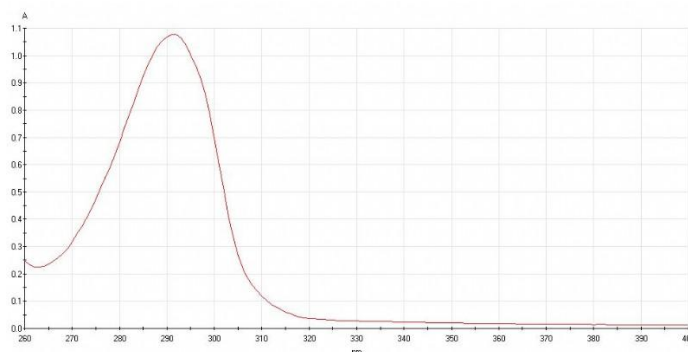
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<sup>1</sup>Department of Chemistry and Chemical Treatment Technologies, Muğla Vocational School of Higher Education, Muğla Sıtkı Koçman University, Muğla, Turkey

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Ultraviolet (UV) rays can cause many disease such as skin cancer and also its one of the main reason of premature aging. Sun protection products, including sunscreen lotions, are designed to absorb, reflect or scatter the sun's ultraviolet radiation to protect the skin from harmful effects of this radiation. The UV-A and UV-B region (400 - 290 nm) is the spectral region that must be blocked for efficacy of the sunscreen. Additionally, regarding the consumer interest on multi-functional products, a product having 2in1 formulation as sun protection and skin care features would be quite interesting for market trend. In this study, Sun Protection Factor (SPF) value of Sesamum indicum oil (SIO) was determined by using UV-Vis spectrophotometer (Fig. 1) according to the absorbance measurement of dilute test solution of SIO between 290-320 nm to determine efficacy against UV-B. Also fatty acid composition of S. indicum oil was identified by using Gas chromatography-Mass spectrometry (GC/MS). Results showed that SIO presence 4.1 value of SPF. The major fatty acids of SIO were determined as linoleic acid (41.70%), oleic acid (41.69%) and palmitic acid (9.34%). According to the results, sesame oil is considered suitable for a good 2in1 formulation having rich fatty acid content. However, UV radiation protection efficiency of SIO must be supported by additional UV filters in order to be more effective in protecting skin against harmful effects of UV radiations.

**Keywords:** UV-Vis, GC/MS, SPF, Sesame oil, Fatty acid



**Fig. 1.** UV-Spectrum of Sesamum indicum oil (SIO)

O-38

**Synthesis and Characterization of Metal Carbonyls [  $M(CO)_6$  (M=Cr, Mo, W),  $Mn(CO)_3$  Cp ] with 3[4-ethyl(phenyl)imino][1H-indol-2-one] (ISE) and 3[4-butyl(phenyl)imino][1H-indol-2-one] (ISB)**

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Four new complexes of  $M(CO)_5(ISE)$  [ M= Mo(1), Cr (2), W (3)], and  $Mn(CO)_3(ISE)$ , where ISE is 3[4-ethyl(phenyl)imino][1H-indol-2-one] have been synthesized by the photochemical reactions of metal carbonyls  $M(CO)_6$  (M= Mo, Cr, W) and  $Mn(CO)_3$  Cp with ISE. Four new complexes of  $M(CO)_5(ISB)$  [ M= Mo, Cr, W ], and  $Mn(CO)_3(ISB)$ , where ISB is 3[4-butyl(phenyl)imino][1H-indol-2-one] have been synthesized by the photochemical reactions of metal carbonyls  $M(CO)_6$  (M= Mo, Cr, W) and  $Mn(CO)_3$  Cp with ISB (Fig. 1). The complexes have been characterized by elemental analysis, FT-IR,  $^1H$  and  $^{13}C$ - NMR spectroscopy. The spectroscopic studies show that, ISE and ISB ligands, behaves as a monodentate ligand and coordinate via C=N donor atom to the central metal atom in  $M(CO)_5(ISE)$  and  $M(CO)_5(ISB)$  where M= Mo, Cr, W, and as a tridentate ligand coordinating via imine nitrogen donor atom (C=N), oxygen donor atom (C=O) and ring NH donor atom in  $Mn(CO)_3(ISE)$  and  $Mn(CO)_3(ISB)$ .

**Keywords:** Isatin; 1,2,4-triazole; Schiff base; Metal carbonyl

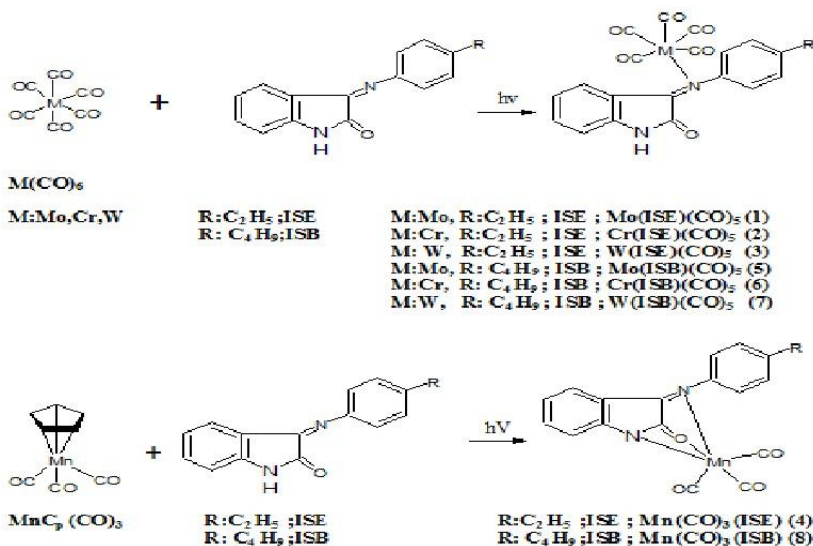


Fig. 1. The photochemical reaction of Metal Carbonyl and ISE and ISB

O-39

## Spectroscopic and Computational Investigation of Some Pyrene Derivatives in Different Solvents

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Pyrene and its derivatives are widely used for photosensitive material design because of their high absorption coefficient, long excited state lifetime and high quantum yield [1]. UV/Vis absorption spectra, fluorescence spectra (Fig. 1) and lifetime measurements of Pyrene and its -OH, -NH<sub>2</sub>, and -CN substituted derivatives have been recorded in different solvents. The computational investigation of Pyrene and derivatives in ground and in excited S<sub>1</sub> states has been carried out in the gas phase and in solution. Geometry optimizations were performed by density functional theory (DFT) at B3LYP/6-311++G(d,p) level. Time-dependent density functional theory (TDDFT) with the same functional and basis set was used for the analysis of excited states of investigated molecules and emission spectra were obtained by using the excited-state geometries. Polarizable Continuum Model (PCM) is used for calculations in solution. Py and its substituted derivatives were not affected from solvent polarity except PyNH<sub>2</sub>. Additionally, PyNH<sub>2</sub> has the smallest HOMO-LUMO gap among all studied molecules. However, it has the shortest fluorescence lifetime in experimental lifetime measurements. Due to this observation, PyCN which has a longer lifetime is more appropriate for use in photosensitive applications.

*We gratefully acknowledge computer time from TÜBİTAK-ULAKBİM Truba Resources and Ege University Faculty of Science Computer Resources (FenCluster). We also thank Prof. Dirk Guldi and his group for lifetime fluorescence measurements in Erlangen University.*

[1] T. Kaya, C. Selçuki, N. Acar, "A DFT and TDDFT investigation of interactions between 1-hydroxypyrene and aromatic amino acids", Computational and Theoretical Chemistry, 1073, 9-19, (2015).

**Keywords:** DFT, intramolecular charge transfer, Pyrene.

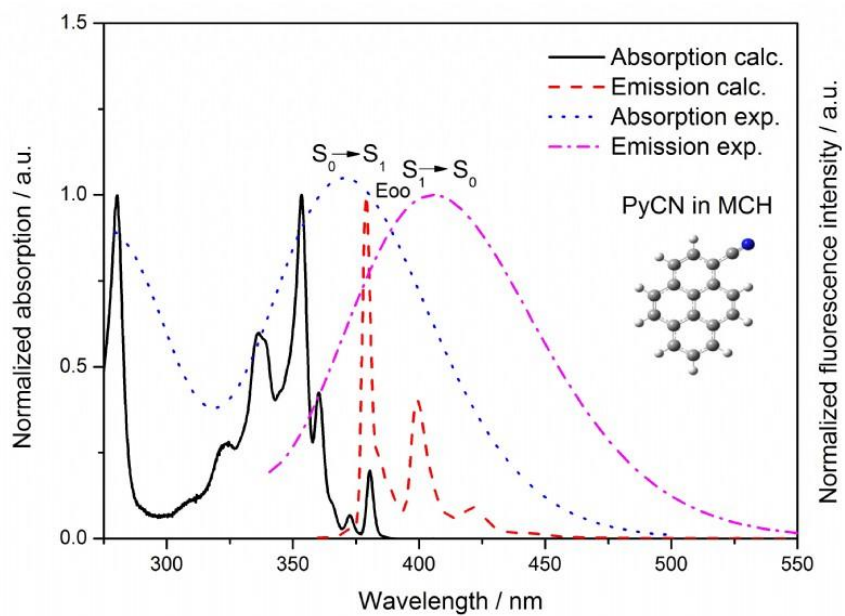


Fig.1 UV/Vis absorption and fluorescence spectra of Cyanopyrene (PyCN) in MCH

O-40

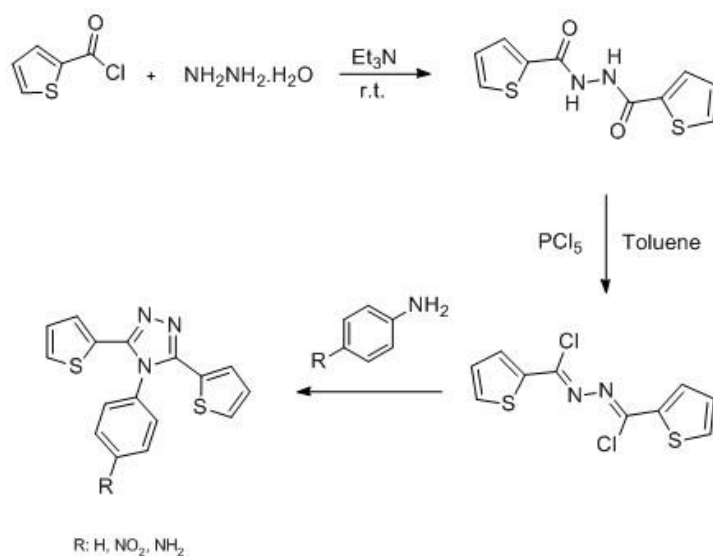
**Synthesis and excited state studies of novel conjugated Triazole compounds for organic electronics**

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Tuning the photo-physical properties of organic molecules is possible by doing some chemical modifications. In this regard, to understand the effect of push-pull group substitution on excited state properties, some novel triazole compounds were synthesized from the reactions of 1,2-bis(chloro(thiophen-2-yl)methylene)hydrazine and some amines (Fig. 1). The structural characterization of the studied molecules were carried out using <sup>1</sup>H-NMR, <sup>13</sup>C-NMR spectroscopic technics. Excited state, IR vibration frequency and <sup>1</sup>H-NMR, <sup>13</sup>C-NMR calculations were carried out in vacuum and different solvents by DFT calculations using B3LYP method 6-31 g (d,p) basis set in Gaussian 09. In addition, the solvatochromic properties and optic band gap energies of synthesized compound were investigated experimentally using UV-Vis and fluorescent spectroscopy. The theoretical data were compared with experimental data and the suitability of the method used for theoretical calculations were discussed.

**Keywords:** Triazole, Optic Band Gap Energy, DFT.



**Fig. 1. Synthetic route of studied triazole derivatives.**



O-41

**Sensor Application of Pristine and M-doped (M = Si, Al or Ge) C<sub>60</sub> Fullerenes in 3-trifluoromethylphenylpiperazine Drug Detection**

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3-trifluoromethylphenylpiperazine (TFMPP) is a recreational drug of the piperazine chemical class as an alternative to the illicit drug ecstasy and its detection is of great importance for police and drug communities. In this research, the absorption mechanism, electronic sensitivity and reactivity of pristine and M-doped C<sub>60</sub> fullerenes (Fig. 1) to the TFMPP were researched by quantum mechanical calculations. Findings suggest that the pristine fullerene displays a worthy electronic sensitivity to TFMPP drug while suffering from a weak interaction and the M-doping process rises the reactivity but decreases the sensitivity of the fullerene to TFMPP. For the M-doped structures, the Al- and Si-compounds are more sensitive in the gas phase and water media correspondingly and they might be used as sensor for detection of this drug.

**Keywords:** Sensor application, Fullerene, DFT, Adsorption, NBO

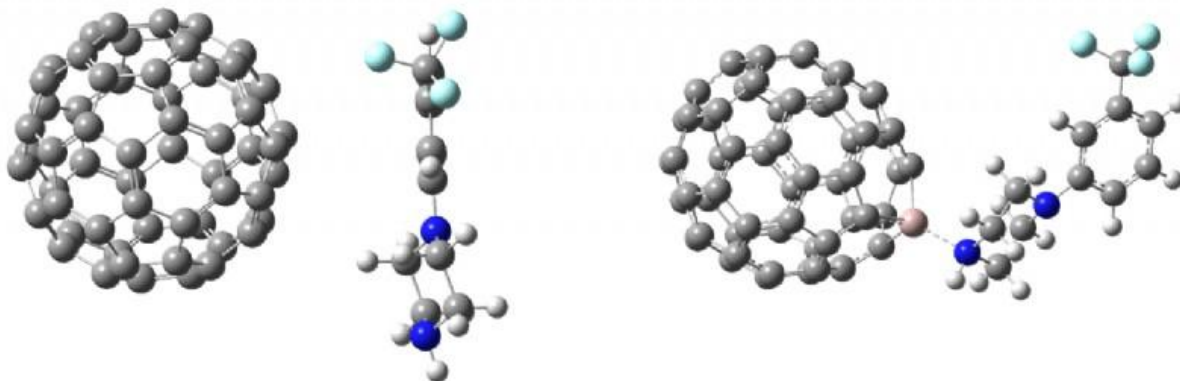


Fig. 1. Optimized structures for the investigated molecular systems



O-42

Synthesis, Spectroscopic and Theoretical Investigation of New Schiff bases of Pyrazole derivatives

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Pyrazoles are important compounds because of their biological and pharmacological activities extensively studied in recent years owing to their great variety of biological activity, ranging from antimalarial, antibacterial, antitumoral, antiviral activities, etc antimicrobial, analgesic, anticancer, antitubercular, anti-inflammatory, antidepressant, anticonvulsant, antipyretic, antihelminthic, antioxidant and herbicidal properties [1,2,3]. In our study we synthesized new Schiff bases including azo and pyrazole group. Their spectroscopic analysis were determined by using IR, UV-Vis, NMR spectroscopic techniques. Density functional theory (DFT) calculations were carried out to obtain the ground state optimized geometries and calculated some electronic and chemical reactivity parameters. The molecular structure of the pyrazole compounds were analyzed by using DFT method. Schiff bases were synthesized by the reaction between p-hydroxy benzaldehyde with (E)-1-phenyl-4-(phenyldiazenyl)-1H-pyrazole-3,5-diamine, (E)-4-((4-nitrophenyl)diazenyl)-1-phenyl-1H-pyrazole-3,5-diamine, (E)-4-((4-methoxyphenyl)diazenyl)-1-phenyl-1H-pyrazole-3,5-diamine, (E)-1-phenyl-4-(p-tolyldiazenyl)-1H-pyrazole-3,5-diamine, (E)-4-((4-chlorophenyl)diazenyl)-1-phenyl-1H-pyrazole-3,5-diamine in THF 1:2 molar ratio as described in the Fig. 1 [4].

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 [4] P. Silku, S. Özkınalı, Z. Oztürk, A. Asan, D. A. Kose, *Journal of Molecular Structure*, 1116 (2016) 72-83

**Keywords:** Schiff bases, Pyrazole, azo-imine; DFT

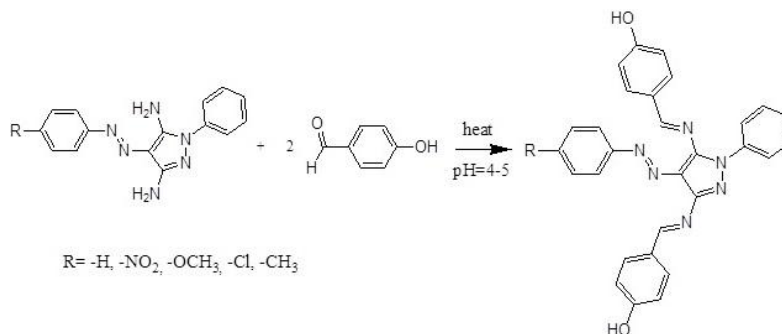


Fig. 1. Synthesis of the Schiff bases of the pyrazole derivatives

O-43

Vibrational Spectroscopy of Hydrogen-Bonded Complexes, Liquids and Solids

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Theoretical model is presented for the X-H(D) stretching vibrations in hydrogen-bonded systems. The model takes into account an adiabatic coupling between the high-frequency X-H(D) stretching and the low-frequency intermolecular X...Y stretching modes, linear and quadratic distortions of the potential energy for the low-frequency vibrations in the excited state of the X-H(D) stretching vibration, resonance interactions between hydrogen bonds, Fermi resonance between the X-H(D) stretching and the overtone of the X-H(D) bending vibrations, and mechanical and electrical anharmonicities. The effects of deuteration and temperature on spectra are successfully reproduced by the model. Comparison between experimental and theoretical spectra is presented for different hydrogen-bonded systems, including ices. We present also the method of Car-Parrinello molecular dynamics used to calculate infrared spectra of crystals.

Proton tunneling in tropone is described by two-dimensional model potentials. The potentials have been fitted to quantum mechanically calculated two-dimensional grid of energies, and used to analyze proton dynamics. The model PES well reproduces experimentally observed promotion of the tunneling by the excitation of the planar modes and suppression by the excitation of the out-of-plane modes.

**Keywords:** hydrogen bond, vibrational spectroscopy, theoretical models

## O-44

### Theoretical studies of molecular structures, infrared spectra and NLO properties of some novel 5-arylazo-6-hydroxy-4-phenyl-3-cyano-2-pyridone dyes

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The arylazo colorants belonging to the azo dyes class are a very important class of colorants. The importance of arylazo pyridone dyes containing pyridone rings have increased due to the use of polyester and nylon as the main synthetic fibers. In this study, the optimized geometrical structures, infrared spectra, molecular electrostatic potential, and nonlinear optical (NLO) properties of azo-hydrazone tautomeric structures (Fig. 1) for 5-phenylazo-6-hydroxy-4-phenyl-3-cyano-2-pyridone (1) and 5-(4-bromophenylazo)-6-hydroxy-4-phenyl-3-cyano-2-pyridone (2) dyes have been investigated by Density Functional Theory (DFT) using B3LYP functional with 6-31G(d,p) basis set. Vibrational modes are assigned with the help of vibrational energy distribution analysis (VEDA) program. Highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) energies of the (1) and (2) compounds with azo and hydrazone forms were calculated with the same method and basis set. Molecular parameters like global hardness ( $\eta$ ), global softness ( $\sigma$ ) and electronegativity ( $\chi$ ) were calculated with the results obtained from the HOMO and LUMO molecular orbital energies. Nonlinear optical parameters [mean polarizability ( $\langle\alpha\rangle$ ), the anisotropy of the polarizability ( $\langle\Delta\alpha\rangle$ ) and the mean first-order hyperpolarizability ( $\langle\beta\rangle$ )] of the title compounds were investigated theoretically. The atomic charges, electronic exchange interaction and charge delocalization of the molecules have been studied by natural bond orbital analysis.

**Keywords:** Arylazo pyridone dyes, Density Functional Theory (DFT), VEDA, Nonlinear optical (NLO) parameters

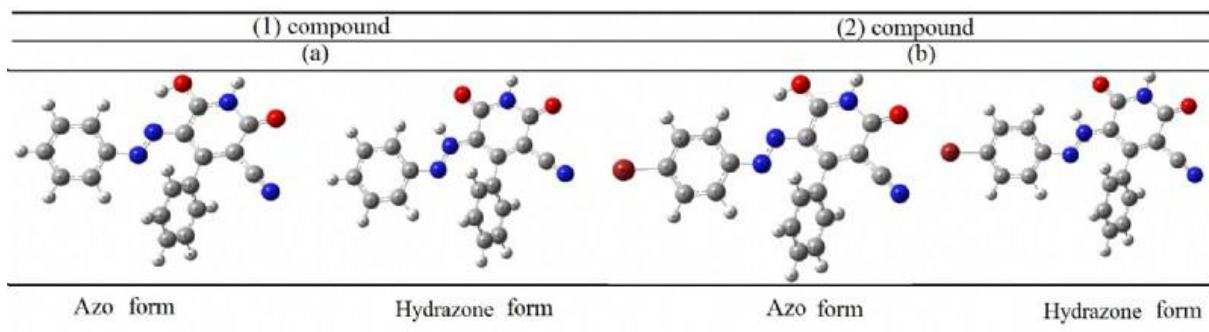


Fig. 1. The optimized molecular structures for the azo and hydrazone tautomers of the aryazo pyridine dyes (1) and (2) using the B3LYP/6-31G(d,p) method.

O-45

**A study of structure and vibrations analysis of the 3-fluoro-4-fomylphenylboronic acid molecule**

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The molecular structure and vibrations of 3-fluoro-4-fomylphenylboronic acid (3-4FPBA) were investigated by infrared spectroscopic technique. The theoretical calculations for the molecular structure and spectroscopic studies were performed with DFT (B3LYP) and 6-311++G(d,p) basis set calculations using the Gaussian 09 program. FT-IR spectra were recorded in the solid phase. Electronic structure properties of in the title molecule such as HOMO-LUMO and Molecular Electrostatic Potential (MEP) were investigated by TD-DFT method. The results of theoretical calculations for the spectra of the title compound were compared with the observed spectra.

*This work was supported by Ahi Evran University Scientific Project Unit (BAP) with, Project No: TBY.E2.17.007.*

**Keywords:** 3-fluoro-4-fomylphenylboronic acid, 3-4FPBA, DFT, HOMO-LUMO.

O-46

## Theoretical Raman Spectra of Carbon Peapods

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Single walled carbon nanotubes (SCNT) can encapsulate small and large molecules, including C60 and C70 fullerenes. Those systems consist of SCNT in which fullerene molecules are inserted and called peapods. Double Walled Carbon Nanotubes (DWCNTs) are also interesting candidates for encapsulating fullerene molecules. Transmission electron microscopy experiments clearly demonstrated that C60 and C70 fullerenes can take different ordered arrangements inside DWCNT with high fullerene filling levels. This hybrid systems between fullerene and carbon nanotubes have generated a lot of interest for electronic applications. Due to their special one-dimensional nanosized structure and their tunable electronic properties. Peapods known a several potential applications from high temperature superconductor to memory element.

Raman spectra calculation are based on the spectral moments method, which has proved to be a powerful approach for determining the infrared, Raman, and inelastic neutron scattering spectra of harmonic systems. This method can be applied to very large systems, whatever the type of atomic forces, the spatial dimension, and structure of the material. A Lennard–Jones potential is used to describe the van der Waals interactions between carbon atoms belonging to two different molecules (tube–tube, fullerene–fullerene or tube–fullerene).

We present the calculation results of the Raman spectra of C60 and C70 encapsulated inside DCNTs as a function of the diameter and chirality of the inner and outer tubes. The evolution of the average Raman intensity ratios between Raman mode of C60/C70 molecules and nanotubes as a function of the concentration of fullerenes has been analyzed. These predictions are useful to interpret the experimental data.

**Keywords:** Raman Spectroscopy, Nanotube, Peapod, Simulation

## O-47

### A study of metallic Fe-Ni-Co alloy and stony part isolated from Seymchan meteorite using X-ray diffraction, magnetization measurement and Mössbauer spectroscopy

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Seymchan, a stony iron meteorite, was found in 1967 in the Magadan District of the former USSR (now Russian Federation) and classified as the main group pallasite (PMG). Fragments of Seymchan meteorite were collected in 2012 by the Meteoritical Expedition of the Ural Federal University. This meteorite consists of Fe-Ni-Co metallic and stony parts containing olivine (Fe, Mg)<sub>2</sub>SiO<sub>4</sub> mainly and some other minerals. A polished slice of Seymchan PMG fragment was characterized by optical microscopy and scanning electron microscopy (SEM) with energy dispersion spectroscopy (EDS). Samples of metallic and stony parts were isolated from Seymchan and then powdered for X-ray diffraction (XRD), magnetization measurements and Mössbauer spectroscopy with a high velocity resolution studies.

Optical microscopy of Seymchan PMG demonstrated the presence of: (a)  $\alpha$ -Fe(Ni, Co) and  $\gamma$ -Fe(Ni, Co) phases, (b) plesite structures consisting of  $\alpha$ -Fe(Ni, Co)/ $\alpha_2$ -Fe(Ni, Co)+ $\gamma$ -Fe(Ni, Co) phases as well as (c) inclusions of silicate and chromite phases. SEM with EDS analysis showed that the Ni content is in the ranges ~5.5–6.5 at.% in  $\alpha$ -Fe(Ni, Co) phase, ~20–25 at.% in  $\alpha_2$ -Fe(Ni, Co) phase and ~28–48 at.% in  $\gamma$ -Fe(Ni, Co) phase. The main iron-bearing component of stony part is olivine with relatively large amount of chromite FeCr<sub>2</sub>O<sub>4</sub> which unusually contains large amount of Mg (~5–6 at.%), and small amounts of troilite FeS and schreibersite (Fe, Ni)<sub>3</sub>P. Some weathered products containing Fe<sup>3+</sup> are also observed. XRD, magnetization and Mössbauer spectroscopy measurements confirmed the main content of olivine and the presence of spinel structure (FeCr<sub>2</sub>O<sub>4</sub> and probably FeMg<sub>2</sub>O<sub>4</sub>), troilite, tiny amount of clinopyroxene (Fe, Mg, Ca)SiO<sub>3</sub> and Fe<sup>3+</sup> compound in the stony part and the presence of  $\alpha$ -Fe(Ni, Co),  $\alpha_2$ -Fe(Ni, Co) and  $\gamma$ -Fe(Ni, Co) phases with small amount of oxidized iron in metallic part of Seymchan PMG fragment. Basing on XRD and Mössbauer results the iron partitioning between the M1 and M2 sites in olivine is estimated.

*This work was supported by the Ministry of Education and Science of the Russian Federation (Project # 3.1959.2017/4.6) and by Act 211 Government of the Russian Federation, contract № 02.A03.21.0006. Contributions from A.A.M and M.V.G. were funded by the RFBR (Project № 16-32-00151 mol\_a).*

**Keywords:** Seymchan main group pallasite, X-ray diffraction, Magnetization measurement, Mössbauer spectroscopy

O-48

**Mössbauer Spectroscopy of Magnetite Nanoparticles for Applications in Biotechnology and Biomedicine**

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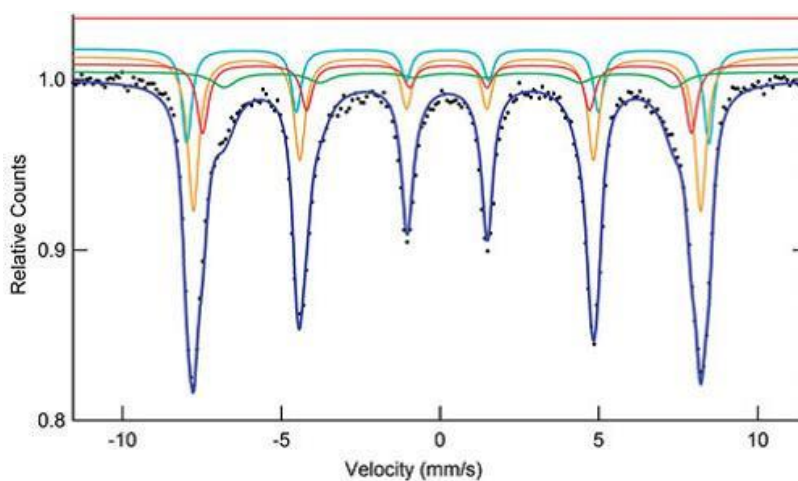
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Nanosized magnetite is less stable than its bulk form and can be more readily oxidized to hematite due to its high surface area (Cornell & Schwertmann, 2006). For this reason, it is important to determine if there is any formation of oxidation product in the magnetite nanoparticles (NPs), as it may affect the reactivity of the NPs and accordingly the state of cellular toxic response. The XRD peaks of magnetite and hematite, which both crystallize in the cubic structure, occur nearly at the same angle and accordingly, it is difficult to distinguish between these two types of iron oxides via XRD. For this reason, Mössbauer spectroscopy, which is a well-known local probe technique for its sensitivity and specificity in investigating Fe containing compounds, was employed to characterize the fine structure and oxidation state of magnetic Fe<sub>3</sub>O<sub>4</sub> NPs. The magnetic phases in the magnetite NPs were identified using aWissel Mössbauer measurement system. The RT Mössbauer spectrum of the magnetite NPs is presented in Fig. 1. According to the Mössbauer spectrum of the magnetite NPs, it can be suspected that there are magnetite, maghemite and hematite crystal phases in the samples.

**Keywords:** Mössbauer Spectroscopy, magnetite, nanoparticle.



**Fig. 1. Mössbauer spectrum of magnetite nanoparticles**



O-49

**Magnetic properties of thermally induced martensite in a  
Fe-27%Ni-4%Mn-1%Zn (wt.%) alloy**

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To examine the thermal induced martensitic transformations, we homogenized the sample at 1200 °C for 12 hours and then quenched into water at room temperature. This sample exhibited austenite phase. Then, we waited for 3 minutes in nitrogen for occurred martensite phase in this austenite sample. As a result of this process, this sample exhibited thermally induced martensite. The single peak of the paramagnetic phase and the six peaks of the ferromagnetic phase of Fe-27%Ni-4%Mn-1%Zn (wt.%) alloy were observed in the Mössbauer spectrum. The effective hyperfine field of ferromagnetic martensite phase was determined as 33.132 T and isomer shift value was determined as 0.0242 mm/s.

*The financial aid of the Amasya University project No. FMB-BAP 16-0174 is gratefully acknowledged.*

**Keywords:** Alloy, Austenite, Martensite, Isomer shift.

**O-50**

**Spectroscopic and structural investigations on Bursa L6 meteorite**

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Bursa meteorite that fell in Bursa Turkey in 1946 (Fig. 1), is a stony olivine-hyperstene chondrite, has been classified as L6 [1]. The aim of this study is a further identification of Bursa meteorite by micro-Raman spectroscopy, Atomic Force Microscopy (AFM) and Thermogravimetric Analysis (TGA). TGA results revealed that very low weight loss of 0.1251 mg (0.3768 %) was observed for the meteorite between 25 and 750 °C. This shows that the meteorite does not lose too much weight in this temperature range so this would be an explanation of low volatilization of the minerals in Bursa meteorite. From AFM results it was possible to extract the detailed surface topography of a small portion of the meteorite and roughness properties. On the other hand, characteristic Olivine signals were detected as a doublet at 820/852 cm<sup>-1</sup> in Raman spectrum. Peaks observed at this doublet refer to ~Fo88 standard [2].

*This study was supported by Ege University Scientific Research Projects Coordination Unit (Project Number: 2017/FEN/050).*

[1] Meteoritics, 5, 1970, 90.

[2] Bhaskar J. Saikia, Gopalakrishnarao Parthasarathy, Rashmi R. Borah, Meteoritics and Planetary Science, 52, 6, 2017, 1146-1154.

**Keywords:** Bursa meteorite, Micro Raman, AFM, TGA



**Fig. 1. Bursa meteorite**

O-51

## The Analysis of Colored Plasters of Saraylı Rural Architecture by UV-VIS Spectrophotometer

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The aim of the project is to analyze traditional rural houses of Saraylı Village in Kocaeli district with archaeometrical methods.

The use of color on building elements plays important role on the perception of rural area. Color is an important component of architectural aesthetics. It is applicable for both modern and traditional rural fabric. Through time, traditional houses in both urban and rural areas have been gone through numerous renovations and paintings resulted in various paint layers on the facades of houses. It is important to study color based on scientific methods for architectural restoration and conservation.

Saraylı is located in Kocaeli, Gölcük district. Rural architecture here has long history back to 14th century AD. Saraylı was one of the earliest towns founded during the conquest. Gölcük district itself has been subjected various civilizations according to archaeological and sources. 51 houses are registered as samples of rural architectural heritage. Four houses, which have well preserved colored plasters, were chosen for this study. Colored plaster samples were collected from these houses.

Solutions of these samples were prepared. The spectra of the samples were analyzed between 200-900 nm wavelengths using UV-VIS spectrophotometer. The peaks obtained from coloring agents were determined in order to compare the structures of coloring agents.

**Keywords:** Rural Architecture, Archaeometry, Colored Plaster, UV-VIS

O-52

Grazing Incidence Small Angle X- ray Scattering (GISAXS) Analysis on Nanostructured Thin Films Synthesized for Optoelectronic Applications

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Thin films have been widely used in optoelectronic devices, in coating technologies and in memory devices. Excellent structural assembling of the thin films may be controlled from atomic dimensions to the nano and micrometer sizes. Thin films can be made of metal, inorganic-organic compounds and biological molecules, according to the research fields and scientific purposes. The physicochemical properties of the films depend on their morphologies and the shapes, sizes and distributions of the appeared nano globules. Many techniques have been developed to obtain accurate structural information on the nanometer scale (1-100 nm). Among these techniques, GISAXS (Grazing Incidence Small Angle X-ray Scattering) is very informative and commonly used modern technique to examine micro- and nano-structured thin films and their inner-outer surfaces.

In the present study, three different types of thin films have been investigated by using GISAXS technique. These films were Ge nanoparticles embedded ZnO thin films, hydrogenated amorphous silicon oxygen alloy ( $a\text{-SiO}_x\text{:H}$ ;  $x < 1$ ) films and poly (chloro-p-xylylene) (Parylene-C, PPX) films. GISAXS data were collected in both of normal and parallel directions to the surface of the samples. Guinier analyses (in small  $q$  region), structural modelling, pair distance distribution calculations and 3D shape determinations were carried out to reach quantitative results with the help of IGOR Pro6 and DAMMIN programs. The effects of external physicochemical conditions, growth parameters and substrate effects on the nanostructural formations were successfully obtained at the end of the work. Fig. 1 shows the fitted GISAXS profiles ( $I(q)$ - $q$ ), the distance distribution histograms and the shapes of the obtained nanoglobules related with PPX film.

**Keywords:** GISAXS, Nanostructured Thin Films, ZnO:Ge, amorphous-crystalline silicon, Parylene-C

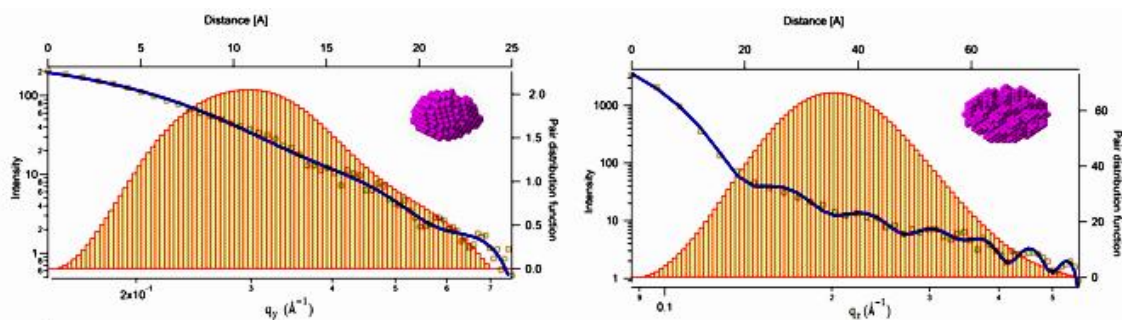


Fig. 1. GISAXS profiles along the surface ( $q_y$ ) and the depth ( $q_z$ ) of a nanocrystalline PPX thin film, Distance distributions and 3D shapes of the nanoglobules assembled inside of the film.

O-53

Concentration and temperature dependent studies of interaction of provitamin D<sub>3</sub> with zwitterionic DPPC model membranes

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Provitamin D<sub>3</sub> (7-dehydrocholesterol) is a common immediate precursor of cholesterol and vitamin D<sub>3</sub> [1]. It is photochemically converted to vitamin D<sub>3</sub> in relatively large quantities in the skin of most vertebrate animals, including humans [2]. Dipalmitoyl phosphatidylcholine (DPPC) is the most studied phospholipid, which consists of two saturated 16-carbon fatty acid chains connected by a glycerol backbone with a zwitterionic headgroup [3]. In the current study, interaction of provitamin D<sub>3</sub> with DPPC multilamellar vesicles (MLVs) (Fig. 1) was investigated as a function of temperature and provitamin D<sub>3</sub> concentration by using Fourier transform infrared (FTIR) spectroscopy and differential scanning calorimetry (DSC). DSC reveals that the addition of provitamin D<sub>3</sub> into pure DPPC liposomes eliminates the pretransition, shifts the main phase transition to lower temperatures and then abolishes it. FTIR shows that in the gel phase, 5, 10 and 20 mol% provitamin D<sub>3</sub> increase the order and decrease the dynamics of DPPC membranes, whereas 30 and 40 mol% provitamin D<sub>3</sub> decrease the order and increase the dynamics. In the fluid phase, 5 mol% provitamin D<sub>3</sub> induces a decrease in the order and the dynamics of DPPC membranes, while 10, 20, 30 and 40 mol% provitamin D<sub>3</sub> cause an increase in the order and a decrease in the dynamics. In addition, provitamin D<sub>3</sub> causes strong hydrogen bonding between the carbonyl and phosphate groups of DPPC membranes and the water molecules around both in the gel and fluid phases.

*This work was supported by Ege University Research Fund 2014 FEN 025.*

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[3] S.E. Feller, Langmuir, 13, 1997, 6555–6561.

**Keywords:** Provitamin D<sub>3</sub>, DPPC, DSC, FTIR spectroscopy.

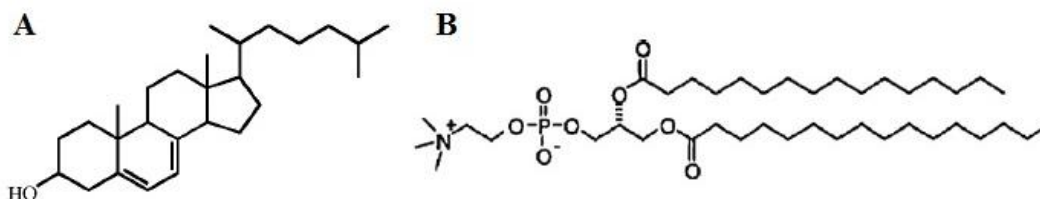


Fig. 1. Chemical structures of provitamin D<sub>3</sub> (A) and DPPC (B).

O-54

**Synthesis, Characterization and Spectroscopic Properties: Schiff Base  
Derivative Bearing Zinc(II) Phthalocyanine**

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Schiff bases are used as ligands in the coordination chemistry. Furthermore these compounds exhibit biological activity as anticancer, antifungal, antibacterial, antiviral and anti-parasitic agents in addition to other biological performances. These compounds have also played a great role in the development of chemistry. Sulfonamides have been widely investigated due to their attractive uses as drugs in the treatment of diseases, and represent an important class of pharmaceutical compounds with a wide spectrum of biological activities, such as, anticancer, antibacterial, antitumor, antihypertensive, anti-inflammatory activities. Metal complexes modify the pharmacology and toxicology of the sulfonamide base ligands. Phthalocyanines (Pcs) are 18  $\pi$ -electron aromatic macrocycles comprising four isoindole units linked together through their 1,3-positions by aza bridges [1]. The particular electron delocalization over these macrocycles gives rise to unique physical and chemical properties. Their bright colors, conductivity, and chemical and thermal stability have made them very desirable for many applications [1]. Pcs continually find their usefulness in contemporary and emerging technologies such as catalysis, photodynamic therapy (PDT), nonlinear optics, gas sensors, thermal writing displays, and solar cells. Specificity in the applications of Pcs can be introduced by modification of the Pc ring or by changes in the central metal or axial ligands[1]. Since then, their outstanding and tailorable properties such as liquid crystallinity, generation of singlet oxygen and redox properties have enhanced their use as efficient agents in several high technology applications including: photodynamic therapy, a technique for which Pcs are currently the most promising class of compounds for photodynamic antimicrobial chemotherapy as sensors including biosensors, for non-linear optical applications, dye sensitized photovoltaic production, semiconductor materials, oxidation or reduction catalysts and photocatalysts among others. The aim of the present study is to produce new synthetic compound combining Pc and benzenesulfonamide derivative containing schiff base (Fig. 1). The novel complex's spectroscopic properties were investigated by IR, UV-vis, <sup>1</sup>H NMR, MALDI-TOF mass spectroscopies and elemental analysis and determined.

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**Keywords:** Zinc(II); phthalocyanine; schiff base, spectroscopic, benzenesulfonamide.

O-55

## Development and Validation of Sensitive Spectrophotometric Method for the Determination of Rilmenidine in Pure and Pharmaceutical Preparations

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Rilmenidine is a novel  $\alpha_2$ -adrenoceptor agonist, used in the treatment of mild or moderate hypertension at the oral dose of 1 mg once or twice daily[1]. In this study, a novel, sensitive and selective spectrophotometric method was developed for the determination of rilmenidine in pharmaceutical preparations. Maximum absorbance of derivative in dichlorometane is measured at 224 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. A linear relationship existed between absorbance and rilmenidine concentration over 50-250  $\mu\text{g}/\text{mL}$  range. The proposed method was successfully applied for the determination of rilmenidine in pharmaceutical preparations and the obtained results were in good agreement with those obtained by the reference method.

*The present work was supported by the Research Project Coordination Fund of Namık Kemal University. Project No. NKUBAP.00.GA.16.02.*

[1] P., Genissel, N., Bromet, J. B. Fourtillan, A. Mignot, H. Albin, The American Journal of Cardiology, 61, 7, D47-D53

**Keywords:** Rilmenidine; determination; spectrophotometric



O-56

**Induction of aggregation of silver nanoparticles via pH variation for sensitive spectrophotometric determination of creatinine in urine**

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Simple, rapid and sensitive method based on surface plasmon resonance (SPR) absorption band of silver nanoparticles (AgNPs) for determination of creatinine was developed. Silver nanoparticles with strong and sharp absorption band around 403 nm was prepared using ascorbic acid and citrate as reducing and capping agents respectively. Addition of creatinine on the AgNPs colloidal solutions induces aggregation of AgNPs that depends on pH. The aggregation of the particles is revealed by observing the color change of the AgNPs colloidal and spectrophotometrically through gradual decrement of the absorption maximum around 403 nm and appearance of new band around 670 nm with creatinine. Aggregation of AgNPs was further confirmed by tunneling electron microscopy (TEM). Absorption ratio of A<sub>670</sub>/A<sub>403</sub> was used for quantitative and qualitative evaluation of the method. The method is selective for detection of creatinine in that the silver nanoparticles are aggregated in the presence of creatinine rather than the species that can be potential interferences available in urine sample. In addition to aqueous creatinine solution, the method was also successfully applied for determination of creatinine in urine sample.

**Keywords:** aggregation, creatinine, silver nanoparticles



O-57

**Preparation of a New Lanthanide-Chelate Cross-Linked, Myoglobin (Mb) Imprinted Affinity Cryogel for Selective Recognition of Myoglobin (Mb) in Blood Serums and Determination of Myoglobin (Mb) by UV-VIS-Near Infrared Spectroscopy (UV-VIS-NIR'S)**

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Myoglobin (Mb) is a 17.6-kDa monomeric hemeprotein exists in the heart and skeletal muscles. Mb is an important biological marker for early detection of some diseases such as myocardial necrosis and acute myocardial infarction (AMI) also known as a heart attack. When muscle is damaged, Mb is rapidly released into the bloodstream from the areas of ischemic injury due to its small size. Large amounts of Mb may cause kidney failure since it can be broken down into toxic compounds. The concentration of serum myoglobin begins to increase within 1 to 3 h after AMI and it reaches the peak levels within 6 to 9 h. Thus, the detection of Mb concentration is crucial for the early diagnosis of AMI.

This study describes the selective recognition of myoglobin in aqueous solutions and human serum in the presence of various proteins by A New Lanthanide-Chelate Cross-Linked Affinity molecularly Imprinted Cryogel polymer. Myoglobin (Mb) imprinted cryogel polymer were prepared by using free radical polymerization technique. For this purpose, N-methacryloylamidoantipyrine-Ce(III) [MAAP-Ce(III)] was used as the functional complex monomer. Myoglobin (Mb) and poly2-hydroxyethyl methacrylic acid were used as the template and cross-linker cryogel polymer, respectively. [P(HEMA-co-MAAP-Ce(III))] cryogel polymer was characterized ultraviolet-visible-near infrared (UV-NIR), scanning electron microscopy (SEM), energy dispersive X-ray (EDX) and swelling tests. The effects of different parameters such as initial myoglobin (Mb) concentration, temperature, pH and ionic strength on binding were investigated. Maximum binding capacity of the cryogel polymer was found to be 68.80 mg/g cryogel polymer at pH 4.0.

**Keywords:** Lanthanide, Imprinting, Acute Myocardial Infarction (AMI), Myoglobin (Mb), Near-IR Spectroscopy

O-58

## Identification of mono- and few-layer graphene films: X-Ray and Raman studies

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The development of new technologies and devices based on the unique properties of graphene requires the accurate determination of the number of graphene layers and low cost methods to prepare them. Raman spectroscopy can be used to provide a rapid, precise and non-destructive analysis to determine the number of layers in graphene thin films.

First, an improved and inexpensive method was used to prepare mono-, bi-, tri- and few-layers graphene thin films [1]. We have found that increasing the volume of graphene solution used in the vacuum filtration results in more sheets of graphene.

The number of graphene layers deposited in the filtration membranes and in Si substrates was determined using Raman spectroscopy. We also used X-ray diffraction (XRD) to compare the patterns from monolayers and few layers graphene in liquid and in the thin films.

In this work, we calculated the non-resonant Raman spectra [2] of graphene films to analyze our experimental results. The first-order resonance Raman scattering mechanisms in graphene was discussed focused on the origin of the G peak, it changes in shape, position and relative intensity as a function of the number of graphene layers. We have found a good agreement to the group theory concerning the number of the Raman-active modes of mono, bi and few-layers [3].

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**Keywords:** Graphene; XRD; Raman Spectroscopy.

O-59

**A comparative study on DNA binding properties of 2,10,16, 24| -tetrakis 4-(4-hydroxyphenyl)-1-phenylethyl) phenoxy) substituted cobalt (II) and Mg (II) phthalocyanine compounds**

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2,10,16, 24-Tetrakis 4-(4-hydroxyphenyl)-1-phenylethyl) phenoxy) phthalocyaninato cobalt (II) and Mg (II) compounds were selected for this study [1]. To determine DNA binding properties of cobalt(II) phthalocyanine 4 and Mg(II) phthalocyanine 5 were used Calf Thymus-DNA. The DNA binding properties of the compounds 4 and 5 were investigated using UV-Vis and fluorescence spectroscopy, cyclic voltammetry, thermal denaturation study, electrophoresis and viscosity measurements in Tris-buffer (pH 7.0). Results showed that the cobalt (II) and magnesium (II) phthalocyanine compounds have strong affinity to Calf Thymus-DNA through intercalation [2].

*This study was supported by the Commission of Scientific Research Projects of Karabuk University.*

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**Keywords:** Phthalocyanine, DNA-binding, UV-Vis spectroscopy, Fluorescence spectroscopy

O-60

The martensitic transformation characteristics on the magnetic properties of  
Fe-27%Ni-4%Mn-2%Zn Alloy

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The focus of the present study was to examine the magnetic properties of thermally induced martensite phase of the Fe-27%Ni-4%Mn-2%Zn alloy by Mössbauer spectroscopy. We homogenized the sample at 1200 °C for 12 hours and then quenched into water at room temperature. This sample exhibited austenite phase. Then, we waited for 3 minutes in nitrogen for occurred martensite phase in this austenite sample. As a result of this process, this sample exhibited thermally induced martensite. The single peak of the paramagnetic phase of Fe-27%Ni-4%Mn-2%Zn (wt.%) alloy were observed both of austenite and martensite phase in the Mössbauer spectrum. Despite the structural transformation occurred, the magnetic transformation not occurred with thermal effect.

NOT

**Keywords:** Martensitic Transformation, Mössbauer spectroscopy, Paramagnetic

PRESENTED

O-61

**Antioxidant and Antiradical Properties of Ruscus hypoglossum L. and Trace elements, Minerals and Vitamin C Levels**

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In this study, Ruscus hypoglossum L. was evaluated for its antioxidant, antiradical properties and contents of trace element (Cu, Zn, Fe, Co, Cd, Cr, Mn, Pb), mineral (Ca, K, Mg, Na) and vitamin C levels. In the study, methanol extracts Ruscus hypoglossum L. leaves of total phenol, flavonoids, total antioxidant capacity, DPPH, ABTS, superoxide, hydrogen peroxide, hydroxyl radicals scavenging activity, reducing power, chelating activity on ferrous ions and vitamin C were determined using spectrophotometer. The results are compared with the reference antioxidants such as trolox,  $\alpha$ -tocopherol BHT and BHA. Trace elements were carried out using method of dry ashing with ICP-OES. All the extracts proved to have free radical-scavenging activity and reducing power, but to different extent. The antioxidant activity was measured against radical species generated in their action system, such as DPPH• (2, 2-diphenyl-1-picrylhydrazyl) and ABTS•+ (2, 2- azinobis - (3- ethylbenzthiazoline - 6-sulphonate)) radicals or by the reducing effect on Fe<sup>3+</sup>/ferricyanide complex (reducing power assay). The results of this study showed that Ruscus hypoglossum L. leaf has a high antioxidant capacity, mineral and vitamin levels. Ruscus hypoglossum L. is thought to be used as additives for food products and pharmaceutical industries with appropriate antioxidant properties and an antioxidant.

*This study was supported by a grant from the Scientific Research Projects Presidency of Yuzuncu Yil University (2015-FBE-YL163).*

**Keywords:** Antioxidant activity, trace element, Vitamin C, Ruscus hypoglossum L.

O-62

**Multicomponent cyclocondensation reaction of  $\beta$ -diketone, arylaldehyde and urea**

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Multicomponent reactions of  $\beta$ -diketones, arylaldehydes with nitrogen containing nucleophiles play an important role in the synthesis of heterocyclic compounds possessing diverse types of physiological activities including antitumour, antimicrobial, antifungal, and analgesic activities. We have been prepared 5-benzoyl-6-phenyl-4-(4-methylthiophenyl)-1,2,3,4-tetrahydro-2-oxopyrimidine via Multicomponent cyclocondensation in acetic acid under reflux condition in this study. The mechanism of the reaction was discussed with quantum chemical methods. The structure of 5-benzoyl-6-phenyl-4-(4-methylthiophenyl)-1,2,3,4-tetrahydro-2-oxopyrimidine was established from their spectral data and elemental analysis. The synthesized pyrimidine derivative has been optimized with Gaussian software in order to obtain information about the 3D geometries and electronic structures (Fig 1).

**Keywords:** Arylaldehyde,  $\beta$ -diketone, Urea

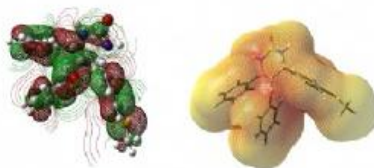


Fig. 1. 3D geometries and electronic structures

**Fig 1. The electronic structures**

O-63

## Synthesis and Spectroscopic Properties Of Newly Peripheral Tetra Substituted Zinc(II) Phthalocyanine Bearing Benzene Sulfonamide Derivative Containing 1,3,4-Thiadiazol, Schiff Base and Bromine

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Schiff bases are considered a very important class of organic ligands possessing diverse applications [1]. Substituted Schiff bases with  $\pi$ -conjugation play a vital role in the development of the new generation electronic and photonic devices due to delocalization of electrons [1]. Schiff bases derived from sulfonamides drug have been acquired interest due to their biological system [2]. Sulfonamide coordination compounds and their derivatives are widely used as antifungal, anti-inflammatory and hypoglycemic agents. Metal complexes modify the pharmacology and toxicology of the sulfonamide base ligands [2]. 1,3,4-thiadiazole derivatives are one of the most important heterocyclic compounds due to their pharmacological and biological properties[3]. As a substituent group, benzothiazoles were used because they enhance the photosensitizer activities of complexes because of synergistic effect [3]. Thanks to their strong delocalized  $18\pi$ -electronic structure, thermal stabilities and optical properties in visible area, phthalocyanines (Pcs) have many potential applications in different areas like as chemical sensors, electrochromic displaying systems, liquid crystals, non-linear optics, solar cells, photo-voltaic optics, molecular electronics, semiconductors, optical storage devices, laser dyes, catalyst and photodynamic therapeutic agents (PDT) [4]. Pcs soluble in polar solvents have strong influence on bioavailability whereas Pcs soluble in nonpolar solvents have a higher tumor affinity [4]. In this work, novel combining four functional materials (phthalocyanines, benzenesulfonamide, 1,3,4-thiadiazol and Schiff base) have been synthesized (Fig. 1) and characterized by common spectroscopic methods and elemental analysis as well.

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**Keywords:** Phthalocyanine; spectroscopy, 1,3,4-thiadiazol, Schiff base, benzenesulfonamide.

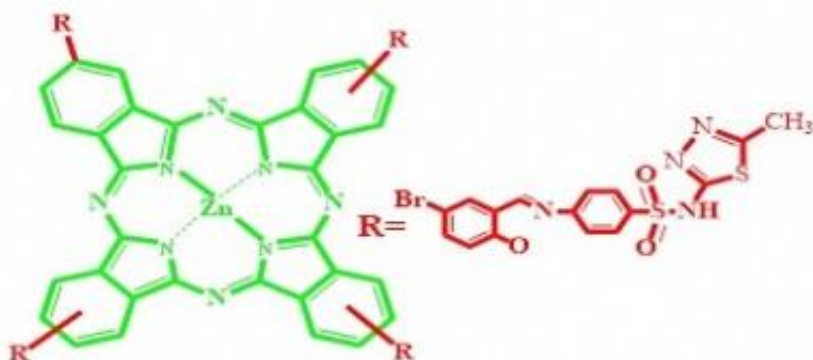


Fig. 1. (E)-4-((5-bromo-2-(λ<sup>1</sup>-oxidanyl)benzylidene)amino)-N-(5-methyl-1,3,4-thiadiazol-2-yl)benzenesulfonamide substituted zinc(II) phthalocyanine



## O-64

### A coumarin-thiophene based fluorescent chemosensors bearing mono and disulfonamide receptoric part for selective determination of fluoride via reaction based mechanism

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Anions are play very important role in clinic, environmental, chemical and industrial processes. For example, DNA is a polyanion cluster which carry genetic data, different anions such as flouride, bromide, iodide, sulfite, phosphate, depends on their environment concentration in biological processes, are caused different disease and side effects in body. Determination of anion can be done with many several spectroscopic (ICP-OES), chromatographic, electrochemical or analytical methods are gave place to faster, more sensitive and easy test methods. By the aid of colorimetric and fluorometric chemosensors, without needing expensive and onerous pre-treatment or equipments, anions determination can be done with using little sample quantity through a UV lamb or even with naked eye. Alternative test methods that provide anion determination by the help of colour/fluorescence alteration are an attractive option as well determination of anions. Although many successful color/fluorescent chemosensors are developed until now there is still a need about the new chemosensors [1, 2].

In this work, we chose coumarin as the fluorophore/chromophore for signaling, and thiophene at the 3-position of the coumarin ring to modify the fluorescence properties of the coumarin core, in order to form a receptor for anions via an mono and disulfonamide functional group. We first studied the photophysical properties of the fluorescence chemosensors. Afterwards, binding properties of the chemosensor toward specific anions such as F<sup>-</sup>, Cl<sup>-</sup>, Br<sup>-</sup>, I<sup>-</sup>, AcO<sup>-</sup>, CN<sup>-</sup>, H<sub>2</sub>PO<sub>4</sub><sup>-</sup>, HSO<sub>4</sub><sup>-</sup> and ClO<sub>4</sub><sup>-</sup> was also investigated by using spectrophotometric, spectrofluorimetic and <sup>1</sup>H NMR spectroscopic titration methods. Interactions between disulfonamide derivative (L2) and floride anion can be shown in Figure 1. Also, upon addition of 1 equiv fluoride anion to L2 then trifloroacetic acid significant flourescence change is observed and can be seen in Figure 2.

*We are grateful to The Scientific and Technological Research Council of Turkey for providing financial support (Project Grant No: 114Z980) for this study.*

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**Keywords:** Fluorescence chemosensors, Coumarin-Thiophene hybrid, Mono and disulfonamide, Fluorescent anion sensors

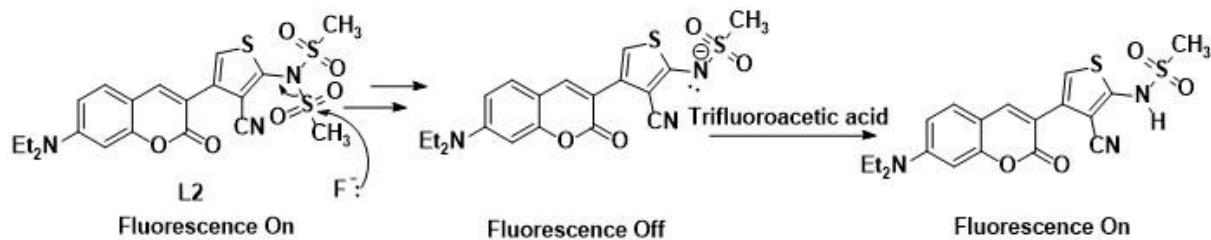


Fig. 1. Proposed desulfonation mechanism of chemosensor L2 with fluoride anion in DMSO solution

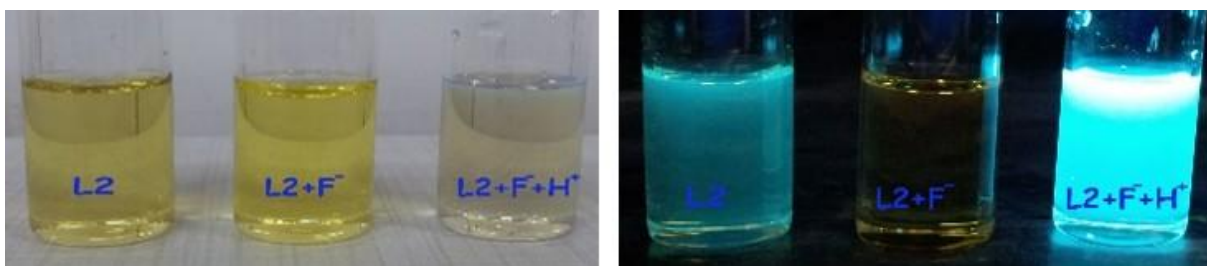


Fig. 2. Photographs of L2 ( $1 \times 10^{-3}$  M in DMSO) upon addition of 1 equiv fluoride anion ( $1 \times 10^{-2}$  M in DMSO) then trifluoroacetic acid under ambient light (above), under UV light (below, 365 nm).

O-65

Synthesis of some novel 3-acetoxy-2-methyl and 2,3-dimethoxy benzamides

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Benzamides are a significant class of amides. These compounds have been broadly studied for their biological and therapeutic activities: antitumor, antimicrobial, antibacterial, antifungal, anti-inflammatory, anticancer [1,2].

Substituted secondary amides were obtained from the corresponding 3-acetoxy-2-methylbenzoic acid and 2,3-dimethoxybenzoic acid which were synthesized using the procedure as described previously [3]. This involved reaction of 2,3-dimethoxybenzoyl and 3-acetoxy-2-methylbenzoyl chloride with the appropriate amine derivatives in the presence of THF to give substituted secondary amides (Fig. 1).

All the structures of these synthesized compounds were determined using IR, <sup>1</sup>H NMR and <sup>13</sup>C NMR spectroscopy, and elemental analysis techniques.

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**Keywords:** Secondary amides, amines, spectroscopic properties

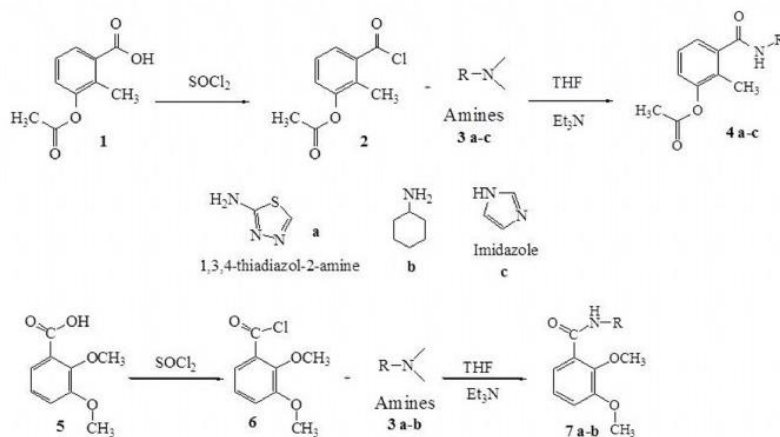


Fig. 1. Synthesis of substituted secondary amides

O-66

The spectroscopic and quantum chemical studies on structural, vibrational, electronic and chemical properties of 2-Chloroquinoline by using density functional theory (DFT)

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This study includes a spectroscopic investigation for 2-Chloroquinoline (2-CQ) obtained through quantum chemical calculations and supported with experimental results from IR, H<sup>1</sup> and C<sup>13</sup> NMR spectra. The optimized energy and geometrical parameters of the molecule (Fig. 1) were calculated by density functional theory (DFT) B3LYP method 6-311++G(d,p) basis set. After the geometric optimization of 2-CQ, vibrational spectral signature were carried out and compared similar structures like quinoline. The assignments of the vibrational spectra were obtained on the basis of the PED via VEDA 4 program. The electronic properties like HOMO and LUMO energies, molecular electrostatic potential surface (MEPs), density of states (DOS) and Mulliken charge analysis were also presented. H<sup>1</sup> and C<sup>13</sup> NMR chemical shift properties that were estimated by using the gauge-invariant atomic orbital (GIAO) method were discussed herein, comparing with the experimental data. Furthermore, NLO and thermodynamic properties were presented for studied molecule.

**Keywords:** 2-Chloroquinoline, DFT, Infrared, NMR, MEP

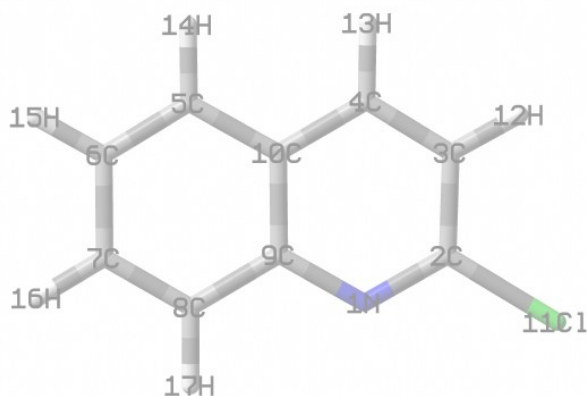


Fig. 1. 2-Chloroquinoline

0-67

## Spectroscopic Characterization and Density Functional Studies of New Thiadiazole 1,1-dioxide Compounds

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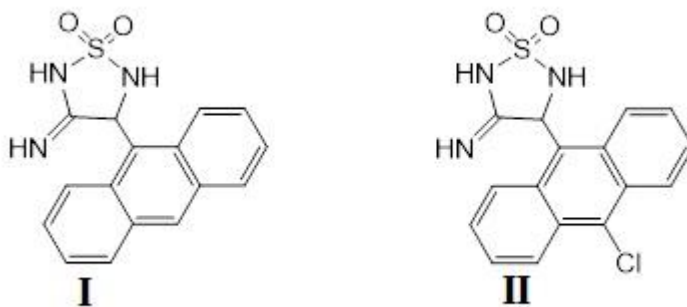
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Thiadiazole 1,1-dioxides are five-membered ring systems, and interesting pharmacophores with low toxicity. They exhibit a wide range of biological activities such as anti-HIV, hypertensive blocker, antiinflammatory antifungal, antiseptic, antiviral, analgesic, antibacterial, antitumor, antianxiety, antidepressant, antioxidant and radioprotective activities [1-3]. In addition, the their metal-complexes derivatives have higher effective [4]. Moreover, some new synthesized imine derivatives have been observed to be more effective than hydroxyurea anticancer drug used in treatment of melanoma, over-cancer and leukemia, and presented as hopeful chemotherapeutic agent [5]. In this study, 3-imino-4-(anthracene-9-yl)-1,2,5-thiadiazolidine 1,1-dioxide (I) and 3-imino-4-(10-chloroanthracene-9-yl)-1,2,5-thiadiazolidine 1,1-dioxide (II) (Fig.1) were synthesized and characterized by FT-IR, <sup>13</sup>C NMR, <sup>1</sup>H NMR and UV-vis spectroscopic techniques. Molecular geometries of the I and II in the ground state, vibrational frequencies, electronic absorption spectra and Gauge Including Atomic Orbital (GIAO) <sup>1</sup>H and <sup>13</sup>C NMR chemical shift values were calculated by using the Density Functional Theory (DFT) method with 6-311++G(d,p) basis set. The computed data were compared with the experimental data. In addition, Molecular Electrostatic Potential (MEP), Frontier Molecular Orbital (HOMO-LUMO) analysis and Non-Linear Optical (NLO) properties of the I and II were investigated using same theoretical calculations.

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**Keywords:** Thiadiazole 1,1-dioxides, NMR, FT-IR, UV-vis, DFT



**Fig.1.** The structure of the compounds (I and II)

0-68

## The exploring of the anion effect on the structure, spectroscopic and electronic features of some imidazolium based ionic liquids

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In this study, theoretical calculations of 1-Hexyl-3-methylimidazolium [HMIM] chloride [Cl], tetrafluoroborate [BF<sub>4</sub>] and hexafluorophosphate [PF<sub>6</sub>] ionic liquids (ILs) were carried out by using DFT/B3LYP method with 6-311++G(d, p) basis set. Primarily, optimized structure, geometric structure parameters, and vibrational wavenumbers were obtained. The UV spectra of the ILs were calculated in gas phase with same basis set using TD-DFT calculations. Then chemical reactivity indices such as atomic charges, dipole moment, HOMO-LUMO energies, chemical potential, chemical hardness and softness of the ionic liquids were calculated. Molecular electrostatic potential maps of the ionic liquids were examined. Furthermore, non-covalent interactions were studied and mapped with reduced density gradient (RDG) analysis. Results of calculation were compared by considering the anion structure dependency.

**Keywords:** 1-Hexyl-3-methylimidazolium chloride, 1-Hexyl-3 methylimidazolium tetrafluoroborate, 1-Hexyl-3-methylimidazolium hexafluorophosphate, DFT, RDG.

0-69

## Investigation of geometrical, electronic and spectroscopic properties of Fluorene-9-phenol molecule

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Fluorene-9-phenol (known as 9,9-bis(4-hydroxyphenyl)-fluorene; BHPF; Bisphenol FL; BPFL) is a kind of bisphenol fluorene with cardo skeleton. BPFL is mostly exploited for the production of polyarylates, polyesters, polyethers, polycarbonates, polyurethanes and epoxy resins since its cardo rings provide unique characteristics. BPFL has been preferred in industrial applications [1, 2] because of their high transparency, thermal stability, insulation and high-refractive index properties. In this study, the physical properties of fluorene-9-bisphenol using the density functional theory (DFT) calculations in both gas phase and different solvents such as ethanol, acetonitrile and water. Solvent effects have been analyzed by using the self-consistent reaction field (SCRF) method based on polarizable continuum model (PCM). In addition, the equilibrium geometry, process of optimization geometry, density of state, charge density, excess charge on the atoms, dipole moment, RDF and FT-IR spectra have been calculated using DFT calculations. Using time dependent (TD)-DFT method based on the optimized structure, the ultraviolet visible (UV-Vis) spectra characteristics, the highest occupied molecular orbital (HOMO), the lowest unoccupied molecular orbital (LUMO) and the frontier molecular orbital energy gap (HOMO-LUMO difference in energy gap, Eg) of Fluorene-9-phenol molecule have been compared with the experimentally measured in the literature and the results have been discussed in detail. Figs. 1 and 2 show Radial Distribution Function (RDF) and Probability Density of studied molecule, separately.

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**Keywords:** Fluorene-9-phenol, BPFL, Density Functional Theory



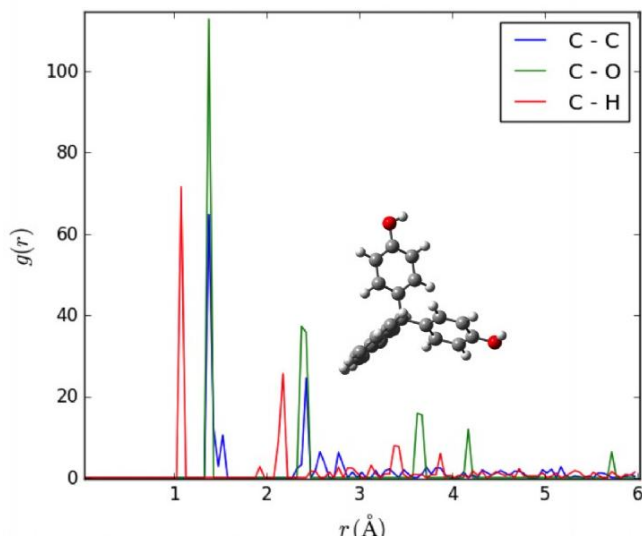


Fig.1. Radial Distribution Function (RDF) of Fluorene-9-phenol

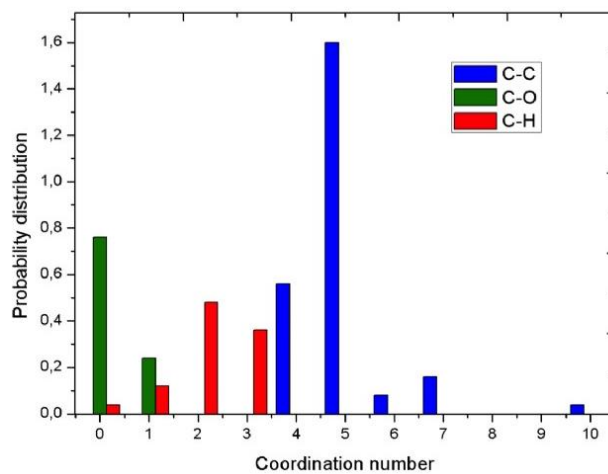


Fig. 2. Probability Density of Fluorene-9-phenol

0-70

## Heteroatom Effect on the Band Gap of Five-Membered Fused Bicyclic Polymers

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Conjugated organic polymers including delocalized  $\pi$ -electron systems have wide applications in optoelectronics (i.e. solar cells, light emitting diodes, field-effect transistors) with intense investigation [1]. One of cyclopentadithiophene derivative has recently been used in organic electronics and optical materials owing to their unique semiconducting and electronic properties, which has high electrical conductivity and low band-gap [2]. In this study, the band gap values of a series of fused bicyclic five-membered polymeric ring structures containing heteroatoms with the same skeletal (Fig. 1) were calculated to see the effects of heteroatoms on the band gaps. The calculations have been carried out by DFT methods (B3LYP and B3PW91) using different basis sets (6-31G(d,p) and cc-pVDZ) with Gaussian 09 program package [3]. Depending on the positions (X, Y and Z) of hetero atom the band gap values showed a systematic change depending on the size and electronegativity of the heteroatoms. It was also noted that the ring containing phosphor in Z positions have higher band gap values.

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**Keywords:** Five-membered fused bicyclic polymer, band gap, heteroatom effect.

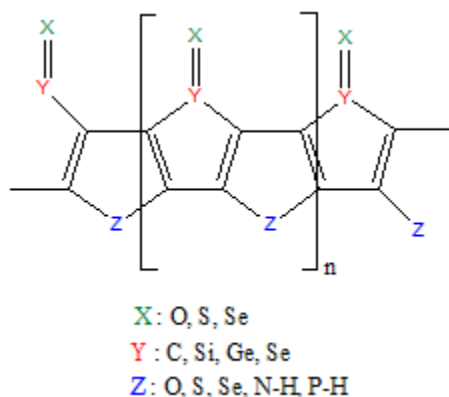


Fig. 1. Repeating structural unit

O-71

Isotopic Effect on Vibrational Spectra of  $TcX_3^+$  and  $TcX_3OH$  (X: O, S and Se):  
A DFT Study

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Technetium-99m has common usage for medical diagnostic studies. So, it would be valuable to make analysis of its compounds, along with its hypothetical compounds which may have potential for some applications. Childs et al. postulated that technetium is transported as  $TcO_3(OH)$  in the gas phase during vitrification, and it was found that it is made up of  $TcO_3^+$  core and OH- ligand bonded to this core [1]. This molecule together with its S and Se analogs have been analyzed theoretically [2]. In this study, these molecules with their cores have been examined from the vibrational (IR and Raman) point of view. All the calculations have been carried out by employing Gaussian 09 program package [3]. The potential energy distributions (PED) were calculated by using VEDA4 program [4]. The structures have been optimized through TPSTPSS with 6-31G(d,p) basis set for X, O, H atoms and Stuttgart RSC 1997 together with its effective core potential (ECP) for Tc atom. It was observed from the spectra that the vibrational frequencies of stretching and bending vibrations decreases with increasing atomic masses down the group of chalcogens (6A) in the periodic table as expected. The same decreases in vibrational frequencies have been obtained for increasing isotopic masses as well.

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**Keywords:** Isotopic effect, vibrational analysis, technetium

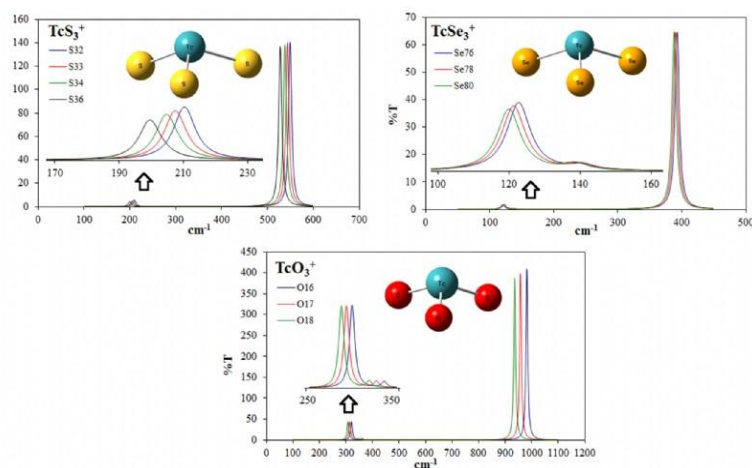


Fig. 1 Calculated IR spectra of  $TcX_3^+$

0-72

## Numerical study and simulation of diffusion of liquid in a long cylindrical packaging material in one-dimensional

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When a cylindrical packaging material is in contact with a liquid, this liquid may enter inside material.

The transfer of a liquid inside a cylinder material is described by considering transient diffusion with a constant diffusivity. The numerical model is developed by using the finite difference method. This model is capable of following the process of transfer by elaborate the concentration profiles with good accuracy.

The effects of the diffusivity, time of simulation and the radius of cylinder on the transfer through this material have been determined, so as to give a better repartition of liquid inside a cylinder.

**Keywords:** Modeling, finite differences, Diffusivity, transfer, Simulation

0-73

## Systematic Vibrational Study of Saturated Chain Alcohols by DFT

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Alcohols are important class of compounds used in several areas in industry, cosmetics and health applications. Production of sweeteners, making perfumes, using as valuable intermediates in the synthesis of other compounds makes them one of the most abundantly produced organic chemicals. They are used particularly in toiletries, pharmaceuticals, fuels, sterilizing hospital instruments, alcoholic beverages, making anesthetic ether, antifreeze, cleaning metals, as solvent, raw material for the manufacture of formaldehyde and resins [1]. Theoretical calculations of vibrational modes of alcohols have been made using molecular mechanical methods and developing force fields for semiempirical methods, extensively [2]. Recently, many new DFT functionals have been improved in which several effects have been considered. Searching the best DFT functional would be a valuable contribution to vibrational spectroscopic studies reproducing better experimental analogs. So, vibrational spectroscopic study of alcohols by a systematic way is aimed including saturated chain and branched alcohols using 10 functionals with different basis sets in this study. All the DFT calculations were performed using Gaussian 09 program package [3]. The scaling factors concerning regional and whole spectrum were improved for each method.

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**Keywords:** Alcohols, vibrational spectrum, DFT, scaling factor.

0-74

## Electronic Underpinnings of the Fascinating Class of Phosphido-Bridged Trinuclear Platinum Clusters

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The compound  $\text{H}(\text{PEt}_3)_3\text{Pt}_3(\mu\text{-PPh}_2)_3$  is the unique example of a  $46e^-$  phosphido-bridged triangular cluster, but its X-ray assigned stereochemistry appears questionable. In particular, the H-free  $\text{P}_3\text{Pt}_3(\mu\text{-P})_3$  metal core is identical to that of the  $44e^-$  cation  $[(\text{PEt}_3)_3\text{Pt}_3(\mu\text{-PPh}_2)_3]^+$  in two salts of the same publication. Also, the lack of a distortional effect due to the upright and strongly-bound hydride ligand is suspicious and intriguing aspects emerge from the inconsistent electronic structure. Although  $\text{H}(\text{PEt}_3)_3\text{Pt}_3(\mu\text{-PPh}_2)_3$  is fully validated by IR and NMR spectra, DFT optimizations (Fig. 1) never reproduced the proposed experimental structure but highlighted a different stereochemistry still consistent with the spectroscopic response. Here, a formal Pt(II) ion is essentially isolated and has square-planar coordination, completed by two trans-axial ligands (H and  $\text{Et}_3\text{P}$ ) out of the  $\text{Pt}_3$  plane. Given the chemical reliability of the silicomolecule, the crystals of the experimental structure have likely contents other than the hydridic cluster and a co-crystallized  $\text{PPh}_2\text{H}$  molecule. As a working hypothesis, the Pt-H and P-H linkages of the distinct components may have reacted together with  $\text{H}_2$  release, and subsequent crystallization of the salt whereas the ion pair  $[(\text{PEt}_3)_3\text{Pt}_3(\mu\text{-PPh}_2)_3]^+ / [\text{Ph}_2\text{P}]^-$ . This would explain the equal geometries of the putative  $46e^-$  cluster and the H-free  $44e^-$  cation. In the lack of any experimental X-ray dataset, the proposed crystal formulation could not be fully validated, but in the paper various aspects support its reliability. Essentially, the problem may arise from the misplacement of two H atoms (those of the mentioned Pt-H and P-H linkages), which does not affect the structural refinement but determines the chemical inconsistency.

**Keywords:** Tri-platinum clusters, Phosphido Bridges, Electronic and Stereochemical Aspects, Structural Reinterpretation

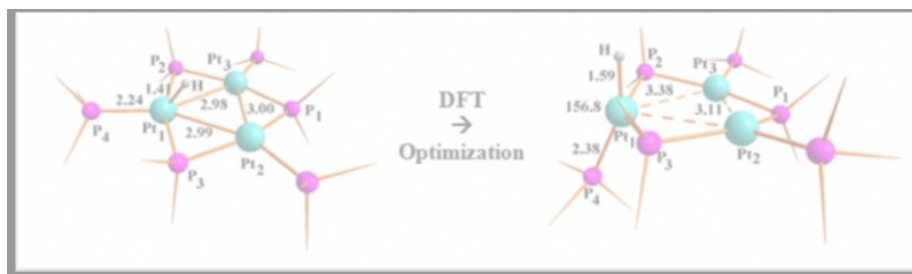


Fig. 1. DFT Optimization

## O-75

### Development of Quartz Crystal Microbalance Sensor by Molecularly Imprinted for Sensitive and Selective Detection of Pesticide in Apple

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2,4-Dichlorophenoxyacetic acid (2,4-D) is a systemic herbicide which selectively kills most broadleaf weeds by causing uncontrolled growth in them. 2,4-D is one of the oldest and most widely available herbicides in the world, having been commercially available since 1945 [1]. Molecularly imprinted polymers (MIPs) involve specific recognition sites in polymeric materials fabricated via the polymerization of the functional monomers and cross linkers in the presence of a template molecule with subsequent extraction of the template molecule [2]. Quartz Crystal Microbalance (QCM) is a simple, cost effective, quick response time, sensitivity, high-resolution and mass-sensitive chemical sensors, which has been used as a transducer in analytical chemistry, biology, environmental assays and others. [3]. In the present study, molecular imprinted QCM sensors were prepared to determine small amounts of 2,4-D. Nanofilms was synthesized in the presence of N- methacryloyl-(L)-tryptophan methyl ester (MATrp) as functional monomers and ethylene glycoldimethacrylate (EGDMA) as the cross linker. 2,4-D was embedded into nanofilm with MIP method. The surface morphology of nanofilm prepared on the sensor surface was determined by ATR-FTIR, contact angle measurements, ellipsometer and atomic force microscopy (AFM) (Figs. 1 and 2). The selectivity studies were made with 2,4-Dichlorophenol and 2,4,6-Trichlorobenzoic acid. The concentrations applied to the sensor were optimized by varying in the range 5-1000 ng/L, as well as denote a limit of detection (LOD) values of 2.18 ng/L. Apple was used as a sample and detected 61.9 ng/L 2,4-D. The results show that imprinted nanofilm have been found to be high selectivity, sensitivity and determine of 2,4-D in both aqueous solution and natural source.

*This study was supported by the TUBITAK project number: 115Z126.*

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3. A. Denizli, (2016) Afinitive Temelli Biyosensörler. ISBN: 978-605-88783-1-0, Ankara.

**Keywords:** Molecularly imprinting, SPR sensor, pesticide

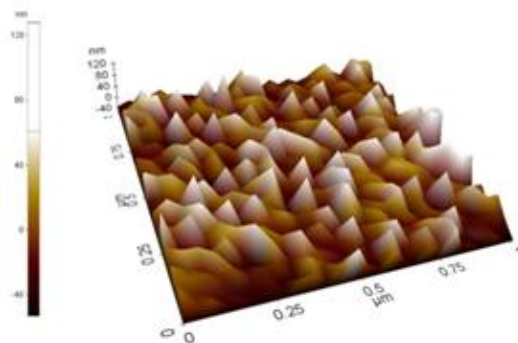


Fig.1 . Atomic Force Microscopy measurements: 2,4-D imprinted QCM sensor surface

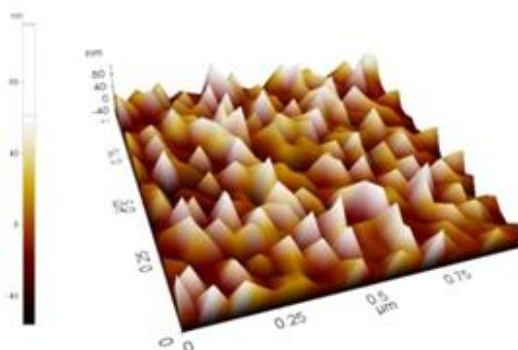


Fig. 2. Atomic Force Microscopy measurements: 2,4-D non-imprinted QCM sensor surface

Surface characterizations values of 2,4-D imprinted and nonimprinted QCM sensors

Surface	Contact angle (o)	Ellipsometer (nm)	Atomic Force Microscopy (nm)
Nonimprinted 2,4-D QCM sensors	$68.3 \pm 0.76$	$131 \pm 1.03$	$80 \pm 2.11$
Imprinted 2,4-D QCM sensors	$74.9 \pm 0.38$	$134.5 \pm 0.92$	$120 \pm 1.67$

Kinetic and isotherm parameters of QCM sensors

Scatchard Analysis	Association Analysis	Langmuir	Freundlich	Langmuir-Freundlich
$\Delta m_{maks}, nM/cm^2$ 3.065	$k_a, nM^{-1} \cdot s^{-1}$ 0.033	$\Delta m_{maks}, nM/cm^2$ 2.646	$\Delta m_{maks}, nM/cm^2$ 1.842	$\Delta m_{maks}, nM/cm^2$ 3.049
$K_A, nM^{-1}$ 2.614	$k_d, s^{-1}$ 0.088	$K_A, nM^{-1}$ 3.287	$1/n$ 0.526	$1/n$ 0.526
$K_D, nM$ 0.383	$K_A, nM^{-1}$ 0.375	$K_D, nM$ 0.304	$R^2$ 0.948	$K_A, nM^{-1}$ 0.460
$R^2$ 0.964	$K_D, nM$ 2.667	$R^2$ 0.998		$K_D, nM$ 2.174
	$R^2$ 0.937			$R^2$ 0.963



O-76

**Structural and spectroscopic analysis of (E)-2-((2,3-dihydroxybenzylidene)amino)-3a,7a-dihydro-1H-isoindole-1,3(2H)-dione**

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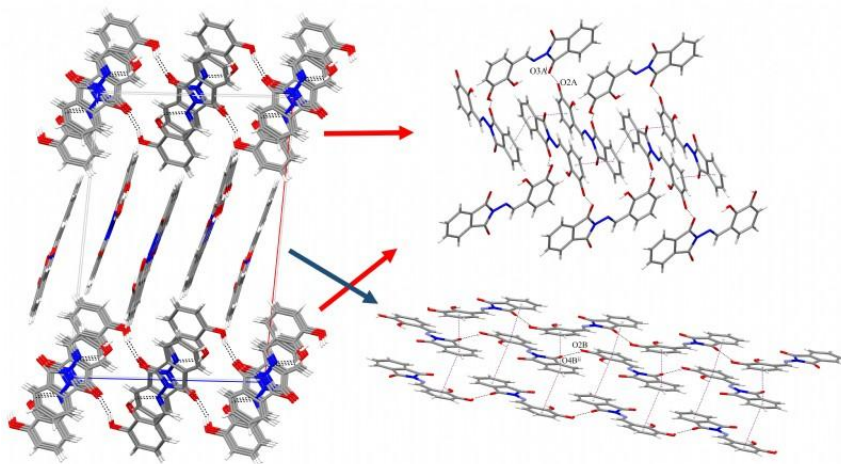
In the present study, the structure of (E)-2-((2,3-dihydroxybenzylidene)amino)-3a,7a-dihydro-1H-isoindole-1,3(2H)-dione was characterized by X-ray diffraction, FT-IR, NMR and UV-vis. spectroscopy. The title compound prefers enol-imin form as to X-ray results. The asymmetric unit of the compound contains two independent molecules. The crystal packing is stabilized by O-H...O type hydrogen bonds forming S(10) zigzag/linear chains. Adjacent chains are connected by  $\pi$ ... $\pi$  interactions (Fig. 1). Electronic structure and spectroscopic properties of the compound were calculated by using density functional theory (DFT) incorporated in B3LYP with 6-311++(d,p) basis set. The detailed vibrational assignments were performed on the basis of the potential energy distributions (PED) of the vibrational modes. Additionally, the Hirshfeld surface was drawn for visualizing the van der Waals distances and to determine the interaction sites.

*This study was financially supported by Giresun University (FEN-BAP-A-140316-36) in Turkey.*

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[2] M.H. Jamróz, *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy* 114 (2013) 220–230.

**Keywords:** X-Ray Diffraction, DFT, Hirshfeld Surface, FT-IR



**Fig.1.** The crystal packing is stabilized by O-H...O and  $\pi$ ... $\pi$  interactions and two independent molecules in asymmetric unit has a different hydrogen bonds forming S(10) zigzag/linear chains

O-77

**Analysis on molecular, spectroscopic and electronic behavior of  
 $C_{30}N_{12}O_2H_{32}Cl_2$  molecule: A theoretical approach**

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1,2,3-triazoles and derivatives such as 1,2,4-triazole have highly effective drug action. The 1,2,3-triazole ring is a core with important biological activities in most drugs. Some of these activities can be listed as antimicrobial, analgesic, anti-inflammatory, local anesthesia, cancer treatment, malaria treatment and antiviral. It is reported that some 1,2,3-triazole compounds are the main DNA interaction agent. In this study  $C_{30}N_{12}O_2H_{32}Cl_2$  (binary structures) molecular geometry (Fig. 1), vibrational frequencies and electronic properties in the ground state were performed by density functional theory (DFT) technique in the B3LYP/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. In addition, electronic properties and molecular electrostatic potential (MEP) are also performed. Calculated results show that the optimized geometry can well reproduce the crystal structure, and theoretical vibrational frequencies show good agreement with experimental values.

**Keywords:** Triazole, DFT, FT-IR, MEP

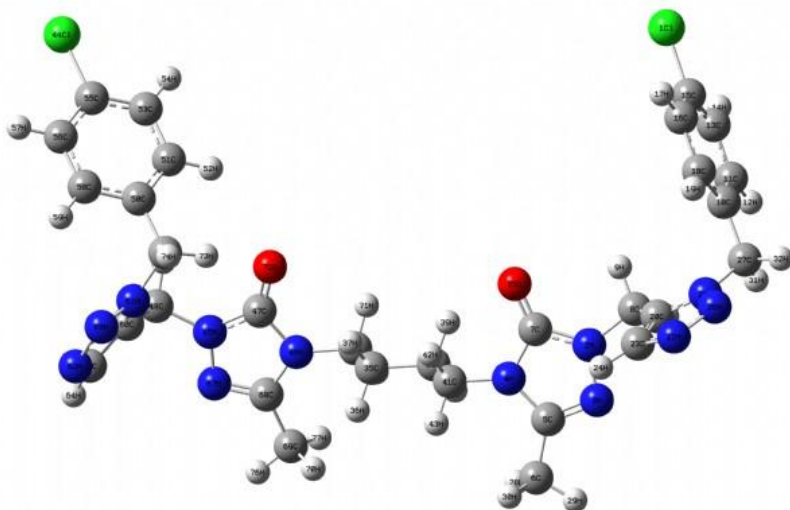


Fig. 1. The molecular structure of the  $C_{30}N_{12}O_2H_{32}Cl_2$  with non atom-labeling scheme.

O-78

**Experimental and Theoretical studies on Conformational, Molecular Docking, FT-IR, NMR and UV-vis spectroscopy of 1-Phenyl-ethanone O-propyl-oxime and 1-(4-Bromo-phenyl)-ethanone O-propyl-oxime**

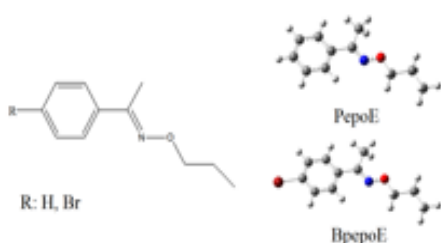
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Oxime molecules as a structure played a significant role in the theoretical chemistry. Since the oxime group possesses two heteroatom such as the nitrogen and oxygen atoms, these molecules show interesting electronic future. These type molecules, structures and electronic properties are important as theoretically or experimentally, due to the fact that they showed versatile antimicrobial activity and they exhibited high DNA binding affinity as well as significant cytotoxic activity.

In this study, two oxime ether molecules, namely 1-phenyl-ethanone O-propyl-oxime (PepoE) and 1-(4-bromo-phenyl)-ethanone O-propyl-oxime (BpepoE) have been synthesized and characterized by IR spectroscopy and elemental analysis. The structural and conformational properties were investigated using the density functional theory (DFT) with the B3LYP method combined with the 6-311++G(d,p) basis set (Fig. 1). The spectroscopic (FT-IR, NMR and UV-vis.) results obtained from DFT calculations were compared with experimental data, and they shows good agreement. In addition, the both oxime ethers have been used to carry out protein docking studies with the protein structure (5FCT which belongs to the class of proteins exhibiting the property as a Dihydrofolate synthase inhibitor) to find the most preferred binding mode of the ligands inside the protein cavity.

**Keywords:** DFT calculation, Molecular docking, Oxime ether, Spectroscopy



**Fig. 1. Optimized structures of PepoE and BpepoE**

## O-79

### Ferric oxide and yttria-stabilized zirconia for dental applications

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The use of ceramic materials such as zirconia, ZrO<sub>2</sub>, alumina, Al<sub>2</sub>O<sub>3</sub>, and glass-based ceramics in dental applications is highly desirable because of their excellent properties, including improved biocompatibility, wear resistance and chemical durability in addition to aesthetics. Biocompatibility is one of the most important advantages of zirconium based ceramics.

At atmospheric pressure, pure ZrO<sub>2</sub> is recognized to adopt three different crystalline structures. Pure zirconia has monoclinic structure below 16700C, tetragonal structure between 1670 and 23000C and cubic structure at high temperature (>23000C). The most stable phase of monoclinic ZrO<sub>2</sub> has limited practical applications due to its 3-5% volume expansion during cooling from the tetragonal phase.

Tetragonal and cubic zirconia is unstable and can be easily translated into monoclinic zirconia crystalline phase at room temperature. The addition of yttria, Y<sub>2</sub>O<sub>3</sub>, can stabilize tetragonal zirconia. In addition, a right amount of Y<sub>2</sub>O<sub>3</sub> has also protective effects on cells and can improve the biocompatibility of materials.

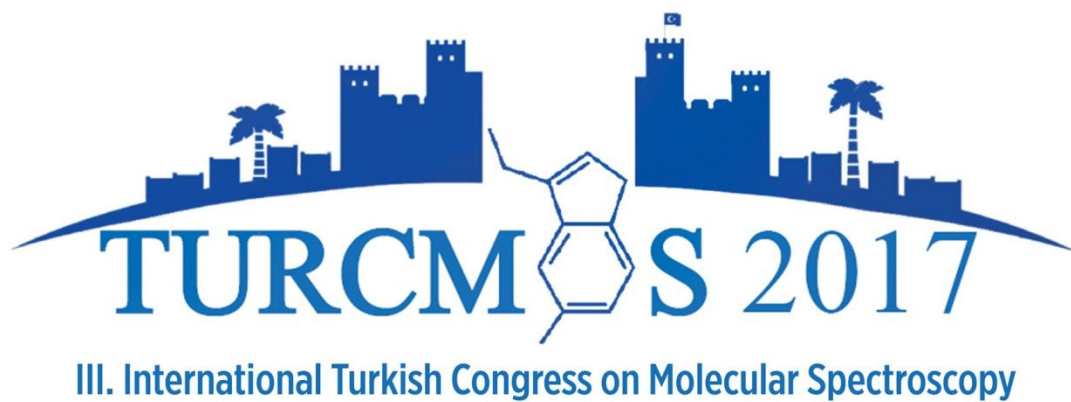
This paper presents for the first time the stabilization of the cubic zirconia phase with a 5 mol% Fe<sub>2</sub>O<sub>3</sub> content in the presence of higher Y<sub>2</sub>O<sub>3</sub> content. The aim of the work was to determine correlations between microstructural changes and spectroscopic properties of the stabilized zirconia. The investigation was realized by X-ray diffraction (XRD), Scanning Electron Microscopy (SEM), Fourier Transform Infrared (FTIR) spectroscopy, UltraViolet-Visible (UV-Vis) spectroscopy, Electron Paramagnetic Resonance (EPR) spectroscopy, Photoluminescence (PL) spectroscopy and density measurements. The obtained information will contribute to the understanding of the mechanisms associated to the formation of cubic zirconia vitroceramics that are highly desirable in technological applications.

The IR data demonstrate that the addition of Fe<sub>2</sub>O<sub>3</sub> significantly improves the cubic ZrO<sub>2</sub> content and increases the amount Zr-O-Fe and Y-O-Fe linkage. UV-Vis and PL data indicate smaller concentrations of oxygen vacancies with addition of higher Y<sub>2</sub>O<sub>3</sub> concentrations.

The EPR spectra are due to the presence of Fe<sup>3+</sup> ions and depend on the Y<sub>2</sub>O<sub>3</sub> content of samples. The increase of the Y<sub>2</sub>O<sub>3</sub> content leads to the decrease of the resonance line centered at g~4.3 and the appearance of a broad line centered at about g~2, characteristic of clustered ions.

*Acknowledgements: This research was supported by the Bridge Program Projects 2016 (PN-III-P2-2.1-BG-2016-0077) and Projects Ro-JINR 2017 Dubna, 59/2017, the phase with No. 4587-4-2016/2017.*

**Keywords:** iron-yttria-zirconia vitroceramics, XRD, FTIR, UV-Vis, PL and EPR spectroscopies.



## Poster Abstracts

P-001

## Theoretical and experimental vibrational spectroscopic study of 3X-thiophene-2-carbaldehyde [X=F, Cl or Br]

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The effects of halogen on the conformer vibrational properties of thiophene-2-carbaldehyde (C<sub>5</sub>H<sub>4</sub>OS) and 3X-thiophene-2-carbaldehyde [C<sub>5</sub>H<sub>3</sub>XOS; X = F, Cl or Br] were investigated employing the DFT method. For theoretical calculation, the B3LYP functional was used with the 6-31++G(d,p) basis set. Computations were focused on the two conformational isomers of the compounds in the gas phase. FT-IR and Raman spectra of 3X-thiophene-2-carbaldehyde have been experimentally reported in the region of 4000-400 cm<sup>-1</sup> and 4000-50 cm<sup>-1</sup>, respectively. Thiophene-2-carbaldehyde and its halogen derivatives were calculated and the effect of halogen on vibrational spectra was investigated.

**Keywords:** 3-halogen thiophene-2-carbaldehyde, FT, vibrational spectra, halogen effect.

P-002

## Experimental Studies on Infrared Spectra and Molecular Structure of the $C_{20}H_{18}N_4O$ Molecule

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Formazans are colored compounds, owing to p bonds and contain azohydrazone conjugated double bonds. Their color ranges from cherry red to red-violet. Experimental studies on infrared spectra and molecular structure of the  $C_{20}H_{18}N_4O$  molecule are investigated. All the data were as expected. Besides, the peaks which were observed in  $825-935\text{ cm}^{-1}$  fingerprint range are the proof of formazans structures. The IR data of formazans given in Table 1 the C=N stretching band appears at  $1505-1535\text{ cm}^{-1}$ . formazans, the C=N stretching band appears at  $1565-1551\text{ cm}^{-1}$ .

*We are grateful to ESOGU for financial support through Research Project No: 2016-1089.*

References

[1] Habibe Tezcan, T. An Uyar, Turk J Spectrosc, V,9,1, 2018-10

**Keywords:** Formazans, IR, Spectroscopy

**NOT  
ATTENDED**

P-003

## Vibrational Spectra and Molecular Structure of The 1-(o-tolyl)-3-(o-hydroxyphenyl)-5-phenylformazans Molecule. Experimental Study

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Formazans are colored compounds. There are important fields of use for formazans such as analytical reagents, trace element determination, photos and thermochromic materials. Vibrational spectra and molecular structure of the 1-(o-tolyl)-3-(o-hydroxyphenyl)-5-phenylformazans molecule were investigated. The FT-IR spectra have been measured for the title compound in the solid state. The vibrational frequencies of the fundamental modes of the compound have been precisely assigned and analyzed. The IR data of formazans given in Table 1 of the C=N stretching band appears at  $1505\text{--}1535\text{ cm}^{-1}$ . It was observed vibration peaks at  $3095\text{--}3100\text{ cm}^{-1}$  for aromatic C-H, at  $1600\text{--}1610\text{ cm}^{-1}$ , C=C, at  $1505\text{--}1535\text{ cm}^{-1}$  for C=N, at  $1450\text{--}1455\text{ cm}^{-1}$  for N=N.

*We are grateful to ESOGU for financial support through Research Project No: 2016-1089.*

[1] Habibe, Tezcan; Eriş, Gülçuk, *Dyes Pigments* 71 (3), 2017, 33-40

**Keywords:** Formazan, Spectroscopy, FT-IR



P-004

## FT-IR Spectroscopic Study of M(Terephthalic Acid)Ni(CN)<sub>4</sub> Complexes (M = Mn, Co, Ni, Cd and Hg)

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In this study, complex of terephthalic acid–tetracyanonickel, given by the formula M(terephthalic acid)Ni(CN)<sub>4</sub> (M = Mn, Co, Ni, Cd and Hg), were obtained for the first time through chemical methods. In literature, several studies were made with the terephthalic acid (TPA) molecule (Fig. 1). The FT-IR spectroscopic data in the region of (4000–400 cm<sup>-1</sup>) was recorded and the IR frequencies were given and explained in detail. The results of spectral analyses of the newly synthesized complexes of terephthalic acid–tetracyanonickel suggest that these complexes are new examples of the Hofmann–type complexes. In title complexes, the Hofmann-type complexes formed by bounding electrons of oxygen–donor atoms of the carboxyl groups of terephthalic acid ligand molecule to transition metal atoms consist of the corrugated |M–Ni(CN)<sub>4</sub>|<sub>∞</sub> polymeric layers which are held in parallel through the chain of (–M–TPA–M–).

**Keywords:** Molecular Spectroscopy, Terephthalic acid (TPA), Fourier Transform Infrared Spectroscopy (FT-IR), Hofmann–type Complexes

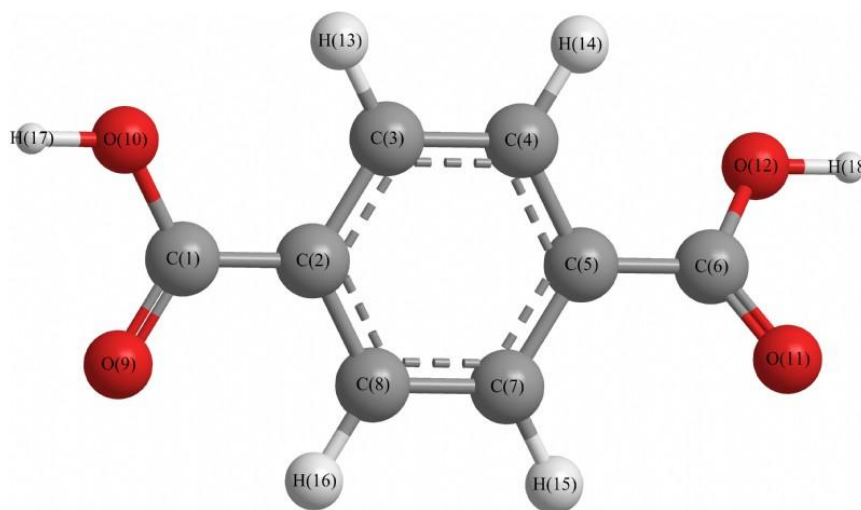


Fig. 1. The molecular structure of Terephthalic Acid

P-005

## Crystal Structure and Infrared Spectroscopic Properties of Redetermination poly-[cobalt (II)(tetraaqua)(fumarato)]

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In the present work; the crystal structure of the title compound,  $C_4H_{10}CoO_8$ , has been reinvestigated with improved precision. The title compound was re-synthesized and structurally characterized by infrared spectral and single-crystal X-ray diffraction methods. The structure of the complex consists of a one-dimensional polymeric chain, in which the Co(II) ion is linked by carboxylate groups of fumarate ion. The Co(II) ion is coordinated with four oxygene atoms of aqua molecules and two oxygen atoms of fumarate ions in a octahedral arrangement (Fig. 1). The x-ray diffraction data of title compound was collected using MoK $\alpha$  radiation on a Bruker APEX-II CCD diffractometer at 296(2) K. The crystal structure of the title compound was determined with direct methods and were refined by the full matrix least squares method to  $R = 0.036$ . The compound crystallizes in the monoclinic, space group P21/c with  $a = 7.4973(9)\text{\AA}$ ,  $b = 14.3932(16)\text{\AA}$ ,  $c = 7.7153(9)\text{\AA}$ ,  $\alpha = 90^\circ$ ,  $\beta = 99.531(4)^\circ$  and  $\gamma = 90^\circ$ . Furthermore, an extensive series of strong Co...O (fumarate), Co...O-H (aqua) and O-H...O (fumarate) hydrogen-bonding interactions involving both the complex molecule and water molecule generate a three-dimensional network.

**Keywords:** cobalt complex, fumarate complex, X-ray; infrared spectra

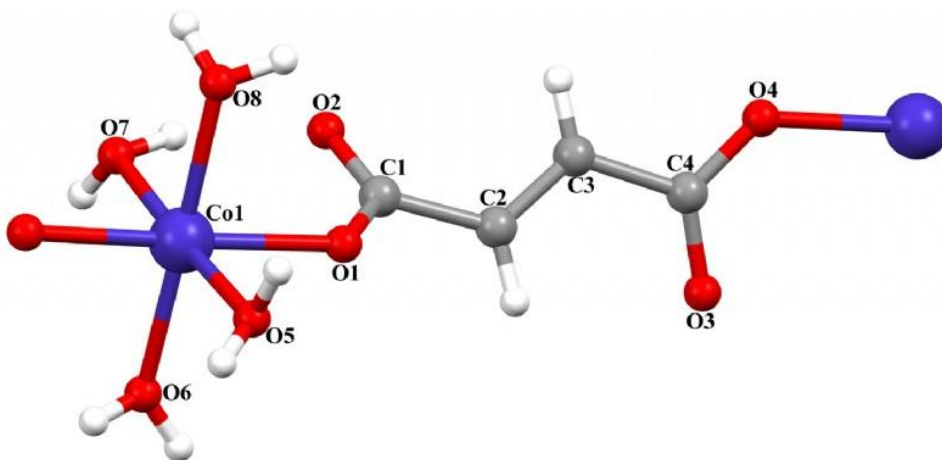


Fig. 1. The molecular structure of poly-[cobalt (II)(tetraaqua)(fumarato)].

P-006

**Removal of Lead(II) by biosorption of Bacillus subtilis ATCC 6051(B1) and two wild strain Bacillus licheniformis (Fl and Fs) with a comparative study from aqueous solutions**

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<sup>3</sup>Unit of Quality and Technology, GAP International Agricultural Research and Training Center, Diyarbakir-Turkey

Biosorption by bacteria is an effective method for the removal of toxic elements from drinking water and waste water [1]. Biosorption of Pb(II) from aqueous solutions was studied in batch method by using death bacteria Bacillus subtilis ATCC 6051(B1) and Bacillus licheniformis (Fl and Fs) sp. [2, 3]. Two types of Bacillus licheniformis (Fl and Fs) sp. was extracted from soil in the area of Tigris River. The concentration Pb was measured by AAS and ICP-OES. The maximum adsorption capacity of Pb<sup>2+</sup> was determined as 40.82, 43.48, 42.92 mg/g, respectively for B1, Fl and Fs (pH 5,5, 50 min. 45 °C with 5.0 mg/L of initial concentration). The isotherm, kinetic and thermodynamic parameters were calculated to describe the adsorption behaviour of bacteria (B1, Fl and Fs) and the data showed that the mechanism of reaction was found to be endothermic from values of  $\Delta G < 0$ ,  $\Delta H > 0$  and  $\Delta S > 0$ . Uptake kinetics follows the pseudo-second-order kinetic equation and the equilibrium is well described by Langmuir model. The chemical composition of the adsorbents were investigated by FTIR, TGA, DTA, SEM and EDX. The analysis shows that the capacity adsorption of Pb (II) by bacteria Fl was found to be higher than bacteria B1 and Fs.

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**Keywords:** Bacillus subtilis, Bacillus licheniformis, Biosorption

P-007

## Determination of Paraben Preservatives in Cream Samples Using Matrix Solid-Phase Dispersion Coupled with Supramolecular Solvent-Based Microextraction and HPLC-UV

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Parabens, or p-hydroxy-benzoate esters, are commonly used as antimicrobial agents and preservatives in the personal care products, pharmaceutical, and food industry. Parabens are thought to break the endocrine system and increase cancer risk. A new analytical method has been presented for the determination of paraben preservatives in semi-solid cream samples by matrix solid-phase dispersion combined with supramolecular solvent based microextraction. Due to matrix effect, parabens were first extracted from the samples by matrix solid-phase dispersion using silica gel as sorbent material with a clean-up performed with tetrahydrofuran in the elution step. The eluate (500  $\mu$ L), n-decanol (120  $\mu$ L) and water (4.5 mL) were then mixed in a polyethylene pipette to form supramolecular solvent. Finally, the analytes in the supramolecular solvent were separated and determined by liquid chromatography with ultraviolet detection. Under the optimized conditions, the limits of detection and limits of quantification for the parabens were in the ranges 30-42 ng/g and 101-140 ng/g. Relative standard deviations based on five replicate extraction of 25  $\mu$ g/g of each paraben were less than 6.7 % for intra-day and 7,9 % for inter-days precision. This method has been successfully applied to analyze the cosmetic samples and satisfactory recoveries were achieved.

**Keywords:** Parabens, matrix solid-phase dispersion, supramolecular solvent, liquid chromatography-UV detection

P-008

## HF and DFT Study of Prism Structure of Water Clusters

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Special geometries of water clusters, such as; cage, prism and ring etc., have been an interesting area due to their different energetics and structural properties at nanoscale [1-4] In the present study, prism structures of water clusters based on trimer, tetramer, pentamer, hexamer and heptamer rings have been investigated by using Hartree-Fock (HF) method and Density Functional Theory (DFT) method with B3LYP and PBE functionals [5]. In the theory, 6-311++G(d,p) basis set has been selected for all (H<sub>2</sub>O)<sub>n</sub> clusters ( for n ≤ 30). The structural and energetic parameters; total energies with zero-point energy corrections, binding energies per molecule and per ring, the highest occupied molecular orbital energy (HOMO), the lowest unoccupied molecular orbital energy (LUMO), HOMO-LUMO gaps and vibrational spectra have been determined and compared with respect to the used methods. It has been shown that the hexagonal prisms of water clusters are relatively more stable in the considered particular prism-like geometries.

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**Keywords:** Water cluster, HF, DFT

P-009

## Synthesis, characterization, spectroscopic properties, DFT calculations and antimicrobial activities of p-toluenesulfonamide,N,N'-1,3-propanediylbis(ptspr) and [Cu(II)(phenanthroline)<sub>2</sub>]ptspr

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In this research, p-toluenesulfonamide,N,N'-1,3-propanediylbis (a disulfonamide compound, ptspr) and [Cu(II)(phenanthroline)<sub>2</sub>]ptspr compounds were newly synthesized. The structure of ptspr was investigated by using elemental analyses; FT-IR, <sup>1</sup>H NMR, <sup>13</sup>C NMR, HETCOR, COSY, LC-MS, and magnetic susceptibility; conductivity measurements. The vibrational frequencies were calculated and scaled values were compared with experimental values. The complete assignments were performed on the basis of the total energy distribution (TED) of the vibrational modes, calculated with scaled quantum mechanics (SQM) methods. The H and C nuclear magnetic resonance (NMR) chemical shifts of the studied molecule were calculated using the Gauge-Invariant Atomic Orbital (GIAO) method. The geometric parameters, vibrational bands and chemical shifts were compared with available experimental data of the molecule. The fully optimized of the molecule were found to be consistent with the X-ray crystal structure. The observed and calculated frequencies and chemical shifts were found to be in very good agreement. Additionally, nonlinear optical properties (NLO), HOMO, LUMO molecular orbital energies were investigated with B3LYP/6-311++G(d,p) level of theory. Further analyses were also made for [Cu(II)(phenanthroline)<sub>2</sub>]ptspr complex by using elemental analysis, LC-MS, magnetic susceptibility; conductivity measurement and FT-IR. The antibacterial activities of synthesized compounds were studied against some Gram-positive and Gram-negative bacteria by using the microdilution and disk diffusion method. The biological activity screening showed that complex have more activity than ligand against the tested bacteria.

**Keywords:** Disulfonamides, Complex, FT-IR, SQM, Antibacterial activity

**P-010**

**Synthesis, Characterization, DFT Calculations and Antimicrobial Studies of Heteroaromatic Diimines and Their Copper(II) Complexes**

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Biologically active copper(II) complexes having  $[Cu(II)L]Cl_2$  formula were synthesized with heteroaromatic diimine ligands; 1,4-bis[3-(tiyofen-2-karboksaldimin)propil]piperazin(L1) and 1,4-bis[3-(furan -2-karboksaldimin)propil]piperazin(L2). Ligands and their Cu(II) complexes were characterized by elemental analysis, spectral methods ( $^1H$ - $^{13}C$  NMR, FT-IR, UV-Vis, LC-MS), magnetic susceptibility and molar conductivity measurements.  $^1H$  and  $^{13}C$  shielding tensors for L1 and L2 were calculated with GIAO/DFT/B3LYP/6-311++G(d,p) methods in  $CDCl_3$ . The vibrational band assignments, frontier molecular orbital energies (FMOs), absorption spectra, nonlinear optical (NLO) activity, reactivity descriptors were performed at B3LYP/6-311++G(d,p) level of theory. Mononuclear metal chelates show distorted tetragonal geometry. Room temperature magnetic moments for  $[Cu(II)L]Cl_2$  complexes are 1.88 B.M. and 2.03 B.M. and their molar conductivities are detected between 142.17-148.10  $\mu S/cm$ . Ligands and  $[Cu(II)L]Cl_2$  complexes were screened for their antibacterial activities as MIC values in mM.

**Keywords:** Diimines, copper(II) complexes, antimicrobial activity, FT-IR, DFT

**P-011**

**Estimation of Bloodstain Age on Linen Fabric by Fourier Transform Infrared Spectroscopy**

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The correct estimation of bloodstains age is a prerequisite to enlighten a crime. Although various techniques in the identification of this trace age have been demonstrated, none of them is established and yet implemented in forensic practice. Among vibrational spectroscopic methods, the utility of Attenuated total reflectance Fourier Transform Infrared Spectroscopy (ATR-FTIR) in the estimation of bloodstain age has been demonstrated. Therefore, the current study was performed to indicate the utility of this spectroscopy combined with chemometric analysis approaches in the estimation of bloodstain age on linen samples with various temperatures (10°C, 20°C, 30°C and 40°C) and time intervals (24, 48, 72 hours, 5 and 10 days). To demonstrate this utility, hierarchical cluster (HCA) and principal component analysis (PCA) were applied to the spectra of the fabric samples with various spectral ranges. To demonstrate the power of the used approach in the age estimation, sensitivity, specificity and accuracy values were calculated from HCA dendrograms. Hierarchical cluster (HCA) analysis revealed that the groups were separated from each other with a very high sensitivity, specificity and accuracy that depend on temperature and time. These discriminations were also supported by the PCA scatter plots. These results imply that ATR-FTIR spectroscopy has potential to accurately and non-invasively determine the age of the bloodstain in routine forensic biological analysis.

**Keywords:** ATR-FTIR, Bloodstain age estimation, Chemometric analysis, Temperature



P-012

## Synthesis and Characterization of Noscapine Loaded Hydroxyapatite Nanoparticles

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Noscapine, a widely used cough suppressant for decades has recently been shown to cause significant inhibition and regression of tumor volumes without any detectable toxicity in cells or tissues. Noscapine nanoparticles offer a promising strategy for drug delivery targeted to tumor cells by improving the bioavailability and distribution of the drug and reducing drug response to the body's response. Hydroxyapatite is a material composed of hard tissues such as bones and teeth. This material has properties such as low solubility in water or body fluids and is attractive for bioceramic application in medicine. In addition, different production methods of particles with hydroxyapatite can be used, and various structures of different materials such as nanoparticles can be synthesized by these methods. Synthetic calcium phosphates are used as bone substitutes because they exhibit good tissue compatibility.

In this study, nanoparticles loaded with noscapine were formed and these nanoparticles were characterized. Hydroxyapatite was synthesized by sol-gel method. In the formation of the sol-gel method, 60% by weight of the natural bone is amorphous/crystallized Hydroxyapatite and theoretically Ca/P molar ratio is 1.67. In the preparation of sol-gel, 8.2 g. (0.0347 mol) of calcium nitrate tetra hydrate was dissolved in 50 ml. of ethanol, then 2.38 g (0.02 mol), diammonium hydrogen orthophosphate was dissolved in 50 ml. of pure water and then noscapine 10 times the mass of calcium was dissolved in 30 ml of methanol. The solutions were prepared by stirring continuously at 70 °C for 4 hours on a magnetic stirrer. Prepared solutions were hydrolyzed by aging for 24 hours. To these different solutions, especially noscapine, which is the third solution, was added dropwise to the medium phosphate solution with constant stirring at 70 °C. The final solution of calcium nitrate was added to these solutions, so that the mixture solution was gelled by continuous stirring at 70 °C for 4 hours.

The obtained hydroxyapatite wet powders were filtered to produce nanoparticles, washed with demineralized water and the product was dried. HPLC, Scanning Electron Microscopy (SEM) and Fourier Transform Infrared Spectroscopy (FT-IR).

**Keywords:** Noscapine, Hydroxyapatite Nanoparticle, Synthesis, Characterization.

P-013

Determination of Progress in Acrylic Acid Modification on Polyvinylidene Fluoride Membrane by Infrared Spectroscopy

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Performances of filtration membranes could be improved by blending with organic/inorganic additives or by treating plasma and radiation induced grafting techniques. In this study, acrylic acid (AA) was applied to surface of the polyvinylidene fluoride (PVDF) membrane by chemical grafting method to obtain better membrane materials (Fig. 1). Changes were investigated by Fourier transform infrared spectroscopy (FT-IR), scanning electron microscopy (SEM) and contact angle measurement techniques. The band of  $1710\text{ cm}^{-1}$  and increase at cross section thickness of AA grafted sample after modification provided information about progress of grafting. Skin layer coated to membrane surface was seen at the SEM images. Water uptake capacities (WU%) of grafted membrane increased to 64% from 57% of PVDF relatively with increasing hydrophilicity. Also it was understood by decreasing contact angles of that AA modified sample. By using easy and low cost method acrylic acid was effectively incorporated on to surface of the PVDF membrane. That is the important method to prepare functional structures which contain specific groups on surface of membrane via acrylic molecules in addition to obtain high performance filtration membranes.

**Keywords:** Chemical grafting, filtration membranes, PVDF, acrylic acid

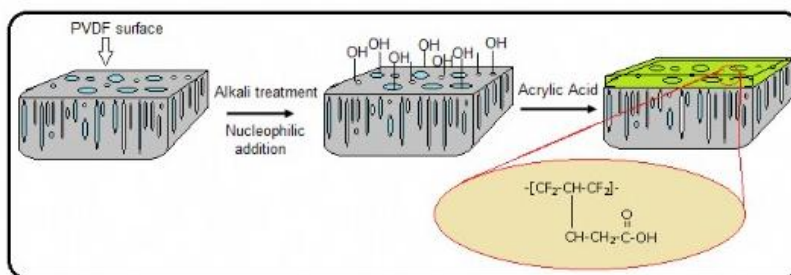


Fig. 1. Representative illustration of AA grafting progress on PVDF membrane surface

**P-014**

## **Investigation of the molecular structure of 3-formylphenylboronic acid molecule by density functional approach**

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3-Formylphenyl boronic acid molecule (3FPBA) were investigated by IR, Raman, UV-Vis spectroscopic techniques, theoretically and experimentally. The theoretical calculations were performed by using GAUSSIAN 09 software. The molecular geometry and vibrational frequencies of 3FPBA molecule were calculated using the density functional methods (B3LYP with 6-311G++(d,p) basis set). In addition we investigated 6 different solvent effect on the vibrational frequencies of the related molecule. The electronic properties, such as excitation energies, oscillator strength, wavelengths, HOMO and LUMO energies, were performed by time-dependent density functional theory (TD-DFT).

### *Acknowledgements*

*This work was supported by Ahi Evran University Scientific Project Unit (BAP) with, Project No: FEF.A3.16.012.*

**Keywords:** 3-Formylphenyl boronic acid, DFT, IR and Raman spectra, UV spectra, HOMO-LUMO.

P-015

**Structural and vibrational spectroscopy investigation of the 4-formylphenylboronic acid molecule**

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*Department of Physics, Ahi Evran University, Kırşehir, Turkey*

4FPBA has  $C_7BO_3H_7$  group,  $C_6H_4$  (phenyl), COH (formyl) and  $B(OH)_2$  group. The possible structures of the title molecule are investigated, due to model system  $B(OH)_2$  and the positions of the hydrogen atoms, whether directed away from or toward the ring. This model offered four conformers/isomers as named C1, C2, C3 and C4. As well as the analysis of the conformation according to the orientation of the oxygen atom in the COH group as named C1A, C2A, C3A and C4A. The computational results diagnose the most stable conformer of 4FPBA. The vibrations wavenumber of 4-formylphenylboronic acid (4FPBA) were investigated by different spectroscopic techniques (such as infrared and Raman). This spectra were recorded in the solid phase. HOMO-LUMO analyses were performed. The theoretical calculations for the molecular structure and spectroscopic studies were performed with DFT (B3LYP) and 6-311++G(d,p) basis set calculations using the Gaussian 09 program. The results of theoretical calculations for the spectra of the title compound were compared with the observed spectra.

*This work was supported by Ahi Evran University Scientific Project Unit (BAP) with, Project No: FEF.A3.16.012.*

**Keywords:** 4FPBA, DFT, FT-IR, FT-Raman, HOMO-LUMO.

P-016

## Characterization of TiO<sub>2</sub> Blended Polyvinylidene Fluoride Composite Materials for the Removal of Organic Substance from Water by Spectroscopic Techniques

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TiO<sub>2</sub> at 2, 4, 6% mass ratio was blended with polyvinylidene fluoride solution in dimethyl formamide and flat sheet TiO<sub>2</sub>-PVDF composites were prepared according to phase inversion technique (Fig. 1). Prepared samples were characterized by Fourier transform infrared spectroscopy (FT-IR), scanning electron microscopy (SEM) and contact angle measurement. Changes in crystallinity of polymer were understood by disappearing of the bands at 975 cm<sup>-1</sup> which represents α-phases of PVDF and emerging of hydrogen bonding. Formation of new channels and finger like structures at SEM images of samples provided information about effect of additive as far as decreasing contact angle values from 74° of PVDF to 58, 61 and 64° for composites. Bovine serum albumin (BSA) was used as a model organic pollutant and BSA rejection performances of composite membranes were investigated. Initial and final concentrations of BSA solution were determined by Ultraviolet-Visible (UV) Spectroscopy at 280 nm wavelength and rejection performances of samples (R%) were calculated. Approximately 37% increase in rejection was obtained with TiO<sub>2</sub>-PVDF composite membranes. TiO<sub>2</sub> acted as a hydrophilic modifier in addition to its multifunctional effects such as inducing the fingerlike structure formation and readjustment of crystallinity.

**Keywords:** TiO<sub>2</sub> additive, filtration membranes, PVDF, BSA rejection

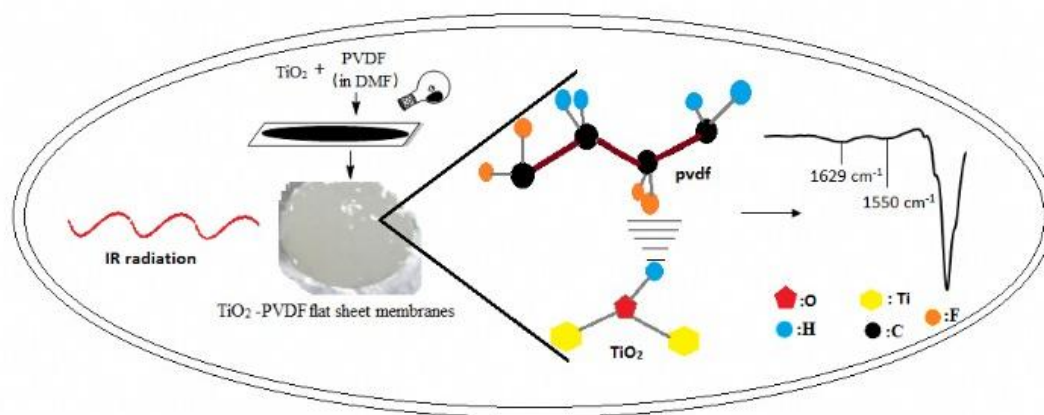


Fig. 1. Representative illustration of TiO<sub>2</sub>-PVDF preparation steps and hydrogen bonding

P-017

## Density Functional Theory and Spectroscopic Studies of 5-Nitro-2-Oxindole

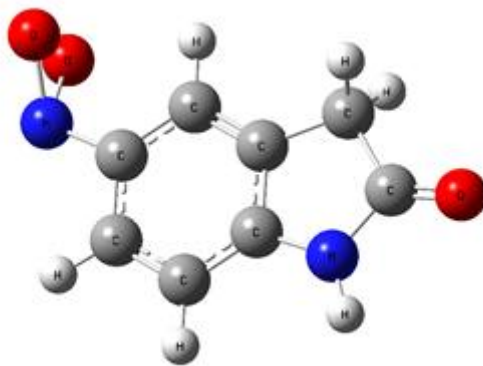
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Isatin, also known as (1H-indole-2,3-dione), has been found to be a heterocyclic motif in a variety of dyes, agrochemicals, and pharmacologically active compounds by virtue of its unique size and privileged electronic properties. Isatin derivatives are also used in variety of pharmacologically active compounds.

In present study, the molecular structure (Fig. 1), molecular electrostatic potential, NBO analysis, linear and non-linear optical properties of 5-Nitro-2-oxindole (5N2O) have been investigated using density functional theory (DFT) calculation with 6-311G++(d,p) basis set. FT-IR ( $4000\text{--}400\text{ cm}^{-1}$ ) and FT-Raman ( $3500\text{--}50\text{ cm}^{-1}$ ) spectra of (5N2O) have been measured and analyzed. The assignment of bands observed vibrational spectra have been made by comparison of its theoretical vibrational frequencies obtained using B3LYP/6-311G++(d,p) basis set. The scaled frequencies resulted in good agreement with the observed spectral patterns.

**Keywords:** 5-Nitro-2-oxindole, FT-Raman, FT-IR, DFT, Hyperpolarizability



**Fig. 1.** Optimized structure obtained using B3LYP/6-311++G(d,p) of 5-Nitro-2-oxindole (5N2O).

P-018

Theoretical and vibrational studies of a tricyclic antidepressant, Imipramine hydrochloride

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Tricyclic drugs act on the central nervous system by blocking the synaptic alpha receptor re-uptake of noradrenaline and serotonin into the neurons, thus prolonging their effects [1]. Imipramine Hydrochloride,  $C_{19}H_{24}N_2.HCl$ , is the prototypic tricyclic antidepressant inhibitor of norepinephrine and serotonin neuronal reuptake [2]. The molecular structure, molecular electrostatic potential (Fig. 1), NBO analysis, linear and non-linear optical properties of Imipramine Hydrochloride have been investigated using density functional theory (DFT) calculation with 6-311G++(d,p) basis set. FT-IR ( $4000-400\text{ cm}^{-1}$ ) and FT-Raman ( $3500-50\text{ cm}^{-1}$ ) spectra have been measured and analyzed. The assignment of bands observed vibrational spectra have been made by comparison of its theoretical vibrational frequencies obtained using B3LYP/6-311G++(d,p) basis set. The scaled frequencies resulted in good agreement with the observed spectral patterns.

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**Keywords:** Imipramine Hydrochloride, FT-Raman, FT-IR.

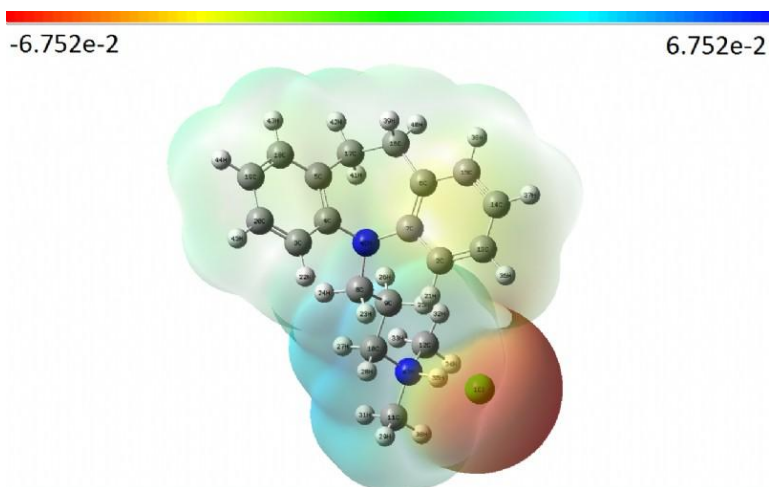


Fig. 1. MEP surface of Imipramine hydrochloride obtained from B3LYP method using 6-311G++(d,p).

P-019

## Determination of the Effect of Polymeric Nanoparticle in Biological Samples with ATR-FTIR Spectroscopy

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Polymeric nanoparticles as compatible materials, which are ever increasing to being explored in biomedical applications such as drug delivery, are able to transport of bioactive agents through target tissues. Fourier transform infrared (FTIR) spectroscopy provides compositional and structural information on a sample concerning the biochemical components like proteins, lipids and nucleic acids. The aim of the study was to reveal the biochemical changes in tissues and body fluids as a result of single dose toxicity test in mice exposed to polymeric nanoparticles using FTIR spectroscopy.

The protocol was approved by the Ege University, Local Ethical Committee of Animal Experiment (28.09.2016, 2016-088). Lys-graft-p(HEMA) nanoparticle was achieved with surfactant free emulsion polymerization and grafting procedure. The characterization and toxicity analyses of nanoparticle were carried out with several methods. The up and down procedures was used to determine the lethal dose (LD50) according to the OECD Guideline 425. Lys-graft-p(HEMA) was administered as limit dose (2.000 mg/kg body weight) to albino mice (15–20g) orally. Animals were also placed in the metabolic cages to collect urine and feces. Mice tissue homogenates prepared from the selected organs (brain, heart, liver, lung, spleen, intestine and kidney) and body fluids were analyzed with attenuated total reflection (ATR)-FTIR spectroscopy. The sample was recorded in the mid-IR spectral region (4000-800  $\text{cm}^{-1}$ ), where the absorbance of biochemical components (i.e., proteins, lipids, carbohydrates and nucleic acids) of biological samples are detected.

In vivo single dose toxicity assay showed that no lethality was detected with oral doses of the nanoparticle. According to the ATR-FTIR results, no structural degradation was observed in the mice tissues and body fluids after 72h of exposition to polymeric nanoparticles.

**Keywords:** Nanoparticle, ATR-FTIR spectroscopy, tissue



P-020

## The Effects of Combined Treatment of Extremely Low Frequency Magnetic Field (50 Hz, 1 mT) and Pterostilbene on Renal Ischemic Injury

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Ischemia occurs when the blood flow and oxygenation of a tissue is disturbed via the clogging of a vein by a physical factor such as a clot or embolism. Ischemia-reperfusion (IR) injury is one of the drastic outcomes observed after organ transplantation, which may become crucial in the end stage of acute or chronic renal failure [1]. Current studies have been focused on the prevention of ischemic injury. Although the application of magnetic field has been proposed as a new treatment strategy for ischemic injury, there have been controversial results reporting magnetic field treatment as being effective or ineffective on ischemic injury [2]. This study aims to detect the therapeutic role of 50 Hz extremely low frequency electromagnetic field (ELF-EMF) application and the administration of pterostilbene, an antioxidant which is chemically related to resveratrol [3], on renal ischemic injury. Rats were divided into control, ischemia-reperfusion (IR), ELF-EMF (50 Hz, 1 mT) treatment and 10 mg/kg dose of pterostilbene injection together with ELF-EMF treatment groups. After the induction of renal ischemia-reperfusion, treatments were applied for 5 consecutive days. Then kidneys were homogenised and analyzed by Fourier transform infrared (FTIR) spectroscopy. Protein secondary structures were predicted using second derivative spectra in amide I region. IR injury caused a decrease in lipid, protein and unsaturated lipid amount, a decrease in lipid/protein ratio and unsaturated/saturated lipid ratio; an increase in membrane fluidity and lipid peroxidation in components of rat kidneys. Moreover, IR injury led to alterations in the structure of proteins and lipids. A higher content of long chained lipids were observed in kidneys of IR group. Although ELF-EMF application (50 Hz, 1 mT) was not sufficient to repair all ischemia-induced alterations; the combined pterostilbene and ELF-EMF treatment successfully restored ischemia-induced changes in all of the investigated parameters, revealing a promising treatment strategy for renal ischemic injury.

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**Keywords:** Renal ischemia reperfusion injury, low frequency magnetic field, antioxidant, pterostilbene, FTIR spectroscopy

P-021

## Raman spectra of C60 confined inside a single-wall boron nitride nanotubes

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In this work, the Raman spectra are computed for infinite boron nitride peapod using the so-called spectral moment's method (SMM). The dependence of these modes has been calculated as a function of the nanotube chirality and diameter. Depending on the diameter of the nanotube, C60 molecules were found to form linear or zigzag chains inside the nanotubes.

In order to obtain the optimal configuration of the C60 fullerenes inside the single walled boron nitride nanotubes (SWBNNT), we calculate the minimum energies of Lennard Jones C60@SWBNNT and C60@C60 interactions. The changes of the Raman spectrum as a function of the configuration of the C60 molecules inside the nanotubes are identified. On the other hand, the effect of the filling factor on the Raman spectrum is analyzed. Finally, these results are useful to the interpretation of the experimental Raman spectra of boron nitride peapod.

**NOT  
ATTENDED**

**Keywords:** C60, SWBNNT, peapod, Raman Spectroscopy

P-022

## Semiclassical line broadening calculations with exact trajectory of NH<sub>3</sub> in collision with He

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Ammonia NH<sub>3</sub>, One of the major tools in the study of the molecular interstellar medium, has interested us and we have calculated the broadening coefficients  $\gamma$  from the semiclassical model of Robert and Bonamy including the accurate 'exact trajectory' for this molecule in collision with He at room temperature. The most crucial point of the calculation of the collisional parameters is the choice of the intermolecular potential describing the interaction. For our study, the potential energy surface for helium-ammonia complex used is the recent one of Koos et al. . The transitions with  $\Delta K = \pm 3n$  (n integer) have been introduced into the expressions of the differential collision cross section  $S(b)$ . A detailed analysis of the contribution of the various anisotropic components of the PES shows that the induced  $\Delta K = \pm 3$  transitions play a crucial role. Calculations performed are in good agreement with the experimental data and correct dependences of the broadening coefficients with the rotational quantum numbers J and K are obtained.

**Keywords:** Ammonia, Ab initio potential energy surface (PES), RB formalism

P-023

## Uniaxial Tensile and Structural Properties of Poly(vinyl alcohol) and Graphene Oxide Composite Films with Different Weight ratios: The Influence of Heating

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Changes in the uniaxial tensile properties and in the structure of poly(vinyl alcohol)(PVA) and graphene oxide (GO) composite films having varying weight ratios of GO to PVA from 0% to 20% were examined at different temperatures from room temperature to 250°C by using tensile testing method for mechanical properties and some spectroscopic methods such as Fourier transform infrared spectroscopy/attenuated total reflectance, differential scanning calorimetry and thermal gravimetric analysis for structural changes. In this study, as it is apparently seen in Fig. 1, the color of the composite films changes from a transparent to darker colors as the content of GO increases. Prominent changes were seen in mechanical properties, that is, Young's modulus, tensile strength and rigidity increased dramatically for the films having GO weight ratio higher than 3.75%. When the samples were heated at 50 °C, strain at break decreased greatly. This tendency continued slower at higher temperatures. Necking behavior was observed at around 5% strain for the GO ratio of 7.5% at room temperature which was shifted to GO ratio of 2.5% at higher temperatures.

**Keywords:** Poly(vinyl alcohol), graphene oxide, mechanical properties, structure-property relationship



Fig. 1. Changing in the color as the content of GO increases

P-024

## Structural and Tensile Characteristics of rGO/PVA Composite Films: Influence of UV Irradiation

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The influence of UV irradiation on the structural and uniaxial tensile characteristics of rGO/Polyvinyl Alcohol (PVA) composite films produced by using reduced graphene oxide (rGO) obtained by microwave-assisted reduction process with varying weight ratio of rGO to PVA from pure PVA to 10% were investigated by using uniaxial tensile tester and Ft-IR/ATR, UV-Visible spectroscopy methods before and after UV irradiation at different times. Great changes in mechanical properties of composite films were seen even after short UV irradiation times such as 2-3 h. For instance, after irradiation times of 3h of pure PVA films, tensile strength and Young's modulus increased 4-5 times and 15-20 times, respectively, whereas strain at break values decreased 7-8 times. Moreover, the tensile strength and Young's modulus of rGO/PVA composite films with rGO/PVA weight ratio equaling 1% increased 3 times and 15-17 times, respectively. The UV irradiation leads to deterioration of strain at break value of these films that is the strain at break value decreased 35-40 times. Therefore, the rigidity of composite films increased significantly. The correlation between the changes in tensile properties and structure of composite films was tried to be obtained by analyzing Ft-IR/ATR and tensile tester results.

**Keywords:** Reduced graphene oxide, polyvinyl alcohol; UV irradiation, tensile strength, Ft-IR/ATR spectroscopy

P-025

**Conformational analysis and h-DFT study of N,N'-phenylene-diylbis[3-(1-aminoethyl)-6-methyl-2H-pyran-2,4(3H)-dione]**

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Conformational analysis of N,N'-phenylene-diylbis[3-(1-aminoethyl)-6-methyl-2H-pyran-2,4(3H)-dione] were performed by using theoretical calculations. The possible stable conformers of title molecule on its potential energy surface (PES) were investigated by semi-empirical methods and appropriate structures were defined with hybrid density functional theory (h-DFT) method along with the basis sets of different size and type. The results of molecular relative energies and population analysis, the more stable form of N,N'-phenylene-diylbis[3-(1-aminoethyl)-6-methyl-2H-pyran-2,4(3H)-dione] was determined

**Keywords:** DFT, PES, Conformational Analysis

P-026

**Density functional theory calculations on spectroscopic and electrical properties of N,N'- propylene-diylbis[3-(1-aminoethyl)-6-methyl-2H-pyran-2,4(3H)-dione]: a potential nonlinear optical material**

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Quantum mechanical calculations of molecular structure parameters, relative energies, vibrational wavenumbers and electronic absorption wavelengths of N,N'- propylene-diylbis[3-(1-aminoethyl)-6-methyl-2H-pyran-2,4(3H)-dione] (C<sub>19.5</sub>H<sub>22</sub>N<sub>2</sub>O<sub>6.5</sub> empirical formula) was performed by using Gaussian 09 program. B3LYP and HSEH1PBE theory levels of density functional theory (DFT) with the 6-311++G(d,p) basis set were used in the performing of above mentioned calculations. The stability of title molecule arising from hyper-conjugative interactions and charge delocalization were analyzed by using frontier molecular orbitals (FMO) and natural bond orbital (NBO) analysis. Nonlinear optical (NLO) behavior of the molecule were examined by determining of electric dipole moment ( $\mu$ ), polarizability ( $\alpha$ ), static first order hyperpolarizability ( $\beta$ ), molecular electrostatic potential surface (MEPs) as well as Mulliken and NBO atomic charges analysis.

**Keywords:** DFT, Nonlinear optic, MEP, Natural bond orbital

P-027

## Influence of UV Irradiation on the Structural and Mechanical Properties of TiO<sub>2</sub>/GO/PVA Composite Films

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The uniaxial tensile and spectroscopic properties of GO/PVA composite films doped with TiO<sub>2</sub> micro particles with changing weight ratio to PVA from %1 to 15% were investigated by using uniaxial tensile tester and FT-IR/ATR, UV-Visible spectroscopy methods before and after UV irradiation at different times. It was apparently seen the color of the composite films changed from darker gray or black colors due to increasing GO concentration from 0.5% to 10% to lighter gray colors as TiO<sub>2</sub> weight ratio increases from 1% to 15% as seen in Fig. 1. With increasing GO and TiO<sub>2</sub> weight ratio, the Young modulus and tensile strength of TiO<sub>2</sub>/GO/PVA films increased from around 1 GPa to 4-5 GPa, and from around 30 to 80 MPa, respectively, whereas the strain at break values decreased dramatically from around 300% to around 10%. The UV irradiation leads to deterioration of especially strain at break value and to changes in spectroscopic properties of the composite films significantly due to photodegradation even after short irradiation times such as 0.5-4 h. The responsible structural changes leading to changes in the uniaxial tensile properties of the studies composite films were tried to be determined by using mainly FT-IR/ATR spectral results and SEM photographs.

**Keywords:** Graphene oxide, UV radiation, tensile strength, FT-IR/ATR spectroscopy

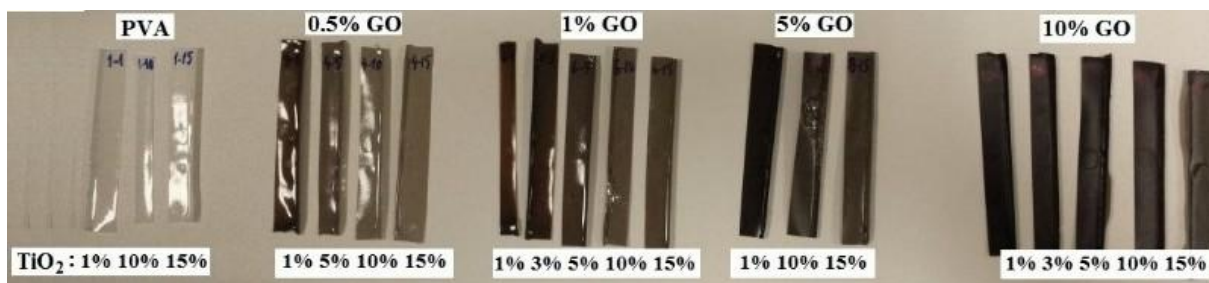


Fig. 1



P-028

## Heating Effect on Spectroscopic and Mechanical Properties of rGO/PVA Composite Films

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The spectroscopic and uniaxial tensile properties of rGO/PVA composite films produced by using reduced graphene oxide (rGO) obtained by microwave-assisted reduction process with varying weight ratio of rGO to PVA from pure PVA to 10% were investigated by using uniaxial tensile tester and Ft-IR/ATR, UV-Visible spectroscopy methods after heating process from room temperature to 200°C. For unheated composite films, with increasing rGO concentration, absorbance intensities in UV-visible and FT-IR spectra of the composite films increased significantly. For unheated composite films, with increasing rGO weight ratio up to 10%, the Young's modulus of rGO/PVA films increased approximately 4 times, whereas the tensile strength and the strain at break values decreased dramatically 4 times and 40 times, respectively. The heating process leads to great decrease in extensibility and significant improvement in tensile strength and the Young's modulus with respect to unheated samples, e.g., tensile strength and Young's modulus increased 2-3 times and 10-13 times, respectively, for the films with rGO/PVA weight ratio of 1% after being heated at 100 °C for 30 min. At the same heating temperature, as rGO concentration increased, similar changing tendency in mechanical properties was observed. Relationship between changes in the mechanical, structural, and thermal properties of the studies composite films were determined by using tensile testing, FT-IR/ATR and UV-visible.

*The authors acknowledge the financial support of Scientific Research Projects Coordinatorship in Yıldız Technical University in Istanbul, Turkey, through the Grant of the Project with the number of 2016-01-01-GEP02.*

**Keywords:** Reduced graphene oxide, poly(vinyl) alcohol, FT-IR/ATR spectroscopy, tensile strength, Young's modulus

P-029

## Spectroscopic parameters of NH<sub>3</sub> in the 2v<sub>4</sub> band

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Line intensities, self broadening coefficients, as well as line mixing parameters and self-shift coefficients have been measured in the 2v<sub>4</sub> perpendicular band of NH<sub>3</sub> at room temperature for about 340 rovibrational lines with rotational quantum numbers  $1 \leq J \leq 11$  and  $0 \leq K \leq J$ . Among these lines studied here, 4 correspond to forbidden transitions. Measurements were made in some branches located in the spectral range from 3100 to 3540 cm<sup>-1</sup> using a high-resolution Fourier transform spectra. These spectroscopic parameters have been retrieved from eight spectra recorded at different pressures of pure NH<sub>3</sub>. These spectra have been analyzed using a multi-pressure non-linear least squares fitting of Rosenkranz profile taking into account line mixing effect. The results of pressure broadening coefficients and line intensities obtained with and without taking into account line mixing effect are compared and analyzed as a function of the branches and the band rotational quantum numbers. Analyzing of overlapped line demonstrates a rather small mixing effect between the inversion doublets components of 2v<sub>4</sub> band. On average the values of these spectroscopic parameters obtained when taking into account line mixing were found to be about 3% smaller than those obtained without taking into account this effect.

On average, the accuracies of self-broadening coefficients and line intensities are estimated to be better than 4 %. The mean accuracies of line-shift data are estimated to be about 13% respectively. Most of the lines have a negative shift coefficient, numerous doublet components have opposite sign of shift values reflecting a mutual line attraction.

**Keywords:** Self-broadening, line mixing, NH<sub>3</sub>, FTIR, Rosenkranz profile

P-030

## Production of Baicalein Containing Electrospun Scaffolds and Characterization through Raman Spectroscopy Thereof

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Synthetic and natural polymeric nanofibers manufactured by electrospinning technique, are one of the promising structures for mimicking the natural extracellular matrix (ECM). In our study, we aim to produce nanofiber-based scaffolds containing an anti-inflammatory, and anticancer Chinese herbal traditional drug called Baicalein, and apply them for using as a bone graft material during the excisional surgical operation of cancer cells especially metastatic prostate cancer. In order to produce nanofibers containing Baicalein, electrospinning method was applied with different polymer solutions such as hyaluronic acid (HA), polyethylene oxide (PEO) and polyvinyl alcohol (PVA) and Baicalein.

In addition, we investigate the characterization of electrospun nanofibers by using Scanning Electron Microscopy (SEM) which showed the morphology of nanofibers. We also used Surface-Enhanced Raman Spectroscopy (SERS) and Fourier Transform Infrared Spectroscopy (FTIR) to investigate the chemical composition of the produced scaffolds in order to reveal that our scaffolds contain the functional groups which belong to the polymers and Baicalein.

In conclusion, we successfully produced biosynthetic functional bone graft containing HA, PEO, and PVA electrospun nanofibers carrying Baicalein which have high anti-inflammatory and anticancer potentials against metastatic prostate cancer.

**Keywords:** Nanofiber, Electrospinning, Raman Spectroscopy, FTIR, Bone graft, Nanomedicine

P-031

Comparison of Extra Virgin Olive Oil (EVOO) and Hypericum perforatum Oil by Using ATR-FTIR Spectroscopy

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Recent developments in Fourier Transform Infrared Spectroscopy (FT-IR) extend the application of this technique to the field of food research, especially to the studies on edible oils and fats. In this study, FTIR spectroscopy is used as an analytical instrument in order to determine changes in the frequency data of some bands and also in the ratios of transmittance of the FTIR spectra during maceration process of Hypericum perforatum in extra virgin olive oil (HP-EVOO) have been studied. H. perforatum L. (St. John's Wort, Hypericaceae) is a member of the genus Hypericum, of which there are 400 species worldwide and is used as a medicinal plant for years [1]. In the result of study, visual examination of spectra revealed that there are no significant differences between spectral features apart from slight changes in the transmittances of some bands as well as some shifts in the exact position of the bands. A band observed at 3003 cm<sup>-1</sup> assigned to the C-H stretching vibration of the cis-double bond of extra virgin olive oil but a slight shift observed to the 3005 cm<sup>-1</sup> after maceration. Changes in the 1700-1480 and 867 cm<sup>-1</sup> spectral region appeared after maceration process. According to the results, there was no spectral shift or widening at 1743 cm<sup>-1</sup> and this information showed that there was no oxidation in EVOO.

[1] P. H. Davis, J. Cullen. Hypericaceae In: "Flora of Turkey and the East Aegean Islands" (Davis PH, Ed.), Vol.10, 1984, pp. 96-103.

**Keywords:** ATR-FTIR, Spectroscopy, Olive oil, {Hypericum perforatum}

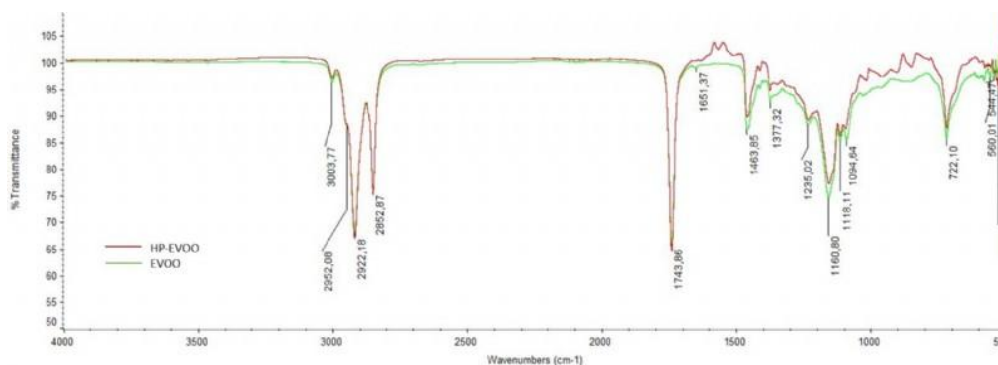


Fig. 1. FT-IR Spectrum of H. perforatum oil and extra virgin olive oil (EVOO)

P-032

## Experimental and theoretical studies of the vibrational and electronic properties of 2-methylimidazole

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In the current investigation, the molecular structure of the 2-methylimidazole molecule was theoretically modelled using density functional theory (DFT) calculations (Fig. 1). The Fourier transform (FT) infrared and Raman spectra of 2-methylimidazole were also recorded. Molecular geometric parameters, vibration frequencies and electronic transition energies of 2-methylimidazole were calculated by DFT-B3LYP, DFT-B3PW91, M06L and MP2 methods via LANL2DZ bases set. The obtained results were compared with experimental ones. As a result of these studies, the most suitable quantum mechanical model for molecular modeling has been determined.

**Keywords:** DFT-B3LYP, DFT-B3PW91, M06L, MP2

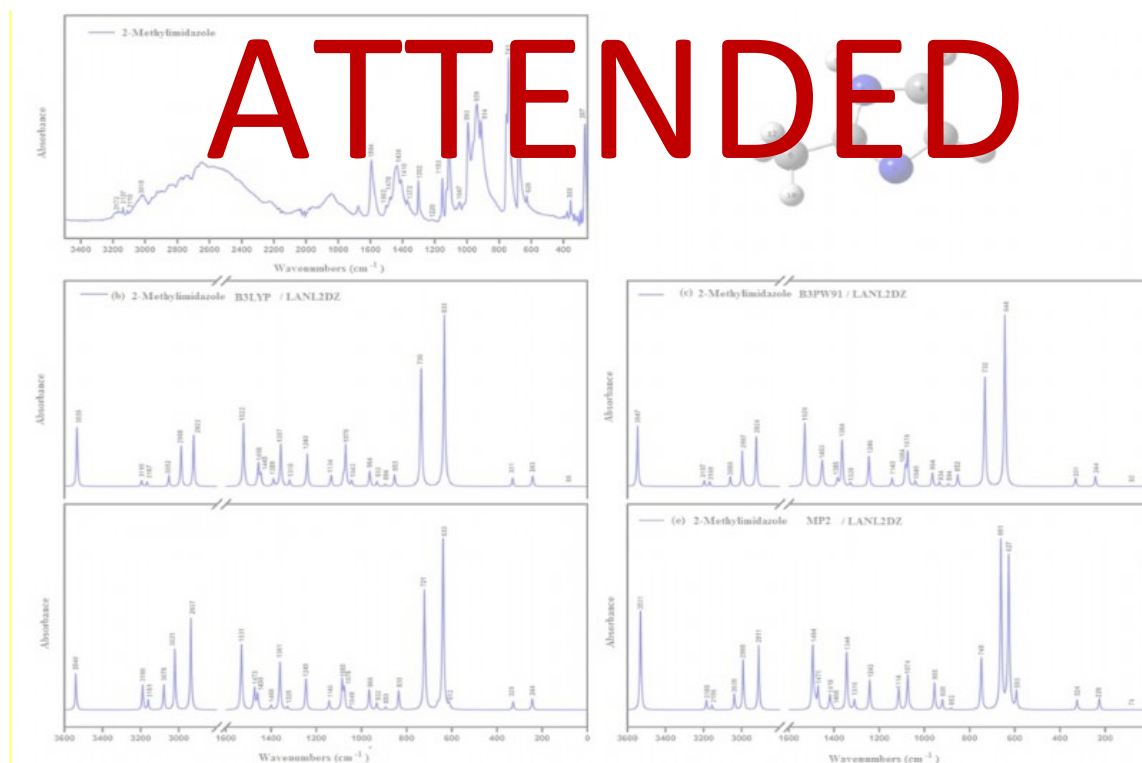


Fig. 1. Experimental and simulated spectra of 2-methylimidazole

P-033

Molecular Geometry, Vibrational Spectra (FT-IR and RAMAN), Vibrational Assignments by Density Functional Theory (DFT) Calculations for Complex  $[\text{Ni}(\text{etim})_4\text{Ni}(\mu\text{-CN})_2(\text{CN})_2]_n$

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In this work, the molecular geometry (Fig. 1) and vibrational spectra of  $[\text{Ni}(\text{etim})_4\text{Ni}(\mu\text{-CN})_2(\text{CN})_2]_n$  were investigated in the ground state using DFT-B3LYP and DFT-B3PW91 methods via LANL2DZ basis set. The vibrational spectra were recorded and fundamental vibration frequencies were assigned on the basis of the potential energy distribution (PED) via VEDA program. The molecular geometry and the vibrational spectral properties of the complex were experimentally reported in the literature. In this study, a theoretical model which well-matched experimental data was suggested using by DFT method. By the way, the agreement between experimental parameters and corresponding ones was demonstrated by plotting of the regression equations. Additionally, HOMO and LUMO energy levels and molecular transition energies of the complex  $[\text{Ni}(\text{etim})_4\text{Ni}(\mu\text{-CN})_2(\text{CN})_2]_n$  has been calculated by time dependent density functional theory with B3LYP and B3PW91 methods with LANL2DZ basis sets.

**Keywords:** DFT-B3LYP, DFT-B3PW91, LANL2DZ, 1-ethylimidazole complex

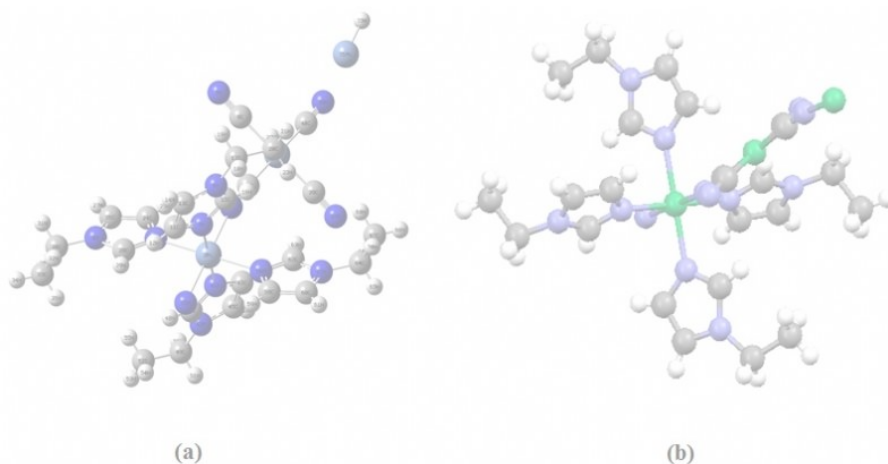


Fig. 1 The molecular structure of the studied complex .

P-034

**Use of EVA Descriptor to Construct Linear QSAR Model for Determining Inhibitory Activity of Sulfonamides against Carbonic Anhydrase and Sweetness Index of Aspartame Derivatives**

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The EVA (vibrational eigenvalue analysis) descriptor can be constructed from either experimental or calculated fundamental IR- and Raman range molecular vibrational frequencies. Although the EVA descriptors are sensitive to 3D structure of molecules, they have advantage over other field-based 3D QSAR methods such as COMFA and COMSIA inasmuch as they are invariant to both translation and rotation of the structures concerned and thus structural superposition is not required.

In this study, by using EVA descriptors, two statistically significant QSAR models were built from two sets of compounds. First linear QSAR model was derived by using inhibitory activity of sulfonamide compounds against carbonic anhydrase isozyme CA II and calculated EVA descriptors. Second QSAR model was constructed by using sweetness index of aspartames and calculated EVA descriptors. Various validation procedures were applied to the obtained QSAR models such as randomization test, determination of application domain using leverage approach, and external validation.

The results of this study showed that EVA descriptors perform well as explanatory and predictive tools for modeling the inhibition activity of sulfonamide compounds against carbonic anhydrase isozyme II and to determine sweetness index of aspartame derivatives.

**Keywords:** EVA, QSAR, DFT, Carbonic Anhydrase Inhibition, Sweetness Index of Aspartame

P-035

## Inhomogeneity of tooth enamel evaluated by vibrational micro-spectroscopy

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Dental enamel is the most crystalline and mineralized hard tissue in the body, composed of biological carbonate-substituted hydroxylapatite containing only traces of organic compounds. UV-Raman (325 nm) and infrared micro-spectroscopy were applied to evaluate the compositional and structural variations in enamel on molecular structural level. Spectral data were collected from fifteen dental cross sections. Enamel was measured in four areas along a line oriented perpendicular to the dentine-enamel junction and parallel to the orientation of apatite rods. UV-Raman spectra were fitted using a pseudo-Voigt profile function and the structural differences were evaluated through the width of the peak at  $960\text{ cm}^{-1}$  ( $\nu_1\text{ PO}_4$ ), changes of the intensity ratio of the peaks at  $960\text{ cm}^{-1}$  ( $\nu_1\text{ PO}_4$ ) and  $1070\text{ cm}^{-1}$  ( $\nu_1\text{ B-type CO}_3$ ) and intensity ratio of the carbonate ( $\nu_1\text{ B-type CO}_3$ ) to hydroxyl peak at  $3570\text{ cm}^{-1}$  ( $\nu_1\text{ OH}$ ). The results reveal that the degree of structural disorder of enamel increases from the surface enamel in depth which is associated with an increase of the degree of carbonate for phosphate isomorphic substitution. In addition the hydroxyl groups in the structure gradually decrease in the same direction. The amount of organic residues in enamel increases significantly in a layer near dentine-enamel junction detected by the change in the intensity of the protein peaks near  $1600\text{ cm}^{-1}$  observed in UV Raman spectra

**Keywords:** Tooth enamel, apatite, UV- Raman, Infrared micro-spectroscopy



P-036

**Molecular Structure and Vibrational Spectroscopic Study of 2-[4-(4-Nitrobenzamido)phenyl]benzothiazole using DFT Method**

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Benzothiazole derivatives show numerous biological activities such as antibacterial, antifungal, antimicrobial, antitumor, anticonvulsant, anti-allergic, anti-inflammatory, antitubercular and antinematode[1,2]. In the present study, a benzothiazole derivative, 2-[4-(4-nitrobenzamido)phenyl]benzothiazole (BSN-011), was investigated from theoretical and vibrational spectroscopic point of view. The molecular geometry optimization, vibrational analysis and HOMO-LUMO analysis have been carried out with the Gaussian 09W software package. All calculations have been performed using DFT/B3LYP functional with 6-311++G(d,p) basis set. The assignment of the calculated wavenumbers of BSN-011 has been obtained by means of VEDA4 program [3] and Potential Energy Distribution (PED) has been achieved. The theoretical spectra have been compared with experimental IR and Raman spectra.

[1] K. Bolelli, I. Yalcin, T. Ertan-Bolelli, S. Ozgen, F. Kaynak-Onurdag, I. Yildiz, E. Aki, Medicinal Chemistry Research 21 (11) (2012) 3818-3825.

[2] O. Unsalan, Y. Sert, H. Ari, A. Simão, A. Yilmaz, M. Boyukata O. Bolukbasi, K. Bolelli, I. Yalcin, Spectrochim. Acta Part A: Mol. and Biomol. Spectroscopy, 125 (May 2014) 414-421.

[3] M.H. Jamroz, Vibrational Energy Distribution Analysis, VEDA4, Warsaw, 2004.

**Keywords:** benzothiazole, DFT, vibrational analysis

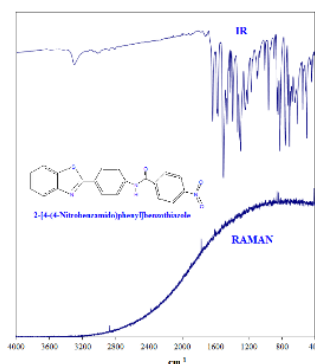


Fig. 1. IR and Raman Spectra of BSN-011

P-037

## Nonadiabatic molecular alignment of linear molecules using circularly polarized femtosecond laser pulses

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We studied the rotational wavepacket evolution of N<sub>2</sub>, CO, and C<sub>2</sub>H<sub>2</sub> using circularly polarized femtosecond laser pulses (Fig. 1 and 2). We showed that circular polarization produces a net alignment along the laser propagation axis at certain phases of the evolution. The results were compared to the calculated nonadiabatic molecular alignment parameter in terms of the effects of electronic structure and symmetry of the molecules.

**Keywords:** Nonadiabatic molecular alignment, strong field ionization, femtosecond laser

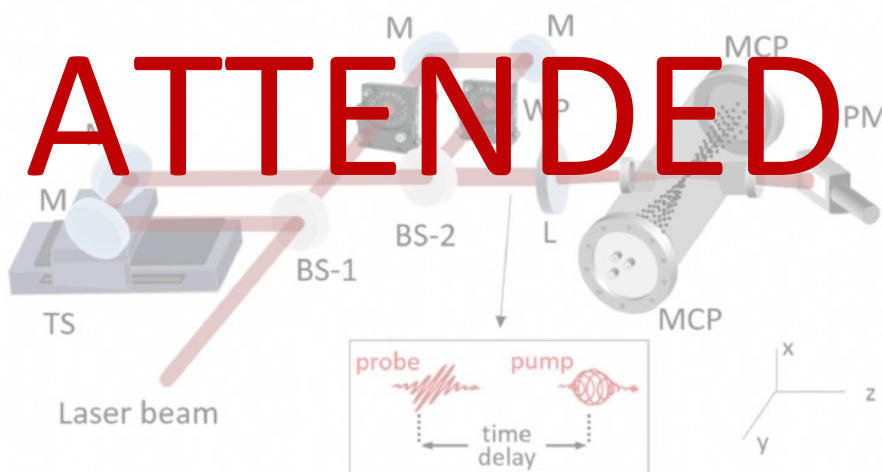


Fig. 1. Experimental setup. BS: beam-splitters, TS: translational stage, WP: wave plates, M: flat mirrors, L: achromatic focusing lens, PM: power meter, MCP: microchannel plates.

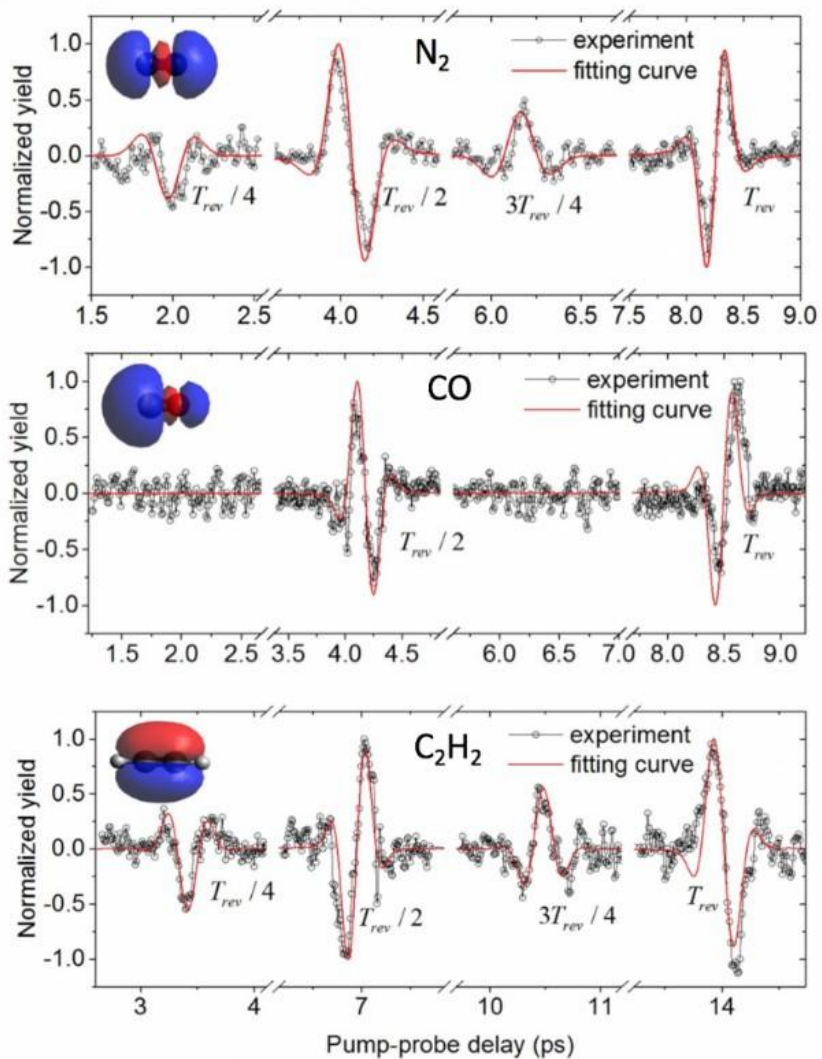


Fig. 2. Strong-field ionization yield of nonadiatically aligned N<sub>2</sub>, CO and C<sub>2</sub>H<sub>2</sub> gas molecules along with the fitting curve as a function of the pump-probe delay time

P-038

## Synthesis and Structural Characterization of 1D Coordination Polymer with Co(II)-3,3-Dimethylglutarate

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The design and synthesis of coordination polymers have been attracted interest due to their fascinating architectures and potential application areas in gas adsorption/separation, catalysis, magnetism, luminescence, sensor, etc. Aliphatic dicarboxylic acids which can be used as a ligand coordinate the metal ions as bridging ligand at the synthesis of coordination polymers. Especially, 3,3-dimethylglutaric acid (H<sub>2</sub>dmg) which can bridge metal ions by oxygen atoms of carboxylate groups is a functional ligand. In this study, [Co( $\mu$ -dmg)(iodophim)<sub>2</sub>(H<sub>2</sub>O)]·H<sub>2</sub>O<sub>n</sub> (1) complex is synthesized with hydrothermal method (140 °C, 4 days) by using 3,3-dimethylglutaric acid (H<sub>2</sub>dmg), 1-(4-iodophenyl)-1H-imidazole (iodophim) and Co(NO<sub>3</sub>)<sub>2</sub>·6H<sub>2</sub>O. The structure of the complex has been characterized by elemental analysis, IR spectroscopy, single-crystal X-ray diffraction and thermal analyses (TG, DTA, DSC) techniques. According to X-ray diffraction analysis result, the structure of [Co( $\mu$ -dmg)(iodophim)<sub>2</sub>(H<sub>2</sub>O)]·H<sub>2</sub>O<sub>n</sub> was obtained with crystallization of two Co(II) centered molecular structures in triclinic crystal system with the space group P-1. In unit cell, asymmetric unit of 1 contains two half Co(II) ions, one dmg<sup>2-</sup>, two iodophim, one aqua ligands and one crystal water molecule. In molecular packing, each Co(II) atom completes its packaging with six coordination. Co(II) ions are bridged by carboxylate oxygen atoms of dmg ligands to form 1D coordination polymer (Fig. 1.).

**Keywords:** Coordination polymer, dimethylglutarate complex, cobalt(II) complex

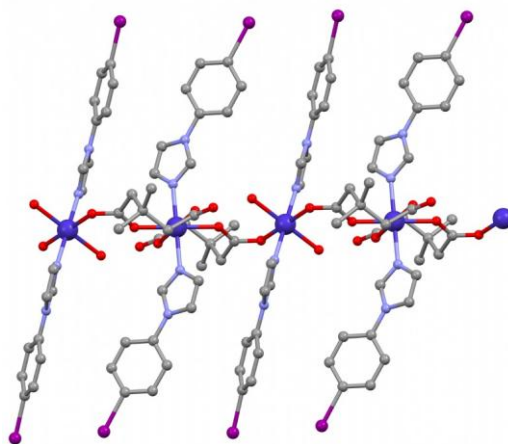


Fig. 1. 1D chain structure of coordination polymer

P-039

## Effect of plant sterol stigmasterol on the physical properties of DMPC membranes: an FTIR study

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Plant sterols, such as  $\beta$ -sitosterol and stigmasterol (Fig. 1) are integral natural ingredients of plant cell membranes [1]. Dimyristoyl phosphatidylcholine (DMPC) is a zwitterionic glycerophospholipid with two saturated acyl chains, containing 14 carbon atoms each [2]. In the present study, the effect of plant sterol stigmasterol on zwitterionic dimyristoyl phosphatidylcholine (DMPC) multilamellar vesicles (MLVs) was investigated for the first time by using Fourier transform infrared (FTIR) spectroscopy. The result of FTIR studies shows that in the gel phase, the addition of low stigmasterol concentrations (1, 5 and 10 mol %) into pure DMPC MLVs increases the order slightly, while high stigmasterol concentrations (20, 30 and 40 mol %) decrease the order of DMPC membranes. In the liquid crystalline phase, all concentrations of stigmasterol induce an enhancement in the order of membranes. In addition, in both phases, 1 mol % stigmasterol has a negligible effect in the dynamics of membranes, whereas other concentrations of stigmasterol cause an enhancement in the dynamics. Stigmasterol also induces a decrease in the wavenumber of the C=O stretching and  $\text{PO}_2^-$  antisymmetric double stretching bands of DMPC in both phases, which points out hydrogen bonding in between the hydroxyl group of stigmasterol and carbonyl and phosphate groups of DMPC membranes. Our findings show that plant sterol stigmasterol has different action on DMPC membranes depending on stigmasterol concentration.

*This work was supported by Ege University Research Fund 2013 FEN 033.*

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**Keywords:** Stigmasterol, DMPC, FTIR spectroscopy.

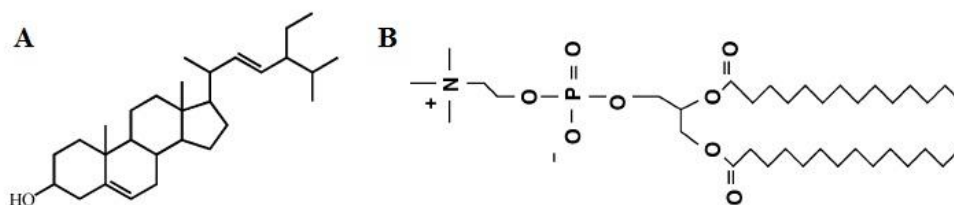


Fig. 1. Chemical structures of stigmasterol (A) and DMPC (B).

**P-040**

**Investigation of physical properties of Betula Pendula (Silver Birch) bark by calorimetric, spectroscopic and microscopic techniques**

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Silver birch bark (Fig. 1) is a substance that has been used for potential treatments of several diseases such as cancer and AIDS [1]. It also has been frequently used as a humidity/heat isolation for Turkish bows which gives them the farthest range in such weather conditions [2]. The aim of this study is to determine some physical properties of the silver birch bark by using Thermogravimetric Analysis (TGA), Attenuated Total Reflectance Fourier Transform Infrared (ATR-FTIR) spectroscopy and Atomic Force Microscopy (AFM). According to TGA results, very low weight loss of 0.01130 mg (0.09303 %) was observed for the bark between 25 and 45°C. This is an indication of low volatilization and shows that the bark does not lose too much of its weight and is not affected by temperature change at all in this temperature range so this might be concluded as an explanation to the farthest range of the bows was reached even at the higher temperatures in the battle field when the bow covered with this material. AFM results also revealed the roughness properties of the bark surface. On the other hand, ATR-FTIR spectrum revealed the structures of pentacyclic triterpene compounds such as lupeol, betulinic acid and betulin and the results are in good agreement with the literature [3].

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**Keywords:** Silver birch, TGA, ATR-FTIR, AFM, Turkish bows



**Fig. 1. Silver birch bark**

P-041

## Mössbauer analysis and Cation distribution of Zn substituted BaFe<sub>12</sub>O<sub>19</sub> hexaferrites

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Barium hexaferrite is a well known hard magnetic material. Doping using nonmagnetic cation such as Zn<sup>2+</sup> were found to enhance magnetization owing to preferential tetrahedral site (4f1) occupancy of the zinc. However, the distribution of cations in hexaferrites depends on many factors such as the method of preparation, nature of the cation and chemical composition. Here, Zn doped Barium hexaferrites (Ba<sub>1-x</sub>Zn<sub>x</sub>Fe<sub>12</sub>O<sub>19</sub>) were synthesized by sol-gel method. In this study, we summarized the magnetic properties of Ba<sub>1-x</sub>Zn<sub>x</sub>Fe<sub>12</sub>O<sub>19</sub> (x=0, 0.1, 0.2, 0.3) BaM, investigated by Mössbauer Spectroscopy. Moreover, cation distribution was also calculated for all the products. Mössbauer parameters were determined from 57Fe Mössbauer spectroscopy and according to it, the replacement of Ba-Zn affects all parameters such as isomer shift, the variation in line width, hyperfine magnetic field and quadrupole splitting. Cation distribution revealed the relative area of undoped BaM, 12k, 2a and 4f2 positions which are close to theoretical values.

**Keywords:** Hexaferrites, superparamagnetism, hyperfine interactions, cation distribution

**P-042**

**The effect of Ti on Mechanical, Morphological and Magnetic Properties in Fe-Ni-Ti Alloys**

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Morphological and magnetic properties in Fe-28.2Ni-0.5Ti, Fe-26.8Ni-1.5Ti and Fe-27.6Ni-4.2Ti alloys are investigated. Scanning electron microscopy (SEM), Mössbauer spectrometer, DSc and Vickers hardness are used to determine the physical properties of alloys. The Mössbauer parameters such as hyperfine field (B<sub>hf</sub>), the quadrupole shift (QS), the isomer shift (IS), the line width (W) and percentage relative area (RA) of the alloys were determined. The morphological changes, M<sub>s</sub>, A<sub>s</sub> and hardness values were determined by depending on Ti content

**Keywords:** Mössbauer, SEM, Hardness



**P-043**

**Magnetic properties of deformation induced martensite in a  
Fe-27%Ni-4%Mn-1%Zn (wt.%) alloy**

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In this study we reported the magnetic properties of deformation induced martensite in the Fe-27%Ni-4%Mn-1%Zn (wt.%) alloy and Mössbauer spectroscopy was used to investigate. We homogenized the sample at 1200 °C for 12 hours and then quenched into water at room temperature and this sample demonstrated the pure austenite phase. The deformed sample 40% with the deformation amount exhibited deformation induced martensite. The single peak of the paramagnetic phase of Fe-27%Ni-4%Mn-1%Zn (wt.%) alloy were observed in the Mössbauer spectrum. In the Fe-27%Ni-4%Mn-1%Zn (wt.%) alloy with deformation effect the six peaks of magnetically ordered martensite phase of were not formed. Despite the structural transformation occurred, the magnetic transformation not occurred with deformation effect.

**Keywords:** Deformation, Fe-based alloy, Magnetic Properties, Phase Transformation.

P-044

## An analysis of orthopyroxene from Tsarev L5 meteorite using X-ray diffraction and Mössbauer spectroscopy

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Tsarev L5 ordinary chondrite consists of various iron-bearing phases such as olivine ( $\text{Fe, Mg})_2\text{SiO}_4$ , orthopyroxene ( $\text{Fe, Mg})\text{SiO}_3$ , troilite  $\text{FeS}$ , clinopyroxene ( $\text{Fe, Mg, Ca})\text{SiO}_3$ ,  $\alpha\text{-Fe}(\text{Ni, Co})$ ,  $\alpha_2\text{-Fe}(\text{Ni, Co})$ ,  $\gamma\text{-Fe}(\text{Ni, Co})$ , chromite  $\text{FeCr}_2\text{O}_4$  and some other minor phases as well as weathering products containing ferric iron compounds. Tsarev L5 was already studied using X-ray diffraction (XRD) and Mössbauer spectroscopy [1, 2]. However, there are some problems which are not solved yet. For instance, it is very important to compare results for the bulk matter and extracted phase(s) for silicates (olivine and pyroxene) and compare results of the estimations of  $\text{Fe}^{2+}$  partitioning between crystallographically non-equivalent M1 and M2 sites in silicates obtained using XRD and Mössbauer spectroscopy. For this reason, we present preliminary results of comparative study of orthopyroxene in the bulk Tsarev L5 and chemically extracted from the bulk sample using both techniques.

The bulk Tsarev L5 sample was powdered for XRD and Mössbauer spectroscopy measurements. Extracted orthopyroxene sample was prepared using a procedure included fine powder of the bulk sample treatment with 20% HCl several times. The obtained washed and dried powder was used for the measurements. XRD demonstrated the main phases in the bulk Tsarev L5 sample while in extracted orthopyroxene sample there were no Fe-Ni-Co alloy, troilite and olivine. Some small amounts of chromite, clinopyroxene, weathered products were detected. Mössbauer spectroscopy showed that in extracted orthopyroxene sample there are small amounts of chromite, probably clinopyroxene and ferric compound in addition to orthopyroxene. The  $\text{Fe}^{2+}$  partitioning between the M1 and M2 sites in extracted orthopyroxene estimated by both techniques was of the same order (0.15 and 0.85 from XRD and 0.09 and 0.91 from Mössbauer spectroscopy for the M1 and M2 sites, respectively).

*This work was supported by the Ministry of Education and Science of the Russian Federation (Project # 3.1959.2017/4.6) and by Act 211 Government of the Russian Federation, contract № 02.A03.21.0006. Contribution from A.A.M. was funded by the RFBR (Project № 16-32-00151 mol\_a).*

[1] M.I. Oshtrakh et al., *Meteoritics & Planetary Sci.*, 43, #5, 2008, 941–958.

[2] A.A. Maksimova et al., *J. Mol. Struct.*, 1073, 2014, 196–201.

**Keywords:** Tsarev L5 ordinary chondrite, Orthopyroxene, X-ray diffraction, Mössbauer spectroscopy

P-045

**Investigation by Mössbauer spectroscopy of magnetic properties in  
Fe-27%Ni-4%Mn Alloy**

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We have studied the austenite-martensite phase transformations which are formed by deformation effect in Fe-27%Ni-4%Mn (wt.%) alloy. In this work used; mössbauer spectroscopy, scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDX) and compression deformation test techniques. From SEM observations, this sample exhibited austenite phase and deformation induced martensite. The six peaks of the ferromagnetic phase of Fe-27%Ni-4%Mn (wt.%) alloy were observed in the Mössbauer spectrum. The effective hyperfine field of ferromagnetic martensite phase was determined as 33.949 T and isomer shift value was determined as 0.0152 mm/s.

*Acknowledgments, the financial aid of the Amasya University project No. FMB-BAP 16-0174 is gratefully acknowledged.*

**Keywords:** Compression deformation, EDX, Martensitic Transformation, SEM.

P-046

## Mössbauer Spectroscopy of Various Iron Compounds

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Various iron compounds such as haematite, wüstite, magnetite, ferrous sulfate, ferrous oxalate and natural iron are examined by using Mössbauer Spectroscopy at  $^{57}\text{Fe}$  resonance. The aim of the experiment was to observe the presence and strength of the hyperfine magnetic field and iron valence of the compounds. The spectroscopy measurements are done under STP. A conventional Mössbauer spectrometer with Co/Rh source and with  $^{57}\text{Fe}$  calibration is used to obtain energy resolved Mössbauer spectrum of natural iron and iron compounds. Also nuclear forward scattering with synchrotron radiation is used to obtain time resolved Mössbauer spectrum.

**Keywords:** Iron, Mössbauer Spectroscopy, Nuclear Forward Scattering and Synchrotron Radiation

P-047

## Solid Phase Extraction Using Modified Magnetic Iron Oxide Nanoparticles for Extraction and Spectrofluorimetric Determination of Carvedilol in Human Plasma Samples

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ATTENDED**

A new analytical approach was developed involving magnetic solid-phase extraction and spectrofluorimetric determination of carvedilol in human plasma samples. A plasma sample was prepared and adjusted to pH 8.2–10, then carvedilol was quickly extracted using iron oxide magnetic nanoparticles modified by the surfactant cetyltrimethylammonium bromide and determined applying spectrofluorimetry at  $354 \pm 3$  nm after excitation at  $241 \pm 3$  nm. Experimental conditions, such as the amount of nanoparticles and cetyltrimethylammonium bromide, pH value, standing time and desorption solvent type and volume have been adjusted to optimize the extraction process and to obtain analytical characteristics of the method. Linearity was observed in the analyte concentration range of 2.0–125 ng/mL with correlation coefficients ( $r$ ) of 0.999. The method showed good precision and accuracy, with intra- and inter-assay precisions of less than 7.0% at all concentrations. Standard addition recovery tests were carried out, and the recoveries ranged from 94.4% to 100.7%. The limits of detection and quantification were found to be 0.67 and 2.24 ng/mL. The method was applied to the determination of carvedilol in human plasma samples.

**Keywords:** Carvedilol, iron oxide Magnetic nanoparticles, plasma, solid phase extraction, spectrofluorimetry

P-048

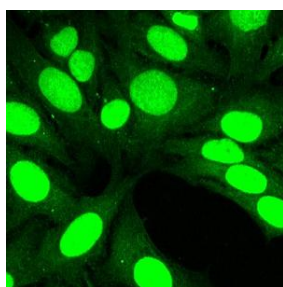
**Fluorescence Spectroscopy: applications in immunology**

Ouadi Ouadi Ibtissem, Gadiri Meriche Sabiha, Meriche Meriche Hacem

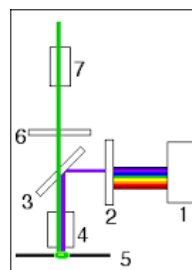
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Optical imaging is unequivocally the most versatile and widely used visualization modality in clinical practice and research. In recent years, fluorescence microscopy and imaging have received particular attention. Although fluorescence microscopy permeates all of cell and molecular biology, most biologists have little experience with the underlying photophysical phenomena. Understanding the principles underlying fluorescence microscopy is useful when attempting to solve imaging problems. Additionally, fluorescence microscopy is in a state of rapid evolution, with new techniques, probes and equipment appearing almost daily. Familiarity with fluorescence is a prerequisite for taking advantage of many of these developments. An important medical use of fluorescence microscopy is to detect, identify and titrate autoantibodies. This is done by the indirect fluorescent antibody (immunofluorescence) test. Certain autoantibodies or anti-tissue antibodies cause diseases in which the body's immune system attacks the body itself. These autoimmune diseases can be detected and identified by indirect fluorescent antibody test. Distinctive patterns of staining are seen in the tissues involved or in other cells that react with specific antibodies in a patient's blood that are characteristic of a disease. In the indirect fluorescent antibody (IFA) test, serum of a patient with suspected disease is incubated with tissue that contains a diagnostic marker antigen. Antibodies present in the patient's serum bind to corresponding antigenic structures on the tissue substrate. The reacted antibodies (e.g Antinuclear Antibodies ANA) are detected with a fluorochrome (fluorescien)-labelled anti-human globulin, normally IgG. The reaction is easily visible under the fluorescence microscope. These techniques are essential to supplement clinical findings and histopathology in the diagnosis of autoimmune disorders. They permit early diagnosis, treatment, and subsequent monitoring of disease activity in patients with these potentially life-threatening disorders. This presentation describes examples of indirect immunofluorescence microscopy used for detecting circulating autoantibodies that can be found in human serum of patients with certain diseases.

**Keywords:** immunofluorescence, autoantibodies, fluorochrome, autoimmune



**Antinuclear Antibodies**



**Fluorescence Microscopy**

P-049

## Imidazole/Benzimidazole-Modified Cyclotriphosphazenes as Fluorescent Probes for Cu<sup>2+</sup>

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Transition-metal ions can cause important environmental and health problems because of their toxicity [1]. Especially, excessive copper content in body can cause serious health problem like liver or kidney damage and high levels of copper is also seriously toxic to environment [1]. In this study, two configurational isomers (cis and trans) of imidazole- or benzimidazole-modified cyclotriphosphazenes (3a, 4a or 3b, 4b, Fig. 1) were designed, synthesized, and investigated as fluorescent probes for metal ions. The newly synthesized compounds were characterized by <sup>1</sup>H, <sup>31</sup>P NMR and mass spectrometry. The configurations of geometric isomers were analyzed by <sup>31</sup>P NMR spectroscopy on addition of CSA. The probes sensing behavior toward metal ions were investigated by UV/vis and fluorescence spectroscopies. Among the examined 20 metal ions, the fluorescence emission of the isomer mixtures were quenched by Cu<sup>2+</sup> together with Fe<sup>2+</sup>, Fe<sup>3+</sup>, Zn<sup>2+</sup> and Ni<sup>2+</sup> ions, but each individual isomer (3a,b and 4a,b) exhibited on-off-type fluorescence response with high selectivity towards only Cu<sup>2+</sup> with the low limits of detection ranging from 1.27 μM to 2.04 μM.

[1] D. T. Quang, J. S. Kim, Chem. Rev. 110, 2010, 6280–6301.

**Keywords:** Fluorescent sensor, copper, imidazole, benzimidazole, phosphazene

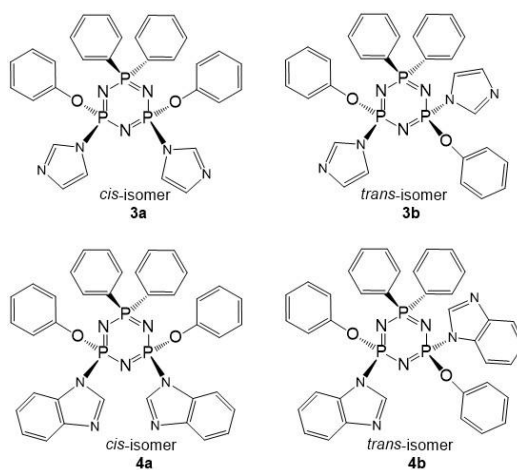


Fig. 1 Benzimidazole-modified cyclotriphosphazenes

P-050

## Three Curcuminoids Upon Inclusion Into (2-Hydroxypropyl)- $\beta$ -Cyclodextrin: An Absorption and Fluorescence Spectroscopic Study

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Curcumin is the main curcuminoid present in turmeric (*Curcuma longa*). In chromatographic studies, it has been proved that curcumin exists with its isomers namely demethoxycurcumin (DMC), and bisdemethoxycurcumin (BDMC) in turmeric samples [1]. Curcuminoids have been linked with many biological activities such as anti-oxidant, anti-alzheimer, and anti-diabetes [2]. However curcuminoids are slightly soluble in aqueous media limiting their bioavailability. The formation of inclusion complexes between cyclodextrins and curcumin is one of the most promising solution for this problem.

In this study, a comparison has been focused on the differences of the UV-VIS absorption and fluorescence properties of three curcuminoids. Inclusion complexes between 2-hydroxypropyl- $\beta$ -cyclodextrins (2-HP- $\beta$ -CD) and curcuminoids improve the water solubility. Through the study, the influence of 2-HP- $\beta$ -CD on the spectroscopic properties of individual curcuminoids was tested. Curcuminoids have native fluorescence but their intensities are very low in aqueous media. However the fluorescence intensities of curcuminoids increase in aqueous solution containing 2-HP- $\beta$ -CD. Furthermore, the fluorescence intensities of each curcuminoid with 2-HP- $\beta$ -CD containing solution were changed. These changes can be attributed to the little differences of the chemical structures of individual curcuminoids. Both the fluorescence and absorption spectra of curcuminoids in aqueous solution containing 2-HP- $\beta$ -CD indicate a strong absorption of the radiation from 300 to 600 nm showing the protection ability of curcuminoids against oxidation and destruction of organisms.

[1] Z. Kalaycıođlu, P. Hashemi, K. Günaydın, F. B. Erim, *Electrophoresis*, 36, 2015, 2516-2521.

[2] Z. Kalaycıođlu, I. Gaziöđlu, F. B. Erim, *Natural Product Research*, 2017, DOI: 10.1080/14786419.2017.1299727

**Keywords:** Curcuminoids, 2-HP- $\beta$ -CD, UV-VIS absorption spectroscopy, fluorescence spectroscopy



P-051

**Determination of Aluminum in Water Resources With New Synthesized N,N'-Bis (2,5-dihydroxybenzylidene)-4,4'-diamino Diphenyl Ether by Using Fluorimetric Method**

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The pollution of water sources from industrial wastes is a major environmental problem. Therefore the precise, sensitive and correct detection of metallic pollution in water is very important. We have synthesized a new Schiff base and used fluorimetric method for a precise, sensitive and correct determination of aluminium in some water sources.

The fluorimetric parameters of the new synthesized macro molecule Schiff base, N,N'-bis (2,5-dihydroxybenzylidene)-4,4'-diamino diphenyl ether (DHDPE), and aluminum complex were determined in acetonitrile. The best fluorescence intensity of DHDPE-Al complex in acetonitrile medium was obtained at  $\lambda_{ex} = 318.59$  nm and  $\lambda_{em} = 482.11$  nm (excitation and emission wavelengths), (Fig. 1). The best pH, time and temperature were 4.0, 20 minutes and 35°C for optimal complex formation, respectively.  $[Al^{3+}]$ -F.I. calibration graphics were linear within 0.027-0.27 and 0.27-2.70 ppm aluminum concentrations. The fluorimetric aluminum determination method with the newly synthesized macro molecule Schiff base DHDPE which was used as the ligand, was applied to various water sources. As a result of the analysis, the Al content in water inlet to KOSKİ was double-fold compared to other water samples.

**Keywords:** Schiff bases; Aluminum; N,N'-bis(2,5-dihydroxybenzylidene)-4,4'-diamino diphenyl ether; Spectrofluorimetry.

P-052

## Photophysical and photochemical properties of an unmetalled phthalocyanine obtained at low temperature

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Unmetalled phthalocyanine was accidentally obtained during the synthesis of diphthalonitrile that was prepared by a nucleophilic aromatic substitution reaction between 4-nitrophthalonitrile and 1,3-benzenediol at 70°C in DMSO. The product was purified by chromatography on a silicagel column with gradient of chloroform, tetrahydrofuran, MeOH, DMSO. The structure of the synthesized compound was characterized using elemental analyzes, and UV-Vis, FT-IR, <sup>1</sup>H-NMR and mass spectroscopies. And then, its photophysical and photochemical properties was investigated.

**Keywords:** Metalfree-phthalocyanines, photodynamic therapy, singlet oxygen, emission spectrum

P-053

## Characterization of some vegetable oils by Fourier transform infrared and Synchronous fluorescence spectroscopy

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This study describes two sensitive, more advantageous and rapid techniques. The method is based on the use of Fourier transform infrared (FTIR) and Synchronous fluorescence spectroscopy (SynFS) for the characterization and differentiation between vegetable oils from different botanical origin, including sunflower, corn, lavender, castor and olive oils. The analysis is made based on absorbance and wave number. FTIR spectra of studied oils show that there are notable differences in the bands around  $3007\text{ cm}^{-1}$  assigned to the C-H stretching vibration of the cis-double bond. The oil composition affects the exact position of the band and yields shifts when the proportion of the fatty acid changes. The height of this band for the olive oil is smaller than other oils. The height of large peak around  $1745\text{ cm}^{-1}$  is attributed to C=O stretching that is varied from oil to another with higher absorbance values for pomace olive oil and lower for lavender oil. For the peak at  $1460\text{ cm}^{-1}$ , the highest value is found for pomace olive oil whereas the lowest is for olive oil. The synchronous fluorescence spectra of oils show a relatively intense band with emission in the range of 300-370 nm has been ascribed to the tocopherols. The fluorescence of pigments of the chlorophyll groups is characterized by the long-wavelength band at 640-680 nm. The intensity of those bands varied from oil to another. Based on these observations, it is possible to differentiate between the different oils. The obtained results suggest that the application of FTIR and FS spectroscopy may be a powerful analytical tool in the characterization, classification and differentiation of vegetable oils and fats.

**Keywords:** Fourier transform infrared spectroscopy, Synchronous fluorescence spectroscopy, Vegetable oils

P-054

## Synthesis, Crystal Structure and Luminescence Properties of 3D Zn(II) Coordination Polymer Constructed from Thiophene-2,5-Dicarboxylate and 1,4-Bis(2-Ethylimidazol-1-yl)Butane

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Coordination polymers (CPs), a class of novel functional hybrid materials, have been received significant attention due to their structural richness and various potential applications in the field of coordination chemistry and material science. CPs are formed by the coordination of metal ions with organic linkers and they have been recently used in many different applications such as gas storage, separation, catalysis, chemical sensor and drug delivery. Heterocyclic dicarboxylic acids which can be used as a ligand coordinate the metal ions as bridging ligand at the synthesis of coordination polymers. In this study,  $[Zn_2(\mu_4\text{-tdc})_2(\mu\text{-betib})]_n$  (1) complex is synthesized with hydrothermal method by using thiophene-2,5-dicarboxylic acid (H<sub>2</sub>tdc) and imidazole derivative of 1,4-bis(2-ethylimidazol-1-yl)butane (betib). The structure of the complex has been characterized by elemental analysis, spectroscopic (IR) and thermal analysis methods (TG/DTA) and X-ray single-crystal studies. Compound 1 was synthesized under hydrothermal conditions (170 °C and 96 hours). The IR spectrum of complex show characteristic bands for antisymmetric-symmetric stretching of the dicarboxylate groups range of 1643-1527 $\text{cm}^{-1}$  and 1413-1377  $\text{cm}^{-1}$ , respectively. The asymmetric unit of complex contains one Zn(II) ion, one tdc ligand, and half betib ligand. The Zn(II) ion displays an square pyramidal geometry ( $ZnO_4N$ ), with equatorial positions occupied by four oxygen atoms of carboxylate groups from four different tdc ligands. The axial position is occupied by a nitrogen atom from a betib ligand. Four different carboxylate groups coordinate two Zn(II) ions to form a paddle-wheel  $[Zn_2(COO)_4]$  secondary building unit (SBU). The axial sites of the paddle-wheel are occupied by betib linkers to form a 2-fold interpenetrated 3D $\rightarrow$ 3D framework with 1D rectangle-like channel. Furthermore, luminescent properties of complex were studied.

**Keywords:** Coordination polymer, thiophene-2,5-dicarboxylate complex, Zinc(II) complex

P-055

**X-ray Absorption Fine Structure Spectroscopic Study of The Chemical Speciation of Mercury and Selenium in Fish-eating Birds: Complexation by Se as a Possible Detoxification Mechanism**

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Mercury compounds are well-known to be common environmental pollutants and neurotoxins. It has been observed that bio-accumulated quantities of Mercury and Selenium often are correlated in the tissues of mercury-exposed animals. We have previously observed using synchrotron radiation based microfocus x-ray fluorescence mapping that in liver tissue slices of marine fish-eating birds (cormorants) Hg and Se spatially co-accumulate in <10 micron-scale clusters, which suggested that the Hg and Se might be chemically bound together, perhaps as a means of immobilizing the Hg and detoxifying it. The chemical complexation was confirmed using Se X-ray Absorption Fine Structure Spectroscopy on a very limited sample of the “hot-spots” and individual birds, demonstrating direct chemical binding of Hg and Se in a disordered Tiemannite-like configuration. The observation raised the question of how broadly these conclusions apply to other individuals and species.

In the current work we report update and extend our previous measurements to other fish-eating individuals and other species, specifically Bald Eagle and Loon. Our results are consistent with the hypothesis that complexation of Hg by Se is an adaptive response to detoxification of mercury.

**Keywords:** X-ray fluorescence, X-ray Absorption Fine Structure (XAFS), Synchrotron Radiation

P-056

## Analysis of Hydrolytic Differences of Free and “Polyacrylic Acid (PAA)-Conjugated Trypsin and Chymotrypsin” by Using Fluorescence Lifetime Distributions

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In this study, the effects of free and polyacrylic acid (PAA) conjugates of the proteases trypsin and chymotrypsin on fluorescence lifetime distribution of PM-BSA complex [N-(1-Pyrenyl)maleimide (PM) – Bovine Serum Albumin (BSA)] were studied by using time resolved fluorescence technique and exponential series method to search out the lifetime distribution profiles from the fluorescence decay data. The results showed that the mole ratio (1:1) used in the PAA-Protease conjugate caused significant decreasing in the activities of the two proteases, probably due to the active sites covered by PAA. Despite the significant inhibition of the proteases by the conjugation, the fluorescence lifetime distribution profiles of the hydrolysates exhibited remarkable differences specific to the conjugates, which are unobservable in the fluorescence spectra, and reveals the sensitivity of the distributional approach model.

**Keywords:** trypsin, chymotrypsin, polyacrylic acid, fluorescence, lifetime, PM-BSA

P-057

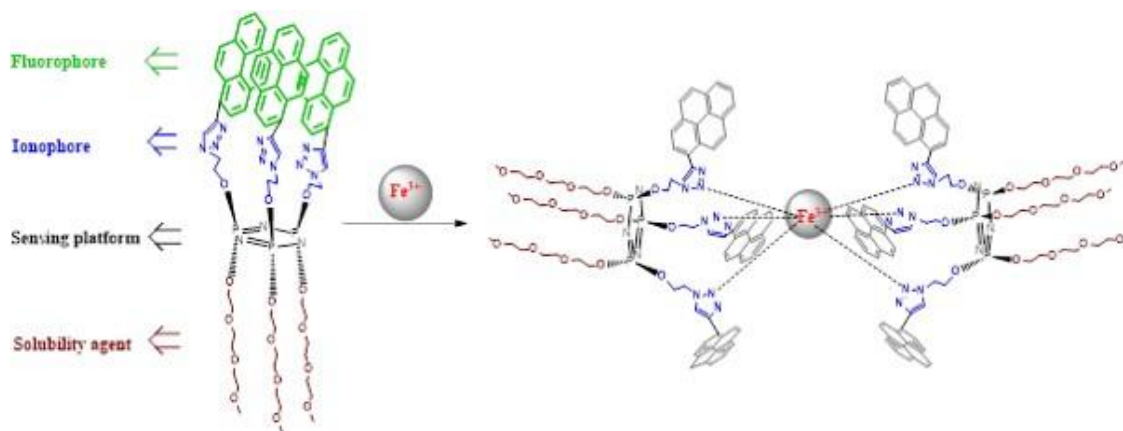
**A highly selective and sensitive fluorescence probe for Iron(III) ions based on a cyclotriphosphazene scaffold**

Serkan Yeşilot, Süreyya Oğuz Tümay, Semiha Yıldırım Sarıkaya, Aylin Uslu

*Gebze Technical University*

Recently, fluorescence sensors have been great interest in environmental monitoring, clinical investigations and control of industrial processes. When compare fluorescence sensors with instrumental methods such as ICP-AES, ICP-MS, AAS, fluorescence sensors have great advantage like high selectivity, sensitivity, instant monitoring, low cost. Iron is one of the most abundant trace elements in lithosphere after oxygen, silicon and aluminium (about 5 % of the earth). Both inadequate iron supply and excessive iron accumulation in the body lead to increased morbidity. However, excessive intake of iron in human body is associated with heart and liver diseases, cancer and neurobehavioral disorders such as Parkinson and Alzheimer's diseases. In this study, the design and synthesis of new cyclotriphosphazene bearing "tripodal" fluorescence sensor system which will be used as selective and sensitive determination of iron in environmental water and drug samples were planned (Fig.1). To reach the main aims of proposal the following objectives will be solved: The synthesis of compounds, the characterization of compounds by using traditional spectroscopic analysis methods, the investigation of photophysically and sensor properties of fluorescent system and real sample analysis after validation of method (response time, continuous variation method (Job's plot), Fluorescence titration study, dynamic range of study etc.)

**Keywords:** Fluorescent sensor, cyclotriphosphazene, iron, pyrene-triazole, real samples



**Fig. 1. Proposed binding mechanism for tripodal" fluorescence sensor system**

P-058

**A water-soluble fluorescence sensor based on a phosphazene platform for Iron(III) ions**

Serkan Yeşilot, Süreyya Oğuz Tümay, Elif Özcan, Aylin Uslu

Gebze Technical University

Fluorescence sensor applications for metal detection can be carried out through the change of emission or absorption peak intensities. Numerous fluorescence sensor studies for metal detection were performed to obtain high selectivity while getting lower detection limits. Among various metal Elements, iron plays an important role and vital element in living organisms because numerous enzymes and proteins include iron in their structures. Also, in biological systems, oxidation states ( $\text{Fe}^{2+}$  and  $\text{Fe}^{3+}$ ) of iron are one of the important redox pairs. In this study, the design, synthesis and investigation properties of new cyclotriphosphazene based which can be used as selective and sensitive fluorescence sensor for  $\text{Fe}^{3+}$  ions were planned. In this way, the disadvantages which appear other determination methods like low detection limits, not allowing real-time detection etc. thought be discarded by means of novel pyrene substituted cyclic phosphazene chemosensors. The novel compounds were fully characterized by the standard spectroscopic techniques such as  $^1\text{H}$ ,  $^{13}\text{C}$  and  $^{31}\text{P}$  NMR, mass spectrometry (MALDI-TOF). The chemosensor behaviors of this thiazole-

PEGME substituted cyclic phosphazene compound against to  $\text{Fe}^{3+}$  ions was determined by UV and fluorescence spectrophotometry (Fig. 1).

*Acknowledgements:* This work was supported by the Scientific and Technological Research Council of Turkey (TÜBİTAK), (Project number: 115Z897).

**Keywords:** Fluorescent sensor, cyclotriphosphazene, iron, thiazole-PEGME

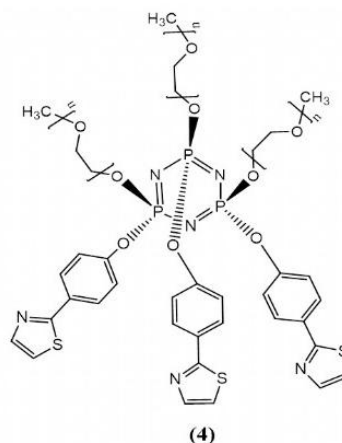


Fig. 1: Chemical structure of thiazole-PEGME substituted cyclic phosphazene compound



P-059

## Spectroscopic Investigation of Synthesized Water Soluble Metallo Phthalocyanines: Absorbance, Fluorescence, Mass and Voltammetric Studies

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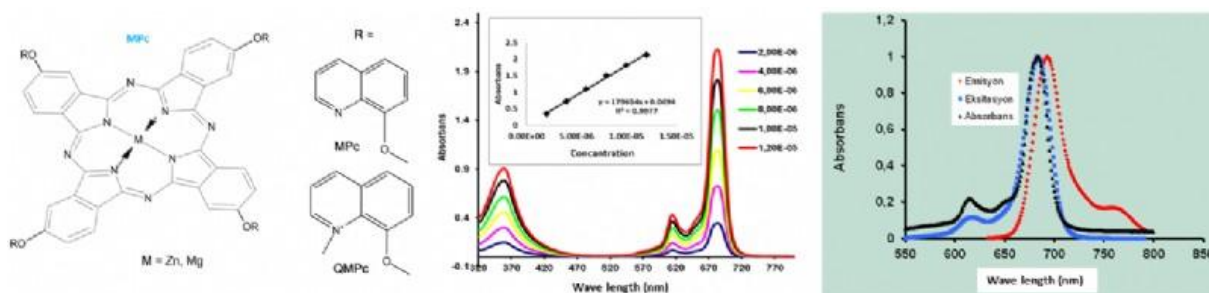
Phthalocyanines (Pcs) are highly conjugated synthetic porphyrin analogs that have been the subject of study due to their intense absorbance in the visible region, electron mobility, thermal, and photo stabilities [1,2]. Although metallophthalocyanines (MPcs) possess great potential due to discrete redox-active, ion-active and photo-active units has been rapidly expanding into several applied fields including biological and material science, they are practically insoluble in common organic solvents and aqueous media, thereby minimizing their applications. In order to reduce phthalocyanine aggregation and to increase their solubility and biological efficacy, phthalocyanine compounds are quaternized via amine groups on substituents such as quinoline moiety at the phthalocyanine macrocycle [3].

In this work, water soluble derivative (3) of tetra-3,4-dicyano-6-quinolin-8-yloxy substituted novel Zn(II) and Mg(II) phthalocyanine (1-2) complexes were synthesized and characterized by UV-Vis, FTIR, <sup>1</sup>H NMR, Fluorescence and Mass Spectroscopies (Fig.1) [4]. MPcs were also investigated by electrochemical techniques such as cyclic voltammetry (CV) and square wave voltammetry (SWV).

*This study was supported by Scientific Research Projects Unit of Yildiz Technical University (Project No: 2015-01-02-GEPO1).*

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**Keywords:** Phthalocyanine, cyclic voltammetry, fluorescence spectroscopy.



**Fig. 1.** The molecular structures of phthalocyanine complexes and UV-vis, Fluorescence spectra

P-060

## Study of the influence of the electromagnetic field on the state of erythrocytes of patients with acute ischemic stroke by the method of UHF dielectrometry

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Electromagnetic fields of anthropogenic origin change the natural electromagnetic background and can lead to the appearance of disorders at the cellular, subcellular and molecular levels [1], that produces various diseases, in particular, weakening of mental activity [2]. The prevalence of acute ischemic disorders among the population, high mortality and rapid "rejuvenation" of the disease cause the urgency of searching and developing informative and accessible methods for early diagnosis and effective prognosis of the state of health. The problem was solved in a diagnostic method, which is performed by examining blood indices using very high frequency dielectrometry at a frequency of 9.2 GHz by comparing the real  $\epsilon'$  and imaginary  $\epsilon''$  parts of the complex permittivity  $\epsilon^*$  of the erythrocyte samples from healthy donors and patients.

In the experiment the heparin stabilized portions of blood of six healthy donors and six patients with acute ischemic stroke have been used. Experimental conditions were: frequency (f) 36.65 GHz, power density (W) at the surface of exposed object  $100 \mu\text{W}/\text{cm}^2$ , exposure time 10 s. The thickness of the cell layer upon irradiation was about 1 mm.

The increase in the dielectric permittivity  $\epsilon^*$  of the irradiated samples of patients to those of donors was established by 16.7% ( $p < 0.02$ ) and the increase in relative  $\epsilon^*$  of patients/donors after the action of the electromagnetic field (restoration effect) was estimated by 4.1% ( $p < 0.02$ ). Objectively, the nature of the relationship between the measured parameters was estimated by the Spearman correlation coefficient:  $r = + 0.34$  ( $p < 0.04$ ). A decrease in the dielectric permittivity means the binding of water in the cell. The results obtained showed that the hydrated environment of the cell is a replica of its structure and reflects any changes that occur at various subcellular disorders.

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2. D. Poljak Electromagnetic Fields: Environmental Exposure/Encyclopedia of Environmental Health, 2011, pp. 259–268.

**Keywords:** microwave dielectrometry, dielectric permittivity, erythrocyte, acute ischemic disorders

NOT  
ATTENDED

P-061

## Magnetic and Microwave Absorption Properties of $\text{Ni}_{0.1}\text{Zn}_{0.8-x}\text{Mn}_{0.1}\text{Cu}_{0.1}\text{Fe}_2\text{O}_4$ Substituted Ni-Zn Nanoparticles

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Mn-Cu substituted spinel NiZn ferrite nanoparticles were prepared by in the form of  $\text{Ni}_{0.1}\text{Zn}_{0.8-x}\text{Mn}_{0.1}\text{Cu}_{0.1}\text{Fe}_2\text{O}_4$  using the conventional solid state reaction method. 1 wt%  $\text{B}_2\text{O}_3$  was added to increase the crystal growth at low temperatures. The structural properties of synthesized samples have been studied using x-ray diffractometry (XRD) and scanning electron microscopy (SEM). Magnetic properties of samples were measured by vibrating sample magnetometer (VSM). The saturation magnetization increases while the nickel concentration increases up to  $x=0.8$ . The samples have low coercivity values of about several oersteds. Ball milling process was applied to the samples to change the domain size of the samples and improve both magnetic and microwave properties. Microwave characteristics were determined by near field measurements using a network analyzer in reflection/transmission mode in 0-20 GHz. The microwave characterization showed that  $\text{Ni}_{0.8}\text{Mn}_{0.1}\text{Cu}_{0.1}\text{Fe}_2\text{O}_4$  nanoparticles have reflection loss value of -24.11 dB at 10.62 GHz with a thickness of 3 mm. The mechanism of absorption is due to the quarter wave cancellation at the matching thickness.

**Keywords:** Microwave Properties, Reflection Loss, Magnetic Measurements, Nanoparticles.

P-062

Line Ratio Diagnostics in Early-Type Galaxies: NGC4710 and NGC5866

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We present interferometric observations of CO lines (12CO(1-0, 2-1) and 13CO(1-0, 2-1)) and dense gas tracers (HCN(1-0), HCO+(1-0), HNC(1-0) and HNCO(4-3)) in two nearby edge-on barred lenticular galaxies, NGC 4710 and NGC 5866, with most of the gas concentrated in a nuclear disc and an inner ring in each galaxy. We probe the physical conditions of a two-component molecular interstellar medium in each galaxy and each kinematic component by using molecular line ratio diagnostics in three complementary ways. First, we measure the ratios of the position-velocity diagrams of different lines, second we measure the ratios of each kinematic component's integrated line intensities as a function of projected position, and third we model these line ratios using a non-local thermodynamic equilibrium radiative transfer code. Overall, the nuclear discs appear to have a tenuous molecular gas component that is hotter, optically thinner and with a larger dense gas fraction than that in the inner rings, suggesting denser clumps immersed in a hotter more diffuse molecular medium. The physical conditions of the molecular gas in the nuclear discs of NGC4710 and NGC5866 thus appear intermediate between those of spiral galaxies and starbursts, while the star formation in their inner rings is even milder.

**Keywords:** galaxy kinematics, lenticular galaxies, star formation, molecular gas, line ratio diagnostics

P-063

## Structural, Spectroscopic and Thermal Characterization of 5-Methylhydantoin: From the Isolated Molecule to Solid State Polymorphism

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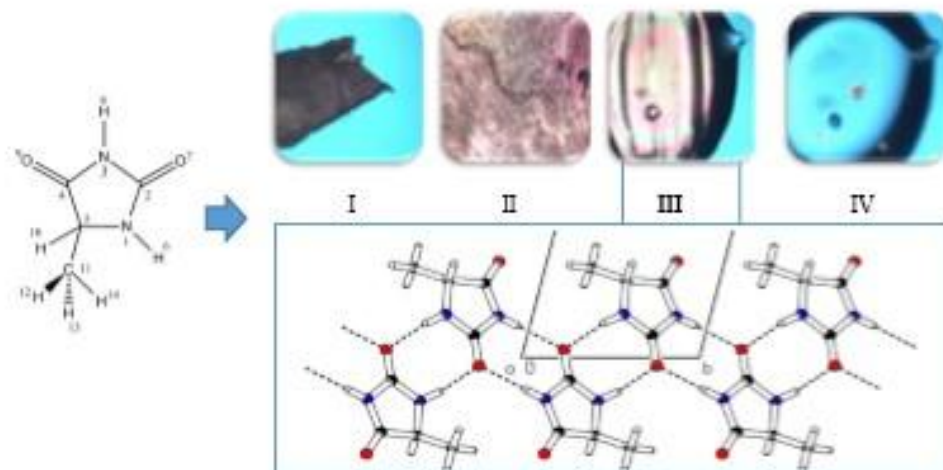
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5-methylhydantoin (C<sub>4</sub>H<sub>6</sub>N<sub>2</sub>O<sub>2</sub>; 5-MH) isolated in argon matrix was studied by using infrared spectroscopy and quantum chemical calculations at the DFT(B3LYP)/6-311++G(d,p) theory level. The electronic structure of the most stable structure of 5-MH was investigated using the Natural Bond Orbital (NBO) method. Upon UV irradiation of matrix-isolated 5-MH, a single photofragmentation pathway was observed, resulting from the cleavage of the hydantoin ring and yielding isocyanic acid, ethanimine and carbon monoxide. This reaction follows the same pattern as those observed before for both the parent hydantoin and 1-methylhydantoin molecules.

The thermal properties of 5-MH were investigated by differential scanning calorimetry (DSC), polarized-light thermal microscopy (PLTM) (Fig. 1) and infrared and Raman spectroscopies. Four different polymorphs of 5-MH were identified. The crystal structure of one of this polymorphs (polymorph III) was determined by single crystal X-ray diffraction (XRD), and two additional polymorphs were characterized by powder XRD.

*Authors thank the Project PTDC/QEQ-QFI/3284/2014 – POCI-01-0145-FEDER-016617, funded by FCT (Lisbon) and FEDER/COMPETE 2020-EU. The CQC and CFisUC are supported by FCT (Projects UI0313/QUI/2013 and UID/FIS/04564/2016), also co-funded by FEDER/COMPETE 2020-EU.*

**Keywords:** 5-Methylhydantoin, Polymorphism, IR and Raman spectroscopies, X-ray analysis, Unimolecular photochemical fragmentation, Thermal analysis.



**Fig. 1.** The molecule of 5-MH (left) and the PLTM images of the four identified polymorphs of the compound (top). The crystal structure of polymorph III (bottom) has been determined by XRD.

P-064

## Conformational Landscape and Polymorphism in 5-Acetic Acid Hydantoin

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The conformational analysis of 5-acetic acid hydantoin 5AAH; [2.(2,5-dioxoimidazolidin-4-yl)acetic acid] was carried out by quantum chemical calculations performed at the DFT(B3LYP)/6-311++G(d,p) level of theory. Thirteen conformers were located in the potential energy surface of the molecule, 6 of them exhibiting the cis configuration (with O=C–O–H dihedral equal to  $\sim 0^\circ$ ) and 7 of them bearing a trans carboxylic group (O=C–O–H dihedral equal to  $\sim 180^\circ$ ). The most stable conformer of 5HAA (cis I) was trapped in a low temperature argon matrix, at 10 K. Assignments of the vibrational modes were done based on normal coordinate analysis. Natural Bond Orbital (NBO) theory was used to study the electronic structure of this conformer.

Thermal properties of 5-AAH were investigated by differential scanning calorimetry (DSC), polarized-light thermal microscopy (PLTM) and Raman spectroscopy, resulting in the identification of four different polymorphs.

Very interestingly, in polymorph A (the most stable polymorph at room temperature), the molecular units of 5AAH assume the conformation that was found to correspond to the highest energy conformer (trans-VI) predicted by the calculations for the isolated molecule.

**Keywords:** 5-Acetic acid hydantoin, Conformational space, Polymorphism, Matrix isolation IR and Raman spectroscopies, X-ray analysis, Thermal analysis.



P-065

## Determination of Ammonia and Nitrite in Exhaled Breath Condensate of Healthy Humans By Using a Sensitive Spectrophotometric Method

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Exhaled breath has recently been identified as an alternative matrix for the detection of drugs and chemical compounds. As a wide variety of chemical and biological substances has already been detected in the exhaled air, the exhaled breath condensate (EBC) was found suitable for non-invasive assessment of the respiratory system. The aim of this work is determination of ammonia and nitrite in EBC. The procedure is based on the derivatization of ammonia using Berthelot reaction. The absorbance of colored compound was determined at  $655 \pm 3$  nm. Nitrite ion is determined after its reduction to ammonia in the presence of Zn/HCl. The method gave calibration curves for ammonia with good linearity in the range of 10– 620 ng/mL, and correlation coefficients ( $R^2$ ) of more than 0.999. The limit of detection (LOD) and quantification (LOQ) and lower limit of quantification (LLOQ) were 1.5, 4.5 and 10.0 ng/mL, respectively. The recoveries of the method were in the range of 94 to 102.5% and the intra- and inter-day precisions were lower than 1.4 and 3.4%, respectively. The method was applied to the determination of the target analytes in EBC samples of healthy volunteers.

ATTENDED

**Keywords:** Ammonia, Berthelot reaction, exhaled breath condensate (EBC), nitrite, spectrophotometry

P-066

## Novel Ideal Soluble And Non-Aggregated Copper(II) Phthalocyanines: Synthesis, Structure, Spectroscopic Properties

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Metallo phthalocyanines (MPcs) are 18  $\pi$ -electron conjugated organometallic macrocycles that typically comprise the usually planar organic ligand and a metal ion or metalloid within the central cavity of the ring. MPcs have attracted considerable attention in solar cells, photodynamic therapy, gas sensors, as liquid crystal, and electrochromic displays because of their remarkable optical, and electrical properties, the conjugated system, as well as chemical and thermal stability. Pcs exhibit strong absorptions in both UV and visible region as expected from the extensively conjugated aromatic chromophore due to their intense  $\pi$ - $\pi^*$  transitions. When Pcs are modified by oxygen-bridged substitution and substitution positions (peripheral or non-peripheral), the compounds have an extended conjugated network of  $\pi$  electrons and their  $\pi$ - $\pi^*$  transitions energy changes. The solubility of Pcs is very important to investigate their physical and chemical properties and it is affected by the substituent positions (peripheral or non-peripheral) and the nature of the substituents on the Pc ring. The solubility of Pcs can be developed by the addition of alkyl, alkoxy, alkylsulfanyl and other bulky groups onto their peripheral or non-peripheral positions. Central metals play a major role in tuning the properties of MPcs; some central metal ions, which increases solubility and reduce molecular aggregation. In this study, 2,6-dimethoxyphenoxy substituted copper(II) Pc molecules were synthesized to soluble, non-aggregated, bifunctional materials to use in various applications. We have tried to determine what molecular structure effect peripheral or non-peripheral position of phenoxy and location of methyl groups on phenoxy unit and nature of metal in Pc cavity was responding to their spectroscopic properties by comparing with 2,6-dimethoxyphenoxy substituted Pcs and their novel analogs (Fig. 1).

**Keywords:** Copper(II); phthalocyanine; soluble, non-aggregated, spectroscopic.

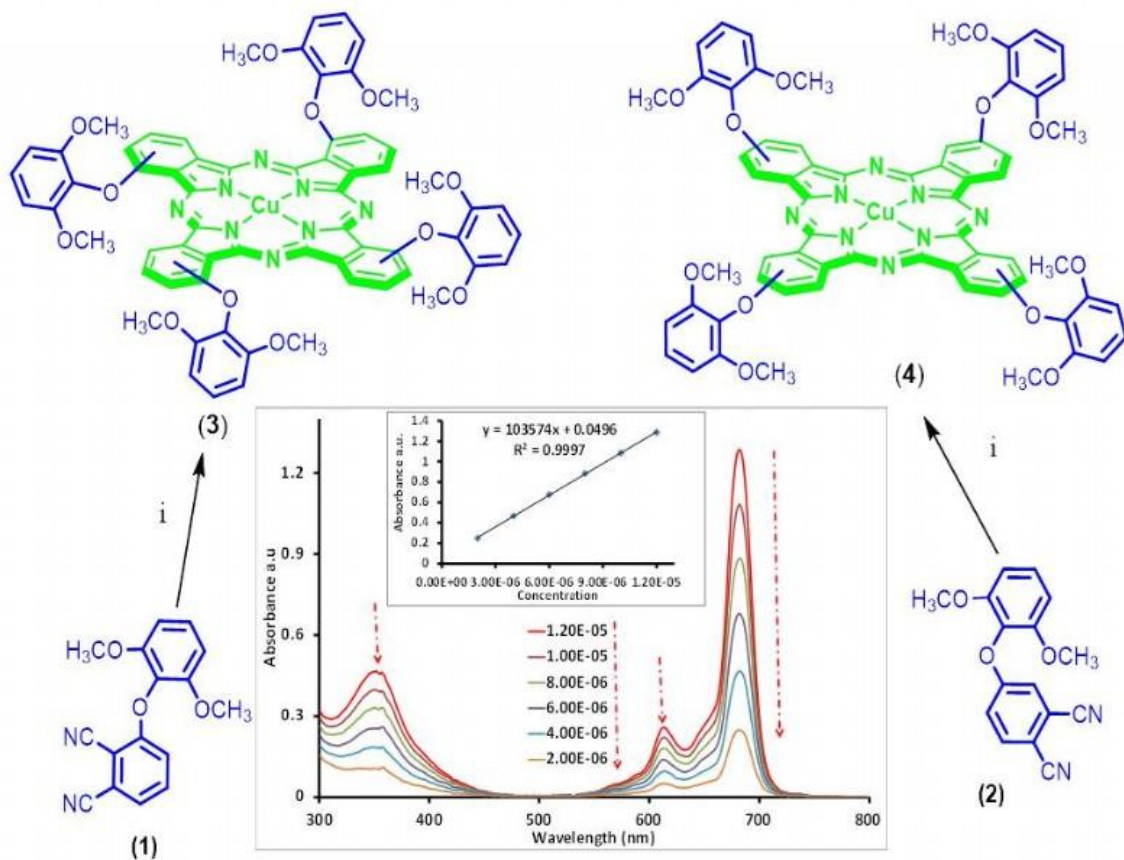


Fig. 1. Synthesis of non-peripheral and peripheral substituted copper(II) phthalocyanines (3 and 4). Reagents and conditions: (i) N<sub>2</sub>, copper(II) chloride, DMF, DBU, 360 °C, 25 min.

P-067

## Boron Compounds with Magnetic Properties and Their Catalytic Applications

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Ferromagnetic substances; the relative magnetic permeability of material is larger than 1. Only the iron, nickel and cobalt are ferromagnetic at room temperature. Many of the alloys containing them carry ferromagnetic properties. Even if in a magnetic field is removed the magnetism continues in this feature. Magnetic separation techniques have advantages that are speediness, high productivity and cost-effectiveness because the magnetic carriers are intense which are metal ions and use determination of coating, drug delivery, enzyme immobilization, protein and cells used in the separation area. Because of this properties ferromagnetic nanoparticles can be use in electric, optical and magnetic fields. Thus, nanoparticles have been synthesized for use in reactions such as reduction, oxidation, degradation. The synthesized nanoparticles have been used in methylene blue degradation reaction and have achieved remarkable results from some nanoparticles.

**Keywords:** Magnetic nanoparticles, nanocatalyst, ferromagnetic

**P-068**

**Nitro compounds reduction reaction with novel synthesized magnetic nanoparticles which are prepared with different metal salts and reducing agents**

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Synthesis of metal-containing boron compound having magnetic properties and the catalytic applications of these compounds include prospective studies. For this aim, it will first give the magnetic properties of boron compounds having different crystal structures will be provided to connect some transition metals. Therefore, the aim of this study has ferromagnetic properties Ni, Fe, Co, such as metal nanoparticles of boron compounds are prepared in their organic reaction (oxidation, reduction, degradation, hydrolysis... etc.), availability will be determined. In this context, metal type and quantity, temperature, magnetic characteristic parameters such as the amount of organic compound will be examined. The structural features of all the products obtained will be elucidated by various spectroscopic techniques. The combination of catalytic quantities of ferromagnetic metal nanoparticles with NaBH<sub>4</sub> and N<sub>2</sub>H<sub>4</sub> smoothly reduces aromatic nitro compounds to amines in aqueous medium.

**Keywords:** reduction, catalytic, magnetic

P-069

## Periferal Tetrakis-Benzenesulfonamide Derivative Substituted Phthalocyanine: Solid State Synthesis, Structure, Spectroscopy

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Phthalocyanines (Pcs) that are synthetic materials are used in energy transfer, electrophotography, optic data collection, gas sensors, laser technologies, dyes and pigments. The rich coordination chemistry of Pc complexes has encouraged researchers to design specific products with certain properties which are required for high technology applications. When a new Pc complex wanted to design, the central metal ion and peripheral substituents are used. We can obtain products with wanted properties when the possibility of inserting different metal ions into the central cavity of Pc is combined with different substituents. A Pc containing metal ions is called metal phthalocyanine (M-Pc). The functions of M-Pcs are based on electron transfer reactions because of the  $\sim 18 \pi$  electron conjugated ring system found in their molecular structure. For many applications the absorption maxima of M-Pcs are best if moved near the infrared region. The strongest absorption of M-Pcs in the visible region, the so-called Q band, can be attributed to the allowed HOMO-LUMO ( $\pi-\pi^*$ ) transition. Also Pc derivatives are known to have potential as second-generation photosensitisers for photodynamic therapy of cancer because they show strong absorption of the far-red light between 600 and 850 nm, which has greater tissue penetration properties and satisfactory photosensitization of singlet oxygen. Schiff bases are considered a very important class of organic ligands and they are capable of forming coordinate bonds with many metal ions and other groups, so they have been used for the synthesis of metal complexes due to their easy formation and strong metal binding ability. Their biological activities make them important antibiotics, anticlerics, antitumor and antifungals. Also their  $\pi$ -conjugation plays a vital role in the development of the new generation electronic and photonic devices due to delocalization of electrons. Especially sulfonamide coordination compounds and their derivatives are widely used important medicines. Metal complexes modify the pharmacology and toxicology of the sulfonamide base ligands. The significant aim of the present research was to synthesize highly soluble and capable of long wavelength absorption maximum new peripherally tetra-substituted zinc(II) Pc complex and characterized by various spectroscopic techniques in this study.

**Keywords:** Phthalocyanine, benzenesulfonamide, electronic spectroscopic.

P-070

## Development and Validation of a New Spectrophotometric Method for the Determination of Rivastigmine in Pharmaceutical Formulations

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Dementia is a progressive brain dysfunction that results in restriction of daily activities and in most cases requires a long term for the need for care. Alzheimer's disease is the most common type of dementia in the old age. Rivastigmine is a carbamate inhibitor of acetylcholinesterase and is used in the treatment of mild to moderate Alzheimer's disease in adults.

In this study, a new sensitive and rapid spectrophotometric method has been developed for the rivastigmine assay in pharmaceutical formulations and validated according to the International Conference on Harmonization guidelines for different validation parameters. Rivastigmine was dissolved in 0.1 N HCl and screened in a 1 cm quartz bath with a double-beam UV-Vis spectrophotometer at the range wavelength of 200-400 nm. Rivastigmine showed a maximum absorbance at a wavelength of 263.1 nm in 0.1N HCl. The method was linear ( $y = 0.0078X - 0.1775$ ) at a concentration range of 10-100 ppm and the correlation coefficient was excellent ( $r^2 = 0.9999$ ). The recovery percentages for Rivastigmine were found to be 98.50, 99.20 and 100.55 when compared to 80%, 100% and 120%, respectively. Relative standard deviations for intraday and inter day reproducibility tests were less than 1%. The limit of detection (LOD) and the limit of quantification (LOQ) were determined to be 0.89 and 2.94 ppm, respectively.

The results showed that the method is simple, cost-effective and less time consuming, as well as accurate, precise and reproducible. The proposed method is suitable for determining the amount of Rivastigmine in pharmaceutical formulations and can be used for routine analysis in quality control.

**Keywords:** Rivastigmine, Pharmaceutical, Spectrophotometry, Validation.

P-071

## Forced Degradation Study on Rilmenidine by first order derivative spectrophotometric method

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Hypertension is a chronic medical condition in which the blood pressure in the arteries is elevated. Today, there are various drug treatment classifications used in the treatment of hypertension, commonly referred to as antihypertensive drugs. Rilmedine's chemical formüle is N-(dicyclopropylmethyl)-4,5-dihydro-1,3-oxazol-2-amine. The stability of a drug product or a drug substance is a critical parameter which may affect purity, potency and safety. Changes in drug stability can risk patient safety by formation of deliver a lower dose than expected. Therefore it is essential to know the purity profile and behaviour of a drug substance under various environmental conditions. Rilmenidine pharmaceutical preparations will be exposed to the stress conditions of acid, base and oxidative in order to calculate to degradation percent by developed UV derivative spectrophotometric method.

*The present work was supported by the Research Project Coordination Fund of Namık Kemal University. Project No. NKUBAP.00.GA.16.02.*

**Keywords:** Rilmenidine, derivative, spectrophotometry, degradation



P-072

**The Novel Zinc (II) Phthalocyanine Substituted With Benzene Sulfonamide Derivative Compound Containing Pyridine And Nitro Units: Synthesis, Structured Lighting, Spectroscopic Features**

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Among the many different families of organic–inorganic chemicals being currently investigated due to their wide-scale applications, sulfonamides and their N-derivatives are one of the outstanding groups [1]. Schiff bases are one of the most widely used organic compounds and unveil a broad array of biological activities [2]. Sulfonamides were the first chemotherapeutic agents to be used for curing and preventing bacterial infection in human beings. They play a vital role as key constituents in a number of biologically active molecules and are known to exhibit a wide variety of biological activities, such as antibacterial, antifungal, anti-inflammatory, antitumor, anticancer, anti-HIV and anti-tubercular activities [3]. In recent years, extensive research studies have been carried out on the synthesis and evaluation of the pharmacological properties of molecules containing the sulfonamide moiety, which have been reported to be important pharmacophores [4]. Phthalocyanines are used in a number of applications due to their increased stability, architectural flexibility, diverse coordination properties, improved spectroscopic characteristics and an extensive delocalized  $18\pi$  electron system [5]. Some technological applications in fields, such as chemical sensors, liquid crystals, semiconductors, non-linear optics, as photosensitizers in photodynamic therapy (PDT), have shown the increased importance of these macrocycles [5]. Pcs soluble in polar solvents have strong influence on bioavailability whereas Pcs soluble in nonpolar solvents have a higher tumor affinity [5]. In this study, we have produced novel combining three functional materials (phthalocyanines, benzenesulfonamid and Schiff base) (Fig. 1) and characterized by IR, UV–Vis, <sup>1</sup>H- NMR, TG-DTA, MALDI-TOF mass spectroscopies and elemental analysis as well.

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**Keywords:** Phthalocyanine; spectroscopy, structure, pyridine, benzenesulfonamide.

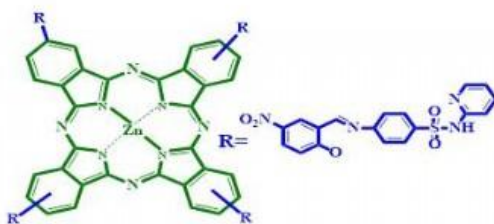


Fig. 1

P-073

Removal of Methylene Blue Dye Using Cerium Based Nano-Photocatalysis

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Nanoceria is implicated in a wide range of applications ranging from fuel cells to cosmetic products. To the best of our knowledge, for the first time, origanum syriacum plant extract was used for the green synthesis of nanoceria particles. In order to produce smaller particles, the agglomeration had to be reduced, thus biomolecules, such as alkaloids, phenols, flavonoids etc., whose contain many O-H functional groups and could bind surface of nanoparticles, were used in initial nucleation stage [1].

In this study, cerium nanoparticles were used in methylene blue colorant treatment (Fig. 1). H<sub>2</sub>O<sub>2</sub>/UV and photocatalytic oxidation as advanced oxidation processes were used for producing hydroxyl radical in order to remove methylene blue [2-3]. Removal efficiencies of experiments those were conducted under UV light and under normal room conditions were compared. As a result of this study, 30% of methylene blue was removed in H<sub>2</sub>O<sub>2</sub>/UV system and the removal rate of methylene blue had reached up 70% in nanoceria/UV system in 90 minute. Nanoceria has produced very rapid degradation of the methylene blue dye with almost to 100% removal in less than three hours.

The authors were grateful to TUBITAK Research Fund for their support to the Project 115Z887.

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**Keywords:** Nanoceria, Photocatalysis, Removal, Methylene blue

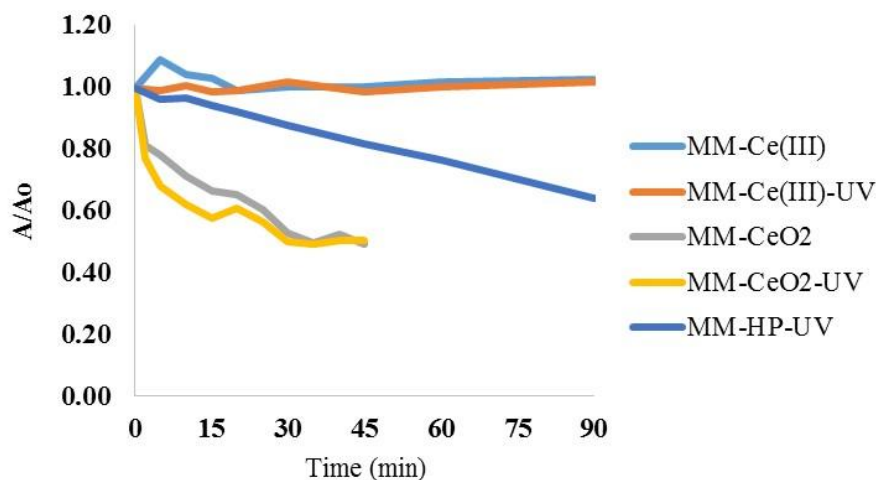


Fig.1 Effects of Ce(III), nanoceria, H<sub>2</sub>O<sub>2</sub> and UV on degradation of the methylene blue dye

P-074

## In Vitro Effects of Fexofenadine on PON1(Q192R) Isoenzymes in Patients with Sleep Apnea Serum

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Paraoxonase 1 (PON1: EC 3.1.8.1) is an antioxidant enzyme that is synthesized by the liver. In serum, it is closely associated with high-density lipoproteins [1-2]. PON1 hydrolyze organophosphate compounds which are widely used as insecticides and nerve gases. Therefore, it plays a major role in the detoxification of these compounds and other artificial substrates, so that it may alter significantly an individual's susceptibility to the toxicity of these chemicals [3]. PON1 exists in 2 polymorphic forms, Q (glutamine) or R (arginine) at codon 192. The Q isoform has a higher activity for hydrolyze of diazoxon, sarin, and soman; whereas the R isoform has a higher activity for hydrolyze of paraoxon and chlorpyrifosoxon. In addition the ability of HDL to protect LDL against peroxidation is significantly lower in HDL particles containing PON1R192 than in those with PON1Q192 [4].

In this study, paraoxonase Q and R isoenzymes were determined in sleep apnea disease bloods. The isoenzymes were separately purified from sleep apnea disease serum by Sepharose4B-L-tyrosine-1-naphthylamine hydrophobic interaction chromatography. The in vitro effect of fexofenadine was determined on purified Q and R. In conclusion, the drug showed inhibitory effect on PON1 isoenzymes under in vitro conditions. It was found that Q phenotype were more resistant to inhibition by fexofenadine than R phenotype. Therefore, PON1 activity was not decreased in patients with Q phenotype who used fexofenadine. Consequently, the side effect of this drug could be less for people with Q phenotype compared to R.

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*This work was supported by Balıkesir University Scientific Research Project (Project No. 2017/082).*

**Keywords:** paraoxonase, polymorphism, sleep apnea

P-075

## Identification and Classification of Polymers Using LIBS and Chemometry

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In the systems that are used for industrial waste disposal, different polymers are sent to the burning tanks without any prior knowledge of their ingredients. There exist also economically high price among the disposal material. Possibility of recycling materials are determined to recycling process before sent the burning tank will be supplied great advantage economy of the country and protection of the nature. Identification and classification of polymers is important for recycling of plastics waste to prevent serious environmental challenges. Laser induced breakdown spectroscopy (LIBS) were used to identify of polymers such as PE, HDPE, PMMA, PP, PVC combined with multivariate data analysis methods (PCA and PLS-DA) to classify the samples for recycling purposes. Nd:YAG laser [EKSPLA, NL 301 HT, 1064 nm, multimode] with 4.4 ns pulse width (FWHM) and ICCD spectrometer was used in LIBS system [1,2]. In polymer samples C2 Swan and CN Violet molecular bands were observed in the UV-VIS spectra and used to classify the polymers.

*This work was supported by the Ministry of Science, Industry and Technology of Turkey and The Scientific and Technological Research Council of Turkey, TUBITAK-TEYDEB, under contracts 404.TGSD.2010 and 9130018 projects, respectively.*

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**Keywords:** LIBS, polymer, chemometry, PCA, PLS-DA.

P-076

**Vortex assisted microextraction followed by UV–Vis spectrophotometric determination of mercury in fish samples**

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Mercury and its organic and inorganic species are toxic to the central and peripheral nervous system, however, this toxicity depends of this chemical form, among which organic mercury compounds are the most toxic. The principal chemical forms of mercury are: elemental mercury ( $\text{Hg}^0$ ), divalent inorganic mercury ( $\text{Hg}^{2+}$ ), methyl mercury ( $\text{CH}_3\text{Hg}^+$ ) and dimethylmercury ( $(\text{CH}_3)_2\text{Hg}$ ). A novel method was developed for the determination of mercury by vortex assisted microextraction (VA-ME) combined with UV–Vis spectrophotometry. The factors influencing the extraction procedure such as type and volume of extracting and disperser solvent, concentration of chelating reagent, pH, salt effect, temperature, and vortex time were systematically investigated. Under the optimized conditions, the analytical characteristics of the method were determined. The calibration graph was linear in the rage of  $0.5\text{--}250 \mu\text{g L}^{-1}$  with a detection limit of  $0.15 \mu\text{g L}^{-1}$ . The relative standard deviation for ten replicate measurements of 10, 50 and  $175 \mu\text{g L}^{-1}$  of mercury was in range of 2.9-4.5%. Enrichment factor was 109. The accuracy of the method was evaluated by analyzing the fish homogenate IAEA-407 certified reference material. This procedure was also used as a novel extraction method for mercury speciation. Moreover, in comparison with other methods, the proposed method, which is applicable for routine analysis of total mercury contents in fish samples, is very simple, easy, rapid, and sensitive for determination of Hg at trace levels in complex matrices.

**Keywords:** Mercury, fishes, microextraction, UV–Vis spectrophotometry, vortex

P-077

## Mn and Al removal from the waste water of hendek industrial zone with adsorption method color and turbidity removal by waste water adsorption method

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Wastes that contain metals are considered to be hazardous to both human life and the environment due to their acute toxicity and non-biodegradability, even when the heavy metals are present at trace concentrations. Most of the heavy metals are bound to particles in sediment, but only a small quantity becomes dissolved in the water and it can spread widely in the food chains. Because of that reason, treatment of waste water was performed by using advance treatment techniques such as adsorption, chemical and photo-oxidation. Adsorption is a very effective process for a variety of applications, and is considered economical and widely applicable. It creates relatively little sludge and is an efficient method for metal ions removal from wastewaters. The most widely used adsorbent is activated carbon, also easy to produce and cheap adsorbent materials such as zeolite were used in Fe and Al removal with adsorption.

Incoming water of Waste Water Facility of Hendek is effluent of metal and food factories. In this study time, speed, pH and amount parameters were examined by using silver doped activated carbon and zeolite adsorbents modified with silver. Mn and Al concentrations of incoming waste water of Hendek Waste Water Facility were found 101.976 ug/L and 175.799 ug/L respectively. Also pH 7.11 and temperature  $25 \pm 2^\circ$  C was identified in laboratory environment. Activated carbon modified with iron was identified as the most suitable adsorbent, Al removal was calculated as 78 % and Al removal was calculated as 72 %

**Keywords:** adsorption, aluminium and iron removal, waste water

P-078

## Color and turbidity removal by waste water adsorption method

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As the synthetic dyestuff was used quite often in textile industry, they increased the high Chemical Oxygen Demand (COD), pH, temperature and toxic solid material content by changing the color of textile waste water. Waste water constitutes an environmental problem because of their toxic characteristics. It is a complicated structure as it contains surfactant and organic-inorganic compounds with complex structure at high concentrations. Because of that reason, treatment of waste water which contained dyestuff, was performed by using advanced treatment techniques such as adsorption, chemical and photo-oxidation. Adsorption has been the highest treatment performance and mostly used among these methods. The most widely used adsorbent is activated carbon, also easy to produce and cheap adsorbent materials such as zeolite, bentonite and wood ash were used in dye removal with adsorption.

22 Pt-Co adsorbent as the result of activated carbon modified with iron was found (A) 0.029, 41 Pt-Co adsorbent as the result of raw data was found (A) 0.054 by measuring at 456 nm wavelength for the determination of color parameter of spectrophotometer device according to European Norm DIN EN ISO 9001: 2008 for the incoming waste water taken from Hendek Waste Water Facility. Also 7.11 pH and 10.6 °C temperature was identified in laboratory environment.

Raw data result for the determination of turbidimeter device parameter according to European Norm DIN EN ISO 9001: 2008 for the incoming waste water taken from Hendek Waste Water Facility was found as 58.4 NTU and the result of activated carbon modified with iron was found 18 NTU. Also 7.11 pH and 10.6 °C temperature was identified in laboratory environment.

In this study color, pH and amount parameters were examined by using activated carbon and zeolite adsorbents modified with iron. Activated carbon modified with iron was identified as the most suitable adsorbent and dye removal was calculated as 90 % and turbidity removal was found 69 %.

**Keywords:** adsorption, color and turbidity removal, waste water



P-079

## Chemical Oxygen Demands (Cod) Removal From The Waste Water Of Hendek Industrial Zone With Adsorption Method

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Chemical Oxygen Demand (COD) is the most important test parameter that is used to identify the degree of the pollution in the water and waste water samples. Various treatment technologies have been used for the reduction of COD, which is a major contaminant in industrial wastewater. Because of that reason, treatment of waste water was performed by using advance treatment techniques such as adsorption, e filtration, ion exchange, coagulation/flocculation, chemical and photo-oxidation. Adsorption of COD has been previously studied to evaluate the overall adsorption behavior in wastewaters.

In this study activated carbons which were synthesized with traditional and microwave method, were used as adsorbent. The determination of structural characteristics of activated carbons was made with FTIR. SEM device was used to identify the morphology. Then COD works were conducted with the characterized activated carbons. High COD containing sample which was collected from the point where the waste water of Hendek district and 2nd Industrial Zone were discharged. 200 mL was taken from pH: 7.11 C: 10.6 sample mixed 1 hour at 150 rpm with traditionally obtained activated carbon. The highest yield among the used adsorbents was in activated carbons. The European Norm of the water taken from the entrance of Wastewater Treatment Facility of Hendek according to DIN EN ISO 9001: 2008, "closed reflux" colorimetric method was used which was identified in the standard methods for COD measurement. pH: 7.11 and temperature 10.6 °C was identified in laboratory and time, speed, pH and amount parameters for chemical oxygen need were examined. Traditional method as the most suitable adsorbent was obtained with obtained activated carbons.

**Keywords:** COD, activated carbon, removal

**P-080**

**Total Organic Carbon Matter (TOC) Removal from the Waste Water of Hendek Industrial Zone with Adsorption Method**

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Waste water constitutes an environmental problem because of their toxic characteristics. It is a complicated structure as it contains surfactant and organic-inorganic compounds with complex structure at high concentrations. Because of that reason, treatment of waste water was performed by using advance treatment techniques such as adsorption, chemical and photo-oxidation. The removal of pollutants from water by adsorption is one of the most promising techniques because of its convenience when applied in current water treatment processes. The most widely used adsorbent is activated carbon, also easy to produce and cheap adsorbent materials such as zeolite, bentonit and wood ash were used in TOC removal with adsorption.

Incoming water of Waste Water Facility in Hendek/Sakarya is effluent of metal and food factories. UV(A) measurements were conducted at 254 nm wavelength with Jenway Model 6105 Spectrophotometry. Incoming waste water taken from Hendek Waste Water Facility, as the raw data result of the TOC parameter identified in accordance with ISO 9001:2008 norm is 34.9 mg/L, it was found as 2.44 mg/L as the result of the adsorption with activated carbon modified with iron. Also pH 7.11 and temperature 10.6 °C was identified in laboratory environment.

**Keywords:** Total organic carbon removal, adsorption, waste water

P-081

Experimental and computational study on furan-3-methanol

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3-FM and its derivatives have been more used to the photochemical reactions. Considering the literature, FT-IR,  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra were presented. On the contrary UV-vis spectrum has been not recorded. Purpose of this study is to provide detailed experimental and theoretical characterization on 3-FM. Ground and excited states calculations by using TD//DFT/B3LYP/6-311G(d,p) level in gas phase and methanol solvent (by using conductor-like polarizable continuum model, CPCM) have been fulfilled. It is concluded that there is a good agreement between experimental and corresponding theoretical results. FMO energies of 3-FM in gas phase and methanol solvent have been calculated by using the B3LYP/6-311G(d,p) level. The occupied and unoccupied MOs being the most active in electronic transition for 3-FM are given Fig. 1. To sum up, it can be said that 3-FM displays a positive solvatochromic behavior within different solvent polarities.

**Keywords:** Furan-3-methanol, UV-vis, TD/DFT, FMOs

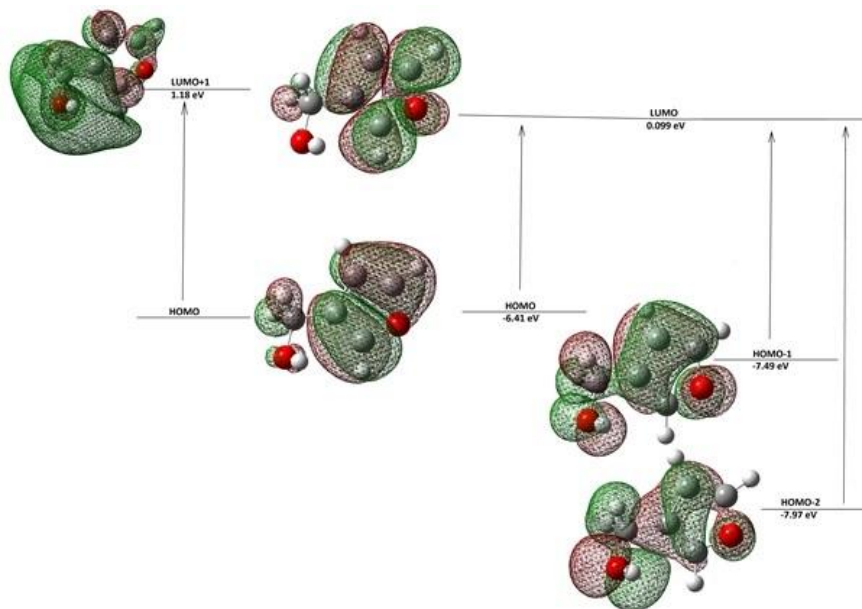


Fig. 1. The FMOs being the most active in electronic transition for 3-FM

P-082

## A new spectrophotometric method for the determination of nicotinamide (vitamin B3) in real samples after microextraction

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Nicotinamide, also known as niacinamide and nicotine amide, are forms of Vitamin B3, which is commonly found in nutritional supplements and added to fortify foods. Vitamin B3 is an essential vitamin required for processing fat in the body, lowering cholesterol levels, and regulating blood sugar levels. A deficiency of nicotinamide leads to pellagra, a condition characterized by diarrhea, dermatitis, perioral inflammation of the mouth, amnesia, delirium, and death [1,2]. In the study, the ultrasound-assisted ionic liquid-based dispersive liquid-liquid microextraction (UA-IL-DLLME) developed for as an ultra preconcentration and/or technique for the determination of nicotinamide (vitamin B3) in beverage, milk and food samples. After optimization, the proposed method performances like excellent linearity (LR), limits of detection (LOD), limits of quantification of 5–800  $\mu\text{g L}^{-1}$  with  $R^2$  of 0.9918, LOD (1.6  $\text{ng mL}^{-1}$ ), LOQ (5.2  $\mu\text{g L}^{-1}$ ), respectively show successful and accurate applicability of the present method for monitoring analytes with within- and between-day precision of 1.9–3.5%. The average absolute recoveries of the nicotinamide extracted from the beverage, milk and food samples were 91.5–104.7%. The proposed method was compared with other methods and its applicability was evaluated by the determination of nicotinamide in these samples.

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**Keywords:** ultrasonic extraction, ionic liquid, nicotinamide, ultraviolet detection

P-083

## Synthesis, Structure and Spectroscopic Properties of Novel Zinc(II) Phthalocyanine Using Sonogashira Cross-Coupling Reaction

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Phthalocyanines (Pc) have received increasing attention for a wide variety of applications due to their unique physical, chemical, biological and spectral properties. Carbon-carbon bond formation is the essential step for the synthesis of complicated organic molecules. Prominent among these procedures is the Pd-catalyzed C-C bond-forming reaction. Based on this methodology, a number of novel Pcs have been prepared with improved their catalytic, photophysical and biological activities. The major drawback is that Pcs have poor solubility in most of the organic solvents and water. The solubility of Pcs in organic solvents can be increased by substitution at the peripheral positions with several functional groups. In this study, we designed and prepared ZnPc bearing N,N-dimethyl-2-propyne amine groups at peripheral positions to obtain novel water-soluble Pcs via Pd-catalyzed Sonogashira coupling reaction and characterized by common spectroscopic properties.

**Keywords:** phthalocyanine, N,N-dimethyl-2-propyne amine, spectroscopic

P-084

## Determination of Total Antioxidant Capacity of Shampoos by Spectrophotometric Method

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Antioxidants are molecules that inhibit free radicals into nontoxic waste products. The body has the antioxidant defense system against free radicals. The antioxidant defense systems of body have influences on the development of cosmetic industry. Currently, cosmetic industry offers variety of products containing antioxidants. The active substances are plants extracts, which are rich in antioxidants and vitamins. Antioxidant in cosmetic products aims to protect biological tissue from damage of free radicals, which ultraviolet radiation, environmental pollution and some factors formed. Free radicals are the main cause for aging in this sense; antioxidants are also used in anti-aging cosmetic products.

Shampoos are probably the most widely used detergents because of their insensitive property to hardness of water. This allows it to rinse well and therefore there are no scum residue. In past, shampoos were only for hair and scalp cleanliness but nowadays they promise much more. Lately antioxidants are used in shampoos too. Researches show that water has metallic compound in it and this compound causes oxidative stress. Shampoos with antioxidants in them, decline copper-induced oxidative stress, protein in hair are better preserved, and hair condition can improve over time and expand the shelf life of product. The aim of this study is related to the plant extracts, vitamins, synthetic antioxidants added to shampoos. However, antioxidant quantity is not written on the packages. Determinations of specific antioxidant activity in cosmetics are difficult and in most cases, it is impossible because of synergistic effect. However, total antioxidant capacity can be determined with many analytical methods. There are special testing methods that consider hydrophobic and hydrophilic part of compounds. In this context the Ferric-Ferrozine method with Sephadex QAE A-25 resin used without pre-extraction processes for measure total antioxidant capacity.

**Keywords:** Antioxidant capacity, solid-phase extraction, ferric ferrozine, spectrophotometry, shampoo

P-085

## Structural and Optical Characterisation of $\text{CuInSe}_2$ Thin Films

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For a long time the scientific literature related to the materials of solar converters with a high efficient conversion factor have been discussed as I-III-VI<sub>2</sub> compounds. In this paper we have presented the structural and optical properties of  $\text{CuInSe}_2$  semiconductor thin films produced by the sol-gel method. First of all, this compound is relatively much more attractive than other candidate of its class compounds. So, its optical properties are relatively close to the maximum of solar activity radiation conversion. According to the x-ray diffraction analyse and optical absorption measurements the  $\text{CuInSe}_2$  thin films have a chalcopyrite phase with high crystalline quality and the width of the forbidden band is approximately estimated as 1.04 eV. These results are highly attractive for optical and solar cell devices.

**Keywords:** I-III-VI<sub>2</sub> compounds,  $\text{CuInSe}_2$  thin film, thin film solar cell

**NOT  
ATTENDED**

P-086

## Effects of Highly Mg dopant level on the structural and optical properties of ZnO thin films

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In this study, the effects of highly Mg dopant levels (5, 10, 20, and 30 %) on the structural and optical properties of ZnO thin films were investigated. X-ray diffraction (XRD) measurements revealed that both undoped and Mg-doped ZnO films had a hexagonal wurtzite crystal structure with (002) preferential orientation. No impurity or secondary phase formation was observed. Scanning electron microscope demonstrated the surface of the nanostructured films was homogeneous and dense. Average crystallite size and grain size of the films were decreased as the Mg content increased. Ultra-violet visible (Uv-vis) absorption spectroscopy studies showed the blue shift in the optical band gap of the subsequent to Mg doping content. Using the optical absorbance and transmittance the refractive index ( $n$ ), extinction coefficient ( $k$ ) and dielectric constants ( $\epsilon_r$  and  $\epsilon_i$ ) were calculated depending on Mg content in Uv-visible region.

**Keywords:** Mg-ZnO thin films, sol-gel, refractive index, dielectric constant



P-087

## Optical Properties of SiO<sub>2</sub>/MPS-Capped CdS Quantum Dots Mixture Thin Films

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The present study aimed at preparation and characterization of the SiO<sub>2</sub>/CdS quantum dots (QDs) mixture thin films for optical applications. First, CdS QDs were synthesized by using (3-mercaptopropyl)trimethoxysilane (MPS) and SiO<sub>2</sub> sol was synthesized by using tetraethyl orthosilicate (TEOS). After that, SiO<sub>2</sub> sol and colloidal MPS-capped CdS QDs were mixed and then were deposited on a glass substrate by spin coating process. In addition, colloiddally produced MPS-capped CdS QDs were self-assembled directly on a glass substrate using spin coating method without introducing any matrix. The films were heat-treated at 150°C in an N<sub>2</sub> atmosphere. Optical properties of the films were characterized by UV-Vis absorption spectrophotometer and NKD spectrophotometer measurements. The refractive index and thickness of the films were obtained by fitting of the measured data to a Drude–Lorentz model using a modified Levenberg-Marquardt procedure in the Pro-Optix™ data analysis software package. The refractive index of the SiO<sub>2</sub>/ CdS QDs mixture thin film was found as 1.51 at 550 nm wavelength. This result shows that the refractive index values of the thin film of SiO<sub>2</sub>/CdS QDs mixture is close to the glass substrate. Therefore, such films can be a good candidate for the planar luminescent solar concentrators.

**Keywords:** CdS quantum dots, Optical properties, SiO<sub>2</sub>, Thin films

P-088

## Thin Films of Fluorescent N-isopropylacrylamide Nanogels: Optical Investigation

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In this study, thermosensitive N-isopropylacrylamide (NIPAM) nanogels were synthesized by free radical precipitation polymerization by using NIPAM (used as monomer), N,N-methylenebis acrylamide (BIS, used as cross linker), ammonium persulfate (APS, used as initiator) and 8-hydroxypyrene-1,3,6-trisulfonic acid (Pyranine) molecules. Having bound pyranine molecules to the polymer strands, nanogels earned fluorescence property and smaller particle size. The results show that the gel size was decreased with increasing amount of pyranine molecules. Spin coating method was used for deposition of the colloidal nanogels on a glass substrate. Optical properties of the films were characterized by NKD spectrophotometer and UV-Vis absorption spectrophotometer measurements. The refractive index, extinction coefficients, dielectric constants and thicknesses of the films were determined. According to the results, it is observed that while the transmittance and the refractive index values of the films increased with increasing amount of pyranine molecules, absorbance values of the films decreased. Also, the thicknesses of the films decrease with increasing amount of pyranine molecules.

**Keywords:** N-isopropylacrylamide, Nanogels, Optical properties, Pyranine

P-089

**Hydrothermal Synthesis and Characterization of New Erbium(III) Complex**

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Lanthanide coordination polymers have various applications since they can be microporous structurally, thermally stable, optically luminescent, electrically conducting, non-conducting and semi-conducting materials [1]. Recent research activities developed in those areas that Erbium coordination polymers put forward industrial products because of their potential applications in NIR luminescent optical devices [2]. In this work, a new Erbium coordination polymer,  $[\text{Er}(2\text{-stp}).3(\text{H}_2\text{O})].3\text{H}_2\text{O}$ , 1 [2-stp = 2-sulfoterephthalate] has been prepared under hydrothermal conditions and characterized by single crystal X-ray diffraction (Fig. 1). Compound 1 crystallizes in the orthorhombic space group Pbcn with the unit cell parameter of  $a= 19.8224(8) \text{ \AA}$ ,  $b= 7.3738(3) \text{ \AA}$ ,  $c= 19.4844(7) \text{ \AA}$  and  $\alpha=\beta=\gamma= 90.^\circ$  Er(III) ions are bridged through three 2-stp ligands in three different directions to form a central symmetrically building unit, and the nearest non-bonding ErIII...ErIII distance is  $5.728 \text{ \AA}$ . The intermolecular Er(III)...Er(III) distances are  $11.232 \text{ \AA}$  in 2D framework.

*This work was supported by BAP 16/108 (Mugla Sıtkı Kocman University, The Scientific Research Projects Coordination Unit).*

[1] G. Oylumluoglu, M. B. Coban, C. Kocak, M. Aygun and H. Kara, "2-and 1-D Coordination Polymers of Dy(III) and Ho(III) with Near Infrared and Visible Luminescence by Efficient Charge-Transfer Antenna Ligand" J. Mol. Struct. 1146, (2017), 356-364

**Keywords:** Er(III) complex, Hydrothermal Synthesis, Crystal structure

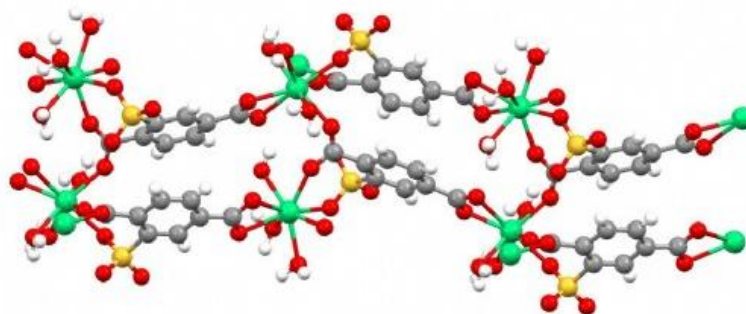


Fig. 1

P-090

## Theoretical studies of structural, optic and electronic properties of polypyrrole (PPy) oligomer

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Since the discovery of polypyrrole (PPy) almost 50 years ago, a myriad of publications are now available, more than 800 this past year alone according to Web of Science. PPy is a prototype conducting polymer that displays unique mechanical, optical, electrical, and biocompatible properties. However, much about the physical properties and structural characteristics of PPy are still not well understood, with data that is often contradictory. With the advent of nanomaterials, today PPy is used as a component at the nanoscale in a variety of sensors, fibers, and coated foams among other nanostructures.

In the present study, First-principles calculations are used to investigate the electronic properties of negatively charged n-pyrrole oligomers with  $n = 1-29$ , and all results were plotted to determine the optimal number of chains ( $n$ ). The molecules were optimized using the density functional theory (DFT) with the B3LYP method combined with the 6-31G(d,p) basis set (Fig. 1). Transition energies and oscillator strengths for the electronic excitation of the first 12 singlet-to-singlet excited states of PPy were calculated using time-dependent (TD) DFT at the same level. In addition, optical properties of PPy were studied as theoretically. It was observed that there is quite compatibility between the calculated and experimental data.

**Keywords:** Band gap, Polypyrrol, TDDFT, UV-vis spectroscopy

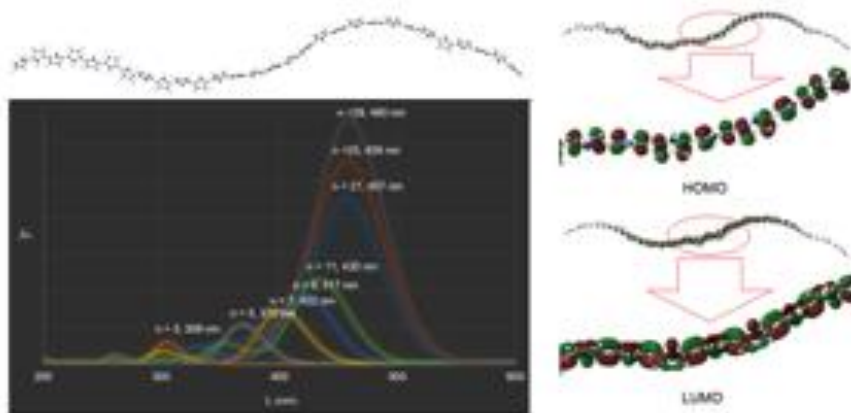


Fig. 1. Optimized structure, HOMO-LUMO orbitals and UV-vis spectra of PPy oligomer ( $n = 29$ )

P-091

## Kinetic Study of Oxidation of Indigo Carmine by Pyridinium Chlorochromate

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Pyridinium Chlorochromate (PCC) is a mild oxidizing agent commonly employed in the oxidation of primary alcohols to aldehyde without further oxidation to corresponding carboxylic acid. However, PCC is considered ineffective reagent for the oxidative cleavage of C-C multiple bond in organic compounds under mild conditions.

The kinetics of the oxidation of the organic dye Indigo Carmine (IC) by PCC in aqueous solution was examined by uv-visible spectroscopy and proton NMR. The progress of the reaction was measured by monitoring the degree of bleaching of the blue color of IC with time. The reaction proceeds readily at room temperature and does not require harsh conditions. The results shows that the rate of oxidation of IC by PCC is strongly dependent on the pH of the medium and the highest rate is achieved at strongly acidic conditions near pH = 2. The reaction was found to be first-order in the concentrations of IC, PCC and H<sup>+</sup>. The study of the reaction kinetics at different temperatures shows that the reaction has an activation energy of 19.54 kJ/mole and is accompanied by a decrease in entropy of activation by -177 J/K mol.

Identification of the products of the oxidation of IC by PCC using uv-visible, NMR and mass spectroscopy demonstrated that the only product formed is isatin sulfonic acid. This product can be formed only by the oxidative cleavage of the olefinic C-C double bond in the chromophoric group of IC. The oxidative cleavage of the olefinic C-C bond of IC was observed previously using strong oxidizing agents such as acidic potassium permanganate and ozone. The above results demonstrate the ability of the mild oxidizing agent PPC to cleave the C-C double bond in IC at room temperature and without the need for harsh conditions.

**Keywords:** Indigo Carmine, Pyridinium chlorochromic acid, Oxidative cleavage

P-092

**Determination of H<sub>2</sub>O<sub>2</sub> and organic peroxides by spectrophotometry using nanoceria particles**

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Organic peroxides are applied in many industrial processes, e. g. as initiators of free-radical polymerization, cross-linking agents and additives for rubber vulcanization. In order to monitor organic peroxides being released into the environment by many industrial processes and products and better understand the processes of formation and degradation of organic peroxides in the atmosphere as well as in biological tissues and food products, detection and quantification of organic peroxides are rapidly gaining practical importance in clinical and environmental fields.

Detection and quantification of organic peroxides are rapidly gaining practical importance in clinical and environmental fields to monitor and understand the processes of formation and degradation of organic peroxides and their products being released in the environment, atmosphere, biological tissues and food products by many industrial processes.

The aim of this study is to investigate a spectrophotometric method for the determination of hydrogen peroxide and several organic peroxides using nanoceria particles. Firstly, we synthesized nanoparticles using green chemistry and then determined hydrogen peroxide and several organic peroxides using N,N-dimethyl-p-phenylenediamine (DMPD) reagent. When it is mixed with a suitable oxidizing solution, DMPD forms a colored radical cation (DMPD•+). Hydrogen peroxide is oxidized using nanoceria particles and then hydroxide radicals formed a stable and colored radical cation (DMPD•+) which shows a maximum of absorbance at 515 nm. A variety of techniques for the determination of peroxides has been developed in the last decade but these methods are applicable only for the determination of hydrogen peroxide and a few organic hydroperoxides.

**Keywords:** Hydrogenperoxide, Organicperoxides, Nanoparticles, Greenchemistry

P-093

## Cyclophosphazene Based-Oligospiranes as New Molecular Rods

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Molecular rods, that is, long molecules with a relatively rigid conformation, claim a continuously growing interest in chemistry, materials science, nanoelectronics and biosciences [1]. Cyclic phosphorus-nitrogen compounds have a wide range of derivatives having diverse applications by virtue of their multifunctional nature [2]. Recently, new types of cyclophosphazenes having very active P-halogen bonds were synthesized from the deprotonation reaction of aminocyclotriphosphazene derivatives contain a P-NHR group in the side chain [3-4]. In this study, the new inorganic-organic heterocyclic compounds in the rod form were prepared by deprotonation reaction in high yield (Fig.1). They have four and two  $PCl_2$  groups in the outer and inner phosphazene rings, respectively, which make them potential precursors for preparation the macromolecular and supramolecular systems or the longer cyclophosphazene based-oligospiranes.

[1] P. F. H Schwab, J. R. Smith, J. Michl, Chem. Rev. 105, 2005, 1197-1279.

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[3] S. Beşli, Simon J. Coles, David B. Davies, Ayşen O. Erkovan, Michael B. Hursthouse, Adem Kılıç, Inorg. Chem. 47, 2008, 5042-5044.

[4] S. Beşli, Simon J. Coles, David B. Davies, Adem Kılıç, Robert A. Shaw, Dalton Trans. 40, 2011, 5307-5315.

**Keywords:** Inorganic-organic heterocyclic rods, cyclophosphazene, oligospiranes, deprotonation.

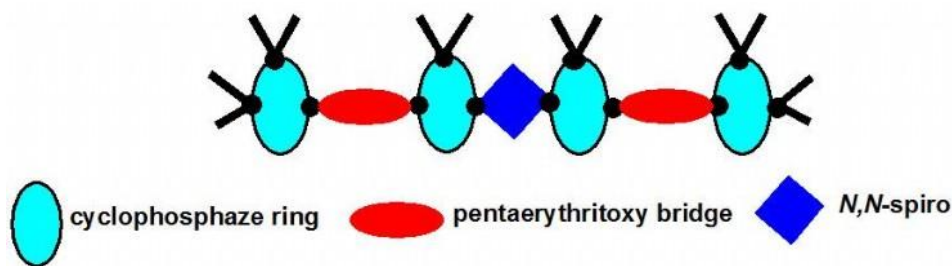


Fig. 1. Schematic illustration of new type of inorganic-organic heterocyclic rods

P-094

Cyclotriphosphazene Derivatives Bearing Glycol Groups

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Cyclophosphazenes are one of the important class of inorganic heterocycles which contain phosphorus and nitrogen atoms alternately [1]. Cyclophosphazene derivatives bearing glycol groups have some significant properties such as thermosensitivity and water solubility [2,3]. In this study, we have synthesized diethylene glycol monomethyl ether (DEGME) and diethylene glycol butyl ether (DEGBE) substituted cyclotriphosphazene derivatives (1-4 Fig.1). All compounds are soluble in water and in most polar organic solvents. Compounds 1-4 were characterized by using  $^{31}\text{P}$  nuclear magnetic resonance (NMR) spectroscopy.

[1] M. Gleria, R. De Jaeger, "Phosphazenes: A Worldwide Insight", Nova Science Pub Inc., New York, 2004

[2] S. B. Lee; S.C. Song; J. Jin; Y. S. Sohn; J. Am. Chem. Soc., 2000, 122, 8315-8316.

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**Keywords:** Phosphazene, water-soluble, glycol

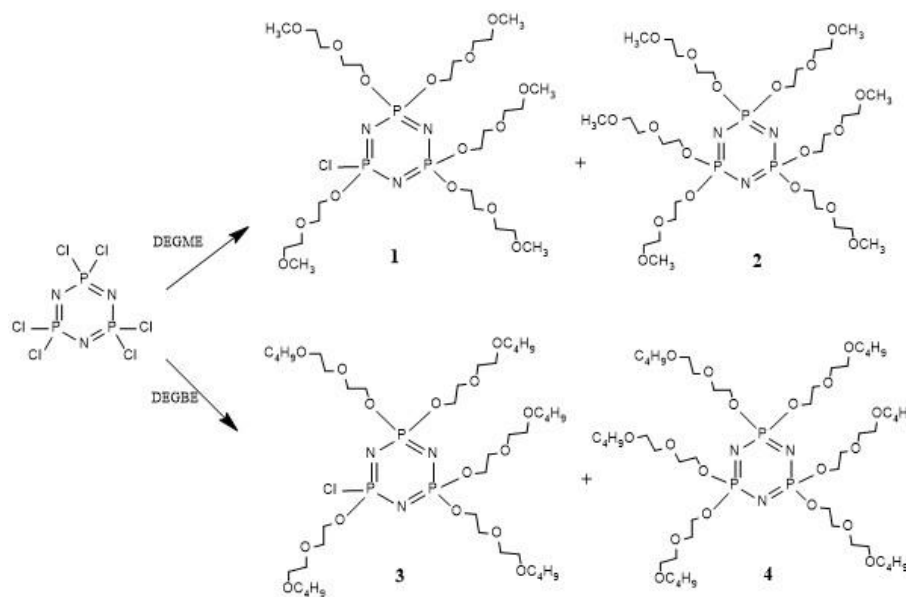


Figure 1



P-095

## Deprotonation Reactions of Fluorodioxy Substituted Cyclophosphazene and Investigation of Thermal Properties

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Deprotonation reactions having an important role in the synthesis of organic compounds [1] unfortunately are less known in the phosphazene chemistry [2]. Recently, interesting cyclophosphazenes that consisted fused ring system were prepared via deprotonation of proton on the exocyclic nitrogen atom in the cyclophosphazene ring [3, 4]. In this study, the mono-spiro, di-spiro, and mono ansa fluorodioxy compounds were reacted with *n*-butylamine and the compounds bearing a P–NH group were obtained. Deprotonation reactions of the compounds containing an *exo*-secondary amino group in the presence of the strong base NaH lead to intermolecular displacement of a chloride and formation of stable di-spiro *cis* and *trans*, tetra spiro and di-ansa fluorodioxy derivatives of N,N-spiro bridged biscyclotriphosphazenes (Fig. 1). Additionally, the thermal stabilities of all new compounds were investigated and found that the thermal stability increases with the formation of N,N-spiro bridge.

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[4] S. Beşli, C. Mutlu, H. İbişoğlu, F. Yuksel, Christopher W. Allen, *Inorg. Chem.* 54, 2015, 334–341.

**Keywords:** Cyclotriphosphazene, fluorodiol, ansa ring, deprotonation, spiro bridge

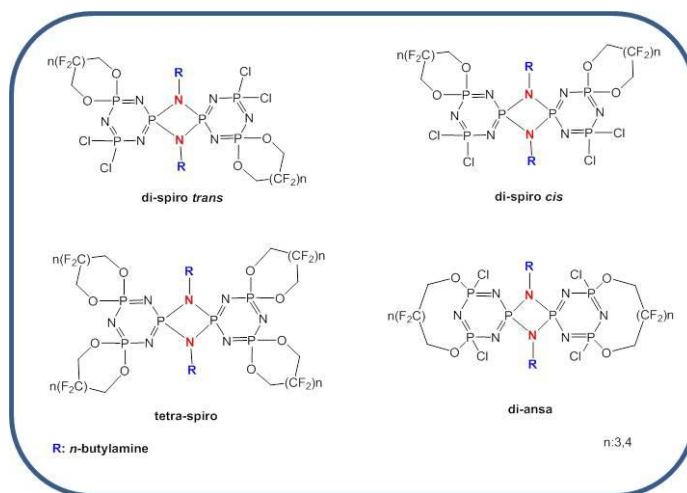


Fig. 1. N,N-spiro bridged biscyclotriphosphazenes

P-096

## Synthesis of Bimetallic Ruthenium Complexes and their Spectroscopic Properties

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Metal complexes play important role as chemotherapeutic agents. Platinum-based drugs have been used in cancer treatment for many years but researches now focus on other metals because of their dose dependent side effects and their resistance. Among metals, ruthenium complexes are new potential candidates for cancer treatment because they have fewer side effects than platinum that allow higher doses for treatment. They have various oxidation states. Ligand exchange rate is an important parameter for anticancer activity and ruthenium have similar ligand exchange kinetics to cisplatin.

In this study, bimetallic ruthenium complexes, represented in Fig. 1, have been synthesized and their spectroscopic properties have been investigated by FT-IR, UV-vis and  $^1\text{H}$  NMR techniques. The compounds, investigated by spectroscopic techniques, was synthesized starting from L1. Dichloro(p-cymene)ruthenium(II) dimer was used as metal complexes. Alkyl groups are butyl, octyl, dodesyl and octadesyl.

**Keywords:** ruthenium, bimetallic,  $^1\text{H}$  NMR

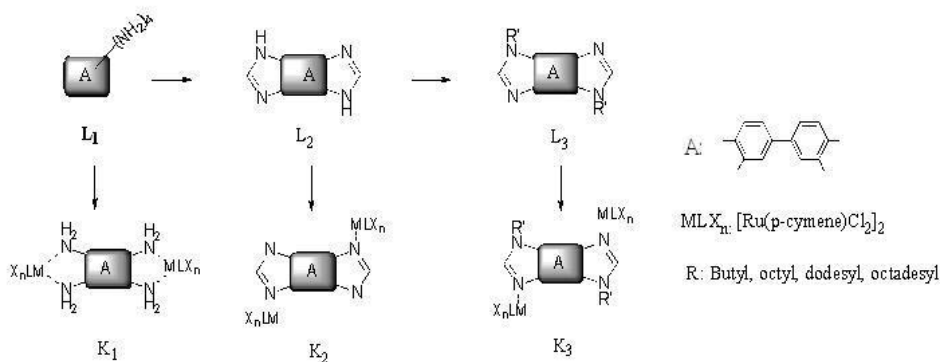


Fig. 1

P-097

The gentisic acid salts of the tetrapyrrolidino and tetrapiperidino mono(4-fluorobenzyl)spirocyclotriposphazenes: spectroscopic and thermal results

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Faculty of Science, Bartın University, 74100 Bartın, Turkey

The fully substituted phosphazenes are also known as strong phosphazene bases, and the pKa' values of a large number of cyclophosphazenes were measured in the literature. Thus, they are able to form stable salts with HCl, HF, HClO<sub>4</sub> and CH<sub>3</sub>COOH. Recently, three articles have been added to the literature by our research group the cyclophosphazene-based salts obtained with bulky organic acids.

The protic molten salts (PMOS) of (1-6) have been prepared from the reactions of tetrapyrrolidino and tetrapiperidino fully substituted phosphazenes with the gentisic acid (Fig. 1). The structures of PMOS (1-6) were characterized by elemental analyses, FTIR and <sup>1</sup>H, <sup>13</sup>C, <sup>31</sup>P- NMR techniques. The thermal properties of PMOS were verified using thermogravimetric instruments.

**Keywords:** Phosphazene salts, Spectroscopy, Thermal analysis

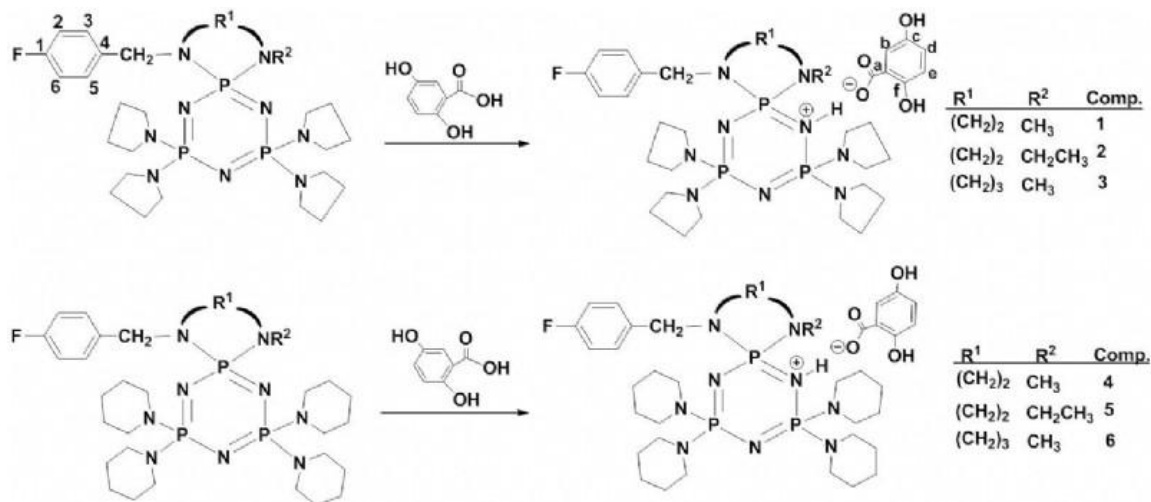


Fig. 1. The gentisic acid salts of the tetrapyrrolidino and tetrapiperidino mono(4-fluorobenzyl)spirocyclotriposphazenes

P-098

## Synthesis of mono metallic Ru (II) arene complexes and spectroscopic properties

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A mononuclear compound of the general formula  $[(\eta^6\text{-p-cymene})\text{Ru}(\text{Cl})(\text{N}(\text{R}1)\text{-N}(\text{R}2)\text{ethane-1,2-diamine})]\text{PF}_6$  has been synthesized from a bidentate N,N-donor ligand as  $\text{R}1 = \text{H}$ ,  $\text{Bu}$  when  $\text{R}2 = \text{naphthalene}$  and  $\text{R}1 = \text{Bu}$ ,  $\text{Mes}$  when  $\text{R}2 = \text{Aniline}$  (Fig. 1). The isolated coordination compounds were characterized by IR, UV-vis, cyclic voltammetry, X-Ray and  $^1\text{H}$ ,  $^{13}\text{C}$ ,  $^{19}\text{F}$ ,  $^{31}\text{P}$  NMR spectroscopies. The complexes of  $\text{K}_1$ ,  $\text{K}_2$  and  $\text{K}_3$  were found to be well soluble and stable in dichloromethane but the complex of  $\text{K}_4$  is slightly soluble in dichloromethane. The single crystal X-Ray analysis of the complexes reveal that  $\text{PF}_6$  molecules are located outside the coordination sphere, thereby the complexes become more stable. Infrared spectra were recorded on a Perkin Elmer Spectrum 100 IR spectrometer using KBr pellet technique. In the IR spectrum, were detected N-H, C-N and M-Cl stretches which specific peaks for the complexes. Electrochemical experiments were performed by cyclic voltammetry to estimate the redox potential of the  $\text{Ru}^{\text{II}}/\text{Ru}^{\text{III}}$  couple in each case. Cyclic voltammetric (CV) studies were carried out using an Autolab204 electrochemical system utilizing three electrode configuration consisting of a glassy carbon (working electrode), platinum wire (auxiliary electrode) and  $\text{Ag}/\text{AgCl}$  (reference electrode) electrodes. The experiments were done in DMSO using 0.1 M tetrabutyl tetrafluoroborate as supporting electrolyte. For UV-vis, the stock solution of complexes ( $1 \times 10^{-3}$  M) was prepared by using spectroscopic grade DMSO solvent.

**Keywords:** Ruthenium (II) arene, Monometallic Ruthenium complex, Spectroscopic properties

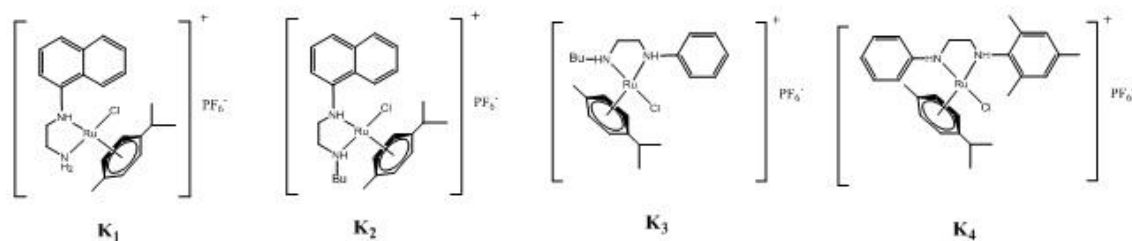


Fig. 1. Synthesized Ru (II) arene complexes

P-099

## Synthesis of some new 1,3,4-thiadiazole compounds derived from butyric acid and Characterization of structures by spectroscopic methods

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<sup>2</sup>Hitit University, Department of Chemistry, Faculty of Science and Literature, Çorum, Turkey

<sup>3</sup>Kastamonu University, Department of Forest Industrial Engineering, Faculty of Forestry, Kastamonu, Turkey

Some new 1,3,4-thiadiazole compounds were synthesized through the cyclisation reaction of 4-phenoxy-butyric acid and N-phenylthiosemicarbazide derivatives with phosphorous oxychloride. The structures of 1,3,4-thiadiazole compounds (1-13) was clarified by using spectroscopic methods such as UV-Vis, IR, <sup>1</sup>H-NMR and <sup>13</sup>C-NMR spectroscopies. Moreover, their antibacterial activities were tested against gram negative bacteria (Salmonella enteritidis, Salmonella typhimurium, Enterobacter aerogenes, Salmonella infantis, Salmonella kentucky, Escherichia coli) and gram positive bacteria (Staphylococcus aureus, Bacillus subtilis, Enterococcus durans) by using disk diffusion method. Furthermore, antifungal activity experiment was carried out against Candida albicans by using disk diffusion method. The all synthesized compounds had antibacterial activity against S. aureus. Also, the synthesized compound (10) showed antibacterial activity against E. durans. However, the synthesized compounds did not showed antimicrobial activity against gram negative (E. coli, E. aerogenes, S. kentucky, S. enteritidis, S. typhimurium, S. infantis) and gram positive (B. subtilis) bacteria and the fungi C. albicans. The results showed that the synthesized compounds could be used as a potential source of antimicrobial agents against S. aureus after investigating of the toxicology studies.

**Keywords:** 1,3,4-Thiadiazole, antimicrobial activity, IR and NMR spectroscopies

P-100

The synthesis and investigation of different cobaloximes by spectroscopic methods

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<sup>3</sup>Harran University, Faculty of Arts and Sciences, Department of Physics, Şanlıurfa, Turkey

In the present work, firstly the novel monooxime and asymmetric dioxime ligand derived 4-(4-Hydroxyphenyl)-2-butanone as ketone was prepared under optimum conditions. Then, the cobaloxime complexes with respect to varied axial groups were synthesized in a two-necked round-bottom reaction flask by direct contact of dioxime ligand, and different neutral base without special requirement of any additional chemical process. The prepared dioxime ligands and its cobaloxime complexes (Fig. 1) were characterized by means of NMR spectra, FT-IR spectra, UV-Vis spectra, LC-MS, melting point and magnetic susceptibility measurements as well as elemental analysis. The spectroscopic results demonstrated that the proposed cobaloxime complexes are a six-coordinated species and octahedral geometry.

\*This study supported by Harran University Scientific Research Project Coordinator (P. No. 16098)

**Keywords:** Multinuclear cobaloxime complexes, Carbon dioxide, Epoxides, Cyclic carbonate

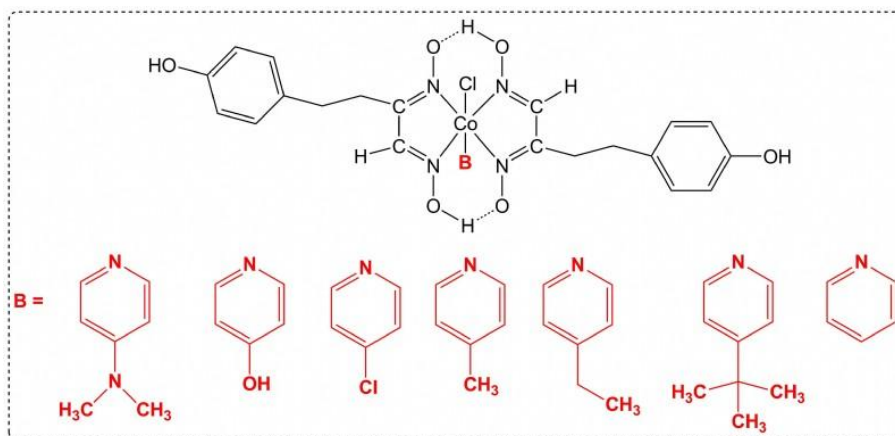


Fig. 1. The structure of cobaloxime complexes

P-101

Synthesis and spectroscopic characterization of bulky hemi-salen ligands and their triboron complexes

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In the present work, the synthesis and spectroscopic properties of a series of various hemi salen ligands and salen-fused triboron complexes have been investigated (Fig. 1). The salen-fused triboron complexes have been designed and prepared from hemi salen ligands (L1H3-L4H3) and BF<sub>3</sub>.Et<sub>2</sub>O or B(Ph)<sub>3</sub> under simple reaction conditions. The hemi salen (L1H3-L4H3) ligands and their BF<sub>2</sub> or B(Ph)<sub>2</sub> chelating triboron complexes characterized by means of NMR (<sup>1</sup>H, <sup>13</sup>C, <sup>19</sup>F and <sup>11</sup>B) spectra, FT-IR spectra, UV-Vis spectra, fluorescence spectra, mass spectra, melting point as well as elemental analysis. The triboron complexes [L(1-4)(BF<sub>2</sub>)<sub>3</sub>] and [L(1-4)(BPh<sub>2</sub>)<sub>3</sub>] were investigated for their absorption and emission properties and these complexes are also good chelates towards boron(III) fragments such as BF<sub>2</sub> or B(Ph)<sub>2</sub> quantum yield in solution reaching up to 51%.

This study supported by Harran University Scientific Research Project Coordinator (P. No. 16047).

**Keywords:** FT-IR spectra, UV-Vis spectra, hemi-salen ligands, Boron complexes

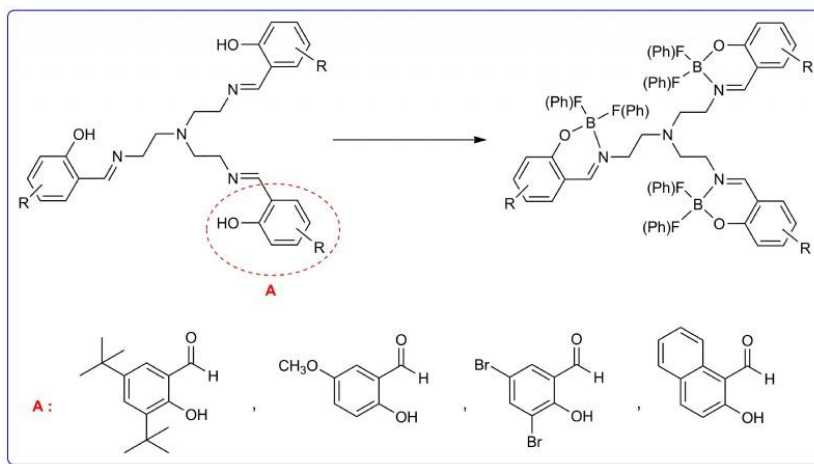


Fig. 1. The structure of hemi-salen ligands and triboron complexes



P-102

## Synthesis of Benzothiazole Derivative Mono Azo Dispers Dyeing, Investigation of Structure Analysis and Absorption Spectrum

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There have been intensive studies in recent years regarding the synthesis and dyeing properties of mono azo dyestuffs which are pyrazole derivatives. 5-aminopyrazoles can be used as starting materials in the synthesis of many poly substitute compounds. 5-aminopyrazoles are heteroaromatic amines which can be diazotized to give a re-coupling reaction.

In this work; firstly a series of carbocyclic amines reacted with 3-aminocrotonitrile to give 2-arylhydrazone-3-ketiminobutyronitrile 1(a-m). On the other hand, the 2-aminobenzothiazole compound treated with hydrazine monohydrate to synthesize the 2-hydrazinobenzothiazole compound. The compounds 1(a-m) synthesized refluxed in ethanol with 2-hydrazinobenzimidazole to give 1-(1,3-benzothiazol-2-yl)-3-methyl-4-arylo-5-aminopyrazole compounds 2(a-m) (Fig. 1). The structures of the synthesized compounds elucidated by using FT-IR, 1H-NMR and 13C-NMR and mass spectrophotometers. The absorption spectra of the resulting dyes investigated in different solvents and their behavior in acidic and basic media evaluated.

**Keywords:** Azo dyes, Heterocyclic compounds, Aminopyrazole.

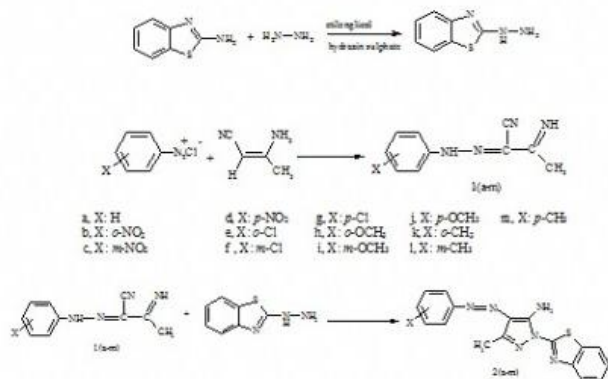


Figure: Synthesis of compounds 2(a-m)

Fig. 1. Synthesis of compounds 2(a-m)



P-103

Synthesis and characterization of 5,6-dihydro-1H-cyclopropa[c]indole-2,7(1aH,3H)-dione by NMR spectroscopy and single crystal x-ray analysis

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Heterocyclic compounds include many of the biochemical material essential to life. Many naturally occurring pigments, vitamins, and antibiotics are heterocyclic compounds. The most common heterocycles are those having five- or six-membered rings and containing heteroatoms of nitrogen (N), oxygen (O), or sulfur (S). the most known of the simple heterocyclic compounds are pyridine, pyrrole, furan, and thiophene. Also, five membered cyclic amides are called  $\gamma$ -lactams and they are very important class of antibiotic compounds<sup>1</sup>. In this work, we synthesized "5,6-dihydro-1H-cyclopropa[c]indole-2,7(1aH,3H)-dione" via the radical reaction using single electron transferable reagent (Fig. 1). Characterization of the compound was performed by <sup>1</sup>H-NMR, <sup>13</sup>C-NMR and 2D-NMR techniques. Also, exact structure of the molecule was determined via single crystal X-ray analysis.

**Keywords:** Heterocyclic compounds,  $\gamma$ -lactam, NMR spectroscopy, x-ray structure

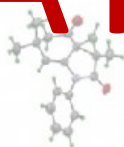
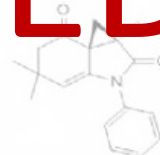


Fig. 1. ORTEP Diagram



structure of molecule

P-104

One-pot Synthesis of 3-(Acylamino)-4(3H)-quinazolinones Utilizing N-(2-Aminobenzoyl)benzotriazoles

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Quinazolinones represent an important class of heterocyclic compounds which have wide usage areas such as anti-bacterial, anti-cancer, anti-fungal, anti-inflammatory. In this study, 3-(acylamino)-4(3H)-quinazolinones were obtained by three component one-pot reaction of N-(2-aminobenzoyl)benzotriazoles with orthoesters and hydrazides in the absent of any catalyst (Fig. 1). The obtained products were purified by using column chromatography. The structures of the products were confirmed by  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR spectroscopy

**Keywords:** 3-(Acylamino)-4(3H)-quinazolinones, N-(2-Aminobenzoyl)benzotriazoles, NMR spectroscopy

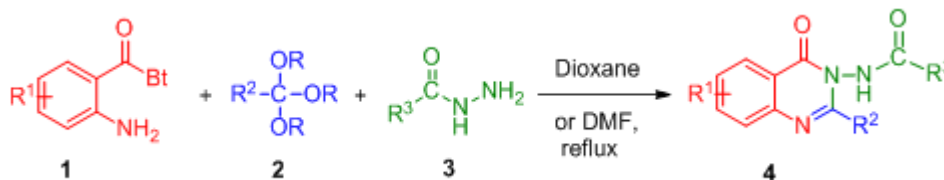


Fig. 1

P-105

Amino acid bounded quinazolinones by a one-pot, three-component reaction of N-(2-aminobenzoyl)benzotriazoles, amino acids and ortho esters

Büşra Demir, Ilker Avan, İlhami Çelik

Department of Chemistry, Faculty of Science, Anadolu University

Quinazolinones are important heterocyclic scaffolds because of their wide range of medicinal and pharmacological properties including anticancer, anti-tumor anti-inflammation, anti-hypertensive, antidepressant, anticonvulsant and antibacterial. Herein, a new method is described for the preparation of amino acid bonded-quinazolinones. Quinazolinone derivatives are obtained by a one-pot, three-component reaction of N-(2-aminobenzoyl)benzotriazoles, amino acids and ortho esters (Fig. 1).

**Keywords:** Quinazolinone, N-(2-Aminobenzoyl) benzotriazole, amino acid, one-pot reaction

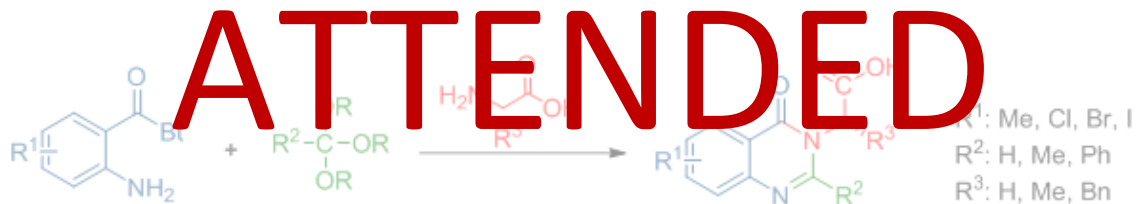


Fig. 1

P-106

Synthesis of novel piperazine derivatives and comparative characterization of their experimental and theoretical NMR spectra.

Sait Sari<sup>1</sup>, Seda Ünalın<sup>1</sup>, Kübra Çakır<sup>2</sup>, Mehmet Yılmaz<sup>1</sup>

<sup>1</sup>Kocaeli University

<sup>2</sup>Marmara University

Piperazine is an organic compound that consists of a six membered ring containing two nitrogen atoms at opposite positions in the ring. Piperazine derivatives are one of the most important heterocyclic class of compounds which have diverse biologic and pharmacologic activities. Many compounds containing piperazine derivatives show anticancer, antioxidant, antibacterial, antifungal, antidepressant and anticonvulsant activities.

In this study several acyl piperazine compounds were synthesized (Fig. 1) and characterized by NMR spectroscopy. Furthermore, theoretical NMR spectra of the compounds were also calculated using Gaussian software and compared with the experimental NMR spectra.

Keywords: Piperazine, NMR, GAUSSIAN

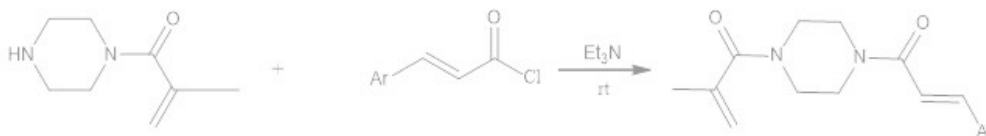


Fig. 1. Piperazine synthesis

P-107

## Synthesis, X-ray Crystal Structure and NMR Study of 3-butyl-4-iodo-6-methoxybenzo[c][1,2]oxaborol-1(3H)-ol via Consecutive Metal-Iodine Exchange of 3,4,5-Triiodoanisole

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3-butyl-4-iodo-6-methoxybenzo[c][1,2]oxaborol-1(3H)-ol was designed and synthesized via successive Metal-Iodine Exchange (MIE) reaction of 3,4,5-triiodoanisole is reported. The reactivity and regioselectivity of the MIE reactions here are remarkably controlled providing the iodinated product in good yield. The synthesized product (Fig. 1) were fully studied by NMR spectroscopy for the open and cyclised forms. This product is also screened for in vitro antimicrobial activity against two Gram-positive strains of bacteria *Micrococcus luteus* (ATCC 934) and *Bacillus cereus* (ATCC 11778) and two Gram-negative strains *Escherichia coli* (ATCC 25922) and *Serratia marcescens* (ATCC 27117) using well diffusion assay and dilution method. The in vitro antimicrobial evaluation indicated a superior antibacterial activity against Gram positive strains.

**Keywords:** 3,4,5-Triiodoanisole, Antibacterial, Regioselectivity, NMR spectroscopy

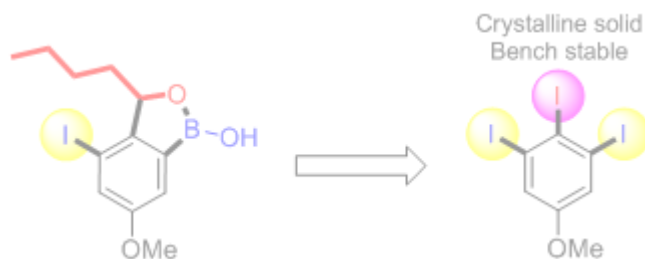


Fig. 1. Retrosynthesis of this target from triiodoanisole via successive metal-iodine exchange reaction

P-108

Investigation of Heavy Metal Contents of Some Spices Sold in Market Places

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The mineral composition, as reflects the soil type and environmental growing conditions, is a powerful tool for food traceability [1]. Food products such as spices, fruits and dry food accumulate heavy metals from the soil, water or air. Besides the useful aspects of these commonly used products, harmful effects can also be seen, especially depending on the metal content. The aim of this study is to determine the amount of some heavy metals in red peppers and black peppers sold at Karaman's market places. The samples were prepared to be 2 parallel for each sample and were solutioned by wet burning method. For this purpose, one gram of the powdered sample washed and dried in a suitable manner is precisely weighed 16 ml HNO<sub>3</sub> and 4 ml HClO<sub>4</sub> are added to it and the solution is slowly heated in the drawer for about 5-6 hours. The heating process close to the end of the acids is cut off and the solution sare cooled. Then 5 ml H<sub>2</sub>O<sub>2</sub> was addedand heating was continued until clear liquid was obtained. Heating was stopped when clear liquid was formed, and the solutions were allowed to cool. Cooling solutions were filtered through blue band fitler paper and 10 ml of the obtained solutions were mixed with distilled water to prepare the analyzed. Concentrations of Co, Ni, Cr, Cu, Zn, Pb, Mn, Mg, Fe and Ca were determined by FAAS instrument. According to the results, Co, Ni, Cr, Cu, Pb, Mn, Fe and Ca elements were found to be above the limit values in Europe and Turkey (Fig. 1a and b). In the prevention of heavy metal pollution sources of contamination must be well defined, these resources must be eliminated and environmental exposure with traceability of hazard conditions must be ensured.

- [1]. S. A. Drivelos and C. A. Georgiou, Multi-element and multi-isotope-ratio analysis to determine the geographical origin of foods in the European Union Trends in Analytical Chemistry, 40 (2012), pp. 38–51.

**Keywords:** FAAS, Heavy metal, Karaman, Spices, Turkey

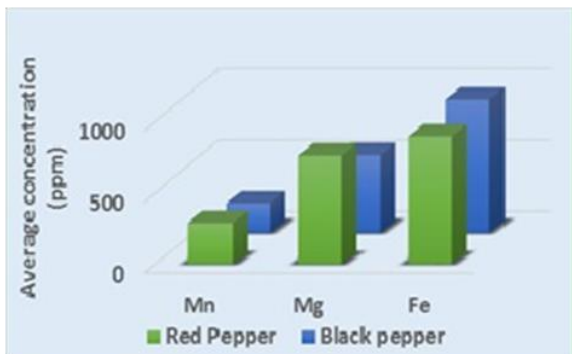


Fig. 1a. Average element contents and evaluation evaluation in red pepper and black pepper (ppm)

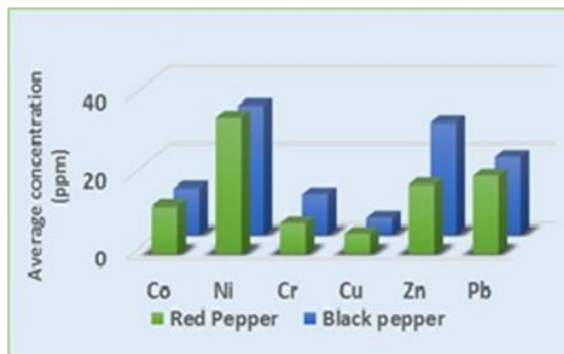


Fig.1b. Average element contents and evaluation evaluation in red pepper and black pepper (ppm)

P-109

Investigation of The Heavy Metal Content of Soil Taken from Field Corn Silage

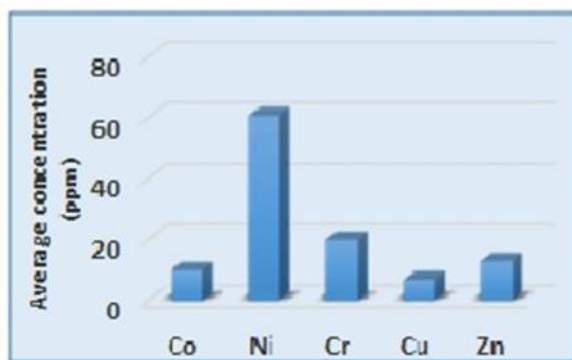
Hacer Sibel Karapınar, Fevzi Kılıçel, Fadimana Ünüvar

Chemistry Department, Karamanoğlu Mehmetbey University, Karaman, Turkey

One of the most important problems brought by industrialization and urbanization in nature is considered environmental pollution. Recently it has been stated that the gases and powders laid by mines, chemical factories and large industrial complexes pollute the soil and plants. Especially heavy metal pollution is a great potential hazard for plants living on this type of soil. Therefore, studies are being carried out to increase the productivity by applying different breeding procedures on the soil where such heavy metal pollution occurs [1]. In this study, the concentrations of heavy metals in silage corn fields produced in Karaman were determined and soil samples from 8 different cultivars were taken. The samples were prepared to be 2 parallel for each sample. Soil samples were ground and dried under suitable conditions. They have been numbered as being put into transparent bags and they have been done ready to weighing. 1 g of soil sample has been weighed and then put into beaker of 50 mL. 15 mL aqua regia has been added on it. It has been waited for 5-hours. After weighing capacity is heated to dryness on oven, 10 mL 2 M HNO<sub>3</sub> has been added and after it has been waited for 2 hours, it has been filtered from blue-band filter paper and it has been done ready to be analyzed as it has been completed to 25 mL. Concentrations of Co, Ni, Cr, Cu and Zn were determined by FAAS instrument. According to the results, Ni element was determined above the permissible limit values. Other elements were observed among the limit values. The high Ni concentration is thought to be due to soil structure, spraying, fertilizing or irrigation (Fig. 1).

[1] G. Geiger, P. Federer and H. Sticher, 1993. "Reclamation of Heavy Metal Contaminated Soils: Field Studies and Germination Experiments", Journal of Enviromental Quality, 22:(1), 201-207.

**Keywords:** FAAS, Heavy metals, Karaman, Soil pollution, Turkey.



Element	Range Found	Acceptable	Evaluation
Co	9.926	20	Normal
Cu	6.842	50	Normal
Cr	19.90	100	Normal
Ni	60.73	30	High
Zn	12.95	150	Normal

Fig. 1. Average heavy metal concentrations (ppm) Average element contents and evaluation in soils (ppm)

**P-110**

**Adsorption of Phenoxyacetic acid on Polymeric Adsorbents Using UV and FTIR spectrophotometer**

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<sup>2</sup>*Istanbul University, Engineering Faculty, Department of Chemistry, Avcılar-İstanbul, TURKEY*

<sup>3</sup>*Istanbul Technical University, Department of Chemistry, Maslak-İstanbul, TURKEY*

<sup>4</sup>*Istanbul University, Engineering Faculty, Department of Chemistry, Avcılar-İstanbul, TURKEY*

Phenoxyacetic acid (PAC) is a herbicide [1]. It is used to control weeds growing in crops such as rice, wheat. It has an adverse effect on soil and water like oxine. Its solubility in water is low but its mobility is high. Because it is bioaccumulated, it can harm biological life. In this study, adsorption of phenoxyacetic acid (PAC) was examined on the resin QP, PVBCIm and DGE. QP obtained with the quaternization of cross-linked ethyl piperazine

modified polystyrene. PVBCIm obtained by modifying polyvinyl benzyl chloride (PVBC) with imidazole. And DGE obtained with modification of glycidyl methacrylate and ethylene glycol dimethacrylate copolymer by N,N-dimethyl ethylenediamine. In the aqueous solution the adsorption of PAC was determined by UV-vis spectrophotometer at the 25°C. Adsorption isotherm experiments of herbicide in aqueous solutions was applied by Freundlich, Langmuir method for five different concentration at 25°C. The characteristic structures of the polymeric adsorbents before and after adsorption were determined by FTIR.

[1] T. Cserhati, E., Forgacs, Journal of Chromatography B, 717, 1998, 157-178

**Keywords:** phenoxyacetic acid, herbicide, adsorption



**P-111**

**Adsorption of Dyes with Natural Resin Functionalized Hollow Silica Sphere  
Bionanocomposite Material**

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Dyes, which are an important place in the chemical pollutant class, have to remove from the water due to the synthetic root and complex molecule structure. Hollow silica spheres have low density, high specific surface and good adsorption performance [1]. Gum arabic, also known as acacia gum. It is a complex mixture of glycoproteins and polysaccharides and it has known as natural resin.

In this work, Acacia Senegal (GA) and hollow silica sphere (HSS) nanoparticles were combined for adsorption of basic blue 3 (BB3) and reactive blue 21 (RB21). The adsorption of dyes onto (GA/HSS) bionanocomposite material was investigated by UVspectrophotometry. HSS was synthesized by using sol-gel method and then functionalized with GA. Characterizations of GA functionalized Hollow Silica Sphere (HSSAG) were done by FT-IR, and SEM technique. The HSAS was demonstrated as the best adsorption capacity ( $q_{max}100 \text{ mg g}^{-1}$ ) for basic blue 3 than reactive blue 21.

[1] Y. Zhang, Z. He, H. Wang, L. Qi, G. Liu, X. Zhang, Front. Environ. Sci. Eng., DOI 10.1007/s11783-015-0811-0.

**Keywords:** hollow silica sphere, basic blue 3, reactive blue 21

**P-112**

**Synthesis and Characterization of Nano Metal Oxides Prepared by Different Methods for Photocatalytic Degradation of Benzoquinone**

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During the past decade, various catalytic techniques have been investigated to solve the increasingly serious environmental pollution problems. Heterogeneous photocatalysis has shown a high efficiency in the photooxidation of many organic pollutants present in air.

Benzoquinone is an important organic pollutants widely found in industrial wastewater. In this study, pure  $\gamma$ -Al<sub>2</sub>O<sub>3</sub>, TiO<sub>2</sub>, ZnO and ZrO<sub>2</sub> nano structure semiconductors were tested in the complete and effective degradation of benzoquinone. The photocatalytic activities of the catalysts were evaluated for the degradation of benzoquinone under UV irradiation. The degradation rate of benzoquinone and its mineralization effectiveness were analyzed by HPLC and TOC measurements.

The structural and surface properties were achieved by employing various techniques (XRD, BET, DRS, SEM/TEM). All oxide structures showed high activity in the decomposition reaction of benzoquinone but  $\gamma$ -Al<sub>2</sub>O<sub>3</sub> catalyst was more active than other photocatalysts and able to provide complete decomposition. It is understood that the particle structure, crystal size and band gap energy of  $\gamma$ -Al<sub>2</sub>O<sub>3</sub> affected the degradation rate of benzoquinone when the structural and optical analysis were evaluated.

**Keywords:** Benzoquinone, degradation, semiconductor, UV irradiation, characterization

P-113

**The Investigation of Physical and Chemical Structure Properties of the (1E,2Z)-1-(4-nitrobenzylidene)-2-[4-(propan-2-yl)benzylidene]hydrazine with Spectroscopic Techniques and Quantum Chemical Computational Methods**

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(S)-perilaldehyde is a monoterpenoid class containing aldehyde group as use flavours and fragrances. We generated multicomponent reaction between hydrazine hydrate, aromatic conjugate aldehyde (4-nitrobenzaldehyde) and aliphatic conjugate aldehyde as perilaldehyde [1]. An excellent  $\pi$ -conjugated system was obtained and it caused fluorescence effect.

In this study, we reported that synthesis via multicomponent reaction of the 1-(4-nitrobenzylidene)-2-(4-(prop-1-en-2-yl)benzylidene)hydrazine and crystal structure determined with single crystal X-ray diffraction analysis (Fig. 1). The structural properties of the compound were characterized by means of FT-IR, <sup>1</sup>H-NMR, <sup>13</sup>C-NMR and fluorescence techniques. Furthermore, the optimized molecular geometry parameters, vibrational assignments, nuclear magnetic resonance chemical shift values of the compound were investigated by Density Functional Theory (DFT/B3LYP) method with 6-311G(d,p) basis set. The frontier molecular orbital energies to determine the charge transfer within molecule, some physical and chemical structure parameters such as ionization potential, electron affinity, electronegativity, chemical hardness or softness, and molecular electrostatic potential (MEP) of the title compound were examined using the same method. Also, dipole moment, polarizability and first hyperpolarizability values were calculated in order to find the non-linear optical (NLO) character of the compound. The computational approaches were performed by using the Gaussian 09 software [2] and GaussView 5.0 molecular visualization program [3].

[1] E. Ruijter, R. Scheffelaar, R. V. A. Orru, *Angewandte Chemie*. 50, 6234–6246, (2011).

[2] M. J. Frisch, et al., *Gaussian 09*, Revision C.01, Gaussian, Inc., Wallingford, CT, (2009).

[3] R. Dennington, T. Keith, and J. Millam, *GaussView*, Version 5, Semichem Inc., Shawnee Mission, KS, (2009).

*Acknowledgement: This work was supported by Amasya University Scientific Research Foundation (FMB-BAP 16-0218).*

**Keywords:** Density Functional Theory (DFT/B3LYP), (S)-perilaldehyde, FT-IR, <sup>1</sup>H-NMR, <sup>13</sup>C-NMR

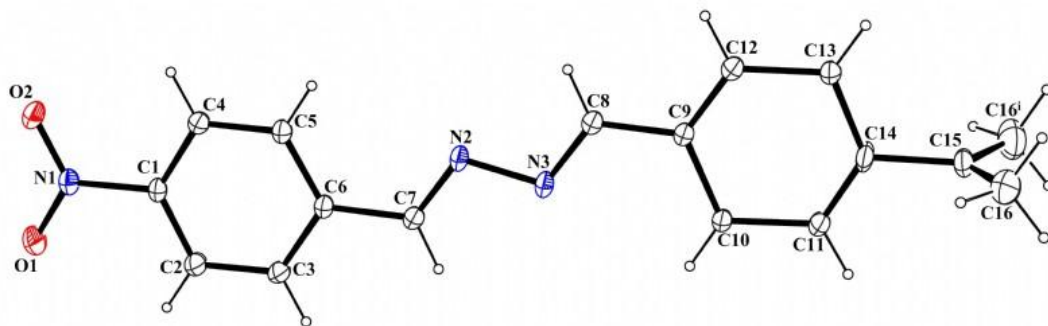


Fig. 1. A view of the title compound showing the atom-numbering scheme

P-114

4-(3-mesityl-3-methylcyclobutyl)-3-(phenylamino)thiazol-2(3H)-thione:  
Experimental and DFT Studies

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<sup>2</sup>Department of Chemistry, Firat University, Elazig, Turkey

<sup>3</sup>Department of Physics, Ondokuzmayis University, Samsun, Turkey

The chemistry of aminothiazoles and their derivatives has attracted the attention of chemists, because they exhibit important biological activity in medicinal chemistry, such as antibiotic, anti-inflammatory, antihelmintic, or fungicidal properties[1]. 2-Aminothiazoles are known mainly as biologically active compounds with a broad range of activities and as intermediates in the synthesis of antibiotics, well-known sulfa drugs, and some dyes. In addition, it has been shown that 3-substituted cyclobutane carboxylic acid derivatives exhibit anti-inflammatory and antidepressant activities and also liquid crystal properties [2].

The aim of the present work was to describe and characterize the molecular structure, vibrational properties and chemical shifts of the title compound (Fig. 1), both experimentally and theoretically. A comparison of the experimental and theoretical spectra can be very useful in making correct assignments and understanding the basic chemical shift-molecular structure relationship. Molecular electrostatic potential (MEP), frontier molecular orbitals (FMOs), conformational flexibility and nonlinear optical properties of the title compound were studied at the B3LYP/6-311G(d,p) and B3LYP/6-311++G(d,p) levels. The computational approaches were performed by using the Gaussian 09 software [3] and GaussView 5.0 molecular visualization program [4].

[1] P. Crews, Y. Kakou, E. Quinoa, J. Am. Chem. Soc. 110 (1988) 4365.

[2] E.V. Dehmlow, S. Schmidt, Liebigs Ann. Chem. 5 (1990) 411.

[3] M. J. Frisch, et al., Gaussian 09, Revision C.01, Gaussian, Inc., Wallingford, CT, (2009).

[4] R. Dennington, T. Keith, and J. Millam, GaussView, Version 5, Semichem Inc., Shawnee Mission, KS, (2009).

**Keywords:** Thiazol, Cyclobutane, DFT

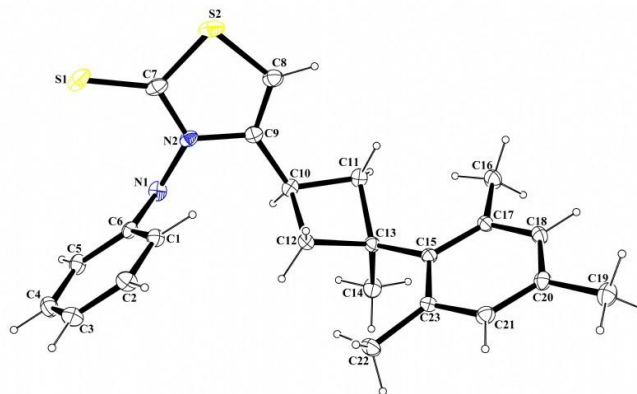


Fig. 1. The molecular structure of the title compound showing the atom-numbering scheme

P-115

**Determination of crystal structure of 2-aminopyridine molecule from X-ray powder diffraction data**

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2-aminopyridine (2AP) molecule has an important role in pharmaceutical applications. The 2AP is one of three isomeric aminopyridines (also 3-aminopyridine and 4-aminopyridine), with chemical formula  $H_2NC_5H_4N$  and a colorless solid powder compound. Knowing the structural properties of this molecule allows understanding its chemical properties and its effects in the production of drugs. In this work, we tried to obtain the structural properties of the 2AP molecule and its crystal structure from X-ray powder diffraction data (Fig. 1). Powder pattern was collected by using an automated Rigaku RINT2500 equipped with the silicon strip Rigaku D/teX Ultra detector and the monochromatic  $CuK\alpha_1$  radiation ( $\lambda=1.54056 \text{ \AA}$ ). The 2theta range of collection was  $7-75^\circ$  with a step of  $0.02^\circ/\text{min}$ . The EXPO2014 package program was used for crystal structure solution. The results of the structural determination of 2AP and the refinement by the Rietveld technique are presented. The 2AP structure has a monoclinic cell with space group P21/c and cell parameters:  $a=11.72423$ ,  $b=5.67841$ ,  $c=7.60252 \text{ \AA}$ ,  $\beta = 95.532^\circ$ . Such a solution agrees with a single-crystal structure determination reported in literature.

**Keywords:** 2-aminopyridine (2AP), crystal structure determination, X-ray powder diffraction

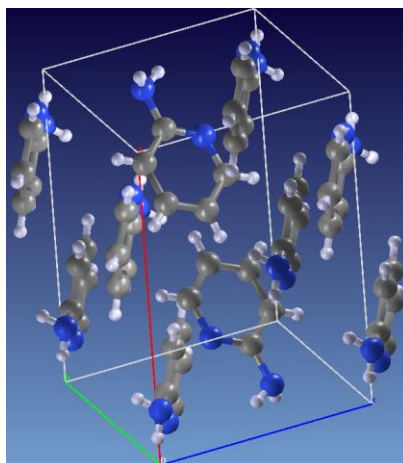


Fig. 1. The unit cell content of the crystal structure of 2-aminopyridine molecule.

**P-116**

**Effects of chemical structures of omega-6 fatty acids on the molecular parameters and quantum chemical descriptors**

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Omega-6 fatty acids are essential polyunsaturated fatty acids (PUFAs) and found in refined vegetable oils, nuts and seeds that play a very important role in heart and brain function, along with normal growth and development. These acids have at least two double bonds and 18 carbon atoms (18:2) that the number of double bonds present refers to the degree of unsaturation of a fatty acid. A first phase of calculations was performed using PM3 semi-empirical method to characterize to potential energy surface of omega-6 fatty acids: Linoleic (18:2),  $\gamma$ -linolenic (18:3), Eicosadienoic (20:2), Dihomo- $\gamma$ -linolenic (20:3), Arachidonic (20:4), Docosapentaenoic (22:2), Adrenic (22:4), Docosadienoic (22:5), Tetracosatetraenoic (24:4) and Tetracosapentaenoic (24:5). Afterwards, the lowest energy conformer of each acid was selected for the geometric optimization step and PM3 geometries were fully optimized using the DFT method at the B3LYP/6-311++G(d,p) level. After the geometry optimizations, the harmonic vibrational frequencies calculations at the same level of theory were carried out to characterize the nature of each stationary point.

The influence of a fatty acid's structure (chain length, degree of unsaturation and also the number of methylene group) on its vibrational frequencies, dipole moment and quantum chemical descriptors such as HOMO/LUMO energies and chemical hardness were discussed.

**Keywords:** Omega-6 fatty acids, conformational analysis, quantum chemical descriptors

P-117

## Synthesis, Characterization and Theoretical Study of N,N'-(oxybis(4,1-phenylene))bis(1-(4-fluorophenyl)methanimine)

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The synthesis, characterization and theoretical calculation of (N,N'-(oxybis(4,1-phenylene))bis(1-(4-fluorophenyl)methanimine) (L2) compound is reported. The structure of the synthesized compound was confirmed by UV-Vis, Raman, IR, <sup>1</sup>H NMR, <sup>13</sup>C NMR, and SEM analysis. The optimized geometric parameters, conformational analysis, normal mode frequencies and corresponding vibrational assignments of L2 was theoretically examined by means of density functional theory (DFT) method using the Becke-3-Lee-Yang-Parr (B3LYP) exchange-correlation functional and the 6-311G++(d, p) basis sets. The DFT based nuclear magnetic resonance (NMR), infrared (IR) and ultraviolet (UV) calculations was performed to compare with experimental data of L2. A good consistency was obtained between the theoretically predicted structural parameters, vibrational frequencies and those obtained experimentally.

**Keywords:** Schiff base, Raman, NMR, Theoretical



P-118

**Synthesis, spectroscopic studies and calculation of 5-benzoyl-6-phenyl-4-(4-methylthiophenyl)-1,2,3,4-tetrahydro-2-thioxopyrimidine**

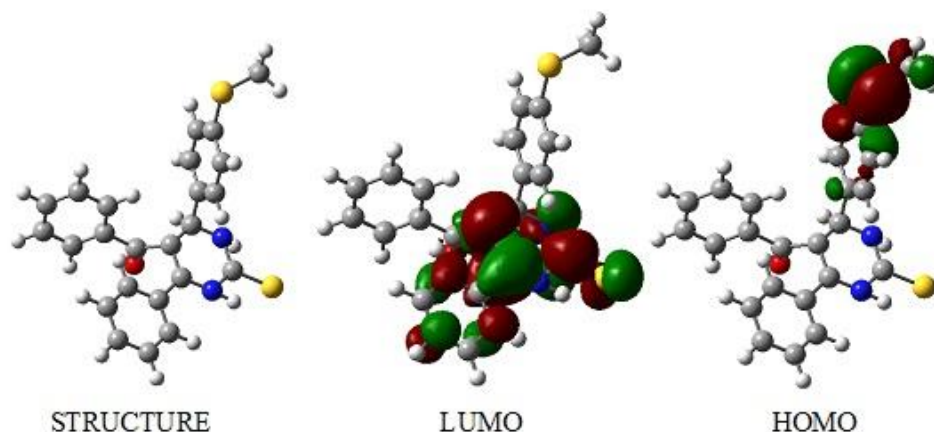
Erdem Ergan<sup>1</sup>, Esvet Akbaş<sup>2</sup>, Metin Çakır<sup>2</sup>

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5-Benzoyl-6-phenyl-4-(4-methylthiophenyl)-1,2,3,4-tetrahydro-2-thioxopyrimidine have been prepared via Biginelli cyclocondensation reaction in acetic acid under reflux condition in good yield. The mechanism of the Biginelli reaction was discussed with quantum chemical methods. The structure of 5-benzoyl-6-phenyl-4-(4-methylthiophenyl)-1,2,3,4-tetrahydro-2-thioxopyrimidine was established from their spectral data and elemental analysis. The synthesized pyrimidine derivative has been optimized with Gaussian software in order to obtain information about the 3D geometries and electronic structures (Fig. 1).

**Keywords:** Biginelli, Thioxopyrimidine, Calculation



**Fig. 1.** The frontier orbitals of 5-benzoyl-6-phenyl-4-(4-methylthiophenyl)-1,2,3,4-tetrahydro-2-thioxopyrimidine

**P-119**

**The solvent effects the C=O stretching vibrations of the  
4-formylphenylboronic acid molecule**

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The effects of 5 solvents on the C=O stretching vibrational frequency of 4FPBA were determined to investigate solvent-solute interactions. Solvent effects on the geometry and C=O stretching vibrational frequency of 4-formylphenylboronic acid molecule were studied theoretically at the DFT/B3LYP method using the default setting for the polarized continuum model (PCM) implemented in the Gaussian 09 program. Molecular electrostatic potential (MEP) and Mullikan charges were also computed.

*This work was supported by Ahi Evran University Scientific Project Unit (BAP) with, Project No: PYO–FEN.4001.15.012.*

**Keywords:** 4FPBA, DFT, Solvent Effect, MEP

P-120

**Synthesis, molecular structure and theoretical calculation of (2-imino-4-(4-(methylthio)phenyl)-6-phenyl-1,2,3,4-tetrahydropyrimidin-5-yl) (phenyl) methanone**

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(2-imino-4-(4-(methylthio)phenyl)-6-phenyl-1,2,3,4-tetrahydropyrimidin-5-yl) (phenyl) methanone were synthesized using three component cyclocondensation reaction of an appropriate  $\beta$ -diketone, arylaldehyde, and guanidine in good yield. The structure of (2-imino-4-(4-(methylthio)phenyl)-6-phenyl-1,2,3,4-tetrahydropyrimidin-5-yl) (phenyl) methanone was established from their spectral data and elemental analysis. The synthesized pyrimidine derivative has been optimized and calculated with Gaussian software in order to obtain information about the 3D geometries and electronic structures (Fig 1).

**Keywords:** Pyrimidine, Imino, Cyclocondensation Reaction



**Fig. 1. Structure, HOMO, LUMO and All for compound**

**P-121**

**Optoelectronic Properties of Donor-Acceptor Type Conjugated Polymers**

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The interaction between alternating donors and acceptors results in a diminished band gap. With determining the proper donor (D) and acceptor (A) groups, it is possible to decrease the band gap (<1.8 eV) as much as possible or to adjust HOMO (highest occupied molecular orbital)-LUMO (lowest unoccupied molecular orbital) levels. Therefore, in this study the theoretical methods were used for the modelling of the donor-acceptor-donor type conjugated polymers. The optical and electronic properties of conducting polymers was investigated with time-dependent density functional theory (TDDFT). A series of donor-acceptor-donor systems with thiophene, and 3,4-ethylenedioxythiophene (EDOT) as donors and benzene, benzo[c][1,2,5]thiadiazole, benzo[c][1,2,5]thiadiazole-5,6-diamine, and naphtho[2,3-c][1,2,5] thiadiazole as acceptors as examples of donor-acceptor systems with increasing donor-acceptor character was studied. Spectral properties were analyzed in terms of differences in ionization potentials and electron affinities of donors and acceptors and charge separations between donors and acceptors in ground and excited states. Studies were performed in the gas and solution phases and the properties of the ground state and excited state for the possible structures were done with the Gaussian 09 program. The results indicate that calculated band gaps are in good agreement with the experimental values in the literature. The theoretical methods used in this study are promising for the modelling of similar donor-acceptor type novel conjugated polymers.

**Keywords:** Donor-acceptor, bandgap, UV spectrum, TDDFT.

**P-122**

**Spectroscopic Study of Furan and Benzofuran Derivatives Combined with DFT Calculations**

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In this study, we aimed to present joint experimental and theoretical studies on newly designed furan and benzofuran-azine derivatives, namely (E)-(furan-2-ylmethylene)hydrazine (1) and (E)-(benzofuran-2-ylmethylene)hydrazine (2). The azine derivatives were prepared by the reaction of the corresponding carbaldehyde with hydrazine. Structural analysis of the synthesized compounds was performed by appropriate spectroscopic methods (UV-vis, FT-IR, LC-MS, <sup>1</sup>H-NMR, <sup>13</sup>C-NMR, and UV-visible spectroscopies and elemental analysis). Our consecutive efforts have been contributed to theoretical studies in order to obtain information about structural properties (bond lengths, bond angles, dihedral angles, and dipole moments), energies (HOMO-LUMO energies and band gaps) and spectroscopic characteristics (UV-vis, FT-IR, <sup>1</sup>H-NMR and <sup>13</sup>C-NMR) of the target compounds. Theoretical data were then used for identifying the structure-activity relationship and determining chemical properties of the studied molecules. Spectral, electrical and structural properties of the compounds have been studied using DFT (density functional theory) quantum mechanical methods. Molecular geometries and energetics of azines in gaseous phase have been obtained using B3LYP/6-31G(d,p) level of theory. The optimized molecular geometry of furan-hydrazine derivative is discussed based on X-ray structural reports from the literature. The assignments of the vibrational frequencies were done on the basis of potential energy analysis using VEDA4 software. The energy gap between highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) was evaluated to study the reactivity and stability of the compounds. Global reactivity and local reactivity descriptors of reactants and the products have been calculated for all the optimized structures. Finally, the region of interaction during the reaction to form azine derivatives was determined using molecular electrostatic potential analysis. The calculated results have been analyzed and compared with experimental values.

**Keywords:** Furan, Benzofuran, DFT, Spectroscopy.

P-123

**Molecular, electronic and spectroscopic, properties of 6-Chloroquinoline by using DFT method**

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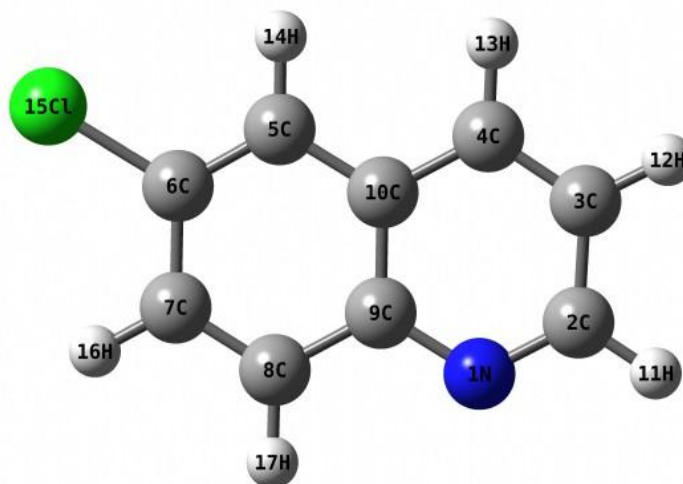
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Structural, electronic, and spectroscopic properties of 6-Chloroquinoline (6-CQ) were analyzed by quantum chemical calculations and supported with experimental results from IR, <sup>1</sup>H and <sup>13</sup>C NMR spectra. The geometrical parameters of the molecule were obtained from the optimized structure determined via DFT/B3LYP method 6-311++G(d,p) basis set calculation and compared with that of structurally similar molecules. The fundamental vibrational assignments were done based on the PED by using VEDA program. The HOMO and LUMO energies, Mulliken charge analysis, electrostatic potential surface, and density of states (DOS) analyses were studied for deep evaluation of electronic properties of title molecule. The chemical shifts of the molecule obtained by using the gauge-invariant atomic orbital (GIAO) method for <sup>1</sup>H and <sup>13</sup>C NMR were compared corresponding experimental data. Moreover, thermodynamic and NLO parameters of the present molecule were carried out. The results were observed to be well-correlated with their experimental results.

**Keywords:** 6-Chloroquinoline, DFT, Infrared, NMR, DOS



6-chloroquinoline

P-124

## Computational Investigation of Metal Complexes of ISE (3[4-ethyl(phenyl)-imino][1H-indole-2-one])

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Isatin and its derivatives which have indole structure are used in drug development as they show antibacterial and antifungal activities [1]. Isatin is also widely used in coordination chemistry as a Schiff base [2]. Metal carbonyl complexes of Schiff bases are used as catalysts in syntheses of organic aldehydes and acids, and hydrogenation of olefins in coordination chemistry [2].

Intermolecular charge transfer processes of  $M(\text{CO})_5(\text{ISE})$  complex formed by the reaction between ISE (3[4-ethyl(phenyl)-imino][1H-indole-2-one]) and  $M(\text{CO})_6$  [ $M=\text{Mo}, \text{Cr}, \text{W}$ ] [3], have been investigated by computational methods. Calculations were carried out using Density Functional Theory (DFT) at B3LYP 6-311++G(d,p) level. For metals LANL2DZ basis set was used. Excited state calculations were carried out with Time-Dependent Density Functional Theory (TDDFT) at the same level using the first 40 excitations. Orbital energies, UV-Vis spectra, and total electron densities were shown for gas phase and for the solvent tetrahydrofuran (THF). All calculations were performed using Gaussian09 [4]. There is a charge transfer (CT) between ISE and  $\text{Cr}(\text{CO})_5$  in gas phase. For  $\text{Cr}(\text{CO})_5(\text{ISE})$  system,  $S_0 \rightarrow S_1$  transition (772 nm) between H $\rightarrow$ L orbitals shows that there is CT from the metal moiety towards isatin ring. The maximum wavelength of the system is at 589 nm ( $S_0 \rightarrow S_3$  transition) and corresponds to CT. On the other hand, the small HOMO-LUMO energy gap (2.48 eV) of the complex indicates that it may have potential use for development of photosensitive materials.

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**Keywords:** Isatin, Schiff base, Metal Carbonyl, DFT

P-125

**Spectroscopic Analysis and DFT Calculation of poy(epichlorhydrin-b- $\epsilon$ -caprolactone) and poy( $\epsilon$ -caprolactone-b-tetrahydrofurane-b- $\epsilon$ -caprolactone) Block Copolymers**

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Theoretical-experimental FT-IR and NMR methods were employed for the spectroscopic characterization of the poy(epichlorhydrin-b- $\epsilon$ -caprolactone) (PECH-PCL) (Fig. 1) and poy( $\epsilon$ -caprolactone-b-tetrahydrofurane-b- $\epsilon$ -caprolactone)(PCL-PTHF-PCL) block copolymers prepared by the ring opening polymerization of  $\epsilon$ -caprolactone, initiated via diethylether-HCl complex in the presence of polyepichlorhydrin and polytetrahydrofuran diol. Isotropic <sup>1</sup>H magnetic shielding constants dimer and trimer form of the diblock or triblock copolymers have been calculated by employing EPRNMR the B3LYP density functional level of theory. Geometric optimizations, NMR and IR calculations were performed using the ORCA 4.0.0[1] quantum chemistry package using one input file in a one step. A graphical user interface for computational chemistry packages named Gabedit [2] was used to prepare the input file and visualize the IR spectrum. Comparison of experimental and theoretical spectroscopic data were carried out via linear regression analyses using QtiPlot program [3]. All calculations were carried out in parallel on a virtual server with 16 CPUs and 30 GB of RAM rented from server4you.com.

[1] F. Neese, "The ORCA program system" Wiley interdisciplinary Reviews - Computational Molecular Science, 2012, Vol 2., Issue 1, Pages 73-78

[2] A.R. Allouche, Gabedit-A graphical user interface for computational chemistry softwares. Journal of Computational Chemistry, 32 (2011) 174-182.

[3] QtiPlot, QtiPlot - Data Analysis and Scientific Visualisation.

**Keywords:** FT-IR, NMR, B3LYP, Block Copolymer



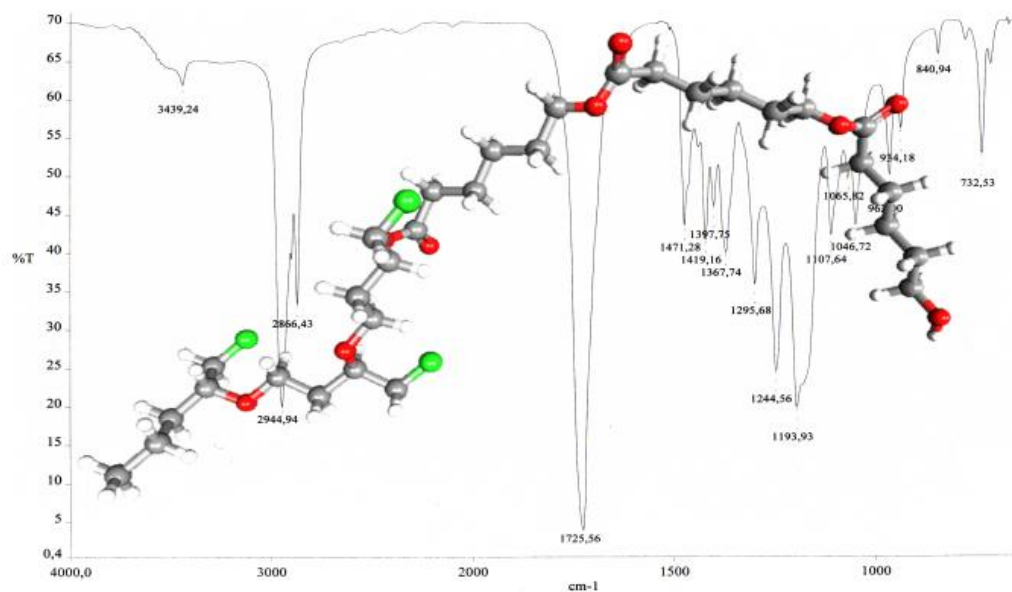


Fig. 1. IR Spectrum of poly(epichlorhydrin-b-ε-caprolactone) block copolymer

P-126

Spectroscopic and Computational Investigation of Selected Porphyrins

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UV/Vis absorption spectra and quantum chemical methods were used to investigate intramolecular charge transfer properties of selected biologically important porphyrins. Ground state geometries and electronic transitions were calculated. Calculations were first performed in gas phase and then were repeated in water to determine the solvent effects. The selected porphyrin derivatives are 5,10,15,20-Tetraphenyl-21H,23H-porphine (TPhP), Octaethyl-porphine, and 5,10,15,20-Tetrakis(4-hydroxyphenyl)-21H,23H-porphine (TPhP-OH). The effects of ethyl, phenyl and phenolic substituents on porphyrin electronic properties were observed. Geometry optimizations were performed by density functional theory (DFT) at B3LYP/6-31G(d,p) level. Time-dependent density functional theory (TDDFT) with B3LYP/6-311++G(d,p) level was used for the analysis of excited states of investigated molecules and emission spectra were obtained by using the excited-state geometries. Polarizable Continuum Model (PCM) is used for calculations in solution. Red shifts in wavelengths were observed in UV/Vis absorption spectra (Fig. 1) in the order OcEtP, TPhP and TPhP-OH. TPhP-OH showed an easier charge transfer at S<sub>1</sub> state. This charge transfer had a  $\pi$ - $\pi^*$  character from the phenyl rings towards porphyrin center. Current results indicate that TPhP-OH is the best candidate for photosensitive material design.

We gratefully acknowledge computer time from TÜBİTAK-ULAKBİM Truba Resources and Ege University Faculty of Science Computer Resources (FenCluster).

**Keywords:** Porphyrine; intramolecular charge transfer; Time-Dependent Density Functional Theory

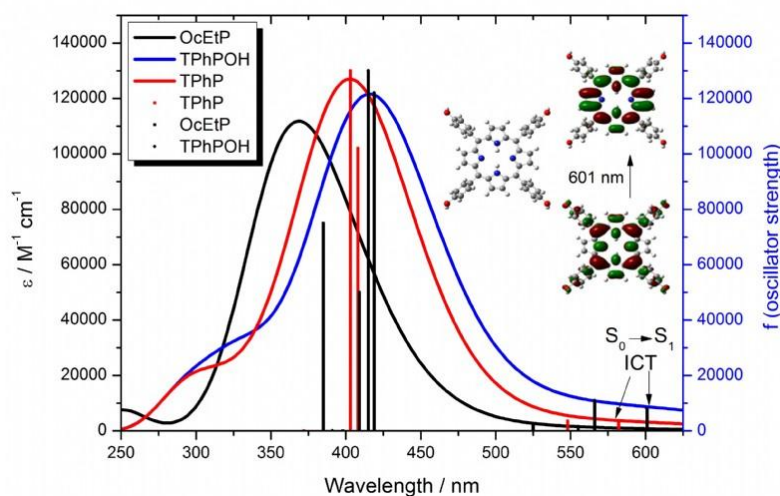


Fig.1 Calculated UV/Vis absorption spectra of investigated porphyrins in the gas phase.

P-127

The spectroscopic properties and theoretical calculation of some new disazo dyes derived from 2,4-Dihydroxyquinoline

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It has been known for many years that the azo compounds are the most widely used class of dyes due to their versatile application in various fields such as the dyeing of textile fibers, the coloring of different materials, colored plastics, biological medical studies and advanced applications in organic synthesis. Many patents and papers describe the synthesis and dyeing properties of azo compounds.

In this work, we report the synthesis of some hetarylazoquinoline dyes resulting from the use of 2,4-quinolinediol as coupling component (Fig. 1) and an evaluation of their visible absorption spectra with respect to the influences of solvent. The effects of concentration as well as acid and base on the visible absorption maxima of the dyes are also reported. The synthesized compounds were characterized by using spectroscopic methods such as FT-IR and <sup>1</sup>H-NMR. Besides, the experimental data was supported by the quantum chemical calculations. The UV-Vis, IR and NMR calculations of the molecules were performed by using PBE1PBE method with 6-311g, 6-311++g(d,p) and cc-pvtz basis sets. Furthermore, dipole moment, polarizability, chemical hardness/softness and electronegativity values of the compounds were also calculated and analysed. The UV-Vis, FT-IR and NMR calculations of the molecules were compared with experimental results, and interpreted in detail.

**Keywords:** 2,4-dihydroxyquinoline, heterocyclic, disazo dyes

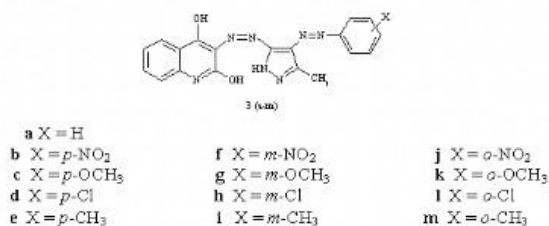


Fig. 1: General structures of compounds

P-128

**NMR and IR Spectroscopy and DFT Calculation of Polymers Bearing Side Chain Aziridine Group**

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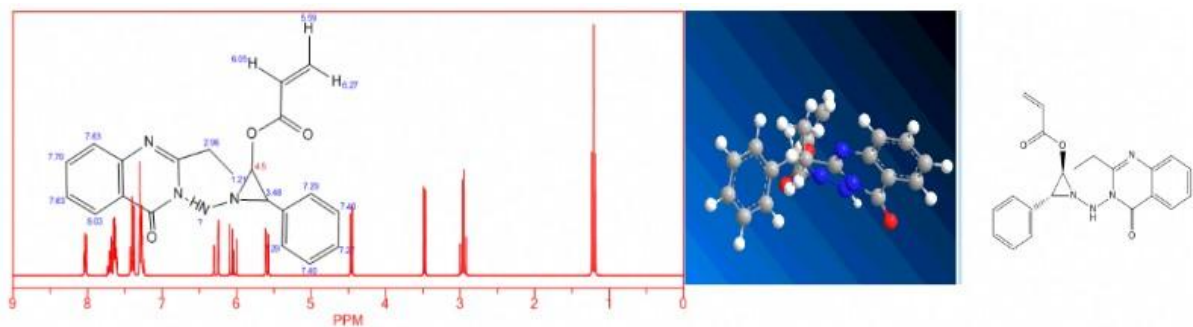
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In this work, some novel aziridine containing monomers were synthesized by the reaction of 3-aminoquinazolinones using hydrazine monohydrate and polymerized by thermal initiated radical mechanism. Spectroscopic characterizations of polymers and monomers were experimentally and theoretically performed using Gaussian G03[1] and Orca[2] quantum Chemical calculation packages. Atomic and orbital populations of monomers were also calculated by a method of 'natural population analysis via Orca and Janpa[3] program packages. The calculated spectroscopic data are then compared with the experimental values. The quality of each correlation was determined with R value, the Pearson correlation coefficient via least square method using QtiPlot software[4].

*The authors garetefully aknowledge financial support from TUBITAK with TBAG-2171 project.*

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- [3] T.Y.Nikolaienko, L.A.Bulavin, D.M.Hovorun, JANPA: an open source cross-platform implementation of the Natural Population Analysis on the Java platform, Computational and Theoretical Chemistry (2014), V.1050, P.15-22,
- [4] QtiPlot, QtiPlot - Data Analysis and Scientific Visualization, <http://www.qtiplot.com/>

**Keywords:** IR,NMR DFT, Aziridine



**Fig. 1. NMR Spectrum and molecular structure of the studied compound.**

P-129

## Morphological Characteristics of 4-n-octyl-4'-cyanobiphenyl (8CB) at the Air/Water Interface as Studied by Molecular Dynamics Simulation

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Some calamitic liquid crystals, which have a long hydrophobic alkyl chain and a strongly polar hydrophilic head group, are able to form stable and compressible monolayers at the air/water (Langmuir films) interfaces. The study on monolayers is a significantly interesting branch of physical chemistry, with considerable implications in many fields of science and technology. Langmuir films are model systems for membrane biophysics, since a biological membrane can be thought of as two weakly coupled monolayers. Therefore, such monolayers are used in biological and chemical reaction studies in interfaces. In the present study, the morphological characteristics of calamitic 8CB molecules at the air/water interface were investigated for different surface coverages by all-atomic molecular dynamics (MD) simulation. Mass density profiles and number density profiles of some selected atoms were obtained. The microscopic behaviour of the mesogen molecules at interfaces of different surface coverages was studied by generating the snapshots of their simulated structures. The thicknesses of 8CB monolayers, the monolayer peak heights and positions were calculated. And it was seen that the results were consistent with the available literature data. The average tilt angles between the water surface normal and various vectors defined in the rigid and alkyl parts of 8CB were calculated. It was concluded that the results are in good agreement with previous experimental data.

**Keywords:** Liquid crystals, molecular dynamics, monolayers

P-130

## Orientalional Order Properties of 4-n-pentyl-4'-cyanobiphenyl (5CB) Molecules at the Air/Water Interface: A Molecular Dynamics Simulation Study

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Interfacial properties of liquid crystals, which have a fundamental interest, are of practical importance for the design of display devices. The molecular tilt should be controlled essentially in many devices and it is recognized that the alignment of liquid crystal molecules is strongly affected by the properties of substrate and interface. It was shown that n-alkyl-cyanobiphenyl (nCB) liquid crystals could form Langmuir monolayers at the air/water interfaces. In this study, the order properties of 5CB molecules at the air/water interface were investigated for different surface coverages by full atomistic molecular dynamics (MD) simulations. Orientalional order properties and bond order parameters for 5CB were calculated. Radial distribution functions (RDFs) in the bulk and interfacial region were obtained. The average tilt angles between the interface normal and various vectors defined in the rigid and alkyl parts of 5CB were calculated. It was determined that the results are consistent with previous experimental data. In addition, the distribution of these tilt angles was computed.

**Keywords:** Langmuir monolayers, molecular dynamics, order parameters, tilt angle

P-131

**DFT Computational Studies of 2-((E)-[4-(Hydroxymethyl)phenyl]-iminomethyl)phenol**

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Schiff bases are used as starting materials in the synthesis of important drugs, such as antibiotics, antiallergic, antiphlogistic, and antitumor substances. Schiff bases have a wide range of industrial uses such as dyes and pigments. They have also been employed as ligands for the complexation of metal ions. Generally, Schiff bases display two possible tautomeric forms, the enol-imine and the keto-amine forms. Depend on the tautomers, two types of intramolecular hydrogen bonds are observed: O-H...N in the enol-imine and N-H...O in keto-amine tautomers.

The Schiff base compound 2-((E)-[4-(Hydroxymethyl)phenyl]-iminomethyl)phenol has been characterized by X-ray determination. In this work, quantum chemical calculations of 2-((E)-[4-(Hydroxymethyl)phenyl]-iminomethyl)phenol have been performed using the DFT/B3LYP method at the 6-31G(d) basis set. Molecular geometry, molecular electrostatic potential (MEP), frontier molecular orbitals, nonlinear optical (NLO) properties were investigated at B3LYP/6-31G(d) level of theory.

**Keywords:** Schiff base, DFT, NLO, MEP

P-132

**A Study on Spectroscopic (FT-IR and NMR) Properties and DFT Computations of N-[4-(diphenylamino)phenyl]methylene-2,3,5,6,8,9,11,12-octahydro-1,4,7,10,13-benzopentaoxacyclopentadecin-15-amine**

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The experimental spectroscopic analyses of the title compound (Fig.1) were performed with proton and carbon-13 NMR chemical shift and FT-IR spectroscopic techniques. Structural, vibrational and magnetic (chemical shifts) analyses were theoretically investigated using DFT/B3LYP method at 6-31++G(d,p) basis set. The computed structural geometric parameters were compared with similar structure in the literature. Additionally, the experimental FT-IR vibrational frequencies and NMR chemical shift values were supported with their computed data. Nonlinear optical (NLO), HOMO-LUMO and MEP analyses were theoretically done in order to understand optical and some electronic properties of the title compound. The calculated and experimental spectroscopic data show that they are in a good agreement.

**Keywords:** Spectroscopy, DFT, Non-linear optic

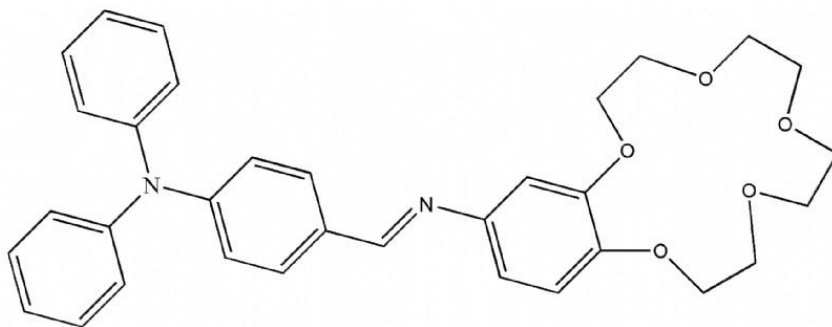


Fig. 1. The structure of the title compound (C33H34N2O5)



P-133

## Theoretical Study on the origins of the gap bowing in $\text{Ca}_x\text{Mg}_{1-x}\text{S}$ alloys

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The structural, electronic properties of three chalcogenide compounds MgS, CaS and their  $\text{Ca}_x\text{Mg}_{1-x}\text{S}$  ternary alloy in the rocksalt phase have been investigated by using the full-potential linearized augmented plane-wave method (FP-LAPW) within density functional theory (DFT). We employed the local density approximation (LDA) and generalized gradient approximation (GGA) for the calculation of exchange-correlation (XC) potential. The equilibrium lattice constants and the bulk modulus are in agreement with the values reported in the literature, their deviation from linearity has been examined and discussed. From the study of the electronic properties, we find that these binary compounds MgS and CaS, have indirect band gaps.

For ternary alloy  $\text{Ca}_x\text{Mg}_{1-x}\text{S}$  the study of these various properties are calculated, particularly the variation of structural and electronic parameters with concentration  $x$ . We focused our attention on the origins of bowing parameters corresponding to these physical properties.

In this study, we compare these predictions to the results already obtained experimentally as well as theoretical work in this regard.

**Keywords:** DFT, FP-LAPW,  $\text{Ca}_x\text{Mg}_{1-x}\text{S}$ , rock-salt phase, bowing parameters

**P-134**

**Investigation of the interactions of Tamoxifen with the estrogen receptor alpha via quantum mechanics methods and molecular docking**

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Triphenylethylenes are developed for the treatment of the estrogen-dependent breast cancer. Tamoxifen (TAM), one of the most important Triphenylethylenes, is widely used for breast cancer treatment, and is a reference compound for prevention and treatment of breast cancer. Estrogens receptors (ERs) display interesting tissue selective action. Therefore, ERs have great biomedical importance in the development of prevention and treatment of breast cancer. One of the estrogen receptor is ER( $\alpha$ ), and is closely associated with breast cancer biology, especially development of tumors. One way of prevention of ER positive breast cancers is blockage of active sites of ER hormones by antagonist Selective Estrogen Reseptor Modulator (SERM) like Tamoxifen. Therefore, the exploration of active structure of SERMs and their interactions with ERs have vital significance.

With this purpose in mind, the optimized structure, geometric parameters, electronic features and chemical environment of the anticancer drug TAM were investigated by the DFT/ B3LYP/6-311G++(d,p) calculations. DFT calculations were analyzed to produce quantum mechanical descriptors that define the active nature of TAM. These descriptors include ESP, Mulliken charges, HOMO-LUMO characteristics, and interaction properties with its environment. Ligand-Enzyme interaction were investigated on the base of TAM-ER( $\alpha$ ) docking properties using AutoDock-Vina and iGEMDOCK. Docking analysis produces the most stable binding between ligand and enzyme and provides details about surrounding interactions in binding site.

**Keywords:** Tamoxifen, DFT, Estrogen receptor alpha, Molecular docking.

P-135

Effect of External Electric Field on Intermolecular Halogen Bond of the  
N-Substituted Imidazoles ••• X<sub>2</sub>/XY Complexes

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Quantum chemical calculations have been performed to study the effect of external electric fields on intermolecular halogen bond of N-substituted imidazoles ••• X<sub>2</sub>/XY (F<sub>2</sub>, Cl<sub>2</sub>, Br<sub>2</sub>, BrCl, BrF, ClF) complexes (Fig. 1) at the MP2/aug-cc-pVDZ level. The main goal of this work is to explain the primary effect of external electric field for the studied complexes on the structure and energetic of the intermolecular halogen N ••• X<sub>2</sub>/XY halogen bond; and to investigate the physical origin of this interaction. A detailed natural bond orbital (NBO) [1], the quantum theory of atoms in molecules (QTAIM) [2], the noncovalent interaction index (NCI) [3], and the symmetry-adapted perturbation theory (SAPT) [4] based energy decomposition analyses have been carried out to clarify interaction strength and properties in these halogen bonded systems. The results show that the stability of the halogen bonding interaction is sensitive towards the strength as well as direction of the applied external electric field. It has been concluded that the strength of the intermolecular halogen bonding interaction formed in the N-substituted imidazoles ••• X<sub>2</sub>/XY complexes can be controlled by external electric field.

[1] A.E. Reed, L.A. Curtiss, F. Weinhold, Chem. Rev. 1988, 88, 899-926.

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*This work was supported by Unit of Scientific Research Projects of Süleyman Demirel University (Project No: 4600-D2-16).*

**Keywords:** Halogen bond, electric field, imidazoles, QTAIM, SAPT

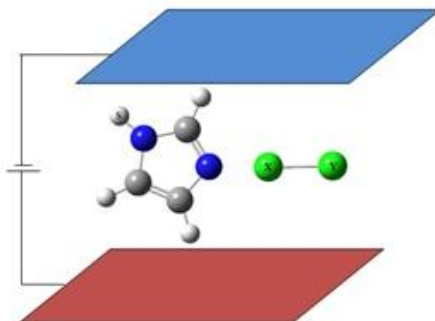


Fig. 1. Illustration of N-substituted imidazoles ••• X<sub>2</sub>/XY (F<sub>2</sub>, Cl<sub>2</sub>, Br<sub>2</sub>, BrCl, BrF, ClF) complexes under external electric field.

P-136

**Salicylaldehyde based a hydrazone compound: Synthesis, crystal structure, a comparison of theoretical and experimental spectroscopic results and the investigation of interaction with Pd(II) and Pt(II) by DFT calculations**

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Hydrazone compounds are noteworthy complexing agents because of their versatile applications in the isolation, separation and extraction of various transition metals. Salicylaldehyde based hydrazone compounds and their metal complexes are potential analytical, spectrophotometric and bioactive agents [1].

In this work, a novel hydrazone compound was obtained from the reaction of isobutyric acid hydrazide with 3,4-dihydroxybenzaldehyde. This compound was analyzed both experimentally and theoretically using X-Ray single crystal diffraction technique, IR and NMR spectroscopy techniques, and quantum chemical computation. The molecular geometry, vibrational frequencies and chemical shift values were calculated using density functional theory (DFT) at B3LYP level 6-311G+(d,p) basis set. It was seen that the computational results obtained were in agreement with the experimental results. In addition, the interaction of the title compound with Pd(II) and Pt(II) salts was investigated by using the values of Charge Transfer ( $\Delta N$ ) and Energy Lowering ( $\Delta E$ ).

*This work was supported by a grant (Project Number: FMB-BAP 16-0206) from Scientific Research Projects Coordination Unit of Amasya University.*

Reference:

- [1] Bandyopadhyay, N., Pradhan, A.B., Das, S., Lu, L., Zhu, M., Chowdhury, S., Naskar, J.P. (2016), Journal of Photochemistry and Photobiology B: Biology, 160, 336-346.

**Keywords:** Hydrazone, IR and NMR spectroscopy, DFT

P-137

## Quantum Chemical Computational Study of N'-((E)-2-(hydroxyimino)-1-phenylethylidene)furan-2-carbohydrazide

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Oximes and hydrazones are the two important classes of compounds owing to their wide applications in industry, medicine, detection and determination of various metal ions. These compounds have a number of potential bonding sites such as carbonyl oxygen, azomethine and imine nitrogens. Therefore, hydrazone and oximes as well as their coordination compounds have been studied extensively [1]. In recent years, much attention has been given to theoretical studies on hydrazones and oximes.

In this study, quantum chemical calculations of the molecular structure, vibrational frequencies, gauge including atomic orbital 1H chemical shift values were carried out using the density functional B3LYP method with the 6-311G+(d,p) basis set for the hydrazone oxime compound N'-((E)-2-(hydroxyimino)-1-phenylethylidene)furan-2-carbohydrazide. The theoretical vibrational frequencies and chemical shift values were seen to be in agreement with the experimental values. UV-Visible spectrum of the compound was recorded and the electronic properties HOMO and LUMO energies were measured by time-dependent TD-DFT approach. To understand the chemical behavior of this compound, the reactivity descriptors such as ionization energy, molecular hardness, electrophilicity, condensed Fukui function and total energy were calculated for N'-((E)-2-(hydroxyimino)-1-phenylethylidene)furan-2-carbohydrazide. In addition, the NBO/NPA atomic charges were performed to explore the possible coordination modes of this compound.

[1] R. Gup and E. Giziroglu, Spectrochim. Acta, Part A, A65, 719-726 (2006).

**Keywords:** Hydrazone, Oxime, DFT

P-138

**Conformational, Structural, Electronic and Vibrational Investigations on 5-Methyl-4-(2-thiazolylazo)resorcinol by FT-IR, FT-Raman, NMR and DFT**

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<sup>2</sup>Department of Physics, Ahi Evran University, Kirsehir, Turkey

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<sup>4</sup>Department of Electrical & Electronic Engineering, Harran University, Sanliurfa, Turkey

Geometry parameters of the 5-Methyl-4-(2-thiazolylazo)resorcinol (MTR) molecule is not in the literature, with the aim of finding a stable structure made of conformational analysis. Conformational distribution of MTR molecule obtained by scanning the potential energy surface were determined using the program Spartan 08 [1]. To do this, Merck Molecular Force Field (MMFF) [2] method was used for. After determining all conformations (Fig. 1) to identify the most stable conformation, geometry optimization calculations were performed with the Gaussian 09W [3] program. Furthermore for the vibrational frequency calculations and calculations of other properties of MTR molecule Gauss View 3.0 [4] graphical interface was carried out with Gaussian 03W program. In all calculations such as geometry optimization, vibrational frequency and other molecular property calculations were performed by B3LYP [5] functional and 6-311G(d,p) basis set. Fundamental vibrational modes of the total energy distribution (TED) calculations and Scaled Quantum Mechanic (SQM) method with Paralel Quantum Solutions (PQS) program has been utilized. Additionally Raman intensities were calculated by Ralnt programs. NMR analysis has been done by using Gauge Independent Atomic Orbital (GIAO) method. The <sup>1</sup>H and <sup>13</sup>C NMR spectra calculations were performed by Gaussian 09 program package. Results compared with experimental results for the identification and characterization of MTR molecule.

The FT-IR spectrum of MTR molecule is recorded in the region 4000-400 cm<sup>-1</sup> on Vertex 80 spectrophotometer. The FT-Raman spectrum of MTR molecule has been recorded using 1064 nm line of Nd: YAG laser as excitation wavelength in the region 50-3500 cm<sup>-1</sup> on the Thermo scientific DXR Raman Microscope. All NMR spectra are measured at room temperature.

[1] Spartan 08, Wavefunction Inc., Irvine, CA 92612, USA, 2008.

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**Keywords:** DFT, FT-IR, FT-Raman, Methyl-4-(2-thiazolylazo)resorcinol;

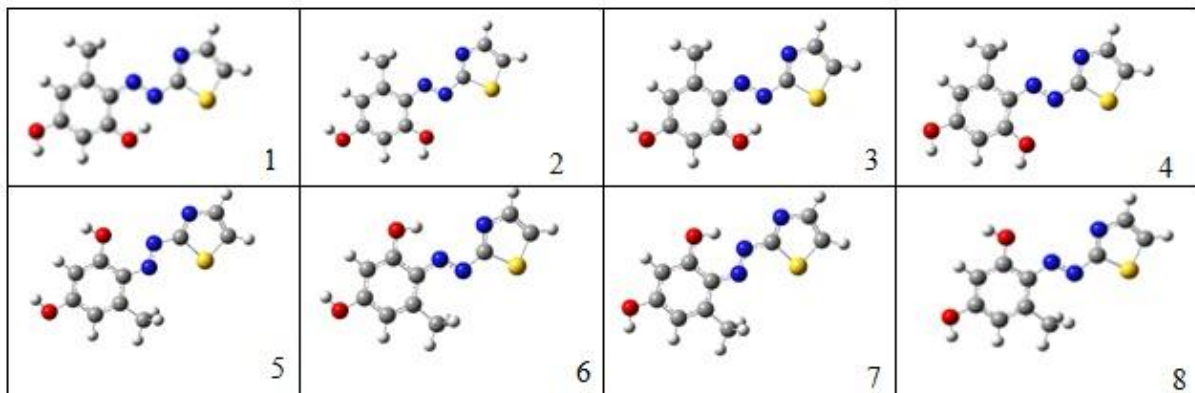


Fig. 1. Conformational analysis results of MTR

P-139

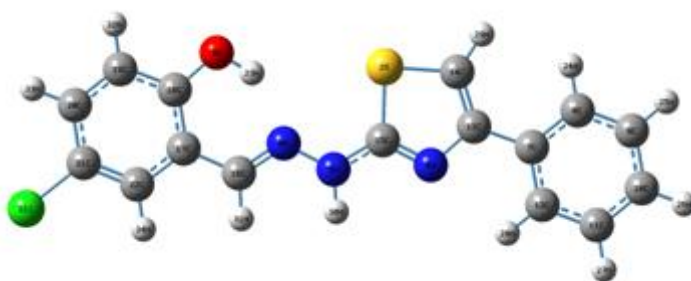
## Investigation of Solvent Effect of Molecular Structures on Molecular Orbital Energies by Density Functional Theory

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The molecular structure of the single crystal structure with heterocyclic compounds and aromatic rings in its structure has been optimized using the Density Functional Theory, which is the most popular method of computational chemistry. In the calculations, the B3LYP base function, which gives good results for organic structures, and 6-311G (split valance) and 6-311G (d, p) (polarized) were chosen as basis sets. Molecular orbital energies of molecular structures were calculated using TD-DFT with ultraviolet spectroscopy technique using structures optimized with different basis sets. First, the molecular orbital energy levels in a gas phase are calculated using a molecular structure, the B3LYP/6-311G and B3LYP/6-311G (d, p) methods, and then the energy levels are calculated in different solvent environments of this molecular structure to determine the molecular energy levels of the solvent effect and dipole moment effect was investigated.

**Keywords:** TD-DFT, solvent effect, molecular structure, UV-vis.



**Fig. 1. Molecular Structure**



**P-140**

**Investigations on the FT-IR, FT-Raman, Conformational analysis, Molecular docking, Fukui function, DFT of 2-Isopropyl-6-methyl-4-pyrimidinol**

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<sup>2</sup>Department of Physics, Gazi University, Ankara, Turkey,

<sup>3</sup>Photonics Application and Research Center, Gazi University, Ankara, Turkey

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Literature reveals that to the best of our knowledge DFT calculations and experimental studies on molecular structure and vibrational spectra of 2-Isopropyl-6-methyl-4-pyrimidinol (IMP) molecule have not been reported so far. Therefore, we have carried out detailed theoretical and experimental investigations on the molecular structure, vibrational spectra and some electronic properties of IMP molecule completely. We have utilized the B3LYP [1-3] with 6-311G(d,p) basis set. The complete vibrational analysis of IMP is performed by combining the experimental and theoretical information using Pulay's Density Functional Theory (DFT) based on the scaled quantum chemical approach. Thus, the present study aims to give a complete description of the molecular geometry, vibrations and electronic properties of the IMP molecules.

The calculations were performed at DFT levels by using Gaussian 09 program package, invoking gradient geometry optimization [4]. In order to establish the stable possible conformations (Fig. 1), the conformational space of IMP 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 IMP 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 6-311G(d,p) basis set, using SQM program [5].

[1] P. Hohenberg, W. Khon, Phys. Rev. B 136 (1964) 864.

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**Keywords:** 2-Isopropyl-6-methyl-4-pyrimidinol, DFT, FT-IR

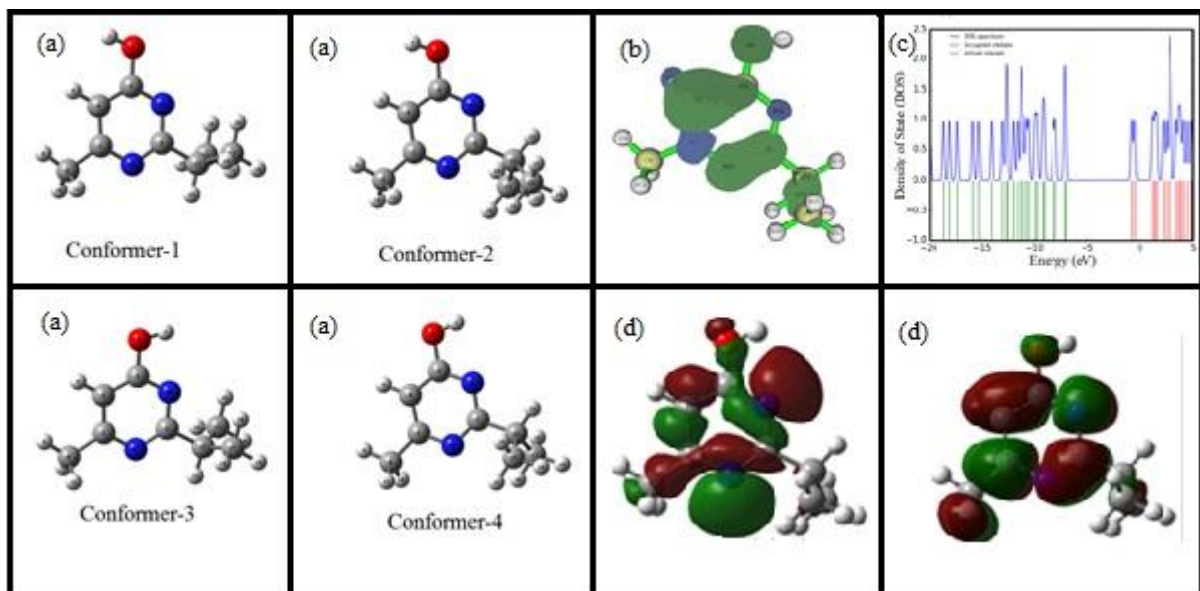


Fig. 1. (a) Conformational analysis results, (b) Fukui function, (c) DOS plot and (d) HOMO-LUMO plots of IMP

P-141

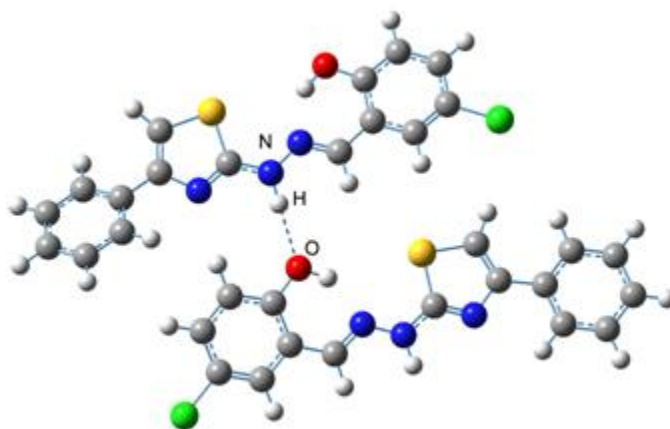
**Investigation of D-H... A Hydrogen Bond Effect on Vibration Frequencies of Molecular Structures by Density Functional Theory**

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The monomers and the different dimeric forms (Fig. 1) of the molecular structure containing the phenyl ring, the hydrazone group, the thiazole and the chlorophenyl ring in the structure are optimized using Density Functional Theory, which is the most popular method of computational chemistry. In calculations, B3LYP was selected as the basis function, 6-311G (split valance) and 6-311G (d, p) (polarized) as the basis sets. Vibrational frequencies of monomer and dimer forms of molecular structures were calculated using different basis sets. First, the vibrational frequencies were calculated to the monomeric form, ie, a molecular structure that does not contain intermolecular hydrogen bonds, using the B3LYP/6-311G and B3LYP/6-311G (d, p) methods and then, vibration frequencies were calculated by selecting two different basis sets of N-H...O and N-H...N type hydrogen bonded dimeric forms and the effect of hydrogen bonding on vibration frequencies was investigated.

**Keywords:** TD-DFT, hydrogen bond, vibrational frequency.



**Fig. 1. Molecular structure**

P-142

## Investigation on spectroscopic and quantum chemical calculation studies of Aloe Emodin molecule

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This work deals with the spectroscopic properties (FT-IR and FT-Raman spectra), structural and some electronic properties as well as theoretical calculations of Aloe Emodin molecule. The vibrational, structural and some electronic properties observations of the Aloe Emodin molecule were reported, which is investigated using some spectral methods and DFT calculations.

The FT-IR spectrum of Aloe Emodin molecule was recorded in the region 4000-400  $\text{cm}^{-1}$  on Vertex 80 spectrophotometer. The FT-Raman spectrum of Aloe Emodin molecule was recorded using 1064 nm line of Nd: YAG laser as excitation wavelength in the region 50-3500  $\text{cm}^{-1}$  on the Thermo scientific DXR Raman Microscope.

In the present work, the quantum chemical calculations were performed by means of the Gaussian 09 software package, using hybrid density functional theory (DFT) at the B3LYP level and with 6-311G (d, p) basis set. All the computations have been carried out in gas phase. In order to establish the stable possible conformations, the conformational space of Aloe Emodin molecule was scanned with theoretical methods. The harmonic vibrational frequencies were calculated at the same level of theory. The vibrational frequencies were calculated and scaled, and subsequently values were compared with the experimental Infrared and Raman spectra. The vibrational modes were assigned on the basis of TED analysis for 6-311G(d,p) basis set, using SQM program. The observed and calculated frequencies are found to be in good agreement [1-3].

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[2] H.B. Schlegel, J. Comput. Chem. 3 (1982) 214-218

[3] G. Rauhut, P. Pulay, J. Phys. Chem. 99 (1995) 3093

**Keywords:** Aloe Emodin molecule, DFT, FT-IR, FT-Raman

P-143

**Supramolecular self-assembly of new benzamide derivatives directed by intermolecular and  $\pi$ -stacking interactions: Crystal structures and Hirshfeld surface analyses**

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We have synthesized and characterized a series of closely related two thiourea derivative molecules (1 and 2), obtained by reaction of 4-R-benzoyl chloride (R: H and OCH<sub>3</sub>) with an equimolar amount of potassium thiocyanate and dibenzilamine in dry acetone (Fig. 1). The crystalline and molecular structures of synthesized compounds have been examined to understand how alter the crystal packing of the substituted different functional groups at para positions on the aromatic ring. Single-crystal X-ray analysis has revealed that molecules of the prepared compounds are assembled into supramolecular units connected via networks of similar intermolecular interactions. The packing arrangements of the compounds, however, were found to be different. We have also conducted an analysis of Hirshfeld surfaces and associated two dimensional fingerprint plots for the synthesized compounds and followed the changes of different properties on these surfaces upon systematic variation of the substituent. Hirshfeld surface analysis and decomposed fingerprint plots show that the structures are stabilized by H $\cdots$ H, H $\cdots$ S, O $\cdots$ H, N $\cdots$ H, C-H $\cdots$  $\pi$  and  $\pi\cdots\pi$  intermolecular interactions. The most significant contributions come from H $\cdots$ H and C $\cdots$ H contacts, which correspond to van der Waals interactions and the C-H $\cdots$  $\pi$  contacts, respectively.

*Acknowledgement: This study was supported by the Research Fund of Mersin University in Turkey with Project Number: 2016-AP4-1426.*

**Keywords:** Hirshfeld surfaces, Non-covalent interactions, Benzamide, X-ray single crystal diffraction, Synthesis.

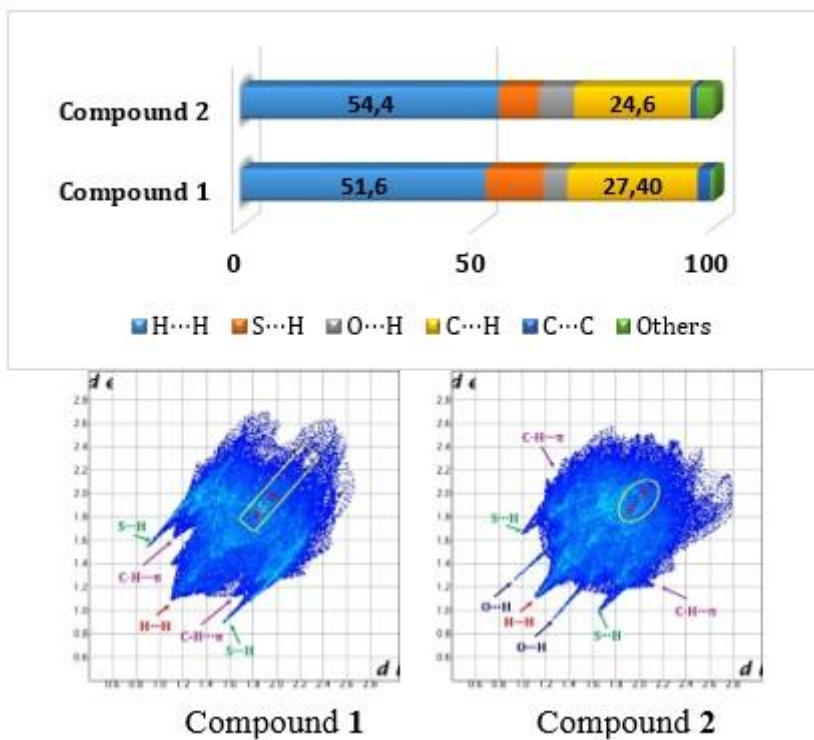


Fig. 1

P-144

**Experimental and theoretical studies of the molecular structure of 7-Methyl-3-[(3-methyl-3-mesityl-cyclobutyl]-5-phenyl-5H-thiazolo[3,2- $\alpha$ ]pyrimidine-6-carboxylic acid ethyl ester**

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In this work, the title molecule, 7-Methyl-3-[(3-methyl-3-mesityl-cyclobutyl]-5-phenyl-5H-thiazolo[3,2- $\alpha$ ]pyrimidine-6-carboxylic acid ethyl ester (C<sub>30</sub>H<sub>34</sub>N<sub>2</sub>O<sub>2</sub>S<sub>1</sub>), was synthesized and characterized by FT-IR spectroscopy and single crystal X-ray diffraction. The compound crystallizes in the triclinic space group P21/c. with Z = 4, a = 14.1988(6), b = 19.0893(5), c = 10.1325(4) Å, V = 2674.56(17) Å<sup>3</sup>. The optimized structure parameters of the studied molecule was determined theoretically using HF/6-31G(d) and B3LYP/6-31G(d) methods for ground state, and compared with previously reported experimental findings. The calculated harmonic vibrational frequencies are scaled and they are compared with experimental frequencies obtained by FT-IR spectra. The electronic properties, such as HOMO and LUMO energies, and molecular electrostatic potential (MEP) are also performed.

*Crystallographic data for the structure analysis have been deposited with the Cambridge Crystallographic Data Centre, CCDC No 899805. Copies of this information may be obtained free of charge from the Director, CCDC, 12 Union Road, Cambridge CB2 1EZ, UK (fax: +44-1223-336033; e-mail: deposit@ccdc.cam.ac.uk or www: <http://www.cede.cam.ac.uk>).*

**Keywords:** B3LYP, DFT and HF calculation, IR spectrum, X-ray

P-145

**Synthesis, Spectroscopic (FT-IR, UV-Vis), Experimental (X-Ray) and Theoretical (HF/DFT) study of: (E)-2-chloro-N-((4-nitrocyclopenta-1,3-dienyl)methylene)benzenamine**

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Schiff Bases are also becoming increasingly important in the dye and plastic industries as well as for the liquid-crystal technology and mechanistic investigation of drugs used in pharmacology, biochemistry and physiology [1,2]. The Schiff Base compound, (E)-2-chloro-N-((4-nitrocyclopenta-1,3-dienyl)methylene)benzenamine was synthesized and characterized by elemental analysis FT-IR, UV-Vis and X-Ray diffraction (XRD) technique. X-Ray diffraction measurements were collected at room temperature (296 K) by using graphite-monochromated Mo-K $\alpha$  radiation ( $\lambda=0.71073$  Å). The intensity symmetries indicate the monoclinic P 21/c space group and  $a=12.022$  (5),  $b=7.1699$  (7),  $c=121.101$  (3) Å and  $\beta=121.101$  (3)° in the unit cell parameters. The molecular structure was optimized at the Hartree Fock (HF) and density functional theory (DFT) methods. The vibrational frequencies and electronic absorption spectra of the title compound were computed at the HF and DFT methods. The electronic structure parameters and energetic behaviours of the title compound in solvent media were studied by theoretical methods. Besides, molecular electrostatic potential (MEP), natural bond orbital (NBO), frontier molecular orbital (FMO), Mulliken atomic charge and natural population analysis (NPA) were computed. Finally, the experimental results show good agreement with theoretical results.

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[2] I. Sheikhshoae, M. A. Sharif, *Acta Crystallogr. E* 62 (2006) o3563-o3565.

**Keywords:** Schiff base, Hartree Fock, Density Functional Theory, MEP, NPA



P-146

**Crystal Structure Analysis, Spectroscopic Characterization and Theoretical Calculations of: (E)-4-bromo-5-methoxy-2-((p-tolylimino)methyl)phenol**

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Schiff bases are used as starting materials in the synthesis of important drugs, such as antibiotics and antiallergic, antiphlogistic and antitumor substances [1-3]. On the industrial scale, they have a wide range of application, such as dyes and pigments [4]. In this study, lots of physicochemical properties of a new Schiff base compound has been characterized and discussed. The crystal structure of (E)-4-bromo-5-methoxy-2-((p-tolylimino)methyl)phenol was determined by FT-IR, UV-Vis and X-Ray diffraction technique. The compound crystallizes in the monoclinic space group P 21/n with  $a = 5.1079 (6) \text{ \AA}$ ,  $b = 10.558 (9) \text{ \AA}$ ,  $c = 25.876 (27) \text{ \AA}$  and  $\beta = 94.965 (9)^\circ$  and  $Z = 4$  in the unit cell. The molecular structure was optimized of the density functional theory (DFT). The vibrational frequencies and electronic absorption spectra of the title compound was computed as theoretically. In addition, the molecular electrostatic potential (MEP), natural bond orbital (NBO), frontier molecular orbital (FMO) analysis, thermodynamic and nonlinear optical (NLO) properties were also performed. The calculated results were compared with the experimental determination results of the compound.

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**Keywords:** X-Ray Diffraction, Density Functional Theory, Spectral Analysis

P-147

**Spectroscopic (FT-IR / NMR) and quantum chemical study on  
3,4-dicyanophenyl 4-methylbenzenesulfonate**

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Phthalocyanines are blue-green in color and for many decades have been used as very stable commercial dyes and pigments.

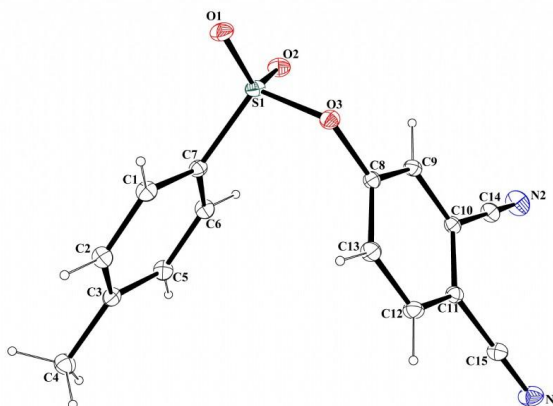
The relative simplify of incorporating substituents onto the macrocyclic ring and introducing a metal ion or metalloid element into the core of the macrocyclic ligand allows tuning of the properties of the system, not simply the color but a range of interesting photophysical and semi-conducting properties. Thus phthalocyanines are important in the area of organic materials development, building on their successfully established applications as charge carriers in photocopiers, as dyes in laser/LED printing and as laser light absorbers for optical data storage in certain CD-ROMs [1].

In this study, we present results of a detailed investigation of the synthesis and structure characterization of 3,4-dicyanophenyl 4-methylbenzenesulfonate using single crystal X-ray (Fig. 1), IR, NMR and quantum chemical methods, besides elemental analysis. The computational details were performed by using Gaussian 09 [2] software and DFT/B3LYP/6-311G(d, p)/6-311++G(d, p) methods.

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**Keywords:** Cyanophenyl, DFT, NMR



**Fig. 1.** The molecular structure of the title compound showing the atom-numbering scheme

P-148

## Experimental and Theoretical Investigation of the Molecular and Electronic Structure of 2,3-dicyanophenyl 4-methylbenzenesulfonate

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Phthalonitrile derivatives are important precursors that have been used for synthesis of phthalocyanines (Pcs). In addition, phthalonitriles are used for synthesis of the high temperature polymers having important properties such as high glass transition, thermal stability and fire resistivity [1]. Pcs having received much attention because of their thermal and photostability, interesting photophysical and photochemical properties, strong electronic delocalization, visible area optical properties. Here, a comparison of the molecular structure, FT-IR and NMR spectroscopic data of the title compound obtained by experimentally and theoretically has been presented. In addition, some electronic properties have been given. The molecular structure of the title compound (Fig. 1) is optimized by the DFT calculations with a hybrid functional B3LYP (Becke's Three parameter Hybrid Functional using the LYP Correlation Functional) at 6-311G (d, p) and 6-311++G (d, p) basis sets and all theoretical computations were carried out using Gaussian 09 program package [2].

[1] H. Saraçoğlu, F. Güntepe, Ç. Yüksektepe, N. Çalışkan, S. Saydam, *Molecular Crystals and Liquid Crystals* 537 (2011) 111–127.

[2] M. J. Frisch, et al., *Gaussian 09, Revision C.01*, Gaussian, Inc., Wallingford, CT, (2009).

**Keywords:** Cyanophenyl, DFT, NMR

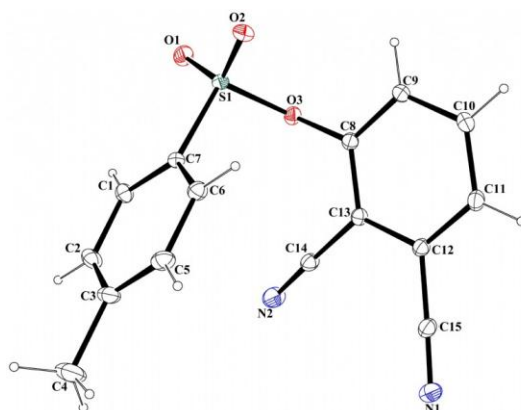


Fig. 1. A view of the title compound showing the atom-numbering scheme

P-149

**Experimental (X-ray, FT-IR and UV-VIS spectra) and theoretical methods (dft study) of N'-(dipyridin-2-ylmethylene)-4-methylbenzenesulfonohydrazide**

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A new hydrazone derivative compound has been synthesized and characterized by IR, UV-vis. spectroscopy techniques, elemental analysis and single-crystal X-ray diffraction (XRD). The title compound N'-(dipyridin-2-ylmethylene)-4-methylbenzenesulfonohydrazide (C<sub>18</sub>H<sub>16</sub>N<sub>4</sub>O<sub>2</sub>S) crystallizes in C 2/c monoclinic space group. The crystal structure is stabilized by C-H...O intermolecular hydrogen bonding. In addition to crystal structure from X-ray experiment, the molecular geometry, vibrational frequencies and frontier molecular orbital analysis of the title compound in the ground state have been calculated by using DFT B3LYP/6-31G (d, p) methods. The computed vibrational frequencies are used to determine the types of molecular motions associated with each of the observed experimental bands. From the analyses of the experimental data the absorption band centered at 3174 cm<sup>-1</sup> is assigned to the ν(N-H) stretching vibration of hydrazone group. Also, this band was calculated at 3284 cm<sup>-1</sup>, which is in good agreement with literature values [1, 2]. UV- vis. absorption spectra of the compound calculated by TD-DFT has been ascribed to their corresponding molecular structure and electrons transitions. The HOMO and LUMO energies were calculated by TD-DFT approach. In this study, we present results of a detailed investigation of the synthesis and structural characterization of N'-(dipyridin-2-ylmethylene)-4-methylbenzenesulfonohydrazide by using single crystal X-ray, IR, UV-vis. and quantum chemical methods. A comparison of the experimental and theoretical spectra can be very useful in making correct assignments and understanding the molecular structure relationship. And so, these calculations are valuable for providing insight into molecular analysis.

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**Keywords:** Crystal structure, DFT calculations, hydrazones.

P-150

**A density functional theory study on geometric, spectroscopic and electronic properties of BTPCA**

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The main purpose of this study is to describe the relations among the geometric, spectroscopic, electronic and nonlinear optical properties for benzotriazole pyridine-2-carboxylic acid (BTPCA) molecule. For this purpose, the optimized geometry, vibration spectrum, frontier molecular orbitals and first order hyperpolarizability parameter ( $\beta$ ) for BTPCA molecule have been calculated by using B3LYP [1,2] level of density functional theory (DFT) in conjunction with 6-311++G(d,p) [3] basis set. It was observed that the calculated geometric parameters and vibrational wavenumbers are in a good agreement with previously reported experimental data [4]. The  $\beta$  parameter for BTPCA has been calculated as  $17.076 \times 10^{-31}$  esu. Fig. 1 demonstrated that the charge transfer occurs in BTPCA from benzotriazole to pyridine-2-carboxylic acid, leading to increase in  $\beta$  parameter. The other factors that allow to the remarkable  $\beta$  parameter are the conjugated heterocyclic rings where the electrons can move freely and COOH functional group which plays important role in the charge transfer interaction [5].

[1] Axel D. Becke, The Journal of Chemical Physics, 98, 1993, 5648.

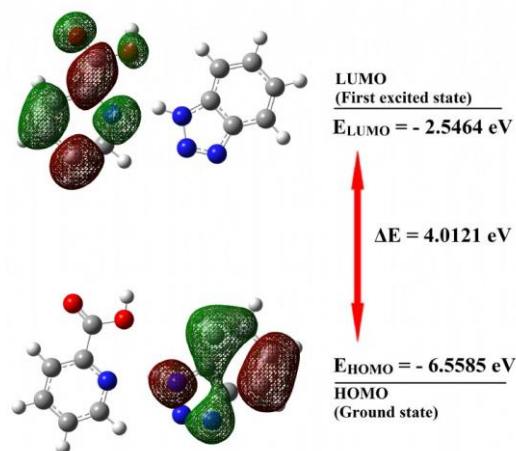
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**Keywords:** BTPCA, DFT, Nonlinear optic, IR, HOMO-LUMO



**Fig. 1.** Frontier molecular orbitals for BTPCA

P-151

**Combined experimental (FT-IR, FT-Raman, NMR) and theoretical studies on the molecular structure, vibrational spectra, reactivity descriptor and molecular docking 4,4/-dimethyl-2-2/dipyridyl**

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In the present work, the quantum chemical calculations were performed by means of the Gaussian 09 software package, using hybrid density functional theory (DFT) at the B3LYP (Becke three parameter hybrid functional combined with Lee-Yang-Parr correlation functional) level and with 6-311G (d, p) basis set. All the computations have been carried out in gas phase. In order to establish the stable possible conformations, the conformational space of 4,4/-dimethyl-2-2/dipyridyl (DMDP) molecule (Fig. 1) was scanned with theoretical methods. The harmonic vibrational frequencies have been calculated at the same level of theory. The vibrational frequencies were calculated and scaled, and subsequently values have been compared with the experimental Infrared and Raman spectra. The vibrational modes were assigned on the basis of TED analysis for 6-311G(d,p) basis set, using SQM program. The observed and calculated frequencies are found to be in good agreement [1-3].

The Hirshfeld charge, Fukui function and molecular docking analysis studies have been reported. The analysis of the all analysis has been well correlated to the spectroscopic studies. Additionally, the highest occupied molecular orbital energy ( $E_{\text{HOMO}}$ ), lowest unoccupied molecular orbital energy ( $E_{\text{LUMO}}$ ) and the energy gap between  $E_{\text{HOMO}}$  and  $E_{\text{LUMO}}$  ( $\Delta E_{\text{HOMO-LUMO}}$ ) have been calculated. The FT-IR spectrum of DMDP molecule is recorded in the region 4000-400  $\text{cm}^{-1}$  on Vertex 80 spectrophotometer. The FT-Raman spectrum of DMDP molecule has been recorded using 1064 nm line of Nd: YAG laser as excitation wavelength in the region 50-3500  $\text{cm}^{-1}$  on the Thermo scientific DXR Raman Microscope. The  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra are taken in solutions and all signals are referenced to TMS on a Bruker Ultrashield NMR Spectrometer. All NMR spectra are measured at room temperature.

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**Keywords:** 4,4/-dimethyl-2-2/dipyridyl, DFT, FT-IR, FT-Raman

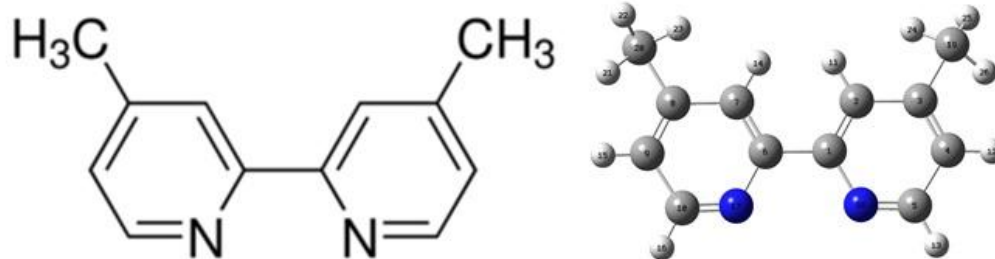


Fig.1. Molecular structure of the 4,4'-dimethyl-2,2'-dipyridyl (DMDP)

P-152

**Optimized geometry, spectroscopic (IR, UV-Vis and NMR) characterization and nonlinear optical properties of 4-(4-methoxy-2-nitrophenylamino)-4-oxobutanoic acid; A DFT study**

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The substitution of aromatic rings with electron donor and acceptor groups has caused to remarkable increase in the first order static hyperpolarizability ( $\beta$ ). The other way for large  $\beta$  parameter is the extension of aromatic rings leading to increase in the number of  $\pi$  electrons as well as their delocalization length. Considering the above mentioned factors, 4-(4-methoxy-2-nitrophenylamino)-4-oxobutanoic acid molecule (Fig. 1) has been seen as a potential NLO material. In this study, geometric parameters, vibrational wavenumbers, electronic absorption wavelengths,  $^1\text{H}$  and  $^{13}\text{C}$  NMR chemical shift values have been calculated by using B3LYP [1,2] level and 6-311++G(d,p) basis set [3]. The obtained theoretical results have been found as consistent with the previously reported experimental data [4]. The  $\beta$  parameter has been calculated as  $22.869 \times 10^{-31}$  esu for the title molecule. The  $\text{OCH}_3$ ,  $\text{NO}_2$ ,  $\text{C}=\text{O}$  and  $\text{COOH}$  functional groups as well as the aromatic benzene ring mainly responsible for the remarkable  $\beta$  parameter [5].

[1] A. D. Becke, The Journal of Chemical Physics, 98, 1993, 5648

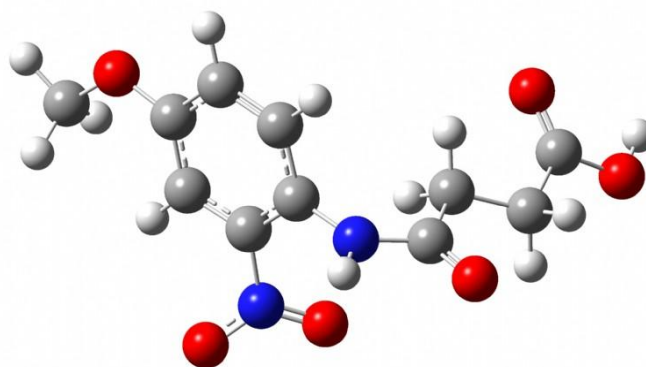
[2] C. Lee, W. Yang, R. G. Parr. Physical review B, 37, 1988, 785.

[3] M. J. Frisch, J. A. Pople, J. S. Binkley, The Journal of chemical physics, 80, 1984, 3265-3269.

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[5] D. Avci, Ö. Tamer, Y. Atalay, Journal of Molecular Liquids, 220, 2016, 495-503.

**Keywords:** B3LYP, IR, NMR, Nonlinear optic, 4-(4-methoxy-2-nitrophenylamino)-4-oxobutanoic acid



**Fig. 1.** The optimized geometry for 4-(4-methoxy-2-nitrophenylamino)-4-oxobutanoic acid



P-153

5-Methyl-2-thiophenecarboxaldehyde: Experimental and TD/DFT study

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It is well known that 5-Methyl-2-thiophenecarboxaldehyde (MTC) is the biological activity effect. In this regard, analysis of MTC by the experimental and theoretical spectroscopic methods is important. In this work, FT-IR (see Fig.1) and UV-vis spectra for MTC were recorded. To determine the optimized molecular geometry and vibrational frequencies of MTC, DFT//B3LYP/6-311++G(d,p) calculations were performed. The detailed assignments of vibrational frequencies were carried out on the basis of potential energy distribution (PED) by using VEDA program. To investigate UV-vis absorption wavelengths and significant contributions to the electronic transitions, TD-DFT/B3LYP/6-311++G(d,p) calculations with the PCM (polarizable continuum model) in ethanol solvent and gas phase in the excited state were employed. In addition, the NLO parameters ( $\beta$ ,  $\gamma$  and  $\chi(3)$ ) and FMO energies of MTC were calculated by using B3LYP/6-311++G(d,p) level. The NLO parameters of MTC were compared with the typical NLO materials (pNA and urea). The  $\beta$  and  $\gamma$  parameters for MTC were calculated as  $4.54 \times 10^{-30}$ ,  $8.64 \times 10^{-30}$  esu,  $12.26 \times 10^{-36}$  and  $30.11 \times 10^{-36}$  esu by using B3LYP/6-311++G(d,p) in gas phase and ethanol solvent. According to the Lorentz-Lorenz equation [5], the relation between linear polarizability ( $\alpha$ ) and refractive index (n) were investigated to observe polarization behavior of MTC in ethanol solvent. To sum up, MTC can be considered as a candidate to NLO material.

**Keywords:** 5-Methyl-2-thiophenecarboxaldehyde, FT-IR and UV-vis, TD/DFT, NLO

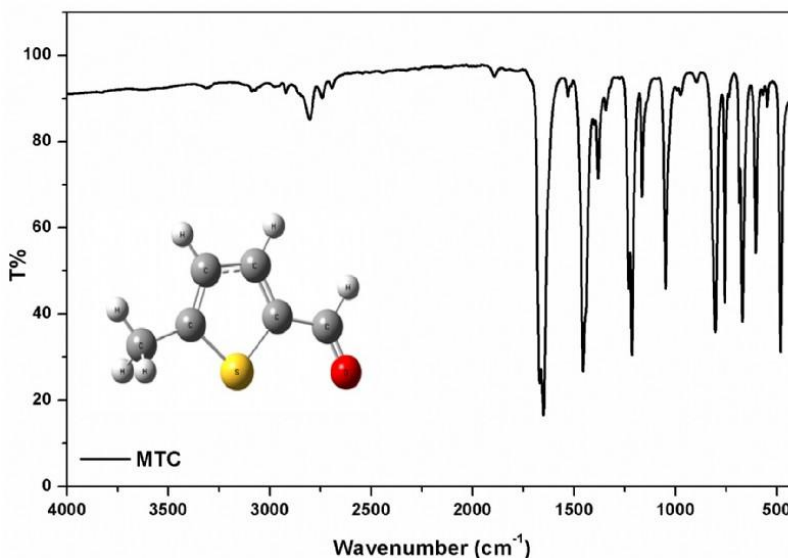


Fig. 1. FT-IR spectrum for MTC

P-154

A theoretical study of solvent effects on 2-acetoxybenzoic acid molecule

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The 2-acetoxybenzoic acid is also referred as aspirin, is a non-steroidal anti-inflammatory drug [1]. The properties of the compounds of the invention can be analyzed using standard assays for pharmacological activity. Thus, understanding of solvent effects of the 2-acetoxybenzoic acid is crucial for the physicochemical and pharmaceutical properties of the studied molecule. In this regards, the aim of the present study is to perform the solubility and solute-solvent interactions of 2-acetoxybenzoic acid using different solvents such as methanol, DMSO, ether and water. Therefore, we investigated the effects of solvents on the geometry and vibrational frequencies with PCM model for 2-acetoxybenzoic acid. We also performed DFT calculations with inclusion of the solvent effects to qualitatively determine the influence of a solvent environment on the structural and electronic structure properties of 2-acetoxybenzoic acid. Moreover, the UV-Vis absorption spectra of aspirin molecule were calculated in different solvents by TD-DFT method [2]. The calculated DFT/B3LYP approach good coherent with the experimental data [1]. Figure 1 and Figure 2 show 2D and 3D chemical structure of 2-acetoxybenzoic acid, respectively.

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**Keywords:** 2-acetoxybenzoic acid, Solvent Effect, Density Functional Theory

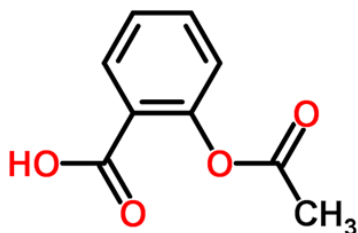


Fig. 1

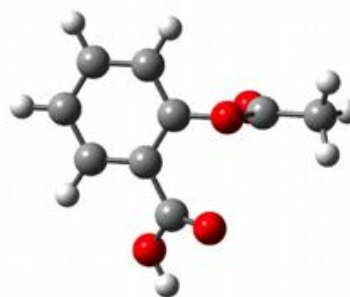


Fig. 2

**P-155**

**Theoretical evaluation of triazine derivatives as steel corrosion inhibitors: DFT**

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Density functional theory (DFT) calculations was performed on hexahydro-1,3,5-triphenyl-s-triazine (Inh1), hexahydro-1,3,5-p-tolyl-s-triazine (Inh2), hexahydro-1,3,5-p-methoxyphenyl-s-triazine (Inh3), hexahydro-1,3,5-p-aminophenyl-s-triazine (Inh4), hexahydro-1,3,5-p-nitrophenyl-s-triazine (Inh5) molecules in order to study their reactivity and adsorption behaviour towards steel corrosion. DFT results indicate that the active sites of the molecules were mainly located on the N atoms of the triazine ring and on the aromatic rings containing substituted polar groups.

**Keywords:** Modelling studies, Acid inhibition, Triazine

P-156

Structural considerations on benzamide derivatives: Synthesis, crystal structure and Hirshfeld surface analysis

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The molecular structure of N-(bis(3,5-dimethoxybenzyl)carbamothioyl)benzamide (1) and N-(bis(3,5-dimethoxybenzyl)carbamothioyl)-4-methoxybenzamide (2) have been and determined by single-crystal X-ray crystallography. The compound 1 crystallize in triclinic P1 space group with Z = 2 while compound 2 crystallize in triclinic space group P1 with Z = 4. A detailed analysis of the intermolecular interactions in synthesized compounds have been performed based on the Hirshfeld surfaces and their associated two dimensional fingerprint plots and mapped with different properties  $d_{norm}$ , shape index and curvedness. The Hirshfeld surfaces analysis revealed that the packing of the molecules in the crystal structure of the compounds shows the linking of two molecules with strong dimeric N-H...S contact. In addition to these interactions, molecules display the weak dimeric C-H...S and strong dimeric C-S... $\pi$  interaction (Fig. 1). These interactions are caused in the formation of a stabilized and strengthening molecular dimer in the crystal structure.

*Acknowledgement: This study was supported by the Research Fund of Mersin University in Turkey with Project Number: 2015-AP4-1162.*

**Keywords:** Hirshfeld surfaces, Non-covalent interactions, Benzoyl thiourea, X-ray single crystal diffraction, Synthesis.

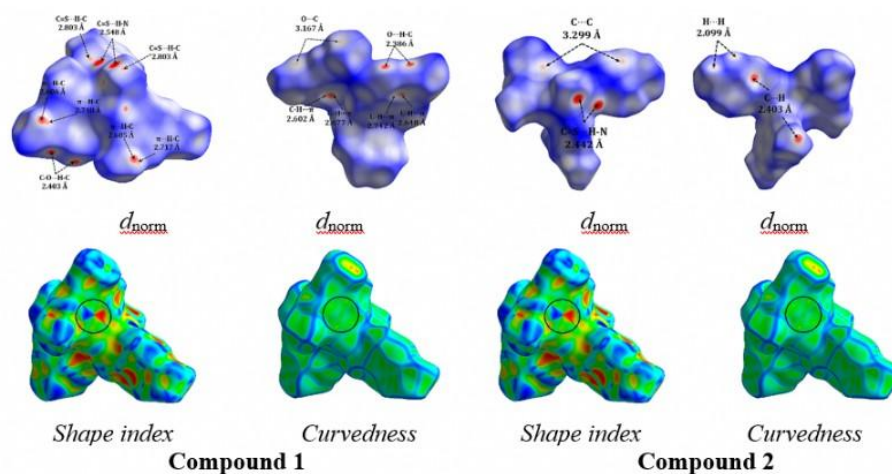


Fig. 1. Hirshfeld surfaces mapped with  $d_{norm}$ , shape index and curvedness for compounds 1 and 2.

P-157

## Computational investigation of Cadmium(II)-Nickel(II) Imidazole Complex: [Cd(imidazole)<sub>4</sub>Ni(μ-CN)<sub>4</sub>]<sub>n</sub>

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The molecular structure of [Cd(im)<sub>4</sub>Ni(μ-CN)<sub>4</sub>]<sub>n</sub> (im = imidazole) was optimized by DFT-B3LYP and DFT-B3PW91 methods in the gas phase using LANL2DZ basis set (Fig. 1). Theoretical vibration frequencies and molecular structure of the complex were calculated by using the same method and basis set on the basis of optimized geometry. The structure and properties of complex [Cd(im)<sub>4</sub>Ni(μ-CN)<sub>4</sub>]<sub>n</sub> were experimentally determined in our previous study [1]. Afterwards, the regression equations and the correlation coefficients were calculated in order to demonstrate a well-matched relationship between experimental and theoretical vibration frequencies. These are following as  $y = 1.009x + 46.851$ ,  $R^2 = 0.9665$  for B3LYP and  $y = 1.0056x + 47.827$ ,  $R^2 = 0.966$  for B3PW91. Additionally, the large amount of the positive charge density is concentrated on the Cd(II) atom in both calculations (which is following as 0.63055 a.u for B3LYP and 0.6973 a.u for B3PW91). The large amount of the negative charge densities was gathered on nitrogen atoms (which is following of calculated as average: -0.7636 for B3LYP and -1.0414 for B3PW91 methods). Furthermore, electronic transition energies, HOMO and LUMO energy levels of the complex has been calculated in singlet and triplet state using by time depended density functional theory B3LYP and B3PW91 methods with LANL2DZ basis set. According to these calculations, the transition energy from HOMO-1 to LUMO+1 of the complex for TD-DFT/B3LYP and TD-DFT/B3PW91 methods was found as 0.0512 eV and 0.5011 eV in the singlet state, respectively (Fig. 2).

*This study was supported financially by Eskişehir Osmangazi University Research fund (Project No: BAP- 201519047).*

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**Keywords:** Imidazole complex, Tetracyanonickelate(II) complex, DFT-B3LYP, DFT-B3PW91, LANL2DZ.

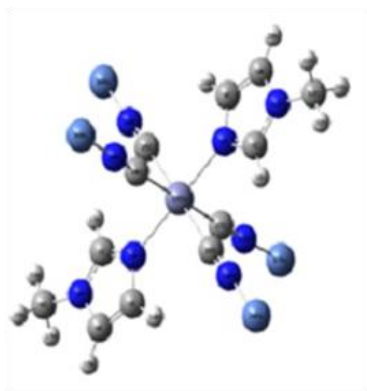


Fig. 1. Optimized molecular structure of the complex

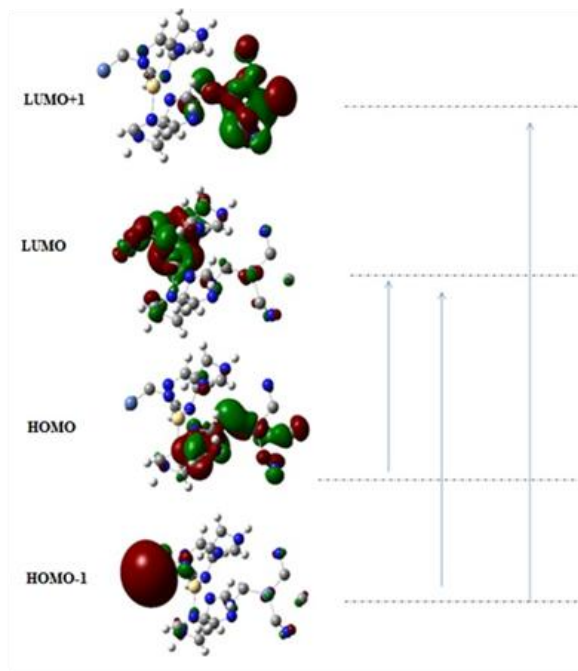


Fig. 2. Electronic transition states of the complex

P-158

**A COPPER-PALADIUM(II) CYANIDE COMPLEX CONTAINING N-METHYLIMIDAZOLE LIGAND: AN AGREEMENT BETWEEN THEORETICAL AND EXPERIMENTAL STUDIES:  $[\text{Cu}(\text{N-Meim})_2\text{Pd}(\text{CN})_4\text{H}_2\text{O}]_n$**

Güneş Süheyla Kürkcüoğlu<sup>1</sup>, Ilkan Kavlak<sup>2</sup>

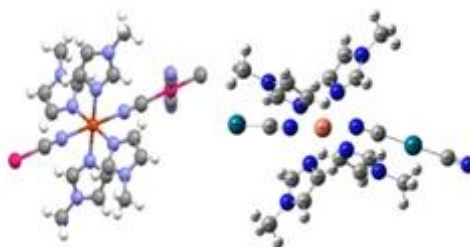
<sup>1</sup>Eskişehir Osmangazi University, Sciences and Arts Faculty, Physics Department, Eskişehir, Türkiye

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In this study,  $[\text{Cu}(\text{N-Meim})_2\text{Pd}(\text{CN})_4\text{H}_2\text{O}]_n$  was optimized using DFT-B3LYP and DFT-B3PW91 methods with LANL2DZ basis set on the ground state and gas phase (Fig. 1). Then, the vibration wavenumbers of the complex were theoretically calculated using the same methods. Theoretical wavenumbers of the complex were compared with experimental ones [1] (Fig. 2). Good agreement was obtained between the experimental and theoretical vibration wavenumbers. At the same time, the regression equations and correlation functions were calculated for the demonstration of observed agreement between the experimental and theoretical vibration frequencies, that is; these values are given for B3LYP and B3PW91 as  $y = 1.0601x - 47.747$ ;  $R^2 = 0.9938$  and  $y = 0.934x + 57.507$ ;  $R^2 = 0.9937$ , respectively. Additionally, electronic transition energies HOMO and LUMO of the complex were calculated by time-dependend density functional theory with B3LYP and B3PW91 methods with LANL2DZ basis set. The transition energies between the HOMO and LUMO levels of the complex were determined as 0.560 eV for B3LYP and 0.564 eV for B3PW91 (Fig. 3).

*(Acknowledgements: This study was supported financially by Eskişehir Osmangazi University Research fund (Project No: BAP- 201519047)*

**Keywords:** N-methylimidazole complex, Tetracyanopalladate(II), Copper(II) complex, DFT-B3LYP, DFT-B3PW91, LANL2DZ



**Fig. 1. Experimental and optimized geometries of the complex**



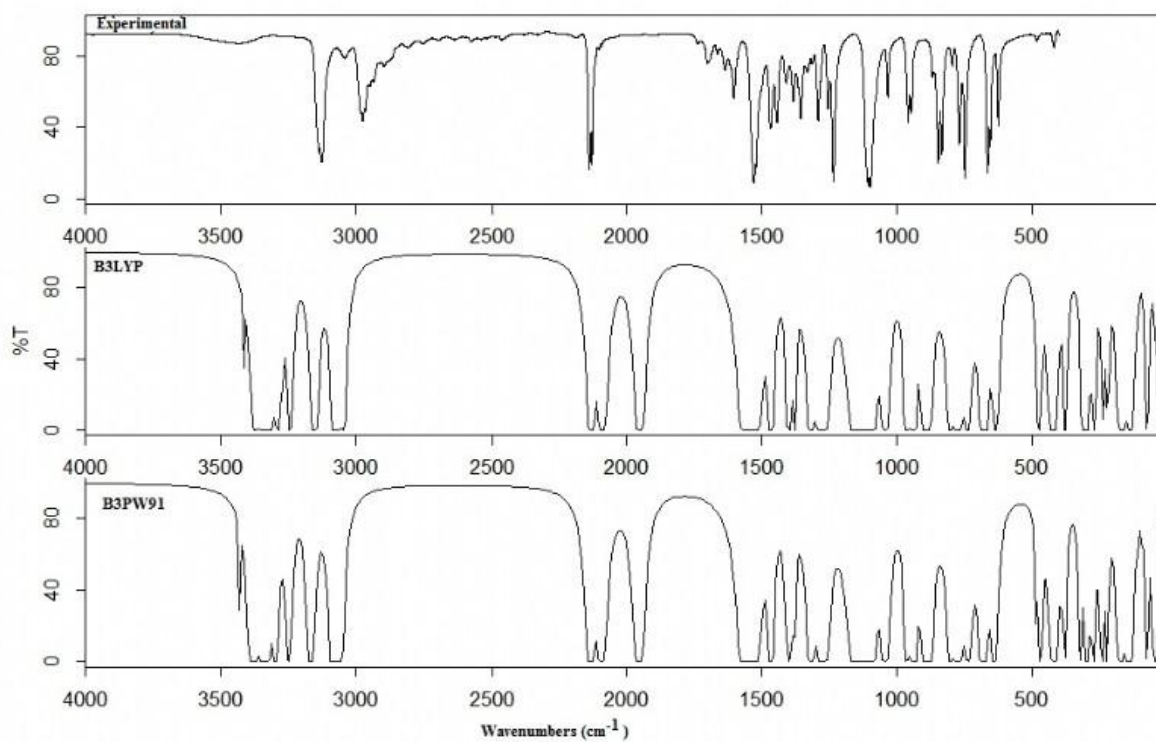


Fig. 2. FT-IR spectra

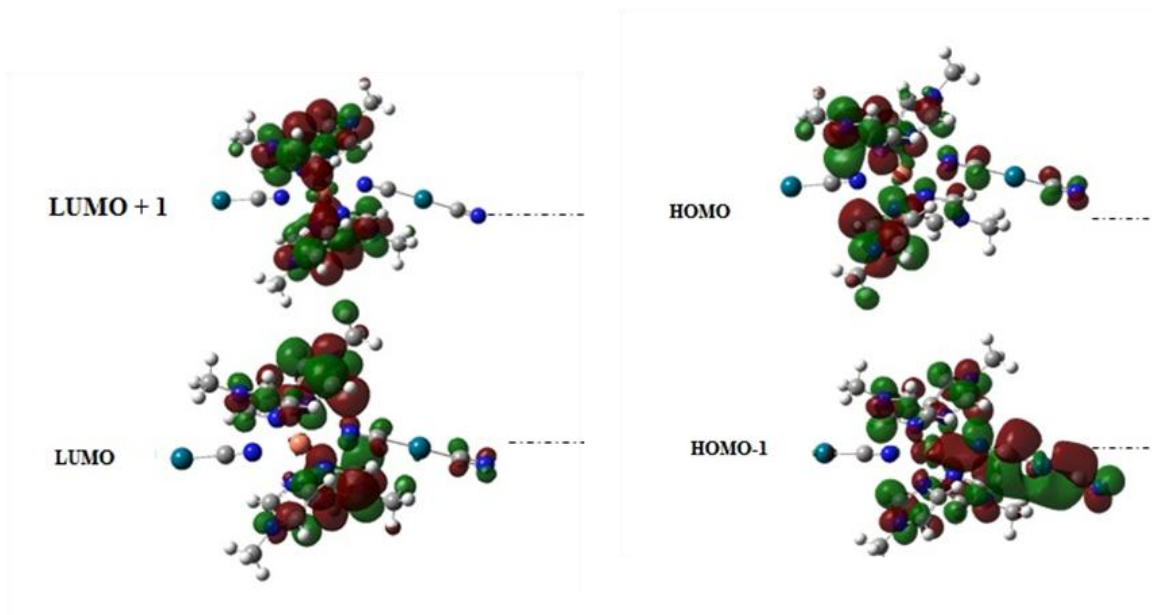


Fig. 3. HOMO-LUMO levels



P-159

## An Investigation of Substitution and Solvent Effects on Intramolecular Proton Transfer in Fluorophenyl Derivatives of (Z)-2,4-di-tert-butyl-6-(((phenyl)imino)methyl)phenol by Means of Spectroscopic Measurements and Quantum Chemistry Calculations

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Schiff bases exhibit unique properties which make them favorable for an array of applications such as liquid crystals, organic dyes, catalysts and intermediates in organic synthesis. They receive a special interest from chemists and physicist due to their rich photochromic and thermochromic properties, most of which are related to intramolecular proton transfer directly connected with the contained hydroxyl groups.

In this study, we investigated solvent effect on tautomeric behavior of the 2, 4, 2,4-difluoro and 2,5-difluoro substituted derivatives of (Z)-2,4-di-tert-butyl-6-(((phenyl)imino)methyl)phenol by using experimental Uv-Visible electronic absorption and fluorescence emission spectroscopy methods and DFT and TD-DFT calculations. The electronic absorption spectra of the compounds in different solvents namely methanol, chloroform and DMSO are similar, whereas their fluorescence emission spectra exhibit very different profiles in the different solvents. Results of quantum chemical calculations were used to rationalize why emission spectrum of the compounds are different in the different solvents.

**Keywords:** Intramolecular proton transfer, DFT, solvent effect, substitution effect, Schiff bases

P-160

Time Dependent DFT Study of UV-Visible Spectrum of Polyselenophene  
Molecular Segment as a H<sub>2</sub>O Sensor

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Conducting polymers can find applications in the production of sensors. They are sensitive to pH, certain inorganic ions and organic molecules as well as gas molecules[1]. Molecular and electronic structure of polymers used as gas sensor and their sensing mechanism can be elucidated by means of theoretical methods. In one of the studies[2], the sensitivity and selectivity of neutral and cationic pyrrole oligomers to NH<sub>3</sub>, CO<sub>2</sub> and CO have been investigated by DFT method.

Polyselenophene which has same skeleton as polypyrrole has been extensively studied in recent years [3]. In this study, the adsorption of H<sub>2</sub>O by -NH<sub>2</sub> and -NO<sub>2</sub> substituted and unsubstituted selenophene oligomers has been studied by DFT calculations to observe the sensing ability. B3LYP hybrid functional [4] with basis set 6-31G(d,p) has been employed for this purpose. All the calculations have been carried out by Gaussian 09 program package [5]. After optimization of the geometries (as seen in Fig.1) with BSSE correction, TDDFT calculations have been done to obtain UV-Visible spectrum. In addition to UV-Visible spectrum, binding energies, charge distributions, frontier molecular orbital energies have been calculated to see the effects upon adsorption of H<sub>2</sub>O. The structure with best sensing ability has been decided based on these results.

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**Keywords:** Sensor, polyselenophene, UV-visible spectrum, TDDFT

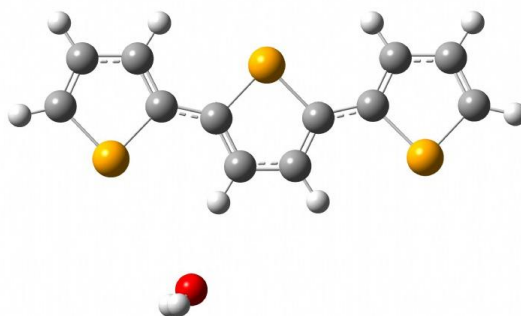


Fig. 1. Optimized geometry of selenophene trimer with H<sub>2</sub>O.

**P-161**

**Analytical solutions to the Kratzer potential in the presence of a constant magnetic field: non-relativistic neutral 2-body system**

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<sup>1</sup>*Department of Physics, Karadeniz Technical University, Trabzon, Turkey*

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Generalized Kratzer-type potential describing the molecular vibrations is important in studying the dynamical variables of diatomic molecules and usually used in applications on the molecular spectroscopies. This potential contains both a repulsive and a long-range attraction parts. The superposition of these parts produces an effective potential pocket and the form of this potential pocket is very important for the correct vibrational and rotational energy eigenvalues.

This study aims to investigate of two opposite non-relativistic charged particles, interacting with each other through the generalized Kratzer-type potential as a neutral system at rest; meaning that the center of mass momentum is zero, under the influence of uniform magnetic field perpendicular to the plane of motion.

We saw that the encountered differential equation is a quasi-exactly solvable, owing to the existence of a hidden  $sl_2$  algebraic structure and in order to solve this differential equation, we applied the power series method. The obtained relation between power series coefficients was a three-step recursion relation instead of the two-step recursion relations so often encountered in exactly solvable cases. It has been seen that the main effect of the magnetic field has revealed a new quantum condition on ro-vibrational energy states, which is required for ensuring normalizability of the wave function.

**Keywords:** Diatomic molecules, Kratzer potentials, Magnetic field, Schrödinger equation

P-162

**DFT Calculations of Hybrid Compound Based on Curcumin and Thalidomide  
for Multiple Myeloma**

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<sup>1</sup>*Department of Physics, Karadeniz Technical University, Trabzon, Turkey*

<sup>2</sup>*Department of Physics, Sakarya University, Sakarya, Turkey*

Cancer is a multifactorial disease that requires treatments able to target multiple intracellular components and signaling pathways. The natural compound, curcumin, was already described as a promising anticancer agent due to its multipotent properties and huge amount of molecular targets in vitro. Its translation to the clinic is, however, limited by its reduced solubility and bioavailability in patients. In order to overcome these pharmacokinetic deficits of curcumin, several strategies, such as the design of synthetic analogs, hybrid molecules have been developed. Compared to the combination of multiple drugs, hybrid molecules may provide certain advantages: (1) enhanced potency by self synergy within one molecule that may not be achievable by a traditional combination of separately dosed agents that may miss the ideal timing window; (2) reduced risk of developing drug resistance; and (3) improved pharmacokinetic properties and reduced toxic side effects compared to the administration of multiple agents. Hybrid molecule based on the structures of thalidomide and curcumin can be given an important example of these newly designed agents. (Thalidomide, an oral agent with antiangiogenic and immunomodulatory properties, is being investigated extensively in the management of advanced cancer). In this study, structural properties, physical properties such as charge distribution and spectroscopic properties; UV-Vis, IR spectrums of novel hybrid compounds of curcumin and thalidomide has been studied theoretically in order to understand structural-activity relationships. Theoretical investigations has been calculated using density functional theory (Gaussian09, Gauss view), utilizing the B3-LYP/ 6-311+G (d,p) basis set.

**Keywords:** Anti cancer agent, Curcumin hybrid, DFT calculations, Thalidomide

P-163

**Crystal structure, Hirshfeld surfaces and DFT computation of (E)-2-(((5-nitrothiophen-2-yl)methylene)amino)benzonitrile**

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In the present study, the structure of (E)-2-(((5-nitrothiophen-2-yl)methylene)amino) benzonitrile was investigated with experimental (X-ray diffraction method and FT-IR spectroscopy) and as well as theoretical (DFT) techniques point of view. In the crystal, 2D supramolecular structure throughout (202) plane is C-H...O type hydrogen bonds. The hydrogen bonds generate adjacent R21(7) and R33(14) ring motives (Fig. 1). Additionally, the Hirshfeld surface was drawn for visualizing the van der Waals distances and to determine the interaction sites. When 2D fingerprint plot are partitioned, H-O/O-H interactions are seen to be the most dominant interactions with percentage of 24.7. Subsequently, N-H/H-N interactions with 20.2% and H-H interactions with 14.7% come. The gas phase geometry optimization and vibrational frequencies calculations were analyzed by using density functional theory (DFT) incorporated in B3LYP with 6-311++(d,p) basis set. The detailed vibrational assignments were performed on the basis of the potential energy distributions (PED) of the vibrational modes. Additionally, HOMO-LUMO energy gap, natural bond orbital (NBO) analysis and nonlinear optical (NLO) properties of the compound were examined.

*This work was supported by the Ahi Evran University Scientific Research Projects Coordination Unit. Project Number: MMY.A3.16.003*

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**Keywords:** X-Ray Diffraction, DFT, Hirshfeld Surface, FT-IR

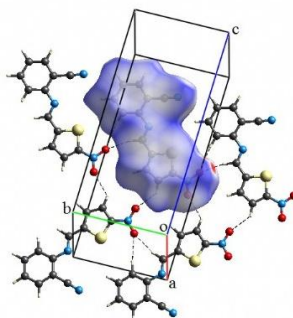


Fig. 1

P-164

Molecular Structure of 4-Amino-3-(thiophen-2-ylmethyl)-1H-1,2,4-triazole-5(4H)one Monohydrate

Hasan Tanak<sup>1</sup>, Meryem Evecen<sup>1</sup>, Levent Semiz<sup>2</sup>, Yasemin Ünver<sup>3</sup>

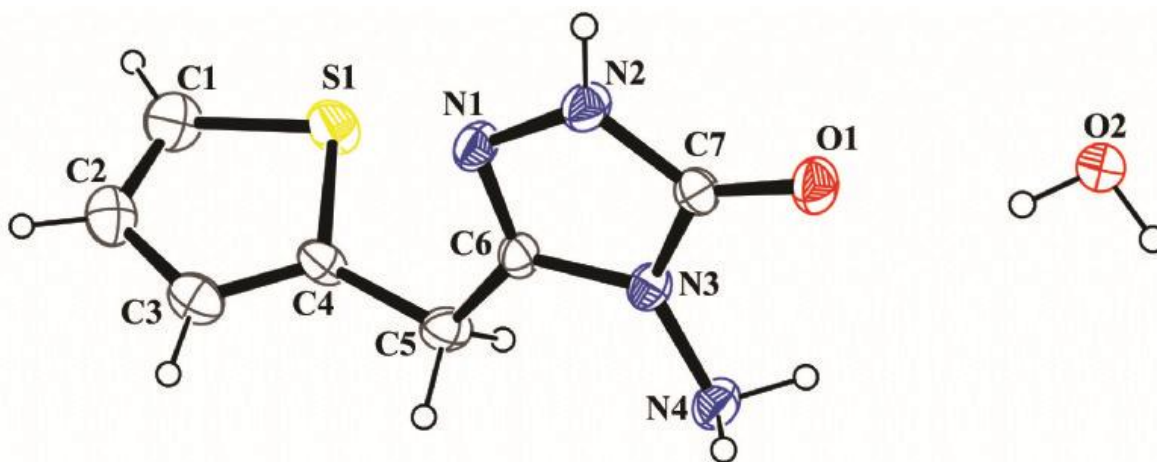
<sup>1</sup>Department of Physics, Faculty of Arts and Sciences, Amasya University, Amasya, Turkey

<sup>2</sup>Department of Chemistry and Chemical Process Technology, Vocational School of Technical Sciences, Amasya University, Amasya, Turkey

<sup>3</sup>Department of Chemistry, Faculty of Sciences, Karadeniz Technical University, Trabzon, Turkey

It has been reported in the literature that thiophene derivatives possess a broad spectrum of biological properties including antimicrobial, anticonvulsant, anti-inflammatory, anticonvulsant, antidepressant, antitumor, and antihistaminic activities. In order to investigate new organic compounds with biological activities, our group has synthesized a novel series of derivatives of 1,2,4-triazole. The molecular structure of the 4-amino-3-(thiophen-2-ylmethyl)-1H-1,2,4-triazole-5(4H)one monohydrate was determined by X-ray diffraction. The compound crystallizes in the monoclinic space group C2/c with Z = 4 in the unit cell (Fig. 1). The title compound is not planar. The dihedral angle between the thiophene and 1,2,4-triazole rings is 73.4(5) deg. In the crystal structure, molecules are connected by intermolecular N-H...O, N-H...N, O-H...O, and C-H...N type hydrogen bonds.

**Keywords:** Triazole, X-Ray, Crystal, Synthesis



An ORTEP-3 drawing of the title compound, with displacement ellipsoids drawn at the 30% probability level.

**P-165**

**Chelate Cross-Linked Affinity Ion-Imprinted Cryogel for Selective Recognition of Ce(III) in Environmental Samples and Determination of Ce(III) by ICP-OES**

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Extraction and preconcentration of rare-earth metals such as cerium have always been of interest over the past several decades, since they have been commonly used as microadditives in functional materials such as high-temperature superconductors, secondary batteries, magnetic, luminescence, and laser materials. Various techniques were proposed for extraction and preconcentration of rare-earth metals such as solvent extraction, precipitation, and ion-exchange chromatography. In recent years, several studies on removal of trace metal ions by Ion-imprinted polymers (IIPs) and Ion-Imprinted Cryogels were reported.

In this study, poly2-hydroxyethyl methacrylic acid- methacryloyl antipyrine [P (HEMA-co-MAAP)] cryogel was produced by free radical polymerization. Prepared this new cryogel was used for the Cerium(III) binding from aqueous solution. P(HEMA-co-MAAP) cryogel was characterized ultraviolet-visible-near infrared (UV-NIR), scanning electron microscopy (SEM), energy dispersive X-ray (EDX) and swelling tests. Effects of flow rate, medium pH, temperature and initial Cerium(III) concentration on the Cerium(III) binding were studied. Maximum binding capacity of the cryogel was found to be 37,00 mg/g cryogel at pH 6.0. Binding studies of Ce(III) in the presence of Nd(III) and La(III) ions were also carried out using Ce(III)-imprinted polymers. The ion-Imprinted Cryogel displayed high selectivity toward Ce(III) ions.

**Keywords:** Cerium(III), Cryogel, MAAP, Ion Imprinting

P-166

**An X-Ray Study for Structural Characterization of cis-Bis(methyl 2-(benzoyl carbamothioyl)-3-(4-chlorophenyl)-5-methyl-4,6-dioxo-1-phenyl-octahydropyrrolo[3,4-c] pyrrole-1- carboxylate)platinum(II)**

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<sup>2</sup>*Department of Chemistry, Faculty of Science, Atatürk University*

Transition metals are an important class of drug discovery studies due to the fact that many transition metal-based drugs have clinically used nowadays [1, 2]. The platinum-based complexes have a very important place in bioinorganic chemistry due to the effectiveness of platinum-containing drugs such as cisplatin used for treatment of many types of cancer [3]. In this study we performed structural characterization of cis-bis(methyl 2-(benzoyl carbamothioyl)-3-(4-chlorophenyl)-5-methyl-4,6-dioxo-1-phenyl-octahydropyrrolo[3,4] pyrrole-1- carboxylate)platinum(II) using X-ray spectroscopic method, one of the most useful molecular spectroscopic methods which are used to determine structure of the new compounds. The X-ray study show that Pt(II) ions created cis-complexes Pt(II) forming distorted square-planar structure in orthorhombic space groups Pnma. The square-planar geometry of the Pt(II) complex form via two sulfur and oxygen atoms and ligands bind to Pt(II) ion fully symmetric to each other. [4].

*We thank Mersin University (project grant BAP-SBE AKB (MG) 2012-8 YL) for financial support.*

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**Keywords:** N-Benzoylthiourea, Pt(II) Complex, X-Ray Study



P-167

NMR-QSAR Model of Some Imidazole Derivatives

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In general, imidazoles and azoles are important family of heterocyclic compounds with a broad interest due to their bioactive properties. Various imidazole derivatives have been reported with a broad range of bioactivities, such as antifungal, antiprotozoal, anti-inflammatory, antiallergic, antihistaminic, antiulcer, antihelminthic, analgesic, antihypertensive, antineoplastic activity and neuroleptic antipsychotic and thromboxane synthetase inhibitory activity. The aim of the present work is to investigate the relationships between the chemical shift of magnetic nuclei obtained from the 1H- and 13C-NMR spectral data and the activity of 2-[(4,5-dimethyl-1-(aryl-amino)-1H-imidazol-2-yl)thio]-1-(aryl)ethanone derivatives (Fig.1) for antibacterial, antifungal and anticancer activities. Geometry and electronic structures of the compounds were optimized in the gas phase by means of the hybrid DFT method at the B3LYP level of theory (Becke three-parameter hybrid correlation functional combined with Lee–Yang–Parr correlation functional) with 6-31G(d,p) basis set. Based on the optimized structures, 13C and 1H NMR shift analysis were carried out at B3LYP/6–311++G(d,p) level. All calculations were performed with Gaussian 09W (D.01) program package and GaussView 5.0.8 molecular visualization program. Finally, EViews statistical program was used for the analysis of data. The multiple linear regression procedure was used to create QSAR models. The obtained NMR-QSAR equations provide a rapid, reliable, and simple way for predicting the antibacterial, antifungal and anticancer activities of the imidazole derivatives.

**Keywords:** NMR, QSAR, Imidazoles, DFT

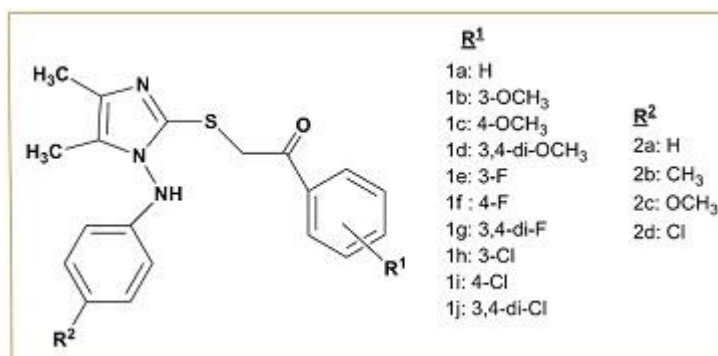


Fig. 1 Structures of the studied compounds

P-168

Quantum mechanical calculated reactivity and molecular docking features of difluoroanilines

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<sup>2</sup>Department of Electronics and Automation, Manisa Vocational School, Manisa Celal Bayar University, Manisa, Turkey

<sup>3</sup>Experimental Science Applications and Research Center, Celal Bayar University, Manisa, Turkey

This study presents a comprehensive investigation of active nature of difluoroanilines (DFA) (2,3-DFA, 2,4-DFA, 2,5-DFA, 2,6-DFA, 3,4,-DFA and 3,5-DFA) by using existing experimental spectroscopic data, and ab initio density functional theory calculations along with molecular docking and quantum structure activity relationship analysis. Reactive natures of DFAs were discussed within dependence on the positioning of fluorine elements i.e. their symmetry and closeness to each other. Essential quantum descriptors obtained for DFAs include electrostatic potential surface, electrophilicity and nucleophilicity from Fukui analysis, aromaticity indexes from nuclear independent chemical shift (NICS) analysis, dipole moment and polarizability tensors, and electronic properties like band gap and ionization potentials from population analysis. Molecular docking and interactional profiles for DFAs were explored on the basis of ligand enzyme interactions between DFAs and T4 Lysozyme Mutant L99A used in model binding site determination for docking calculations (Fig. 1). Docking energies and the type of interactions were visualized, and the variations in ligand-enzyme interactions were discussed depending on the effect of fluorine.

**Keywords:** Difluoroaniline, quantum mechanical calculated reactivity, molecular docking

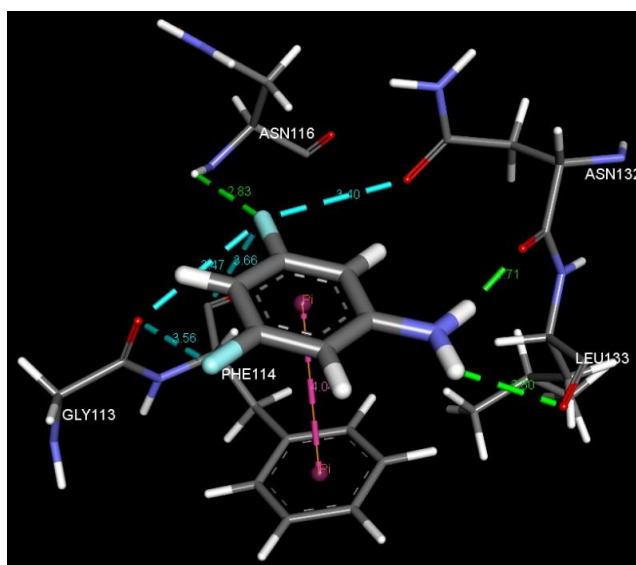


Fig. 1. Interaction profile of 3,5 PDA

**P-169**

**Theoretical evaluation of triazine derivatives as steel corrosion inhibitors:  
Monte Carlo simulation approach**

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Atomistic Monte Carlo simulations was performed on hexahydro-1,3,5-triphenyl-s-triazine (Inh1), hexahydro-1,3,5-p-tolyl-s-triazine (Inh2), hexahydro-1,3,5-p-methoxyphenyl-s-triazine (Inh3), hexahydro-1,3,5-p-aminophenyl-s-triazine (Inh4), hexahydro-1,3,5-p-nitrophenyl-s-triazine (Inh5) molecules in order to study their reactivity and adsorption behaviour towards steel corrosion. Monte Carlo simulations were applied to search for the most stable configuration for the adsorption of the inhibitor molecules on Fe(110) surface both in vacuum and in aqueous solution. The investigated molecules exhibited strong interactions with iron surface. In aqueous solution all the investigated molecules displaced water molecules and were strongly attracted to the Fe surface as evident in their large negative adsorption energies compared to that in vacuum. the adsorption strength from the outputs of Monte Carlo simulations of the studied molecules on Fe(110) surface in vacuum and in the presence of water follow the trend: Inh4>Inh3 >Inh2 >Inh1 >Inh5. The theoretical data obtained are in good agreement with the experimental inhibition efficiency results earlier reported

**Keywords:** Steel, Modelling studies, Acid inhibition, Triazine

P-170

**Synthesis and spectroscopic studies of substituted  
5,6,7,8-tetrahydroquinazolin-2-amine compounds via one-pot method**

F. Tülay Tugcu, Kadir Turhan

*Department of Chemistry, Yildiz Technical University, İstanbul, Turkey*

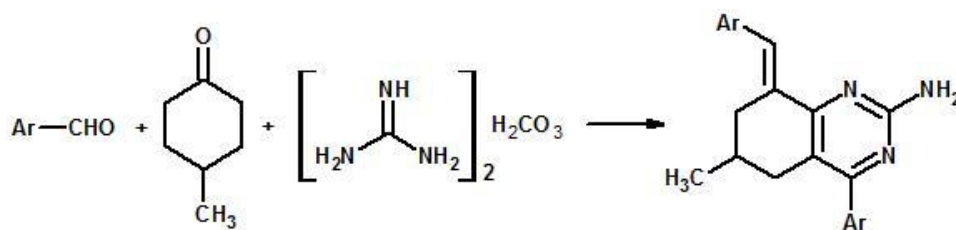
Quinazolines are considered to be an important chemical synthon of various physiological significance and pharmaceutical utility. They possess variety of biological effects including antihypertensive, antimicrobial, antihyperlipidemic, anti-inflammatory and anticonvulsant activities. Moreover, many quinazolines have an important place in the area of heterocyclic compounds because of their presence in the structures of macrocyclic complex drugs, their applications in industry and usage in pharmaceutical researches due to their biological properties [1,2].

Therefore, in this study, some new substituted quinazoline derivatives which are considered that may possess biological activity have been obtained via one-pot multicomponent method by using hetaryl carboxaldehydes, guanidine carbonate and 4-methylcyclohexanone (Fig. 1); and structures of all the synthesized compounds have been determined and characterized by ultraviolet, infrared, nuclear magnetic resonance, mass spectral data.

*Thanks for Yildiz Technical University Scientific Research Projects Coordination's support in this study. Project No: 2012-01-02-GEPO5.*

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**Keywords:** Quinazoline derivatives; one-pot method, nitrogen-containing heterocycles, guanidine carbonate, spectroscopic analysis.



Ar= Thiophen-2-ly, 3-methylthiophen-2-ly, 5-methylthiophen-2-ly

Fig. 1. Synthesis of substituted 5,6,7,8-tetrahydroquinazolin-2-amine compounds

P-171

**Synthesis and spectroscopic studies of substituted  
6,7-dihydrocyclopentapyrimidin-2-amine compounds via one-pot method**

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*Department of Chemistry, Yildiz Technical University, İstanbul, Turkey*

Pyrimidine derivatives as the nitrogen-containing heterocycles, continue to attract considerable attention because of their great practical usefulness, primarily due to very wide spectrum of biological activities such as antimicrobial, anti-inflammatory, antihypertensive, antihyperlipidemic, analgesic, anticancer, antihelminthic, antioxidant, herbicidal and anticonvulsant properties. They have an important place in the area of heterocyclic compounds because of their presence in the structures of macrocyclic complex drugs, their applications in industry and usage in pharmaceutical researches due to their biological properties [1,2].

In this study, some new substituted pyrimidine derivatives which are considered that may possess biological activity have been obtained via one-pot three-component reactions. These reactions, which are carried out using the method of multicomponent reactions (MCRs), proceed as domino processes, making them easier to occur than the conventional multistep organic reactions. This method enables new organic molecules to be synthesized in a single step, using a minimal amount of time and number of trials.

The study consists of one steps. Cyclocondensation of each of the previously substituted cyclic ketones with hetaryl carboxaldehydes and guanidine was achieved by the technique of one-pot multicomponent reaction; and structures of all the synthesized compounds have been determined and characterized by ultraviolet, infrared, nuclear magnetic resonance, mass spectral data.

*Thanks for Yildiz Technical University Scientific Research Projects Coordination's support in this study.  
Project No: 2012-01-02-GEP05.*

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**Keywords:** Pyrimidine derivatives; one-pot method, nitrogen-containing heterocycles, guanidine carbonate, spectroscopic analysis.

P-172

**Application of Fluorescence Intercalator Displacement (FID) Method for Determination of G-quadruplex DNA Binding Selectivity of Water Soluble PIP and HPIP Analogs**

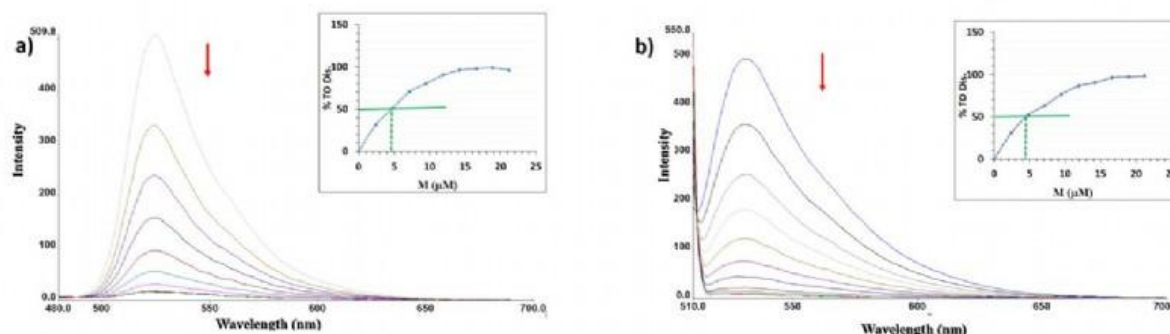
Ufuk Yildiz, Burak Çoban

*Bülent Ecevit University, Faculty of Science, Department of Chemistry, Zonguldak, TURKEY*

To further clarify the nature of the interaction between the compounds and q-DNA and ds-DNA FID was carried out. FID is a simple and fast method to evaluate the affinity of a compound for q-DNA. This assay is based on the loss of fluorescence of thiazole orange (TO) upon competitive displacement from DNA by a putative ligand. Upon interaction with q-DNA, TO exhibits high affinity and displays a significant increase in its fluorescence, whereas when free in solution, the fluorescence is quenched. Therefore, displacement of TO by another molecule provides an approximate measure of the affinity of the given compound for duplex and q-DNA by evaluating the DC50 which corresponds to the required concentration of complex to induce a 50% fluorescence decrease.

The emission spectra of TO bound to ds-DNA and q-DNA in the absence and presence of water soluble PIP are shown in Fig. 1. It can be seen that the addition of PIP to DNA pretreated TO causes appreciable reduction in the emission intensity.

**Keywords:** DNA selectivity, g-quadruplex DNA, FID assay



**Fig. 1. Fluorescence spectra of a) TO (2  $\mu$ M) with ds-DNA (15  $\mu$ M) and b) TO (2  $\mu$ M) with q-DNA (1  $\mu$ M) with increasing amounts of water soluble PIP**

**P-173**

**EPR Investigation of Heating Process on Carob**

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Carob is a traditional food in the Mediterranean region. It has been used in food industry as additive or as coating material and in pharmaceutical industry for drug delivery purposes. Carob with its high content of phenolic compounds has important antioxidant properties. Previous studies have shown an increase in the antioxidant activity of carob powder depending on roasting time and temperature [1, 2]. In the present study, preliminary results of heating process on carob were given. Whole carob flour, carob seeds and pods roasted in the range of 60 °C- 120 °C using various time intervals. Time dependent changes were followed in the EPR spectra. The changes in the peak heights were smooth in 60 °C-100°C region and after that, a sharp increase was observed. The shape of the spectrum has also changed with temperature.

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**Keywords:** EPR, antioxidant, carob

P-174

**ESR dating of fossil mollusc shells from Sarıcalar, Konya Closed Basin (Turkey)**

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The age of nine fossil shells from the Sarıcalar district of Konya closed basin Turkey, is determined by the Electron Spin resonance (ESR) method. All fossil shells samples were collected systematically from four different geological splittings in Sarıcalar district. After physical and chemical sample preparation procedures, the powder form of fossil shells were irradiated in the gamma dose range of 10-1100 Gy. Accumulated doses (DE) of the fossil samples were determined by using the dose response curves of stable isotropic CO<sub>2</sub><sup>-</sup> radical signals ( $g=2.0007$ ). The ESR signal growth curves of fossil shells on additional gamma irradiation have been best fitted by a single exponential saturation functions. Based on this model, the accumulated doses (DE) of L1A3SK, L1A5K, L1B5KS, L1B6KS, L1B7KS, L1C2KS, L1C3KS, L1C4KS and L1D1KS fossil samples were determined as 236.5±38, 224.9±46, 205.1±29, 173.4±20, 143.8±15, 45.68±3, 42.9±3.41, 65.67±5 and 96.28±9 Gy, respectively. ICP-MS technique has been used to determine the annual dose rates (D) of each fossil sample by using the amount of natural radioactive elements in the shell and surrounding sediments samples. The ESR ages of the fossil samples are consistent with the estimated ages from stratigraphic and paleontological expectations.

*Acknowledgement: This work was supported by TUBITAK 114Y237 Research Project.*

**Keywords:** ESR dating, Konya basin, Sarıcalar, CO<sub>2</sub><sup>-</sup> radical, irradiation



P-175

A new phenolic sulfate ester from the aerial parts of *Tamarix balansae* J. Gay

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The n-BuOH soluble fraction of the MeOH (80%) extract of dried aerial parts of *Tamarix balansae* J. Gay, (Tamaricaceae), collected in Algerian Sahara, was fractionated and purified by combination of chromatographic methods (VLC, CC, flash chromatography, HPLC) to obtain a new phenolic sulfate (1) and nine known compounds (2-10) (Fig. 1). Structures elucidation was performed by comprehensive 1D and 2D NMR analyses, mass spectrometry and by comparison with literature data. The new compound (1) was obtained as a white amorphous powder. The positive ESI-MS spectrum showed an  $[M+Na]^+$  ion at  $m/z$  339, compatible with the molecular formula of  $C_9H_9O_8SK$ . The UV spectrum revealed an absorption band at 276 nm (MeOH). In the IR spectrum, in addition to the obvious evidence for a hydroxyl ( $3324\text{ cm}^{-1}$ , carbonyl ( $1708\text{ cm}^{-1}$ ) and aromatic ring ( $1600-1517\text{ cm}^{-1}$ ), the strong absorption at  $1232$  and  $1094\text{ cm}^{-1}$  was indicative of the presence of a  $-O-SO_3^-$  group. The presence of the sulfate group was confirmed by precipitation with  $BaCl_2$ , after acid hydrolysis of 1.

**Keywords:** *Tamarix balansae*, Tamaricaceae, flavonoids; 1D and 2D NMR analyses

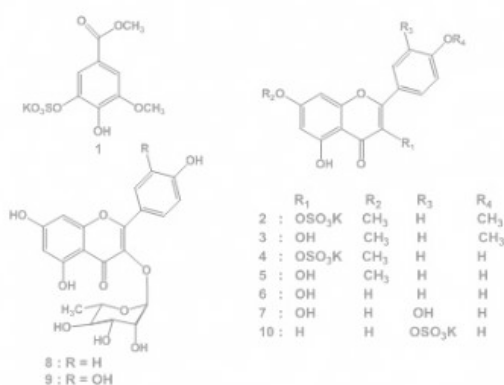


Fig. 1. Chemical structures of compounds 1-10 isolated from *Tamarix balansae*

P-176

A new sulfonlated flavonoid and other compounds isolated from the aerial parts of *Cotula anthemoides* L

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The n-BuOH extract of the aerial parts of *C. anthemoides* L., collected from Algerian Sahara, was separated by combined chromatographic methods (CLC, CC, Flash chromatography, HPLC) to obtain a new sulfonyl flavonol glucoside (1) (Fig. 1), in addition to twelve known compounds (2-13). Structures elucidation was performed by comprehensive 1D and 2D NMR analyses, mass spectrometry and by comparison with literature data. The positive HR-ESI-MS of 1 showed a molecular ion peak  $m/z$  681.0744  $[M+Na]^+$  enabling to determine the molecular formula  $C_{26}H_{28}O_{15}S$ .

**Keywords:** *Cotula anthemoides*, Asteraceae, flavonoids, 1D and 2D NMR analyses

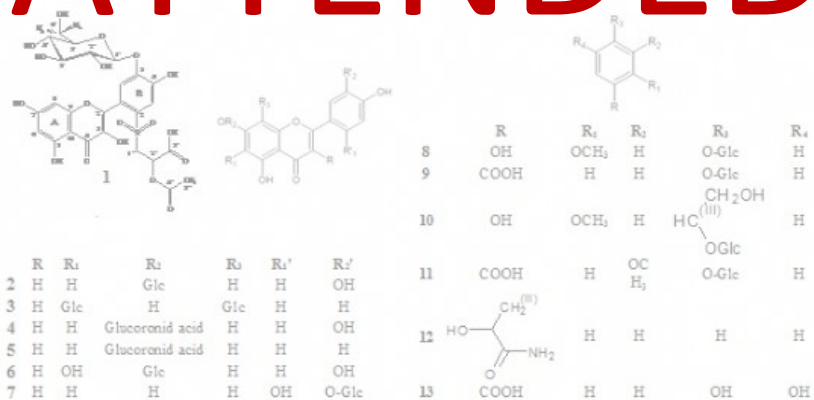


Fig. 1. Chemical structures of compounds 1-13 isolated from *anthemoides* L.

P-177

## Phenolic Profile and Antiproliferative Activity of *Carduncellus helenioides* (Asteraceae) Extracts

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<sup>6</sup>Varenbimol, Chemistry Department, University of Constantine1, 25000, Constantine, Algeria

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This study aimed to quantify phenolic compounds in ethyl acetate and n-butanol extract of *Carduncellus helenioides* (Asteraceae) leaves and flowers; compare the antiproliferative activity of their extracts, identification and quantification of their phenolic acids and their flavonoids. HPLC-TOF/MS analyses were carried out to identify and quantify a lot of compounds. In butanolic extract a total of 12 compounds corresponding to phenolic acids and the flavonoid family were identified from *Carduncellus helenioides* in only 18 min. The phenolic profile showed the presence of nine phenolic acid derivatives (Gallic acid, Gentisic acid, Chlorogenic acid, 4-hydroxybenzoic acid, caffeic acid, vanillic acid, p-coumaric acid, Ferulic acid and Salicylic acid), and three flavonoids (Rutin, quercetin and apigenin-7-O-glucoside).

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In ethyl acetate extract, the HPLC-TOF/MS analysis reveals the presence of 4-hydroxybenzoic acid, gentisic acid, chlorogenic acid, caffeic acid, vanillic acid, p-Coumaric acid, ferulic acid, salicylic acid, Quercetin-3- $\beta$ -D-glucoside, Apigetrin and protocatechuic acid. The ethyl acetate extract and the n-butanol extract have moderate anti-cancer activity compared to 5-FU.

**Keywords:** *Carduncellus helenioides*, phenolic acids, HPLC-TOF/MS, Antiproliferative activity

**P-178**

**Determination of essential and toxic microelements in the bran and wheat flour grown in Southeastern of Turkey by ICP-OES**

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The study involves the analysis of Ca, K, Mg, Fe, Zn, Mn, Si, Sn, Cu, Cr, Cd, Ni, V, Pb, As and Se in wheat flour and its bran separated after milling process. Two types of wheat have registered by GAP International Agricultural Research and Training Center. Analysis were carried out by ICP-OES following digestion in a closed-vessel microwave system. Hydride system of ICP-OES was employed for the determination of As and Se. A standard reference material GBW-10010 (wheat) was used to verify the accuracy and validity of the studied method. The results were in good agreement with the certified values [1-3]. The study indicated that the Ca, Fe, Zn, Mn, Ni, Cd, Cu, Sn, Pb, V and Se values in bran were higher than those in flour while there was no significant difference in two resources with regard to also Mg, K and Cr contents. In conclusion, analysis indicated that microelement contents in the samples of bran and flour were within acceptable levels suggested by Turkish standard and FAO/WHO and therefore the wheat with specific registration is not harmful for public health with regard to its toxic metal contents.

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**Keywords:** Wheat flour, bran, ICP-OES

**P-179**

**Determination of Multielement in the Grains Grown Around Karacadağ and Tigris River of Southeastern Turkey by ICP-OES**

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Both cultivation and consumption of local rice, lentil, chickpea, bread wheat and barley are very high in the South-eastern Anatolia of Turkey. This study aims to determine of trace elements such as K, Na, Ca, Mg, Zn, Fe, Cu, Cd, Pb, Cr, As, Se, V, Sn, Mn, Si and Ni in grains by ICP-OES following the sample digestion in a closed-vessel microwave system. Hydride system of ICP-OES method for the determination of As and Se were used. A certified reference material was used to verify the accuracy of the method [1-3]. The results obtained are in agreement with the certified values. The analysis of element show that Ca, Mg and K values in the rice were found to be lower than the lentil, chickpea, wheat and barley which for Lentil and chickpea were found to be higher than those. The concentration of toxic element such as Pb in the barley and chickpea was found to be higher than the lentil, wheat and rice while the As concentration was found to be blow of the detection limits of ICP-OES. The mineral nutrient ranges in grains did not exceed the dietary reference intake suggested by the Turkish standard and FAO/WHO. The results show that local rice, lentil, chickpea, wheat and barley are safe for human consumption by these are highly nutritional and very low toxic metal values.

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**Keywords:** Grains, ICP-OES, Microwave

**P-180**

**Removal of Hg(II) from aqueous solution by *Bacillus subtilis* ATCC 6051(B1) biomass**

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Hg (II) has been as one of the most toxic metals on health hazards. The biosorption of heavy metals from aqueous solution by biomass is effective as an alternative method in recent years[1-3]. Therefore, the biosorption of Hg(II) from aqueous solutions using *Bacillus subtilis* ATCC 6051(B1) biomass was investigated in this study. For the analysis of Hg (II) were studied by using ICP-MS. The adsorbent was characterized by FTIR. Various factors including solution pH, initial concentration of Hg(II), contact time and reaction temperature were taken into account and promising results were obtained. An initial solution with pH of 4.5 was most favourable for Hg(II) removal. The kinetic data was also analysed using pseudo first order and pseudo second order equations. The results suggested that Hg(II) bioadsorption was best represented by the pseudo second order equation. Freundlich and Langmuir isotherms for the present data were analysed. The most satisfactory interpretation for the equilibrium data at different temperatures was given by the Langmuir isotherm. In present study also was investigated some thermodynamic parameters. While  $\Delta H_o$  and  $\Delta S_o$  was obtained as 76.01 kJ/mol and 239,11 kJ/mol respectively,  $\Delta G_o$  had a low value (4.76 kJ/mol). This study demonstrated that *Bacillus subtilis* having low cost can be used as a effective biosorbent for Hg(II) removal from aqueous solutions.

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**Keywords:** Biosorbent, FTIR, Hg(II)

P-181

**Preparation and Application of Surface Plasmon Resonance Sensors Based on Molecularly Imprinted for Detection of Pesticide in Green Pepper**

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Pesticides have been widely used in many fields such as agricultural products control. Although these substances contribute to increasing of agricultural products, they have also many negative effects on the health due to contamination. Thus, detecting pesticides will have a great impact on their management, as well as improve their toxicity effects over humans [1]. Molecularly imprinted polymers (MIPs) involve specific recognition sites in polymeric materials fabricated via the polymerization of the functional monomers and cross linkers in the presence of a template molecule with subsequent extraction of the template molecule [2]. Surface plasmon resonance (SPR) biosensors are used to characterize and quantify biomolecular interactions. Real-time and fast measurement, high sensitivity and specificity, no need of labeled reagents are the unique properties of SPR biosensors. SPR biosensors have been used for detection of several analytes. Recently, molecular imprinting technology is used for creation of biorecognition surfaces on the SPR biosensors [3]. Here, we fabricate molecularly imprinted polymers nanofilms and integrate with surface plasmon resonance (SPR) sensors for sensitive, selective, fast and real-time detection of amitrole. The molecularly imprinted nanofilms onto the SPR gold surface are prepared via UV polymerization reactions, which consist of N-methacryloyl-L-tryptophan methyl ester (MATrp) as a functional monomer and ethylene glycol dimethacrylate (EGDMA) as a cross-linker. The surface morphology of nanofilm prepared on the sensor surface was determined by ATR-FTIR, contact angle measurements, ellipsometer and atomic force microscopy (AFM). The concentrations applied to the sensor were optimized by varying in the range 0.06-11.9 nM, as well as denote a limit of detection (LOD) values of 0.037 nM. Furthermore, we were performed that the selectivity studies made with dinoseb and benzotriazole which are similar structure to amitrole. Green pepper was used as a sample and detected 0.684 nM amitrole in SPR sensor. The results show that amitrole imprinted SPR sensors have been found to be high selective, sensitive and accuracy to determine amitrole in both aqueous solutions and natural source.

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*This study was supported by the TUBITAK Project number: 115Z126.*

**Keywords:** Molecularly imprinting, SPR sensor, pesticide, amitrole



P-182

Synthesis, Crystal Structures, Spectral FT-IR, NMR and UV-Vis Investigations and Theoretical Studies of N-phenyl-2-imino-5-methylthiophene and N-(4-chlorophenyl)-2-imino-5-methylthiophene

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Two new thiophene derivatives, have been synthesized and characterized by FT-IR, <sup>1</sup>H and <sup>13</sup>C NMR and UV-Vis spectroscopy. Crystal structure of the compounds were determined by single crystal X-ray diffraction method. The data were collected and integrated using Oxford Diffraction CrysAlisPro software[1]. Utilizing OLEX2[2], structures were solved by direct methods in SHELXT[3] and refined by full-matrix least-squares on F2 in SHELXL[4]. Crystal structures are stabilized by mainly van der Waals forces in addition to the pi···ring stacking interactions. The molecular geometries, vibrational frequencies, chemical shifts, frontier molecular orbitals (Fig. 1), Mulliken charges and molecular electrostatic potentials have been calculated for both compounds using the Density Functional Theory (DFT) method. Comparing with the experimental data, it was seen that the theoretical results support the experimental parameters.

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**Keywords:** Crystal structure, DFT calculations, FT-IR, Thiophene derivatives, UV-Vis.

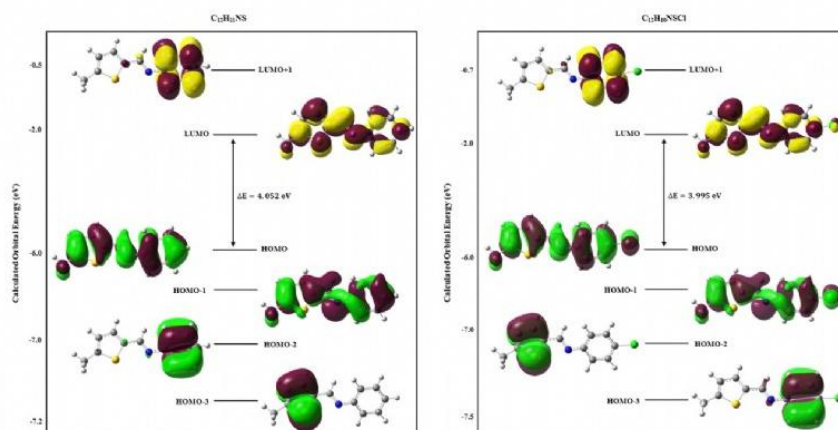


Fig. 1. Molecular orbital surfaces and energy levels



P-183

## Electrochemical Determination of Rivastigmine Hydrogen Tartrate in Pharmaceutical Samples at $\beta$ -Cyclodextrine/Multi-walled Carbon Nanotubes Modified Electrode

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Rivastigmine hydrogen tartrate is a drug used to treat Alzheimer's disease, which is a progressive, degenerative brain disorder that affects reason, judgment and memory. Over a period, people with Alzheimer's disease lose their ability to think and reason clearly, judge situations, solve problems, concentrate, remember useful information, take care of themselves, and even speak. People with mild Alzheimer's disease usually require close supervision and help with everyday tasks; and those with severe disease can do little on their own and require complete full-time care. Alzheimer's disease severely impacts the quality of life of the patient, their family and caregivers.

A glassy carbon electrode modified with  $\beta$ -cyclodextrine ( $\beta$ -CD) and multi-walled carbon nano tubes (MWCNTs) was fabricated and applied to the determination of rivastigmine hydrogen tartrate (RIV) in pharmaceutical preparation. The electrochemical feature of RIV hydrogen tartrate at the modified electrode was investigated using cyclic voltammetry and square wave voltammetry. Characterization of the functionalized electrode was realized with electrochemical impedance spectroscopy and scanning electron microscopy. The calibration curve was linear from 10 to 1500  $\mu$ M and the detection limit was obtained as 2.0  $\mu$ M (S/N=3). The results showed that this electrochemical sensor has good sensitivity and selectivity. Finally, the proposed sensor was applied for determination of RIV hydrogen tartrate in commercially available drug samples with good recoveries.

**Keywords:** Rivastigmine, voltammetry, carbon nanotubes, pharmaceutical

P-184

## High-Resolution Infrared Spectroscopy of Field Red Horizontal Branch Stars

Melike Afşar<sup>1</sup>, Christopher Sneden<sup>2</sup>, Zeynep Bozkurt<sup>1</sup>, Gamze Böcek Topcu<sup>1</sup>, Gregory N. Mace<sup>2</sup>,  
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We obtained the surface abundances of more than 20 elements from H- and K-band observations of three Red Horizontal Branch (RHB) stars. High-resolution ( $R = 45,000$ ) infrared spectra were obtained using IGRINS (the Immersion Grating Infrared Spectrograph) on the 2.7m Smith telescope at McDonald Observatory. IGRINS has the capacity of making simultaneous observations with a wavelength coverage of essentially the entire H- and K-bands (1.5 to 2.4 microns). High S/N ( $>200$ ) IGRINS data serve as a laboratory of molecular bands. A large number of OH, CO and CN molecular bands provided us invaluable information on the abundances of C, N and O, which can be altered as stars evolve from birth to death. OH bands confirmed and greatly strengthened the oxygen abundances previously measured from visible [O I] lines. Carbon and nitrogen abundances were determined from CO and CN molecular bands, respectively. IGRINS also made it possible to achieve more robust abundances of light elements such as Na, Mg, Al, and Si than obtained from their visible counterparts, and allowed S, P and K abundance determination mostly for the first time. Most importantly, we were able to detect  $^{12}\text{C}/^{13}\text{C}$  isotopic ratios from the CO (2-0) and CO (3-1) band-heads present in the K-band, which give us important clues about the evolutionary status of the stars and mixing processes that take place in the interiors of these RHB He core-burning stars.

**Keywords:** Stellar evolution, RHB stars, chemical abundances, molecular bands

P-185

## Synthesis and Evaluation of Antioxidant Activity of Some Pyrimidine compounds

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Pyrimidine compounds were synthesized and evaluated in vitro antioxidant activity. Their antioxidant properties were investigated by various assays including DPPH• (2, 2-diphenyl-1-picrylhydrazyl), ABTS•+ (2,2-azinobis-(3-ethylbenzthiazoline-6-sulphonate) radical scavenging assay, PhNHNH<sub>2</sub> (phenyl hydrazine) induced haemolysis of erythrocytes and metal chelating activities and compared to synthetic antioxidants, such as α-tocopherol and trolox. In this study results demonstrated that pyrimidine compounds 2-thioxopyrimidine (1), pyrimido [3, 2-a]thiazole (2), pyrimido [3,2-a] thiazole (3), [2,1-b] [1,3] thiazin- 4(6H)-one (4) and malonate (5) exhibit a remarkable DPPH• assay, ABTS•+ assay, metal chelating effect assay and PhNHNH<sub>2</sub> (phenyl hydrazine) induced haemolysis of erythrocytes. Compound 4 and 5 showed superior activity over other molecules in DPPH• and ABTS•+. 1,1-diphenyl-2-picryl-hydrazyl (DPPH•) scavenging activities was found to be in the order of α-tocopherol>trolox> 5 >4 >3>1>2. ABTS•+ (2,2-azinobis-(3-ethylbenzthiazoline-6-sulphonate) scavenging activities of pyrimidine compounds was found to be in the order of α-tocopherol>trolox>5> 4 >3>1>2. The metal chelating effect assay indicating 5 better free radical scavenging capacity. The metal chelating effect was found to be in the order of α-tocopherol>5> trolox>4>3>1>2. Compounds 4 and 1 inhibited phenyl hydrazine induced haemolysis of erythrocytes revealing their ability to scavenge most of the free radicals generated. The phenyl hydrazine induced haemolysis of erythrocytes was found to be in the order of trolox>4>1> α-tocopherol >5>3>2. Consequently, compounds 1, 4 and 5 have exhibited scavenging activity ability to act as standard antioxidants.

**Keywords:** Pyrimidine, Antioxidant Activity DPPH, ABTS, PhNHNH<sub>2</sub>, metal chelating activities

P-186

## Synthesis, characterization of polymer-graft-calixarene molecules in different structures and interactions with volatile organic compounds

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Calixarenes that are cavity-containing macrocyclic molecules are very suitable materials for sensor applications with their excellent sorption capabilities and stable structures. The hollow bowl-shaped structure which formed by the aromatic rings has the ability to trap ions or molecules in the environment.[1] If appropriately functionalized, calixarenes may act as a gas sensor for volatile organic compounds (VOCs) because of their potential for forming host-guest complexes.[2]

This study aims to investigate the ability of pvc-g-calixarenes to capture, detect and select VOCs such as toluene, chloroform and acetone in nanograms for surface acoustic wave (SAW)-based gas sensors, therefore a computer controlled gas flow and gas mixture system has been used. For this purpose, we have prepared and characterized polymer-graft-calixarenes which are obtained by click reaction with alkyne functionalized calixarenes and the polymer chain containing the azide end group. These compounds have been investigated in their chemical sensing properties against VOCs using SAW transducers as a sensitive film. The sensing layer material has been coated on the SAW at different thicknesses to determine how the electrical and sensor properties change depending on the film thickness. The responses to six different VOCs in dry and humid air have been studied. The compounds were found to exhibit excellent sensing properties against some VOCs. The host-guest interactions of all coated compounds on SAW will be investigate in detail.

[1] V. I. Kalchenko, et al. "Calixarene-based QCM sensors array and its response to volatile organic vapours." Materials Science 20.3, 2002, 73-88.

[2] L. J. Bauer, and C. D. Gutsche. "Calixarenes. 15. The formation of complexes of calixarenes with neutral organic molecules in solution." Journal of the American Chemical Society 107.21, 1985, 6063-6069.

**Keywords:** Calixarene, SAW sensor, VOC

P-187

**Spectroscopic Details of the Synthesized Novel Benzofuran compound with Experimental and Quantum Chemical Studies: F-TIR, <sup>1</sup>HNMR, <sup>13</sup>CNMR and DFT**

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Benzofuran is considered as an important class of heterocyclic compounds. The benzofuran ring system, although by no means as common as indole, is incorporated into many natural products and into synthetic pharmaceuticals and polymers [1]. Several derivatives of benzofurans have been recognized as biologically and pharmacologically relevant molecules[2]. Moreover benzofurans occur in a great number of natural products [3].

In the present study, the novel benzofuran compound, 1-(3-Aminobenzofuran-2-il)etanon, had been synthesized and its structure was determined by the use of elemental analysis, IR and <sup>1</sup>H-NMR, <sup>13</sup>C-NMR spectroscopy, single-crystal X-ray diffraction techniques and DFT/B3LYP level with 6-311G (d, p) basis set. The calculated molecular geometrical parameters, IR frequencies, <sup>1</sup>H and <sup>13</sup>C NMR chemical shift values are compared and seen in good agreement with experimental XRD, IR (Fig. 1) and NMR chemical shift values. In addition the title compound (C<sub>14</sub>H<sub>13</sub>NO<sub>3</sub>) crystallizes in the monoclinic space group P21/c with a=11,6442(5) Å, b=15,5404(9) Å, c=8,0269(4) Å, β=102.95(3)°, V=1445,83(12) Å<sup>3</sup>, D<sub>calc</sub>=1,279 g/cm<sup>3</sup>, Z=4.

[1] H. Khanam, Shamsuzzaman, 2015, European Journal of Medicinal Chemistry, 97, 483-504.

[2] T.L. Gilchrist, 1985, Heterocyclic Chemistry, 174.

[3] M. Kamal, A.K. Shakya, T. Jawaid, Benzofurans: a new profile of biological activities, Int. J. Med. Pharm. Sci. 1 (2011) 1-15.

**Keywords:** Benzofuran, quantum chemical studies, NMR, F-TIR

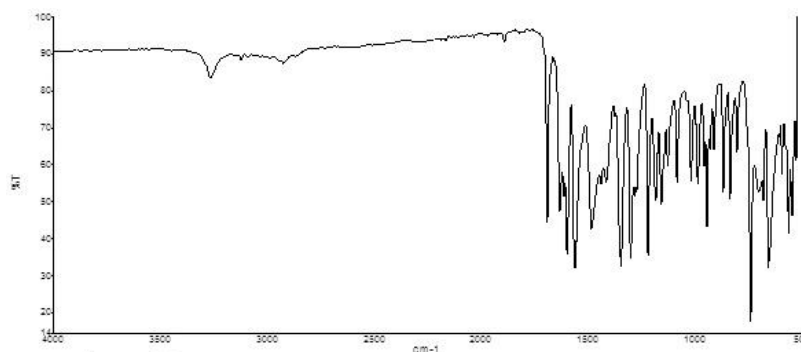


Fig. 1. FT-IR spectrum of the compound.

P-188

## AXS Analyses on Nanostructured Chocolates which have Different Cocoa Ratios

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It was known that chocolate is an important industrial food because of its significant economic value in the food industry with their effective usage potential (8 kg for a person in a year). This food material has been widely used in different structural forms and its taste, roof time etc. are directly related with its molecular, nanoscopic and microscopic structures. Cocoa butter is the basic structure of this food ingredient. This material, which has different crystalline forms, undergoes different physico-chemical effects during the chocolate processing. For this reason, Research and Development activities on these materials continuously increase. On the other hand, the modern experimental methods such as SR (Synchrotron Radiation) based SAXS-WAXS (Small and Wide Angle X-Ray) measurements supply valuable knowledge in the range of molecular-nano scales to follow structural changes. In the present study, SAXS and WAXS analyses on the nanostructured chocolates were performed (Fig.1) and the following results were obtained.

1. Size, shape and distance distributions of the nano globules were determined by using IGOR Pro6 and DAMMIN programmes.
2. WAXS analyses were also completed to reach structural knowledge on crystalline content of the nano aggregations which have 1D, 2D and 3D forms.

**Keywords:** SAXS, WAXS, Nanostructured Chocolate

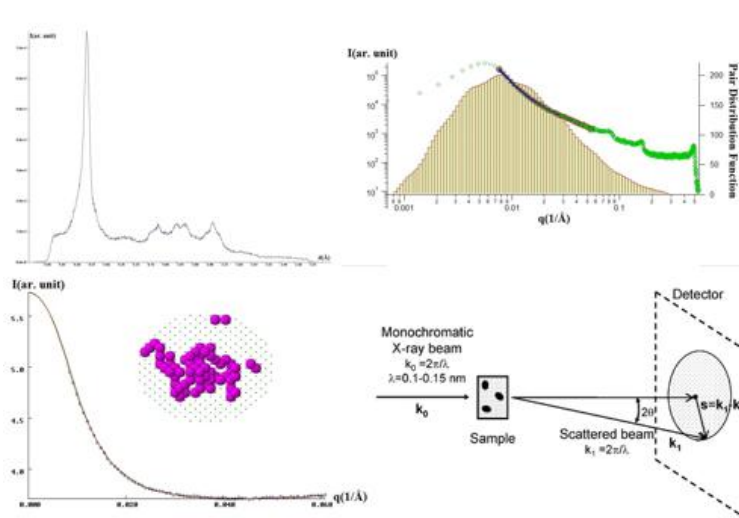


Fig. 1

P-189

## Preparation and Characterization of Crosslinked Polymer Hydrogel Microbeads by Copolymerizing Ethylene Glycol Dimethacrylate with n-Vinyl Imidazole

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Hydrogel microbeads made of polymers include imidazole rings find a wide range of applications in the food industry, agriculture, biomedicine and the pharmaceutical and cosmetic industry owing to their low toxicity, biocompatibility, biodegradability, high binding capacity to specific chemical species, and the ability to adsorb or release molecules in response to external signals or stimuli. For this purpose, poly(ethylene glycol dimethacrylate-n-vinyl imidazole) [poly(EGDMA-VIM)] hydrogel microbeads was prepared by copolymerizing ethylene glycol dimethacrylate with n-vinyl imidazole. The structure of the [poly(EGDMA-VIM)] hydrogel microbeads was characterized by Fourier transform infrared spectroscopy (FTIR), thermogravimetric analysis (TGA), vibrating-sample magnetometer (VSM), scanning electron microscope (SEM), transmission electron microscope (TEM), X-Ray diffraction (XRD) and equilibrium swelling experiment. The specific surface area of the [poly(EGDMA-VIM)] hydrogel microbeads was found to be 304.4 m<sup>2</sup> /g with a size range of 10–250 μm in diameter and the swelling ratio was 53%. The approximate IEP value for the [poly(EGDMA-VIM)] hydrogel microbeads was at pH 4.0. SEM image of the [poly(EGDMA-VIM)] hydrogel microbeads are presented in Fig. 1.

**Keywords:** hydrogel microbeads, n-vinyl imidazole, poly(ethylene glycol dimethacrylate)

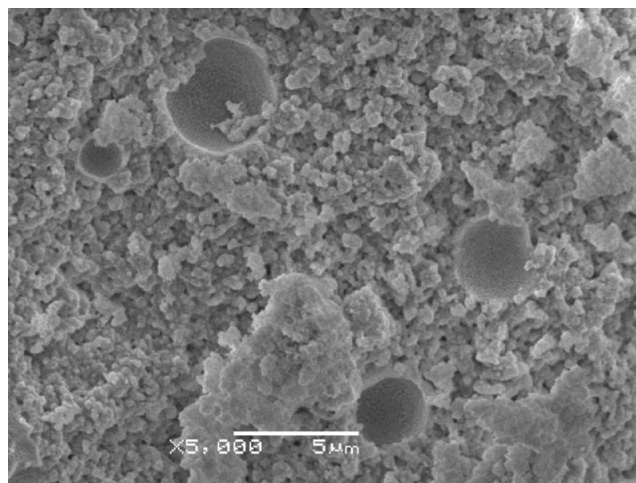


Fig. 1. SEM image of the [poly(EGDMA-VIM)] hydrogel microbeads



P-190

FTIR Spectroscopic Studies of Spider Dragline Silk of Different Species

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Spider dragline silk is fibrous biomaterial and an important model for biomimetic and industrial applications due to its outstanding mechanical properties. The molecular structure of dragline silk primarily consists of proteins that possess large quantities of nonpolar and hydrophobic amino acids and this structural content directly affects its stiffness, toughness and failure strength. Vibrational spectra of biological samples are rich in information on biochemical constituents. In this study, Attenuated Total Reflectance Fourier Transform Infrared (ATR-FTIR) Spectroscopy was used to obtain structural information about spider dragline silk produced by seven different spider species. *Aculeperia ceropegia*, *Araneus diadematus* (Fig.1), *Araneus quadratus*, *Argiope bruennichi* and *Argiope lobate* spiders were collected from the Blacksea region of Turkey. *Cyrtophora moluccensis* and *Nephila maculate* spiders were collected from Taiwan. The spectral analysis revealed that the silk protein is dominated by  $\beta$ -sheet structures. In order to find structural similarities and differences among silks, the infrared bands related to amide A, amide I, II and III, CH<sub>2</sub> and CH<sub>3</sub> vibrational modes were investigated in detail. Hierarchical Cluster Analysis (HCA) was applied to classify the species based on the spectral differences. Our findings show that dragline silks have spectral differences among species. The results indicate variation in the silk structure even within the same species.

*This study is currently being supported by the Scientific and Technological Research Council of Turkey (TUBITAK) under the project number KBAG 214Z049*

**Keywords:** Spider dragline silk, FTIR, protein

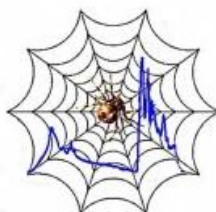


Fig. 1 *Araneus diadematus* spider



**P-191**

**Proficiency Testing by Inductively Coupled Plasma Mass Spectrometry Multi-Elemental Analysis in the Chilli Powder**

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This study presents an international proficiency testing (07217, Lab ID 53) on three trace elements, arsenic, cadmium and lead in chilli powder. Proficiency testing aims to provide an independent assessment of the competence of participating laboratories. Together with the use of validated methods proficiency testing is essential element of laboratory quality assurance. This proficiency-test exercise was registered with a total of 55 laboratories. The assigned reference values of the analytes for performance assessment were provided by the organizers. z-Score was used as the numerical indicator to interpret participants competence. We have assessed an overview of analytical methods used by PT participants, where possible looking for correlations between performance and choice of method. The certified reference material (NIST Tomato Leaves 1573a and ERM-BC084 Tomato paste) was digested with nitric acid and hydrogen peroxide in a microwave oven. The calibration was accomplished by adding the standards prepared in the concentrations of 0.5, 1, 2, 5, 10, 25 and 50  $\mu\text{g L}^{-1}$  from the 10  $\text{mg L}^{-1}$  stock standard solution on the matrix. The procedure follows that recommended in the IUPAC International Harmonised protocol for the Proficiency Testing of Analytical Chemistry Laboratories. According to the results was calculated z score 0.9, 0.3 and 1.1 for As, Cd and Pb, respectively.

**Keywords:** Chilli powder, heavy metals, ICP-MS, proficiency test

P-192

## Adsorption of Arsenic(V) on Adsorbents Produced from Solid Wastes

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The removal of arsenic(V) from aqueous solutions by the adsorbents produced from solid waste of edible oil industry was studied. The adsorbents were produced from solid waste obtained from an edible oil plant. Chemical method was used to prepare adsorbents. Experiments were performed as a function of time, initial concentration and temperature. The values of the Langmuir and Freundlich constants were determined. The experimental data points were fitted to the Langmuir equation in order to calculate the adsorption capacity (Q<sub>0</sub>) of the adsorbent. The adsorption kinetic process was followed the first order Lagergren equation. Mass transfer coefficients and rate constants intraparticle diffusion were calculated. The effect of some anions (NO<sub>3</sub><sup>-</sup>, SO<sub>4</sub><sup>2-</sup>, Cl<sup>-</sup>, Br<sup>-</sup>) on the adsorption of arsenic(V) was studied. The presence of these anions did not affect the adsorption of arsenic(V) significantly. The boundary layer and intraparticle diffusion played important roles in the adsorption rate. Thermodynamic parameters were calculated. The total arsenic(V) content in solution was analyzed on a GTA-110 graphite furnace atomic absorption spectrometer equipped with autosampler cups (Varian SpectrAA220). The current of the As hollow cathode lamp is 12 mA. The As spectral line is 193.7 nm, and the spectral bandpass is 0.5 nm. The values of all the constants calculated in this study were compared to the published data in the same field and were found to be greater than most of them.

**Keywords:** Arsenic(V), adsorption, adsorption isotherms, thermodynamic parameters

**P-193**

**Structural Properties of Fe-27%Ni-4%Mn-2%Zn alloy**

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The specimens used in the present study are Fe-27%Ni-4%Mn-2%Zn (wt.%) alloy. The alloy was produced by melting the component metals in a high frequency induction furnace under argon atmosphere. In the present work, morphology and crystallography in the athermal transformation in Fe-27%Ni-4%Mn-2%Zn (wt.%) alloy have been studied in detail by scanning electron microscopy with energy-dispersive X-ray spectrometry (SEM-EDX) and X-ray diffraction (XRD). From SEM observations, the Fe-27%Ni-4%Mn-2%Zn (wt.%) alloy show thermally induced "lath martensite" morphology. X-ray diffraction analysis revealed the face centred cubic (f.c.c.) of austenite phases and body centred cubic (b.c.c.) thermal induced martensite phases for the studied alloy.

*The financial aid of the Amasya University project No. FMB-BAP 16-0174 is gratefully acknowledged.*

**Keywords:** Martensitic Transformation, Morphology, SEM, XRD.

**P-194**

**Development of a fast analytical microextraction method for the determination of Sudan (II) in foodstuffs by spectrophotometry**

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Synthetic Sudan dyes (I, II, III, and IV) are non-authorized and illegally used in the food industry to enhance and maintain the appearance of food products such as in chilli-, curry-, curcuma-, and palm oil-containing foodstuffs. In this study, we describe application of a high-sensitive cloud point microextraction procedure coupled to spectrophotometry for determination of sudan (II) the presence of Triton X-45 at pH 6.5 in food samples. Analytical parameters, such as pH, volume of extraction solvent, volume of Triton x-45, volume of sample, and extraction time, temperature were optimized. Matrix effects were also investigated. Preconcentration factor was found to be 75. Detection limit and relative standard deviation (RSD) were 3.9  $\mu\text{g kg}^{-1}$ . Validation data show a good repeatability and within-lab reproducibility with relative standard deviations < 8.5%. The overall recoveries are in the range of 91–107% in foods and in the range of 88–102% in beverage depending on the dye involved. Calibration curves are linear in the 10-750  $\mu\text{g kg}^{-1}$  range for foods and in the 50–575  $\mu\text{g kg}^{-1}$  range for beverages. The proposed method is specific and selective, allowing the analysis of over 10 samples per working day.

**Keywords:** Sudan dye, spectrophotometry, extraction, Green chemistry

**P-195**

**Isotopic and elemental markers for the differentiation of Transylvanian vegetables**

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The market of organic food and beverages has been extensively developed over the past decade. At the same time, the increasing demand for organically grown food, characterized also from economical point of view by premium prices, have created a financial enticement to mislabel and try to pass off cheaper conventional products as organic.

This work presents the isotopic composition and elemental profile of more than 150 Transylvanian vegetables samples grown under different agricultural practices. The sample set was tested from stable isotopes ratios ( $2\text{H}/1\text{H}$ ;  $18\text{O}/16\text{O}$ ;  $13\text{C}/12\text{C}$  and  $15\text{N}/14\text{N}$ ) and elemental profile point of view. For these purposes, the used techniques were: Isotope Ratio Mass Spectrometry (IRMS) for isotope measurements and Coupled Plasma Mass Spectrometry (ICP-MS) for elemental content determination. The best markers association for the differentiation of organic from and conventional vegetables, as well as for geographical origin discrimination were made by applying chemometric techniques first ANOVA and then, for a more clearly identification, LDA.

Our main objectives were the identification of the best markers combination that are able to classify vegetable samples according to growing conditions organic vs. conventional and also greenhouse vs. field.

**Keywords:** Vegetables, Isotope ratios, elemental profile.

**P-196**

**Discrimination markers for geographical and species origin of raw milk produced in three Romanian farms**

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In this work, cow and sheep milk samples along with the feed and water used for animal breeding, were investigated from stable isotope ratios ( $1\text{H}/2\text{H}$ ;  $18\text{O}/16\text{O}$ ;  $13\text{C}/12\text{C}$ ) and metal content point of view. Milk was collected from three Transylvanian farms, localized at different altitude; sheep milk being produced only in two farms. It should be mentioned that the feeding regime were similar for sheep and cows, breeding in the same farm.

The obtained experimental results were statistically processed, in order to find the best markers that could individualized both, milk geographical provenance and also, animal species. By applying chemometric analysis, it was shown that main markers that can differentiate the origin farms of milk samples were isotope ratios of oxygen ( $18\text{O}/16\text{O}$ ) and carbon ( $13\text{C}/12\text{C}$ ) combined with Sr and Mn concentrations. Also, the species differentiation between cow and sheep was made by the corroboration of Sr concentration with isotope ratio of hydrogen. The results obtained from cross-validation, showed that resulted models of Discriminant Analysis (DA) allowed the correctly classification of 90.9 % samples related to geographical origin, while for speciation the percent was 96.4%.

**Keywords:** Milk, Isotope ratios, elemental profile

P-197

## The Spectroscopy of Environmental Structure Caused The Winds of CW Cep Eclipsing Binary Star

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In this study, the velocities of the material forming of the blue, red wing edges and center wavelengths of H-alpha and He I (6678,15) lines of the early-type eclipsing binary CW Cep (B0.5V-B0.5V) was examined.

We obtained the reduced spectrum of <http://basebe.obspm.fr/basebe/>. The edge and center velocities of the H-alpha and He I (6678,15) lines of these strains were found using the SPLAT spectral analysis program.

The source of the H-alpha line is the disk surrounding the CW Cep. This is why the emission line is observed. He I (6678,15) is the absorption lines on the surface of the stars. CW Cep double - lined spectral binary. The wing limit speed of the H-alpha line reaches its maximum value during eclipsing. However, the wing limit speeds of the He I (6678,15) line have reached maximum values except for the eclipsing.

**Keywords:** CW Cep, eclipsing binary stars, stellar winds, environmental structure, stellar spectroscopy

**P-198**

**Development of a robust ultrasonic assisted ionic liquid-based dispersive liquid–liquid microextraction for preconcentration of Pb in vegetable samples**

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Lead (Pb) is classified as prevalent toxic metal which tend to be concentrated in environmental systems and humans. Absorption from the air in the local environment and intake from the diet are the major sources of human exposure. Pb has been demonstrated to be accumulated in bone and in some soft tissues, such as liver, kidney and brain, A new ultrasonic assisted ionic liquid-based dispersive liquid–liquid microextraction (UA-IL-DLLME) method was developed for preconcentration and determination of Pb in vegetable samples by flame atomic absorption spectrometry (FAAS). This method can solve the problems associated with the limited application of the conventional IL-based DLLME in this samples After optimization of the complexation and extraction conditions, enhancement factor of 60 was obtained for Pb. Under the experimental conditions used, preconcentration of only 10 ml of sample in the presence of 100  $\mu$ L of ionic liquid (IL) permitted the detection of 0.04  $\mu$ g L<sup>-1</sup> of Pb. The calibration graphs were obtained in the range of 0.1–350  $\mu$ g L<sup>-1</sup>. The relative standard deviations (R.S.D.) of 1.6–2.4% for Cu were obtained. The method was applied to the determination of Cu, Fe and Pb in river and wastewater samples. The proposed method has been validated by analyzing a certified reference material and successfully applied to the preconcentration and determination of Pb(II) in vegetable samples with satisfactory results.

**Keywords:** Microextraction, FAAS, Vegetable sample, Lead



P-199

## INFRARED SPECTROSCOPY AND THERMOSTATIC ANALYSIS ON NEW GENERATION PLASTIC ADDITIVES INCLUDING TRANSITION METAL(II) COMPLEX WITH STEARIC ACID

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Plastics based on polyvinyl chloride (PVC) dry blend are composed in PVC, fillers, stabilizers and the other plastic additives such as impact modifiers, strength enhancers, shifters... etc. However, the plastic additives as fillers (specially calcite) and stabilizers are more important than the other one. Therefore, PVC decompositions are prevented or delayed by using PVC additives. Used calcite as filler material is formed calcium carbonate, and this form modified at using transition metal(II) in this study. Thus,  $\text{Cu(II)CO}_3$  and  $\text{Ni(II)-Cu(II)CO}_3$  metallic complex were synthesized with chemical ways. The chemical formulation of stearic acid as saturated fatty acid is  $\text{CH}_3(\text{CH}_2)_{16}\text{COOH}$ . Stearic acid is used in drug cosmetics as lubricants, and producing granule and compound for detergents. Additionally, chemicals which are including stearic acid (str) are known good thermal stabilizers in plastic industry. Therefore,  $\text{Ni(II)-str-Cu(II)CO}_3$  metal complex was synthesized and characterized via vibrational spectroscopy in this study (Fig. 1). Afterwards, Plastic dry blend was composed with adding 10 Phr  $\text{Ni(II)-str-Cu(II)CO}_3$ , and mixed at 70 °C temperature. Then new dry blend which is including new generation plastic additives was plasticized using gelation methods in the mold at 180 °C during 15 minutes. Subsequently, dehydrochlorization (DHC) tests were performed on plastic materials getting by plastic dry blend in which including  $\text{Cu(II)CO}_3$ ,  $\text{Ni(II)-Cu(II)CO}_3$  and  $\text{Ni-str-Cu(II)CO}_3$  plastic additives. DHC test results show that stearic acid is contributed to increase in thermal stability of PVC as shown in Fig. 2.

*This study was supported financially by Eskişehir Osmangazi University Research fund (Project No: BAP 2017-1588).*

**Keywords:** PVC, stabilizers, calcite, filler materials, infrared, DHC test

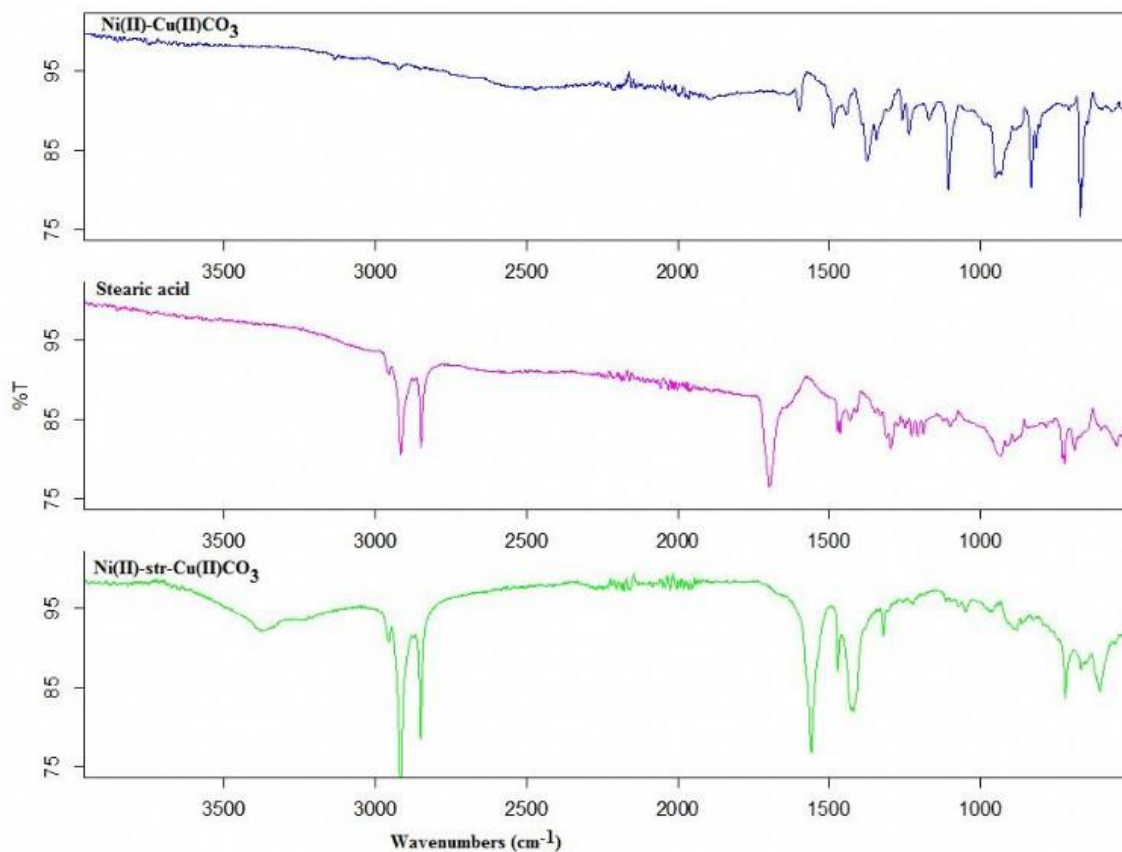


Fig. 1. FT-IR spectra of Ni(II)-Cu(II)CO<sub>3</sub>, stearic acid and Ni(II)-str-Cu(II)CO<sub>3</sub>

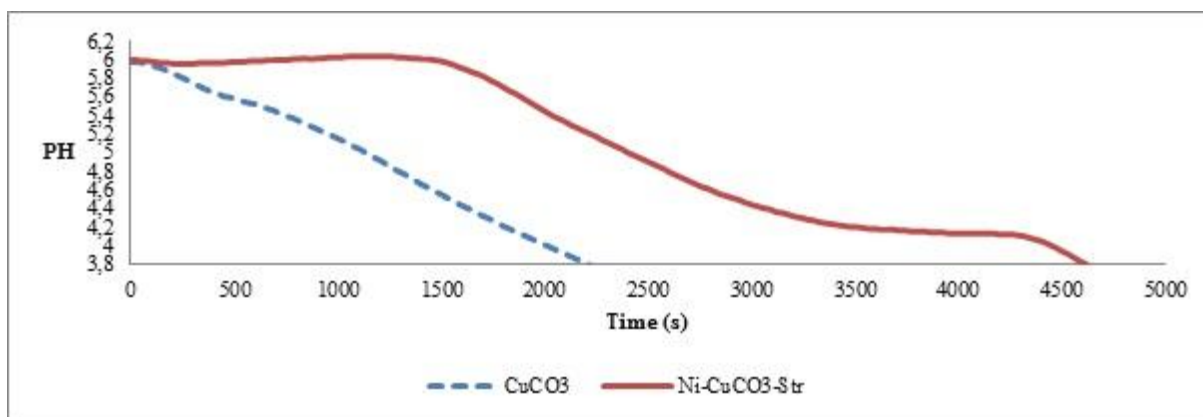


Fig. 2. Comparison of the DHC curves of Cu(II)CO<sub>3</sub> and Ni(II)-str-Cu(II)CO<sub>3</sub>

P-200

**VIBRATIONAL SPECTRAL ANALYSIS AND THERMOSTATIC PROPERTIES OF THE PVC DRY BLENDS CONSISTING OF TRANSITION METAL BORAX COMPLEX WITH STEARIC ACID**

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In this study, heteronuclear transition metal(II) borax complexes are synthesized, characterized by FT-IR spectroscopy (Fig. 1), and investigated thermostatic properties of the plastic materials consisting of the new generation plastic additives as these complexes via dehydrochlorination test. One the one hand boron element is situated in third group of the periodic system, and it consists of two stable isotopes with mass numbers 10. Borax, boric acid and sodium perborate are boron products and they are used in the coatings on the surfaces of the ceramics in the production of special glassware where properties such as heat resistance, surface hardness and durability are required. Principally, boric acid and borates provide fire resistance of the cellulosic materials, remove water molecules from cellulose without are reached the ignition temperature, and prevented further burning by covering the surface of the formed carp. On the other hand, stearic acid is used in drug cosmetics as lubricants, and producing granule and compound for detergents. Additionally, chemicals which are including stearic acid (str) are known good thermal stabilizers in plastic industry. In this study,  $Mn(B_2O_4)_nH_2O$  and  $Ni(II)-str-Mn(II)(B_2O_4)_nH_2O$  metal complex were synthesized and characterized with using infrared spectroscopy (Fig. 1). Afterwards, plastic dry blend were composed with adding 10 Phr these complexes in the PVC dry blends, and mixed at 70 °C temperatures. Then new dry blend which is including new generation plastic additives was plasticized using gelation methods in the mold at 180°C during 15 minutes. Subsequently, dehydrochlorization (DHC) tests were performed on plastic materials getting by plastic dry blend in which including  $Mn(B_2O_4)_nH_2O$  and  $Mn(II)-str-Ni(II)(B_2O_4)_nH_2O$  plastic additives. DHC test results shown that stearic acid is contributed to increase in thermal stability of PVC as shown in Fig. 2.

*"This study was supported financially by Eskisehir Osmangazi University Research fund (Project No: BAP 2017-1588). "*

**Keywords:** PVC, stabilizers, borax, FT-IR, DHC test

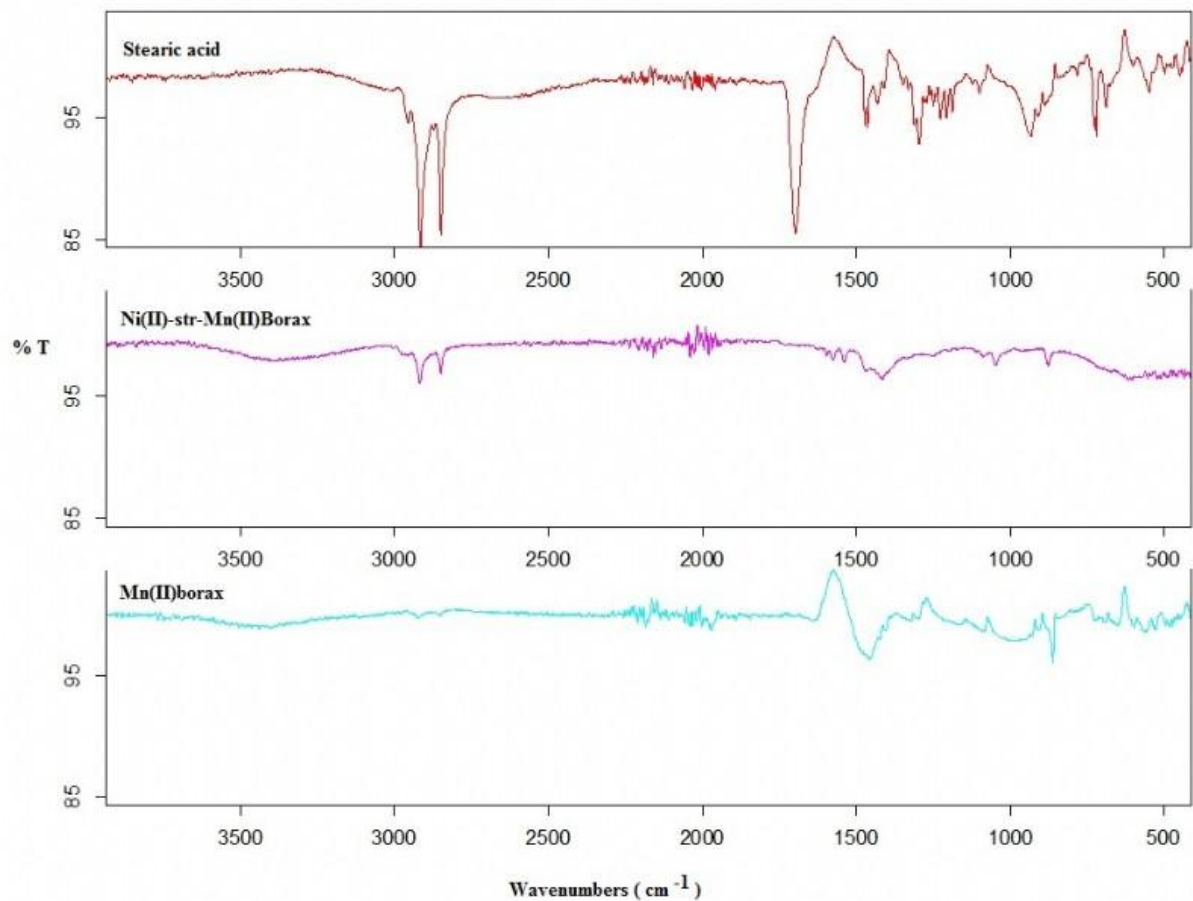


Fig. 1. The FT-IR spectra of stearic acid, Ni(II)-str-Mn(II)borax and Mn(II)borax

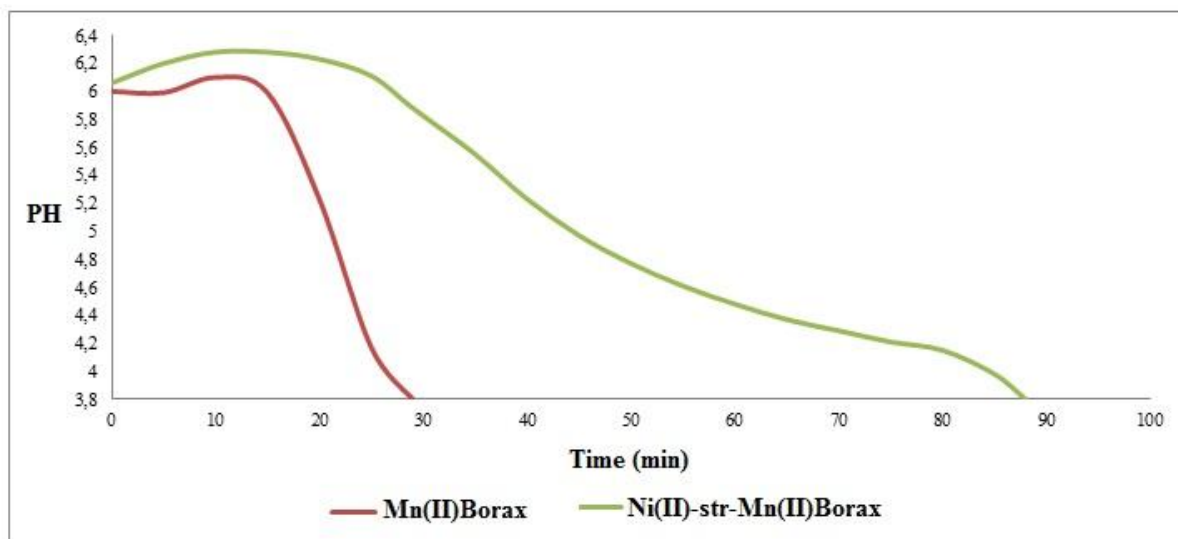


Fig. 2. Comparison of the DHC curves of Mn(II)borax and Ni(II)-str-Mn(II)borax

P-201

**Synthesis, Spectroscopic and Thermal Investigation of  
Poly(triethoxyvinylsilane-co-vinyltris(trimethylsiloxy)silane-co-  
divinylbenzene)**

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Crosslinking in polymers is important especially from a commercial point of view. Many commercial polymers owe their superior property to their crosslinked structures [1]. Crosslinked polymers are frequently presumed to enhance the thermal stability of polymeric systems [2]. Organosilicon polymers are potentially useful materials such as photoresists, semiconductors, hole-transporting materials, and precursors of silicon carbide [3]. The crosslinker divinylbenzene (DVB) have been radically reacted on the chain group of triethoxyvinylsilane (TEVS) and vinyltris(trimethylsiloxy)silane (VTTMSS) for the synthesise of novel crosslinked copolymers. The end products were further examined by IR, Raman, <sup>1</sup>H-NMR and <sup>13</sup>C-NMR spectroscopies to characterize them. Thermal behaviors (TGA&DSC) were showed that these copolymers (Fig. 1) can be used as thermoset materials having high temperature resistant property for industrial applications.

*This study was supported by Erciyes University Scientific Research Project Coordinatorship (Project no: FYL-2017-7415).*

[1] C.S. Patrickios, *Macromol Symp.*, 291–292, 1, 2010, 1-370.

[2] F.M. Uhl, G.F. Levchik, S.V. Levchik, C. Dick, J.J. Liggat, C.E. Snape, C.A. Wilkie, *Polymer Degradation and Stability*, 71, 2001, 317-325.

[3] J.M. Zeigler, F. W. G. Fearon, American Chemical Society: Washington, DC, 1990.

**Keywords:** Alkoxysilane, crosslinked polymer, spectroscopic, thermal behavior.

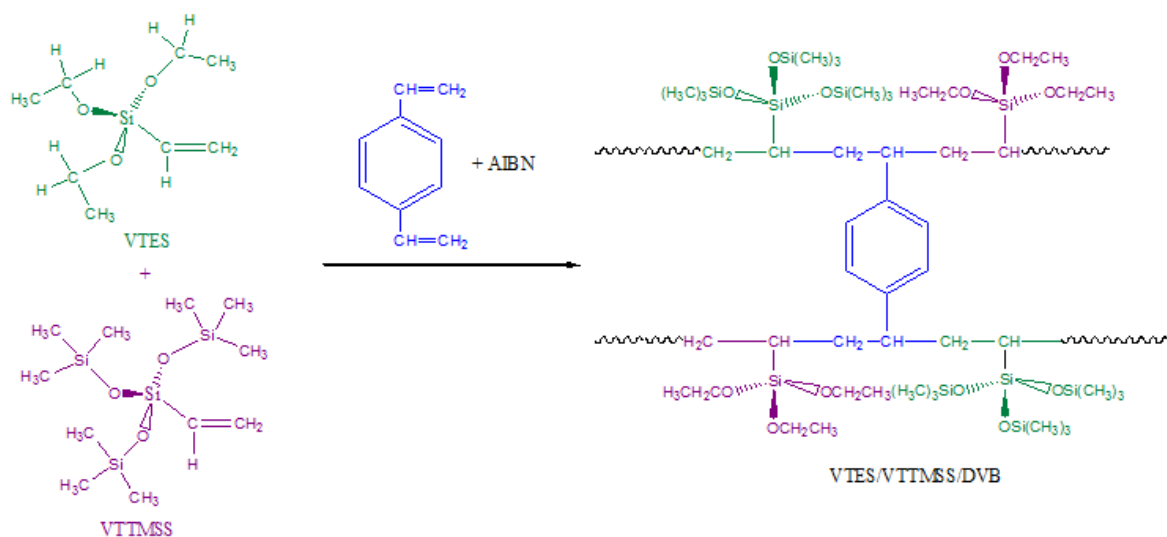


Fig. 1. Reaction scheme of (TEVS/VTMSS/DVB)

P-202

**Synthesis of Poly(triacetoxyvinylsilane-co-trimethylvinylsilane-co-divinylbenzene) and Determination of Spectroscopic and Thermal Behaviors**

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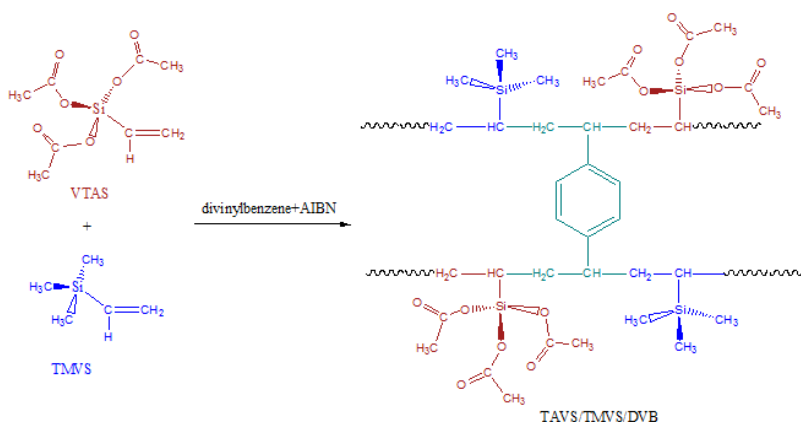
Crosslinked polymers are pretty important in multiple applications such as super-absorbent materials, ion-exchange resins, chromatography packings, additives in surface coatings, dental restorative materials, and several areas including biotechnology, medicine, and agriculture. These kind of polymers are also used in pharmaceuticals and cosmetics, drug-delivery systems, artificial organs, sensors, optics and electronics [1]. The copolymers of silane containing acrylamide derivatives have usually high thermal stability and fire resistance [2]. In this study, novel crosslinked polymers have been synthesized by radical polymerization technique using triacetoxyvinylsilane (TAVS), trimethylvinylsilane (TMVS) monomers and divinylbenzene (DVB) as crosslinking agent. The reaction scheme is shown in Fig.1. The synthesized crosslinked copolymers were further investigated for their spectroscopic (IR & Raman, <sup>1</sup>H-NMR and <sup>13</sup>C-NMR), elemental analysis and thermal behaviors (TGA&DSC) to be used as a thermoset material having high temperature resistance.

Authors wish to thank Erciyes University Scientific Research Project Coordinatorship (Project no: FYL-2017-7415).

[1] C.S. Patrickios, *Macromol Symp.*, 291–292, 1, 2010, 1-370.

[2] W.J. Shua, J.C. Ho, L.H. Perng, *European Polymer Journal*, 41, 2005, 149-156.

**Keywords:** Silane derivative, crosslinked polymer, spectroscopic, thermal behavior.



**Fig. 1. Reaction scheme of (TAVS/TMVS/DVB)**



P-203

**Polyethylene imine/Fe[NiFe]O<sub>4</sub> and Polyethylene imine/Fe<sub>3</sub>O<sub>4</sub> Magnetic Composite nanoparticles: An application for enzyme technology**

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The scope of this study is to synthesize polyethylene imine/Fe[NiFe]O<sub>4</sub> (PINM) and polyethylene imine/Fe<sub>3</sub>O<sub>4</sub> (PIM) magnetic nanoparticles and to achieve carrier-bound immobilization of urease onto this nanoparticles. The morphologic characterization of magnetic nanoparticles was analyzed with transmission electron microscope (TEM) and scanning electron microscope (SEM), (Fig. 1). Also, the surface groups and chemical structure of the particles were determined by using attenuated total reflectance fourier transform infrared spectroscopy (ATR-FTIR). The optimum immobilization conditions were found for urease: adsorption time (30 min), the initial enzyme concentration (1 mg/mL), amount of magnetic particles (50 mg), polyethylene imine amount (75 mg) and glutaraldehyde concentration (3%). The activity reaction conditions (optimum temperature, optimum pH, pH stability, thermal stability, operational stability, and reusability) were characterized. Also kinetic parameters were calculated by Lineweaver–Burk plots. The optimum pH values were found to be 7.5, 6.0 and 6.0 for free enzyme, PIM and PINM, respectively. The optimum temperature values were found to be 35, 30 and 30°C for free enzyme, PIM and PINM, respectively. Reusability studies showed that PIM can be used 9 times with 65% loss in original activity, while PINM lost 48% of activity after the same number of uses. Furthermore, immobilized urease systems exhibited improved thermal and pH stability. The results transparently indicate that it is possible to have binding between enzyme and magnetic nanoparticles.

**Keywords:** polyethyleneimine, Fe[NiFe]O<sub>4</sub>, Fe<sub>3</sub>O<sub>4</sub>, urease

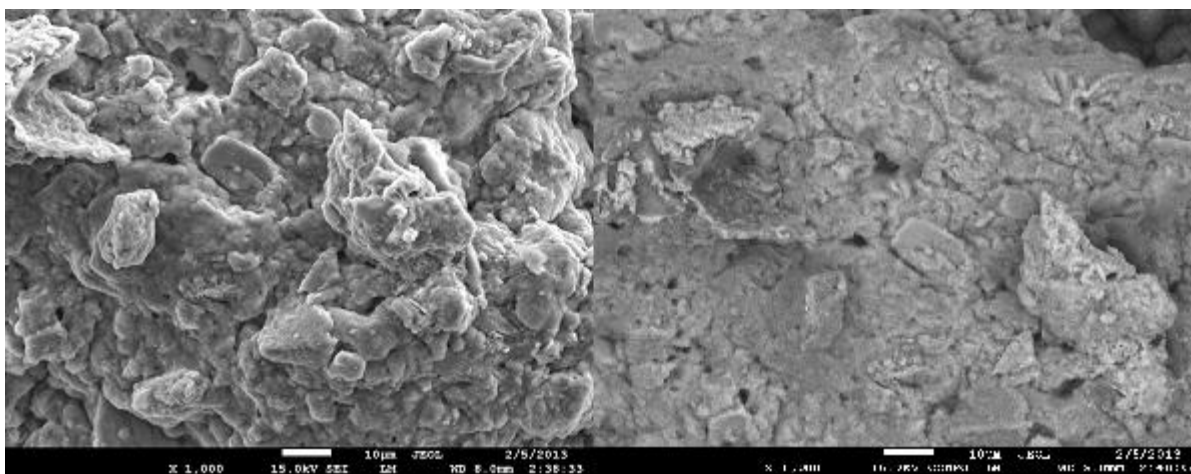


Fig. 1. SEM images of PIM and PINM



P-204

Characterization of Chitosan/TiO<sub>2</sub> Composite Beads: An Application for Enzyme Technology

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The purpose of the present work is improving stability properties of porcine pancreatic lipase by immobilization on chitosan/TiO<sub>2</sub> composite beads. The structural characterization of chitosan/ TiO<sub>2</sub> composite beads (Fig. 1) was analyzed with scanning electron microscope (SEM), X-ray diffraction (XRD), thermal gravimetric analysis (TGA), and attenuated total reflection Fourier transform infrared spectroscopy analysis (ATR-FTIR). The optimum temperature (20–60 °C), optimum pH (3.0–10.0), kinetic parameters, thermal stability (4–70 °C), pH stability (4.0–9.0), and reusability (9 times) were investigated for characterization of immobilized lipase system. The optimum temperatures of free and immobilized lipase were 30 °C. The temperature profile of the immobilized lipase was spread over a large area. The optimum pH values for the free lipase and immobilized lipase were found to be 6.5 and 7.5, respectively. The thermal stability of immobilized lipase was evaluated, and it maintained 45 % activity at 70 °C. But, at this temperature, soluble lipase protected only 15 % activity. Also, The significance of this study is improving of stability properties of lipase for the industrial usage especially production of biodiesel and dairy products.

**Keywords:** Lipase, TiO<sub>2</sub>, chitosan, composite

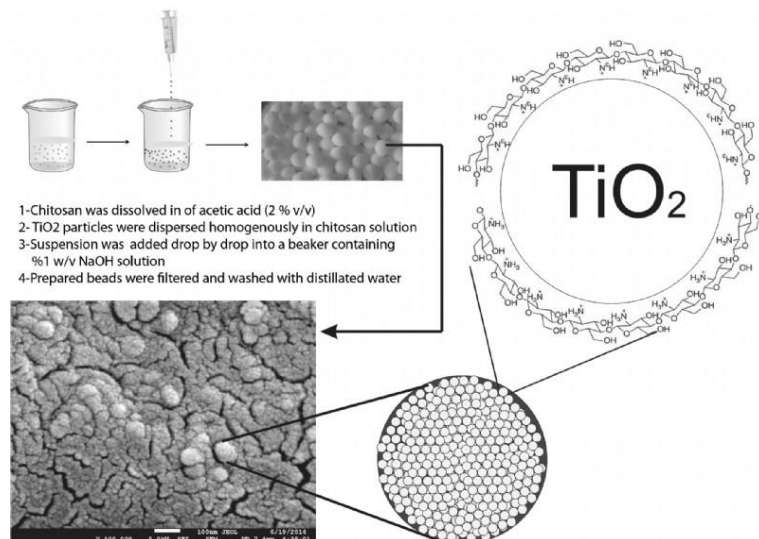


Fig. 1. TiO<sub>2</sub>-chitosan

P-205

**Synthesis, Crystal Structure and Spectroscopic Properties of New Co(II/III) Complex**

Umut Güzel<sup>1</sup>, M. Burak Çoban<sup>2</sup>, Yasemin Acar<sup>2</sup>, Elif Güngör<sup>2</sup>, Görkem Oylumluoğlu<sup>1</sup>, Hülya Kara<sup>1</sup>

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A new tetranuclear cobalt(II/III) complex [C<sub>60</sub>H<sub>68.5</sub>Co<sub>4</sub>N<sub>4</sub>O<sub>17.5</sub>] has been synthesized using tridentate Schiff base ligand which is prepared by reaction of 3 amino-1-propanol (1mmol) with 2-hydroxy-1-naphthaldehyde (1mmol) in hot ethanol. This cobalt complex has been characterized by element analysis, FT-IR, solid UV-Vis spectroscopy and single crystal X-ray diffraction. The crystal structure determination (Fig. 1) shows that all the cobalt ions have a distorted octahedral geometry. Co...Co distances on different cubic faces of complex is also different, vary from 3.035 to 3.206 Å. Molecules interacting through C-H...O hydrogen bonds in complex give rise to a 2D coordination network. The structure of cobalt complex is further stabilized by π...π stacking interactions which lie in the ab-plane.

**Keywords:** Crystal structure, Tetranuclear cobalt(II/III) complex, Synthesis

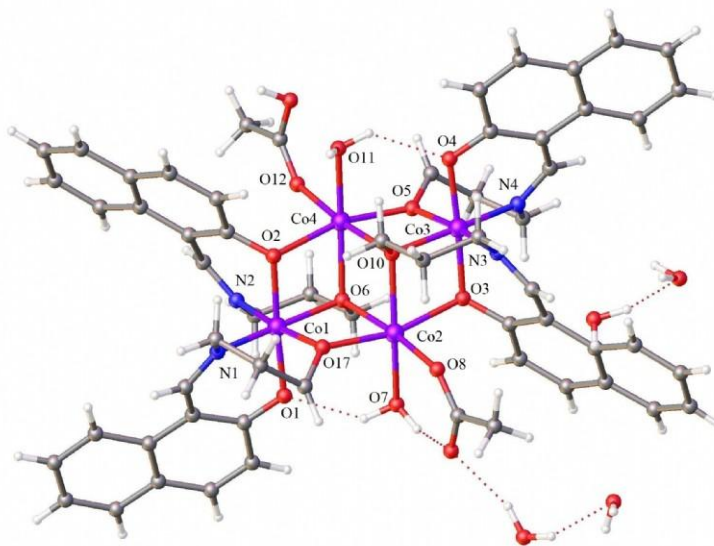


Fig. 1. Structure of the studied compound

P-206

Single Crystal Structure of Holmium(III) Based Porous Coordination Polymer

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The exponential growth of the field of coordination materials, particularly porous coordination polymers (CPs), can be attributed to their excellent network topologies coupled with their many potential applications such as gas storage/separation, catalysis, luminescence sensing, telecommunication, non-linear optic and so on [1]. In this work, a novel lanthanide coordination polymer crystallized in the monoclinic space group P21/n. The asymmetric unit of the compound consist of a Ho(III) ion, a 2-stp chromorphic ligand, three coordinated water molecules and one free water molecule. Each Ho atom is eight coordination and adopts a distorted square-antiprismatic geometry with four oxygen atoms from carboxylate groups, one oxygen atom from sulfonate group and three oxygen atoms from coordinated water molecules (Fig. 1). The crystal packing reveals that the compound is one-dimensional structure and contains extensive hydrogen bonding which play key role in the constructing the 3D-network topology.

*This work was supported by BAP 16/043 (Mugla Sitki Kocman University, The Scientific Research Projects Coordination Unit).*

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**Keywords:** Ho(III) complex, Hydrothermal Synthesis, Crystal structure

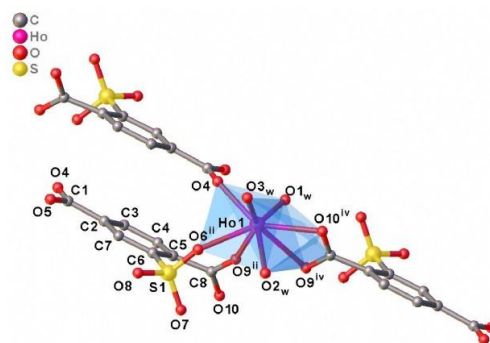


Fig. 1. Crystal structure

P-207

## Structural Characterization of Electrospun PVA/ZnO Composite Nanofibers

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Due to wide direct band gap of ZnO, it is an photonic and electronic material. So, it has attracted many research areas like nanoclusters, solar cells and high functional devices. ZnO can be produced by many methods, for example microemulsion hydrothermal process, wet chemical method, high-temperature physical evaporation, the template-induced method.

In this submitted work, Polyvinyl alcohol (PVA)/ZnO nanofibers were synthesized by electrospinning technique. The operational parameters of nanofibers were PVA concentration (%), Zn concentration (%), voltage (kV), needle tip -collector distance (cm) and injection speed (ml/h). The criteria used in deciding the best PVA/ZnO nanofiber structure were the taylor cone formation during electrospinning, fiber formation, no formation of polymer droplets at the needle tip or on the collector, stable system, easy removal of fiber from the collector, mechanically stable fiber. According to these criteria, the most appropriate operational parameters as electric voltage, distance between tip and collector, concentration of PVA, injection speed were found as 13 kV, 17 cm, 9% PVA and 0.3 ml/h respectively. The morphology and structure of the nanofibers was characterized by scanning electron microscopy (SEM), X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR) and thermal gravimetric analysis (TGA). According to our results, ZnO were successfully embedded in the hybrid fibers due to chemical interactions between ZnO and PVA.

SEM is powerful technology for investigating the morphology of the nanomaterials. The effect of operational parameters was investigated for optimizing the PVA/ZnO nanofiber morphology by using SEM technique. Obtained nanofibers were randomly-organized, smooth and round-shaped. SEM results showed that resulting nanofibers had the narrow diameter distribution.

**Keywords:** nanofiber, electrospinning, SEM, FTIR

P-208

**Determination of chemical composition of *Petroselinum crispum* L. seed by GC/MSD**

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*Petroselinum crispum* L. is an aromatic and medicinal plant that originated from the Mediterranean regions of Europe. It is a biennial plant which is widely cultivated as an annual plant. The leaves are used for garnishing and seasoning while the seed oil is an important flavoring agent for meat and sausages. Traditionally, roots of *P. crispum* has been used as a powerful diuretic, seeds have been used as antimicrobial, antiseptic, antispasmodic, and in the treatment of gastrointestinal disorders, inflammation, halitosis, kidney stones, and amenorrhea. Leaves of *P. crispum* have been employed in the treatment of hemorrhoids, gastrointestinal disorders, diuretic, and as a food-flavoring agent in addition to its common usage as vegetable. *P. crispum* has been found to possess many pharmacological effects including, antioxidant, antibacterial, antifungal, hepatoprotective, antidiabetic, analgesic, spasmolytic, immunosuppressant, and gastroprotective properties.

In the present study, *P. crispum* seed oil was obtained by cold press process. The following method was used to obtain chemical composition from seed; 100 µL of the seed oil was taken and dissolved in 9.800 mL of hexane in a 10 mL volumetric flask. It was mixed for 1 minute by vortex. Then 100 µL of 2 N KOH (prepared with methanol) was added. It was mixed by vortex again. It was centrifuged at 4000 rpm. 1 µL of filtrate was injected into GC/MSD.

GC/MSD and DB-1 MS capillary column were used. According to results of study; the major compounds were determined elaidic acid, linolelaidic acid, apiol, 1-allyl-2,3,4,5-tetramethoxybenzene, palmitic acid and myristicin, respectively. The rich fatty acid composition makes seeds of *P. crispum* valuable for the consumption.

**Keywords:** *Petroselinum crispum*, Fatty acid, GC/MSD, Elaidic acid, Apiol

P-209

**The Determination of Some Trace Elements (As, Be, Cd, Co, Cr, Cu, Li, Mn, Pb, Se, Sr, Ti, V, Zn) and Mineral (Mg) Levels of *Dactylorhiza umbrosa* (Kar. & Kir.) Nevski (Orchiaceae) Plant**

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There are about 75 species of *Dactylorhiza* (Orchidaceae) in the World that are mainly distributed in the Northern Hemisphere. Species of this genus occupy a wide range of open habitats from dune slacks to Alpine meadows and including swamps and peat bogs [1]. In Turkey Orchidaceae species are being used to obtain salep and is known as a drug used for aphrodisiac since the ancient times. It is also known that humans benefit from the protection of the mucous membrane and the removal of respiratory tracts and diseases such as bronchitis and stomach ulcer [2]. The medicinal plants have positive effects on human health as they are rich in trace elements and minerals. N, P, K, Ca, Mg, Na, Fe, Mn, Cu, Zn, B, Mo and Se are important for plant production and are vital for growth and development of all living bodies. However, Co, Cd, Cr, Ni, and Pb are toxic heavy metals and they could be harmful to health according to international references [3, 4]. In this study the concentration of all metals were determined by using inductive paired plasma-optical emission spectrometer (ICP-OES). It was determined that the *Dactylorhiza umbrosa* (Kar. & Kir.) Nevski plant element levels were ordered Sr>Mg>V>Mn>Li>Ti>Cu>Se>Cr>Pb>Co>As>Be>Zn>Cd respectively. It was found that the level of important trace elements Mn, Cu and Se were high and also the quantity of the Mg mineral was quite high. Co and Pb quantities from toxic elements were found to be higher than international reference values.

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- [3] Bihter Çolak Esetlili, Tülin Pekcan, Özgür Çobanoğlu, Erol Aydoğdu, Sevim Turan, Dilek Anaç, Journal of Agricultural Science, 20, 2014, 239-247.
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**Keywords:** *Dactylorhiza umbrosa*, trace elements, mineral



## P-210

### The effect of the sodium oxide in the silicate-yttria-zirconia vitroceraamics

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Zirconia exists in three crystalline polymorphs forms depending on the temperature: monoclinic, tetragonal and cubic phase. The latter two crystalline phases are high-temperature modifications. The low temperature formation of the tetragonal or cubic ZrO<sub>2</sub> crystalline phase was attracted substantial attention because is responsible of these extraordinary properties (mechanical, electrical, catalytic and optical properties).

To stabilize high temperature ZrO<sub>2</sub> crystalline phase, two main methods were used: one is the reduction of the crystallite size, and another is doping of the dopants. Compared to the reduction of the crystallite size, using dopants to stabilize tetragonal or cubic ZrO<sub>2</sub> crystalline phase is more common for various potential industrial applications. Glass ceramics with ZrO<sub>2</sub>-SiO<sub>2</sub> composition are of great interest, in which amorphous SiO<sub>2</sub> matrix can retard the tetragonal-monoclinic transformation and the grain growth of ZrO<sub>2</sub>.

The aim of this study was to clarify some dominant factors for the stable formation of the high temperature ZrO<sub>2</sub> crystalline phase. Then, the objective of the present study is to investigate how the processing temperature and the yttrium (III) oxide, silicon dioxide and sodium oxide contents can influenced the formation of cubic zirconia crystalline phase in vitroceraamics by using investigations of X-ray diffraction (XRD), Scanning Electron Microscopy (SEM), Fourier Transform Infrared (FTIR), UltraViolet-Visible (UV-Vis) and photoluminescence (PL) spectroscopy.

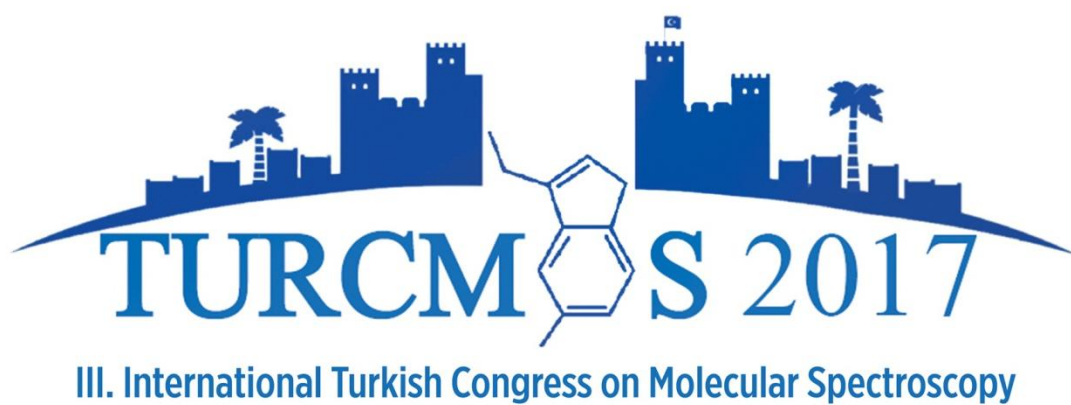
Two cubic zirconia ceramics with the 5Na<sub>2</sub>O·10SiO<sub>2</sub>·xY<sub>2</sub>O<sub>3</sub>·(85-x)ZrO<sub>2</sub> composition where x=10 and 15mol% Y<sub>2</sub>O<sub>3</sub> were obtained for first time at low processing temperature. IR analysis indicates the prominent IR bands situated between 400 and 670cm<sup>-1</sup> which can be due to Zr-O stretching vibrations from cubic ZrO<sub>2</sub> crystalline phase, in agreement with XRD data.

It is impossible to obtain high temperature zirconia phases directly from its pure melt or using only low Y<sub>2</sub>O<sub>3</sub> and/or SiO<sub>2</sub> contents (1 - 3 mol%) in the host matrix. We showed that addition of stabilizers such as Na<sub>2</sub>O, SiO<sub>2</sub> and Y<sub>2</sub>O<sub>3</sub> with a concentration of 5mol% and higher up to 15mol% forms numerous vacancies in the oxygen lattice of ZrO<sub>2</sub> and thus products the formation of the cubic zirconia phase.

The analysis of UV-Vis and PL spectroscopic investigations reveals that with increase in the Y<sub>2</sub>O<sub>3</sub> concentration, yttrium ions leads to the breakdown of silicate network resulting non-bridging oxygen atoms which will decrease the gap energy and the PL intensity.

*This research was supported by the Bridge Program Projects 2016 (PN-III-P2-2.1-BG-2016-0077) and PNCDI III, European and International Cooperation, Partnership Cooperation, Contract no. 67/BM/2016.*

**Keywords:** zirconia vitroceraamics, cubic zirconia, XRD, SEM, FTIR, UV-Vis and PL spectroscopy.



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The organisation of the International Turkish Congress on Molecular Spectroscopy (TURCMOS 2017) would not possible without the generous support of our sponsors and supporting organisations. Therefore, our particular thanks go to the following organisations and companies:

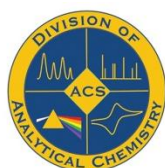
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