TURCMOS 2013

International Turkish Congress on Molecular Spectroscopy

September 15-20, 2013 / Istanbul / Turkey

Harbiye Cultural Center & Museum

BOOK OF ABSTRACTS

Editors

Ozan ÜNSALAN, Gülce ÖĞRÜÇ ILDIZ, Sevgi H. BAYARI

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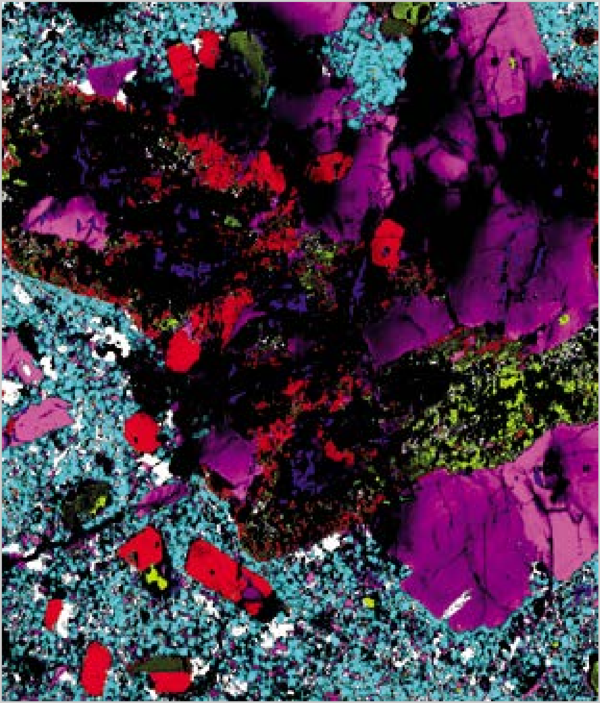
TURCMOS 2013

International Turkish Congress on Molecular Spectroscopy

PROGRAMME AND ABSTRACTS



WELCOME TO TURCMOS 2013

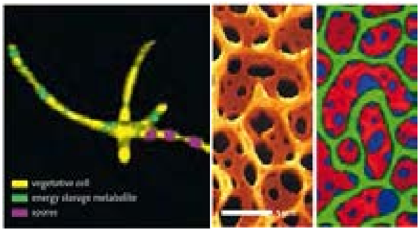
On the behalf of the Scientific Committee and Organizing Committee, we would like to welcome you all to the “International Turkish Congress on Molecular Spectroscopy (TURCMOS2013)”. The scope of the congress is to encourage the exchange of ideas and future collaborations all around the world, introduce new techniques and instruments, and present recent developments in this field of research. In the congress, all aspects of spectroscopic methods as well as related computational and theoretical approaches will be considered. Contacts between young researchers (M.Sc. and Ph.D.) and prominent experts will be particularly stimulated, aiming at the development of future collaborations.

We hope that the congress will provide you intellectual and social experience. We wish you enjoyable week in İstanbul where the continents meet.

Ozan ÜNSALAN
President of TURCMOS2013

Gülce ÖĞRÜÇ ILDIZ
Vice President of TURCMOS2013

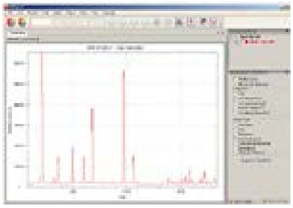
Konfokal Raman ve Scanning Probe Mikroskopi

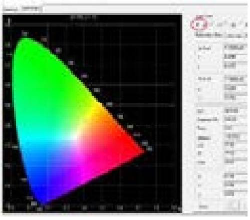


Çalışma Modları

- **Konfokal Mikro Raman Spektroskopisi**
  - ✓ 2D-3D Konfokal Raman Görüntüleme
  - ✓ Derinlik profili
  - ✓ Floresans Görüntüleme
  - ✓ Fotolüminesans Görüntüleme
- **AFM**
  - ✓ Contact, AC, dPFM,ve diğer modlar
- **SNOM**
  - ✓ TERS
- **Time Correlated Single Photon Counting**
  - ✓ FLIM & TLM

Portatif Raman & UV-VIS-NIR Spektrometreler





Portatif Raman Spektrometre Sistemleri

Uyarım : 532, 785, 830, 1064 nm
Resolüsyon : 3 nm'ye kadar
Dedektörler : TE soğutmalı CCD ve InGaAs
Aksesuarlar
- ○ Reaksiyon probları
- ○ Hücre tutucular
- ○ Akış hücreleri
- ○ Mikroskop

Modüler UV - VIS - NIR Spektrometreler

Bölge : UV-VIS & NIR
Resolüsyon : 0.3 nm
Dedektörler : TE soğutmalı CCD, PDA, InGaAs
Aksesuarlar
- ○ Reaksiyon probları
- ○ Hücre tutucular
- ○ Akış hücreleri
- ○ Integrating Sphere
- ○ Multiplexer

TETRA TEKNOLOJİK SİSTEMLER LTD. ŞTİ.

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List of Topics

The congress will include the scientific topics below:

1. Vibrational (IR and Raman) and Electronic Spectroscopies
2. Electron Spin Resonance (ESR) Spectroscopy
3. Mössbauer Spectroscopy
4. Fluorescence Spectroscopy
5. Microspectroscopy and Imaging
6. Surface Enhanced Raman Spectroscopy (SERS)
7. Microwave Spectroscopy
8. Terahertz Spectroscopy
9. Applied Spectroscopies (Archaeology, Geology, Astrophysics, Mineralogy, Arts & History, Environmental Analysis, Food Analysis and Processing, Applications on Biology, Forensic Sciences)
10. Matrix Isolation Infrared Spectroscopy and Low Temperature Spectroscopy
11. Theoretical and Computational Methods
12. Analytical Methods and New Instrumentation
13. Spectroscopy in Drug Design and Drug Discovery
14. New Materials (Nanostructured and Supramolecular Systems, Molecular Electronics and Optoelectronics, Magnetic Materials)

Countries of Participants

Turkey
Russia
Netherlands
Bosnia and Herzegovina
Algeria
Azerbaijan
United States
Sweden
Germany
Malaysia
Hungary
Portugal
Greece
Czech Republic
Austria
South Korea
Poland
United Kingdom
Bulgaria
Romania
Japan
Ukraine

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(Names are in alphabetical order)

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TURCMOS 2013

International Turkish Congress on Molecular Spectroscopy

PROGRAMME

PROGRAMME

HALL 1

Monday, the 16th of September	
09:00 09:30	OPENING CEREMONY
09:30 10:20	Chair: Rui FAUSTO PL1-Peter PULAY
10:20 11:10	PL2-Weitao YANG
11:10 11:30	CB
11:30 12:20	PL3-Juergen POPP
12:20 14:00	LB
14:00 14:20	Chair: E.J. BAERENDS O1-György MAROSI
14:20 14:40	O2-Iryna GONCHAROVA
14:40 15:00	O3-Young Mee JUNG
15:00 15:20	CB
15:20 15:40	Chair: Igor REVA O4-Özgür BİRER
15:40 16:00	O5-Stephan KUPFER
16:00 16:20	O6-Attila FARKAS
16:30 18:30	COCKTAIL (WELCOME PARTY)

Tuesday, the 17th of September	
09:00 09:50	Chair: Peter PULAY PL4-Rui FAUSTO
09:50 10:40	PL5-Michael OSHTRAKH
10:40 11:00	CB
11:00 11:50	PL6-Maral SÜNNETÇİOĞLU
11:50 13:00	LB
13:00 13:20	Chair: James DURIG O7-Igor REVA
13:20 13:40	O8-Hinrich GROTHE
13:40 14:00	O9-Maria MIERZEJEWSKA
14:00 14:20	CB
14:20 14:40	Chair: M. SÜNNETÇİOĞLU O10-Semira GALIJASEVIC
14:40 15:00	O11-Mustafa KOCADEMİR
15:00 15:20	O12-Iryna GONCHAROVA
15:20 15:40	O13-Theodore GANETSOS
15:50 16:20	RENISHAW PRESENTATION (Pierre GRAVE)
16:20 18:20	POSTER SESSION 1

Wednesday, the 18th of September	
09:00 09:50	Chair: W.YANG PL7-E.J. BAERENDS
09:50 10:40	PL8- Feride SEVERCAN
10:40 11:00	O14-Hamit YURTSEVER
11:00 11:30	LB
	EXCURSION Istanbul City Tour Sultanahmet Avenue Topkapı Palace Hagia Sophia Beyazıt Tower Çemberlitaş Grand Bazaar Suleymaniye Mosque

Thursday, the 19th of September	
09:00 09:50	Chair: Juergen POPP PL9-James DURIG
09:50 10:40	PL10- Mustafa BÖYÜKATA
10:40 11:00	CB
11:00 11:20	Chair: F. SEVERCAN O15-Irina ALENKINA
11:20 11:40	O16-Michael OSHTRAKH
11:40 13:00	LB
13:00 13:20	Chair: M. OSHTRAKH O17-Mizuki TSUTA
13:20 13:40	O18-Hinrich GROTHE
13:40 14:00	O19-Artem SMOLENTSEV
14:00 14:20	CB
14:20 14:40	Chair: M. BÖYÜKATA O20-Dilek YONAR
14:40 15:00	O21-Volker STRAUSS
15:00 15:20	O22-Güventürk UĞURLU
15:20 15:40	O23-Semiha BAHÇELİ
15:50 17:50	POSTER SESSION 2
19:00 21:00	GALA DINNER

Friday, the 20th of September	
09:00 09:20	Chair: H. GROTHE O24-Marc RUDOLF
09:20 09:40	O25-Rabia YERLİ
09:40 10:00	O26-Sergei VDAVENKO
10:00 10:20	O27-Emre ERDEM
10:20 10:40	CB
10:40 11:00	Chair: H. YURTSEVER O28-Güventürk UĞURLU
11:00 11:20	O29-Cem LİDER
11:20 11:40	O30-Emine ER
11:40 12:00	CB
12:00 12:20	Chair: S. BAHÇELİ O31-Yunus ÇELİK
12:20 12:40	O32-Tayyibe BARDAKÇI
12:40 13:00	O33-Balázs BUCHHOLCZ
13:00 13:20	O34-H. BERRICHE
	CLOSING CEREMONY ANNOUNCEMENT OF TURCMOS2015

PL: Plenary Lecture
O: Oral Presentation
CB: Coffee Break
LB: Lunch Break

Monday, the 16th of September, 2013

09:00-09:30	Opening Ceremony
09:30-10:20	**PL1 -** Ultrafast QM/MM simulations of molecular spectra: The conformation of 5 bromo-uracil in aqueous solution, and other applications ***by Peter Pulay, György Tarczay***
10:20-11:10	**PL2 -** Exchange-Correlation Energies from Paring Matrix Fluctuation and Particle-Particle-Random Phase Approximation ***by Weitao Yang***
11:10-11:30	Coffee Break
11:30-12:20	**PL3 -** Raman-based approaches for biomedical diagnosis ***by Juergen Popp***
12:20- 14:00	LUNCH (Lunchbox)
14:00-14:20	**O1 -** Raman spectrometry assisting the investigations of pharmaceutical products and processes ***by György Marosi***
14:20-14:40	**O2 -** Bioactivity of silver(I) complexes: study by electronic and vibrational circular dichroism spectroscopy ***by Iryna Goncharova***
14:40-15:00	**O3 -** 2D correlation spectroscopy in protein research ***by Young Mee Jung, Boguslawa Czarnik Matusewicz***
15:00-15:20	Coffee Break
15:20-15:40	**O4 -** Infrared Spectroscopy of HCl and H2O Aggregates at Ultracold Temperatures ***by Anna Gutberlet, Gerhard Schwaab, Ozgur Birer, Marco Masia, Anna Kaczmarek, Harald Forbert, Martina Havenith, Dominik Marx***
15:40-16:00	**O5 -** Electron storage in noval 4H-imidazol Ruthenium complexes assessed with TDDFT simulations and resonance Raman spectroscopy ***by Stephan Kupfer, Linda Zedler, Inês Rabelo De Moraes, Sven Krieck, Rainer Beckert, Michael Schmitt, Jürgen Popp, Benjamin Dietzek***
16:00-16:20	**O6 -** Investigation of trace amounts of drug by surface enhanced Raman chemical imaging supported by MCR-ALS method ***by Attila Farkas, Tamás Firkala, Balázs Vajna, György Marosi***
16:30-18:30	Coktail (Welcome Party)

Tuesday, the 17th of September, 2013

09:00-09:50	**PL4 -** Strategies for Conformational Selection in Cryogenic Inert Matrices: Case Studies ***by Rui Fausto***
09:50-10:40	**PL5 -** Applications of Mössbauer Spectroscopy with a High Velocity Resolution ***by Michael I. Oshtrakh, Vladimir A. Semionkin***
10:40-11:00	Coffee Break
11:00-11:50	**PL6 -** Electron Paramagnetic Resonance (EPR) spectroscopy in biological sytems ***by M. Maral Sünnetçioğlu***
11:50-13:00	LUNCH (Lunchbox)
13:00-13:20	**O7 -** Light-Induced Reactions of Matrix-Isolated Heterocycles ***by Igor Reva***
13:20-13:40	**O8 -** Matrix isolation studies of carbonic acid - the vapour phase above the two polymorphs ***by Hinrich Grothe, Roland G. Huber, Klaus R. Liedl, Jürgen Bernard, Thomas Loerting***
13:40-14:00	**O9 -** Photochemical transformations of 5-methyltetrazole. FT-IR matrix isolation and DFT studies ***by Maria Wierzejewska, Magdalena Pagacz Kostrzewa, Justyna Krupa***
14:00-14:20	Coffee Break
14:20-14:40	**O10 -** Melatonin interactions with copper (II) ion: Spectroscopic and DFT theoretical studies ***by Semira Galijasevic, Vedran Ljevarevic, Vera Dugandzic***
14:40-15:00	**O11 -** Determination of structural and vibrational properties of quinoline-7-carboxaldehyde using experimental FT-IR, FT-Ra and dispersive-Ra techniques and theoretical HF and DFT calculations ***by Mustafa Kumru, Mustafa Kocademir, Levent Sarı***
15:00-15:20	**O12 -** Bioactivity of silver(I) complexes: study by electronic and vibrational circular dichroism spectroscopy ***by Iryna Goncharova***
15:20-15:40	**O13 -** Raman investigation of (CdZn)Te, (CdTe)In and (CdTe)Cl bulk single crystals for Gamma-ray Detectors ***by Theodore Ganetsos, Eduard Belas, Lukas Cedivy, Bill Kotsos, Nikolaos Laskaris***
15:50-16:20	RENISHAW PRESENTATION (Pierre GRAVE)
16:20-18:20	Poster Session 1

P1	Comparison of Thermal and IR Spectroscopy Methods for Determination Amount of Residual Monomer in Dental Composite Materials	Ceren Koser, Sevi Öz, Adil Nalçacı, Orhan Atakol
P2	The Use of Vibrational Spectroscopy in Biophysical Characterizations of Novel Non-Viral Lipoplex Gene Delivery Systems	Nuraniye Eruygur, Erhan Süleymanoğlu
P3	Effects of Thalium Element on Radiation Absorption and Microstructures Properties the Casting Al-Zn Alloy	Emine Aldırmaz, Betül Mavi, Iskender Akkurt, Ilhan Aksoy
P4	Experimental Investigations of Linear Attenuation Coefficients at 662, 1173 and 1332 keV Energies in Cu-Mn-Al alloy	Betül Mavi, Emine Aldırmaz, Iskender Akkurt, Ilhan Aksoy
P5	Analytical Studies of The Thracian Tomb Wall Paintings at Alexandrovo	Zornitza Glavcheva, Denitsa Yancheva, Evelina Velcheva, Bistra Stamboliyska, Georgi Lalev, Valentin Todorov

Tuesday, the 17th of September, 2013

P6	Synthesis, Structural Characterization, Thermal and Biological Analyses of (C14H18N2O4)Cu+2(C7H7SO3) Complex	Akif Arslan, Ömer Çelik, Sevtap Keser, Sedat Köstekçi, Tuba Kıyak, Mehmet Aslantaş
P7	The Spectroscopic characterization of some Ru(III) complexes with Schiff bases derived from salicyladehyde and investigation of interaction with CT DNA	Adnan Zahirovic, Sabina Begic Hairlahovic, Nevzeta Ljubijankic, Emir Turkusic, Emira Kahrovic
P8	Optical luminescence studies of the ethyl xanthate adsorption layer on the surface of sphalerite minerals	Radu Todoran, Daniela Todoran, Zsolt Szakacs
P9	Nonionic and Zwitterionic Forms of Glycylglycylarginine Part of Spider Silk Protein: Structural and Vibrational Spectroscopic Search	Hatice Arı, Talat Özpozan
P10	Structural and Vibrational Studies on Nonionic and Zwitterionic Forms of Glycylglycylglutamine Part of Spider Silk Protein	Hatice Arı, Talat Özpozan
P11	Spectroscopic analysis of the impact of oxidative stress on the structure of human serum albumin (HSA) in terms of its binding properties	Malgorzata Maciazek Jurczyk, Joanna Równicka Zubik, Agnieszka Szkudlarek Hasnik, Anna Sulkowska
P12	Determination of Natural Radionuclide Concentration of Some Metamorphic Rock in Turkey	Kadir Günoğlu, İskender Akkurt
P13	The photon attenuation coefficients of Self Compacting Concrete (SCC	İskender Akkurt, Hüseyin Yılmaz Aruntaş, Ahmet Beycioğlu, Kadir Günoğlu
P14	FTIR-Chemometric methodology for the prediction of the heat stability of extra virgin olive oil	Soraya Nigri, Rabah Oumeddour
P15	Mineralogic characterization of Limestone, Jebel Kellel, north-east Constantine	Mounia Benguedouar, Merzoug Bouchear, Chaouki Benabbas, Chaouki Benabbas
P16	Mineralogic characterization of sandstone and clay, Jebel Kellel, north-east Constantine	Mounia Benguedouar, Samia Kherfi, Merzoug Bouchear
P17	Explanation of 3d ions behavior in the aqueous solution of MgSO3.6H2O: M (M = Cr, Co or Cr+Co)	Ivaylo Parushev, Petya Petkova, Petko Vasilev, Veselin Nedkov, Jordanka Tacheva, Mohamed Toufik Soltani, Youri Tzukrovski
P18	Temperature Effect on the Recovery Process of Stretched Bombyx Mori Silk Fibers	Baki Aksakal
P19	Pollutant identification on the walls of "Valence Aqueduct" (Bozdoğan Kemeri, İstanbul) by portable handheld Raman, SEM-EDX, Far-infrared and Mid-infrared techniques	Ozan Unsalan, Alpaslan Kuzucuoğlu, Ayberk Yılmaz, Olcay Bölükbaşı, Gülder Emre

Tuesday, the 17th of September, 2013

P20	Far-infrared, Mid-infrared, Raman and SEM-EDX investigations on pigments from pallette of old paintings by Feyhaman Duran and comparison with organic pigments	Ozan Unsalan, Gülder Emre, Ayberk Yılmaz, Alpaslan Kuzucuoğlu, Gözem Yaşayan
P21	FT-IR spectroscopic investigation of bipolar patients' blood samples	Gülce Öğrüç Ildız, Ozan Unsalan, Ayberk Yılmaz
P22	The EPR Study Of Mn2+ Ion Alloyed KBr and VO2+ Ion Alloyed KH2PO4 Single Crystals Under High Pressure	Ümit Ceylan, Recep Tapramaz
P23	The EPR Study Of Mn2+ Ion Alloyed DADT Single Crystal Under High Pressure	Ümit Ceylan, Recep Tapramaz
P24	EPR study of Cu2+ ion doped orotato(nicotinamid) cobalt(II) single crystal	Ilkay Yildirim, Bünyamin Karabulut, Orhan Büyükgüngör
P25	Diffusion Energies and Oxygen Diffusion Coefficients of Porous Silicon	Önder Yargı, Süreyya Aydın Yüksel, Ali Gelir, Kenan Koç
P26	FRET study and G-quadruplex folding ability of fluorescent oligonucleotide probes at the Langmuir monolayer interface	Bernard Juskowiak, Angelika Swiatkowska
P27	Transport of gliclazide by serum albumin altered in diabetes: Spectroscopic analysis	Agnieszka Szkudlarek Hasnik, Joanna Równicka Zubik, Malgorzata Maciazek Jurczyk, Anna Sulkowska
P28	Elucidation of the Porous Size Dependence of the Oxygen Diffusion into Porous Silicon by Using Fluorescence Technique	Önder Yargı, Ali Gelir, Süreyya Aydın Yüksel, Kenan Koç
P29	New fluorogenic substrate for DNAzyme with peroxidase-like activity	Bernard Juskowiak, Yu Tang Wu, Joanna Kosman
P30	Spectrofluorimetric determination of Nateglinide in pure and pharmaceutical preparations through derivatization with 4-chloro-7-nitrobenzo-2-oxa-1,3-diazole	Ayça Karasakal, Sevgi Tatar Ulu
P31	New Spectrofluorimetric Method for the Determination of Nizatidine in bulk form and in Pharmaceutical preparations	Ayça Karasakal, Sevgi Tatar Ulu
P32	FTIR matrix isolation and DFT studies of thermal decomposition and photochemistry of (tetrazol-5-yl)acetic acid	Magdalena Pagacz Kostrzewa, Justyna Krupa, Maria Wierzejewska
P33	Ultraviolet-Tunable Laser Induced Transformations of Matrix Isolated Safrole. The First Example of the Allyl Group Photorotamerization	Justyna Krupa, Maria Wierzejewska
P34	Ultraviolet-tunable Laser Induced Phototransformations of Matrix Isolated Isoeugenol and Eugenol	Justyna Krupa, Adriana Olbert Majkut, Igor Reva, Rui Fausto, Maria Wierzejewska

Tuesday, the 17th of September, 2013

P35	Conformational properties and photochemistry of allyl tetrazoles in low-temperature matrices	Magdalena Pagacz Kostrzewa, Malgorzata Mucha, Marek Weselski, Maria Wierzejewska
P36	Low Temperature Matrix-Isolation of Methyl Paraben: FTIR, DFT and Photochemistry Studies	Nihal Kuş, Sevgi Haman Bayarı, Rui Fausto
P37	Matrix Isolation Infrared Spectra and Photochemistry of Hydantoin	Gulce Ogruc Ildiz, Claudio M. Nunes, Rui Fausto
P38	Some projects at the infrared microspectroscopy beamline D7 at the MAX IV laboratory	Anders Engdahl
P39	Study of Ferritin Iron Cores in the Rhizobacterium Azospirillum Brasilense Sp245 Using Mössbauer Spectroscopy with a High Velocity Resolution	Alexander Kamnev, Irina Alenkina, Michael Oshtrakh, Anna Tugarova, Borbála Biró, Vladimir Semionkin
P40	A Comparative Study of Troilite Extracted from Sikhote-Alin Iron Meteorite and in Some Bulk Ordinary Chondrites Using Mössbauer Spectroscopy with a High Velocity Resolution	Michael I. Oshtrakh, Zoltan Klencsár, Evgeniya V. Petrova, Victor I. Grokhovsky, Ernö Kuzmann, Zoltan Homonnay, Vladimir A. Semionkin
P41	Structural and Optical Properties of Si3N4 Thin Films Deposited by RF Magnetron Sputtering	Ümran Ceren Başköse, Gürkan Kurtuluş, Saime Şebnem Çetin, Semran Sağlam, Süleyman Özçelik
P42	Structural characterization, spectroscopic, magnetic, and electrochemical studies of monomer N-substituted-sulfanilamide copper(II) complex with 2,2'-bipyridine	Filiz Öztürk, Ahmet Bulut, İclal Bulut
P43	Phonon and magnetic properties of Ni(II) and Fe(III) doped CoCr2O4	Maciej Wojciech Ptak, Miroslaw Maczka, Jerzy Hanuza
P44	Optic Absorption of GaSe<B,Dy> Thin Films	Alim Dinçer, Nizami Mammadov, Elara Mammadova, Hüseyin Ertap, Hasan Mammadov, Mevlüt Karabulut
P45	Effect of UV-light on the Uniaxial Tensile Properties of TiO2 coated Bombyx Mori Silk Fibers by Sol-Gel Method	Baki Aksakal, Kenan Koç, Önder Yargı, Katherina Tsobkallo
P46	Investigation of Structural and electronic properties of ternary Co-Pt-B clusters	Meryem Evecen, Mustafa Böyükata, Ziya B. Güvenç
P47	Synthesis and Characterization of Halogen Containing Aryl Amide Polymer-Clay Composites	Murat Alparslan, Ali Delibaş
P48	Rutherford Backscattering Spectroscopy Study Of Antimony Electrical Activation In Si(111) Samples	Rebiha Labbani, Hamza Serrar, Chawki Benazzouz
P49	An open three-dimensional Paul trap for the separation of the calcium isotopes at King Khalid University	Mustapha Said Herbane, Hamid Berriche, Gadha Al Shahrani, Gilles Ban

Tuesday, the 17th of September, 2013

P50	Detection of DNA mutations using novel surface-enhanced Raman spectroscopy (SERS) diagnostic platform	Agnieszka Michota Kaminska, Evelin Witkowska, Arumugam Sivanesan, Janusz Weyher, Igor Dziecielewski, Jakub Go&;&6;b, Dominika Nowis
P51	Detection and identification of bacterial cells in blood samples on gold-silver hybrid SERS substrate	Evelin Helena Witkowska, Agnieszka Michota Kaminska, Lukasz Dziewit, Sivanesan Arumugam, Jacek Waluk
P52	Concentration Based Measurement Studies of L-Tryptophan using THz-Time Domain Spectroscopy	Zeynep Özer, Seher Gok, Hakan Altan, Feride Severcan
P53	The DFT and Vibrational Studies of Sudan Red G	Aslı Eşme, Seda Güneşdoğdu Sağdınç
P54	Theoretical and Experimental IR Studies on a Series of Azophenols and their Respective Ester Molecules Serving in Nonlinear Optics	Siham Naima Derrar, Majda Sekkal Rahal, Badra Bensekrane, Kaddour Guemra
P55	Molecular structure and vibrational and chemical shift assignments of 3'-chloro-4-dimethlamino azobenzene by DFT calculations	Mehmet Toy, Hasan Tanak
P56	Theoretical investigation of 2'-chloro-4-dimethlamino azobenzene: MEP, FMO and NLO analysis, FT-IR, UV-Vis and NMR spectra	Mehmet Toy, Hasan Tanak
P57	Spectrocopic investigations (FT-IR, NMR and UV-Vis) and quantum chemical studies of 4'-chloro-4-dimethlamino azobenzene	Hasan Tanak, Mehmet Toy
P58	Molecular structure and vibrational assignment of 1-[N-(2-pyridyl) aminomethylidene}-2(1H)-Naphtalenone by density functional theory (DFT) and ab initio Hartree-Fock (HF) calculations	Hasan Tanak, Mehmet Toy
P111	Experimental and Quantum Chemical Study on 1-Methylindole	Çağlar Karaca, Ahmet Ataç, Mehmet Karabacak
P116	The natural radioactivity of some soil sample of Pamukkale region by using gamma spectroscopy	İskender Akkurt, Kadir Günoğlu, Feride Kulalı
P117	Investigation of Gamma-Ray Shielding Properties of Plasters Containing Different Boron Compounds	İskender Akkurt, Kadir Günoğlu, Raşit Altındağ, Hakan Sarıkaya
P136	Theoretical self-broadening and self-shifting coefficients of 12C2H2 transitions in the 3v5, (2v4+v5)I and (2v4+v5)II bands	Souhail Galalou, Hassen Aroui
P147	Micro-Raman, Mid-IR, Far-IR and DFT studies on 2-[4-(4-Fluorobenzamido)phenyl]benzothiazole	Unsalan, O., Sert, Y.b, Ari, H., Simão, A., Yilmaz, A., Boyukata M., Bolukbasi, O., Bolelli, K., Yalcin I.

Wednesday, the 18th of September, 2013

09:00-09:50	**PL7 -** Beyond DFT: density matrix functional theory for ground state and excited state energy surfaces ***by Evert Jan Baerends***
09:50-10:40	**PL8 -** Infrared Spectroscopy and Imaging in Diagnosis and Screening ***by Feride Severcan***
10:40-11:00	**O14 -** Temperature Dependence of the Bragg Peak-Intensity Close to the Alpha-Incommensurate-Beta Transition in Quartz ***by Hamit Yurtseven, Koray Kaymazlar***
11:00-11:30	LUNCH (Lunchbox)
	EXCURSION (Istanbul City Tour) - Sultanahmet Avenue - Topkapı Palace - Hagia Sophia - Beyazıt Tower - Çemberlitaş - Grand Bazaar - Suleymaniye Mosque

Thursday, the 19th of September, 2013

09:00-09:50	**PL9 -** Conformation determination by Raman and infrared spectra of variable temperatures of xenon solutions ***by James Durig***
09:50-10:40	**PL10 -** Structural and Energetic Stability of Metal Doped Wheel Boron Clusters ***by Mustafa Böyükata, Ziya B. Güvenç***
10:40-11:00	Coffee Break
11:00-11:20	**O15 -** A Possibility to Distinguish Different Microenvironments in the Nanosized Iron Cores in Human Liver Ferritin and its Pharmaceutical Model Ferrum Lek on The Basis of Temperature Dependent Unusual Line Broadening of Mössbauer Spectra ***by Michael Oshtrakh, Irina Alenkina, Ernö Kuzmann, Zoltan Klencsár, Vladimir Semionkin***
11:20-11:40	**O16 -** Study of Chelyabinsk LL5 Ordinary Chondrite Fragments Using Mössbauer Spectroscopy with a High Velocity Resolution ***by Michael Oshtrakh***
11:40-13:00	LUNCH (Lunchbox)
13:00-13:20	**O17 -** Hyperspectral scatter imaging for the spectral decomposition of multi-layered materials ***by Mizuki Tsuta, Kaori Fujita, Mario Shibata, Masatoshi Yoshimura, Mito Kokawa, Junichi Sugiyama***
13:20-13:40	**O18 -** Observing the Microstructure of Bitumen by Fluorescent Spectroscopy and Microscopy ***by Hinrich Grothe, Florian Handle, Daniel Grossegger, Suanna Neudl***
13:40-14:00	**O19 -** Fluorescent properties of azacrown-containing styryl derivative of naphthopyran: ion-binding response and photochemical switching ***by Artem Smolentsev, Evgenii Glebov, Valerii Korolev, Olga Fedorova***
14:00-14:20	Coffee Break
14:20-14:40	**O20 -** Investigation of cis-(Z)-flupentixol dihydrochloride (FLU) interaction with PC liposomes in presence and absence of cholesterol by EPR spin labeling and DSC techniques ***by Dilek Yonar, M. Maral Sünnetçioğlu***
14:40-15:00	**O21 -** Ultrafast Time-Resolved Spectroscopy with Supramolecular Assemblies based on Carbon Nanostructures – Insights into Charge Transfer Reactions ***by Volker Strauss, Thomas Chamberlain, Andrei N. Khlobystov, Dirk M. Guldi***
15:00-15:20	**O22 -** Electronic Structure, Non-Linear Properties and NMR-Structural Analysis of Nicotinic Acid (ortho, meta and para –Hydroxy-Benzylidene)-Hydrazides: Computational Studies ***by Güventürk Uğurlu, Burcu Özcan, Hacali Necefoğlu***
15:20-15:40	**O23 -** Spectroscopic (Vibrational, NMR and UV-Vis.) and Quantum Chemical Investigations on 4-Hexyloxy-3-methoxybenzaldehyde ***by Halil Gökce, Semiha Bahçeli, Ashgar Abbas***
15:50-17:50	Poster Session 2

P59	Laser Flash Photolysis- Time Resolved Infrared Spectroscopy on the Photooxidation of Triarylphosphines Combined with DFT Computations	Shinro Yasui, Md. Mizanur Rahman Badal, Shinjiro Kobayashi, Masaaki Mishima
P60	Validity of HOMO/LUMO approach calculations: DFT study of chemical reactivity of melatonin and its metabolites: N1-acetyl-N2-formyl-5-methoxy kynuramine and N1-acetyl-5-methoxykynuramine	Semira Galijasevic, Elvisa Hodzic
P61	Computational Investigation of Interactions Between Some Polyaromatic Hydrocarbons and Porphyrin	Zeliha Gamze Alp, Nursel Acar

Thursday, the 19th of September, 2013

P62	Vibrational and Theoretical Investigation of [6,7-bis(2-methoxy-ethoxy)quinazoline-4-Yl]-(3-ethynylphenyl)amine (erlotinib)	Talat Özpozan, Özlem Mıhçıokur
P63	Conformational Analysis and Vibrational Study of n-(3-chloro-4fluoro-phenyl)-7-methoxy-6-(3-morpholin-4-ylpropoxy)-quinazolin-4-amine (gefitinib)	Özlem Mıhçıokur, Talat Özpozan
P64	Intermolecular hydrogen bonding interactions of dimethyl sulfoxide, ethylene and pyrrole with water	Turgay Polat
P65	Theoretical Studies on 1-(2,6-Dimethylphenylamino) propone-1,2-dione Dioxime	Serpil Eryılmaz, Aysin Zulfikaroglu
P66	Synthesis, Characterization and Theoretical Calculations of Bicylic Monoterpens α- pinene and Nitrile Oxide Compounds 1,3-Dipolar Cycloaddition Reaction	Serpil Eryılmaz, Melek Gul, Ersin Inkaya, Murat Tas
P67	Experimental and DFT Computational Studies on Bis[1-(2,6-dimethylanilino)propane-1,2-dionedioximato]nickel(II)	Aysin Zulfikaroglu
P68	Density functional theory studies and vibrational spectra of Tribromomesitylene	Soumia Ghanemi, Jean Miennel, Ali Boudjada
P69	Computational characterization of aromatic hydrocarbons involved in non-bonded interactions	Igor Reva
P70	The redox behavior of uranium metallocene complexes. A relativistic DFT/ZORA study	Belkhiri Lotfi, Zaiter Abdellah, Boucekkine Abdou
P71	Theoretical Analysis of Phenolic Components from the Extracts of Walnut (Juglans regia) Leaves	Lütfiye Aydın, Talat Ozpozan
P72	Electronic properties of II-VI semiconductor nanocrystals	Bariza Ellagoune
P73	FTIR and DFT Quantum Chemical Studies on Aurin	Sevgi Haman Bayarı, Semran Sağlam, Ümran Ceren Başköse
P74	Structural Study of 4-(2-morpholinoethanoylamino)-benzenesulfonamide by X-Ray Diffraction Experiment and DFT Calculations	Erol Eroğlu, Mustafa Durgun, Hasan Türkmen, Şerife Pınar Yalçın, Mehmet Akkurt
P75	Vibrational Spectral Analysis and Theoretical Investigation on the Molecular Structure of Isopropyltriphenylphosphonium Iodide (1-Methylethyl) triphenylphosphonium iodide)	T Raci Sertbakan
P76	Molecular Geometry, Vibrational Spectra (FT-IR, Raman, and NMR), Vibrational Assignments and Density Functional Theory (DFT) Calculations for 2,2/- Ethylenedianiline Molecule	Demet Kahraman, Hilal Sarikaya, M. Tahir Güllüoğlu
P77	Time-Dependent Density Functional Study on Variation of UV-Visible Spectrum of Poly(phospolo[3,4b]phosphole) as a Function of Substituent	Zeki Büyükmumcu, Ilknur Koçyiğit
P78	Theoretical Analysis of Substituent Effect on UV-Visible Spectrum of Poly(pyrrolo[3,4b]pyrrole)	Ilknur Koçyiğit, Zeki Büyükmumcu
P79	Structural and energetic analysis of ethyl 2-(3-benzoylthioureido)-acetate: a DFT study	Meryem Evecen, Mustafa Böyükata, Yusuf Sert
P80	Gaussian Calculations Of 3-Methyl-4-(3-Sinnamoyloxybenzylidenamino)-4,5-Dihydro-1H-1,2,4-Triazol-5-One Molecule	Haydar Yüksek, Murat Beytur
P81	The Investigation Of Spectroscopic Properties Of 3-Ethyl-4-(4-Sinnamoyloxybenzylidenamino)-4,5-Dihydro-1H-1,2,4-Triazol-5-One Compound Using B3LYP And Hf Basis Sets	Murat Beytur, Haydar Yüksek, Murat Tolga Kayalar
P82	Computation of Antimony Atoms Transmission Through Nanometric Foils	Rebiha Labbani

Thursday, the 19th of September, 2013

P83	Hydrogen bonds in sucrose crystal and its contribution to optical nonlinearity studied by IR, polarized Raman, IINS and NMR spectroscopy	Katarzyna Piela, Magdalena M. Szostak, Ireneusz Natkaniec, Krystyna Holderna Natkaniec
P84	Conformational and structural studies of n-propylamine from temperature dependent Raman and far infrared spectra of xenon solutions and ab initio calculations	Ikhlas D. Darkhalil, James R. Durig
P85	FT-IR and computational study of raffinose and melezitose	Boutasta Amel, Benosman Abdelhalim, Bekhti Nabila, Rahal Sekkal Madjda
P86	Study of the solvent effect on the molecular structure and C=O stretching vibrations of Michlers' ketone	Marta Sowula, Tomasz Misiaszek, Wojciech Bartkowiak
P87	Infrared, Raman and NMR spectra, conformational stability and vibrational assignment of 7-Hydroxy-4-(Trifluoromethyl)coumarin	Yusuf Erdogdu
P88	Structural and Vibrational Properties, Quantum Chemical Calculation of 2-(Triphenylphosphoranylidene) butyraldehyde	Yusuf Erdogdu
P89	Combined experimental-theoretical characterization of chelidamate nickel complex with 4-methylpyrimidine	Hatice Vural, Ibrahim Uçar, Serkan Soylu
P90	Synthesis, spectroscopic, thermal and structural properties of [M(3-Aminopyridine)2Ni(μ-CN)4]n (M = Co and Cu) heteropolynuclear cyano-bridged complexes	Zeki Kartal
P91	Comparing the effects of Valdecoxib, Rofecoxib and Celecoxib drugs on the model membrane properties using infrared spectroscopy, DSC and Turbidity techniques	Richardas Rachkauskas, Feride Severcan, Sreeparna Banerjee
P92	Characterization of the effect of selective COX-2 inhibitor Valdecoxib on the colon cancer cell lines using ATR-FTIR spectroscopy	Aysun Inan Genç, Sreeparna Banerjee, Feride Severcan
P93	Raman characterization of “Yannis Papadellis” colour’s collection	Thomas Katsaros, Theodore Ganetsos, Pavlos Samios
P94	FT-IR, FT-Raman and Molecular Structure Studies of Mirtazapine and its Comparison of Mianserin	Seda Sağdınç, Ayşe Erbay Şahintürk
P95	Synthesis, FT-IR spectroscopic, thermal and structural properties of M(4-Pyridinecarboxaldehyde)Ni(CN)4 complexes (M = Mn, Co, Ni, Cu and Cd)	Ömer İlhan Karatepe, Zeki Kartal
P96	Molecular structure and vibrational spectra of 7-Methylcoumarin by density functional method	Ebru Karakaş Sarıkaya, Ömer Dereli
P97	Vibrational spectral investigations of glyoxime	Ebru Karakaş Sarıkaya, Ömer Dereli, Fatih Sevgi
P98	Molecular structure and spectral investigations of 3-Aminocoumarin	Ömer Dereli
P99	Comparison of Experimental and Theoretical IR and UV Spectra of Some Benzimidazole Derivatives	Lütfiye Aydın, İbrahim Aydın, M. Orhan Püsküllü, İbrahim Narin
P100	Near-infrared spectroscopy for Co doped (80-x)Sb2O3-20Na2O-xWO3	Petya Petkova, Ivaylo Parushev, Petko Vasilev, Mohamed Toufik Soltani
P101	An Experimental and DFT Study on 1,3-Bis[2-(2-hydroxybenzylideneamino)phenoxy]propane: Vibrational Analysis and Solvent Effect on Prototropic Tautomerism	Hatice Arı, Selen Bilge, Hatice Kanbur Çavuş, Erol Eroğlu
P102	Molecular Structure and Vibrational FT-IR, FT-Raman, FT-NMR spectra Investigations of (2-hydroxyel) triphenylpphosphonium chloride	M Tahir Gulluoglu
P103	Experimental (FT-IR, FT-Raman, UV, 1H and 13C NMR) and computational (Density functional theory) studies on 3-bromophenylboronic acid	Ahmet Ataç, Etem Köse, Mehmet Karabacak, Mustafa Kurt

Thursday, the 19th of September, 2013

P104	Molecular structure, spectroscopic characterization (FT-IR, FT-Raman, UV and NMR), HOMO and LUMO analysis of 3,3Diaminobenzidene with DFT quantum chemical calculations	Mehmet Karabacak, Sibel Bilgili, Ahmet Ataç
P105	Differentation of Different Inbreed Obese Mouse Lines at Adipose Tissues By ATR- FTIR Spectroscopy With Chemometric Tools	Fatma Küçük, Ilke Sen, Onur Baloglu, Mete Severcan, Gudrun Brockmann, Feride Severcan
P106	FT-IR, FT-Raman, surface enhanced Raman scattering and computational study of 2-(p-fluorobenzyl)-6-nitrobenzoxazole	Y. Sheena Mary, Y. Sheena Mary, K. Raju, Tuğba Ertan Bolelli, Kayhan Bolelli, Ilkay Yıldız, Helena I.s. Nogueira, Carlos M. Granadeiro, Christian Van Alseony
P107	FT-IR, NMR, UV And Structural İnvestigations of 4-(2,5-Dİ(THİOPHEN-2-YL)-1H-PYRROL-1-YL)Aniline By Usıng Ab-Inıtıo Calculations	A. Ebru Tanboğa, Sevgi Özdemir Kart, Metin Ak, Hasan Hüseyin Kart
P108	Crystallographic, Spectroscopic and Computational Studies on (E)-2-(((3-bromophenyl)imino)methyl)-5-(diethylamino) phenol	Güneş Demirtaş, Necmi Dege, Erbil Ağar, Sümeyye Gümüş
P109	A First Look into Phenylephrine’s Conformational Landscape	C. Cabezas, A. Simão ,M. Varelaa and J. L. Alonso
P110	Infrared Reflection Absorption Spectroscopy for Characterization of Monolayers on Ceramic Surfaces	Xia Stammer
P112	Oxidative Effect Of Algerian Olive Oil Using Derivatives FTIR Spectroscopy and Chemometrics methods	Rabah Oumeddour
P113	Experimental and Theoretical Study of Novel Pyrrolo[1,2-α] perimidin-10-one dyes	İrfan Koca, Yunus Oruç, Mustafa Böyükata, Salih Cınaklı
P114	Investigation of N,N’ –’-Bis(salisiliden)-1,9-diamino nonane Schiff Base Complexes with different Ions by 1H-NMR Relaxation Time Measurements and Computional Studies	Arzu Ekinci, M. Zafer Köylü, Mustafa Böyükata, Hamdi Temel
P115	Molecular Structure Investigation And Spectroscopic Studies On 5-Bromo-2-Chlorotoluene: A Combined Experimental And Theoretical Analysis	Mehmet Karabacak, Tuğba Maviş, Ahmet Ataç
P118	Study of Interaction Metal Ion With Carbohydrates	Faiza Boukli Hacene, Meriem Merad, Wassila Soufi, Said Ghalem
P119	Interpretation of acoustics properties of Tellurite-based glasses	Touati Ibtissem, Hadjoub Zahia, Doghmane Abdelaziz
P120	Effect of nitrogen addition on the acoustical properties and the structure of oxynitride bioglasses	Hadjoub Fatiha, Boumaza Fatima
P121	Optoelectronic properties of SrxCd1-xO mixed crystals: FP-LAPW investigations	Labidi Salima, Labid Malika
P122	Density functional theory investigation of energy gaps and optical properties of SrTe1-xOx	Labidi Salima, Labidi Malika
P123	The effect of strontium concentration upon optical and dielectric properties of Pb1-xSrxS	Labidi Malika, Labidi Salima
P124	Calculation of structural, electronic, optical and thermodynamic properties of PbS, PbSe and their ternary alloy PbS1-xSex	Labidi Malika, Labidi Salima
P125	Single Cristal Materials Growth for Scintillation Applications	Farhi Hayet, Saida Chouf, Soliman Belkahla
P126	Impact of higher order effects on soliton pulse dynamics in optical fiber systems	Triki Houria, Hamaizi Yamina, El Akrmi Abdulsseltar
P127	Inhibition of the phosphathase Cdc25 by methods of molecular modeling	Wassila Soufi, Meriem Merad, Faiza Boukli, Said Ghalem

Thursday, the 19th of September, 2013

P128	The role of the trifluoromethyl group in reactivity and selectivity in polar cycloaddition reactions. A DFT study	Sobhi Sobhi Chafia, Djerouorou Abdelhafid
P129	TEM diffraction study of T1 phase precipitated in an Al-Li-Cu-Mg (Zr)	Halima Djaaboube, Djamila Thabet Khireddine
P130	The study of the order-disorder transition and hardening behavior in AuCuAg alloy	Amiour Leila, Hamana Djamel, Marie Noëlle Avettand Fénoë
P131	Radiative transport in a high pressure discharge using discrete ordinates method on a line-by-line basis	Elloumi Hatem, Ghrib Basma, Bouaoun Mohamed
P132	Fabrication and characterization of the Polystyrene / CdS nanocomposite	Harieche Barkahoum, Ouili Zeineddine, Boudjada Fahima, Boudine Boubekeur, Halimi Ouahiba, Sebais Miloud
P133	Analysis of Eucalyptus Essential Oils by Capillary Gas Chromatography / Fourier Transform Infrared Spectroscopy (GC / FTIR)	Yazid Foudil Cherif, Noureddine Yassaa, Brahim Youcef Meklati
P134	Detection and Characterization of Antioxydants from Artemisia herba-alba growing in Algeria	Nacéra Dahmani Hamzaoui, Sofia Salido, Pablo Linares Palomino, Aoumeur Baaliouamer, Joaquin Altarejos
P135	Study of surface chemistry of an oxidized activated carbon by spectroscopy FTIR, Boehm titration and methylene blue adsorption	Khelifi Aissa, Addoun Abdelhamid, Tamedrara Larbi
P137	Analytical transfer by rapid liquid chromatography method for quality control of a series of pharmaceuticals	Lynda Lamoudi, Kamel Daoud, Nassima Chérifi, Lamia Draoui
P138	An X-ray Absorption Study of Two GeCl3-Modified Silicas	Ziyad A. Taha, Susannah L. Scott
P139	Synthesys, Antimicrobial Activities And Spectroscopic Properties Of New Lanthanides Complexes With Furan hydrazone ligand Based	Abdulaziz M Ajlouni, Ziyad A Taha, Waleed M Al Momani
P140	Spectroscopic studies on N-((2-hydroxynaphthalen-1-yl) metylene)nicctinohydrazide (L) Lanthanide complexes in solid and solution	Ahmed Kamal Hijazi, Ziyad Taha, Abdulaziz Ajlouni, Fritz Kuehn, Eberhardt Herdtweck
P141	Fluorescence spectra of discharged obelin in the presence of exogenous compounds	Nadezhda Belogurova, Nadezhda Kudryasheva
P142	A comparative study on synthesized tricyclic pyrrolidinyl alcohol ligands: Determination of absolute configuration, spectroscopic and chiroptic properties	Mehmet Çinar, Engin Şahin
P143	The spectroscopic characterization of 5-methoxyindole-2-carboxylic acid: A combined density functional and experimental (NMR, UV, FT-Raman and FT-IR) study	Mehmet Çinar, Mehmet Karabacak
P144	Synthesis, characterization of nanostructured iron and manganese mesoporous molecular sieves catalysts	Adel Saadi, Kahina Lanasri, Khaldoun Bachari, Djamila Halliche, Chérifa Rabia
P145	Study of the stability of polymeric membrane by FTIR spectroscopy characterization	Sofiane Bensaadi, Mourad Amara, Omar Arous, Hacène Kerdjoudj
P146	Quantum-chemical, spectroscopic and X-ray diffraction studies on Diethyl [5-(4-methylbenzoyl)-4-(4-methylphenyl)-2-oxo-pyrimidin-1(2H)-yl] dithiocarbonimidate	Ersin İnkaya, Muharrem Dinçer, Emine Şahan, İsmail Yıldırım, Elif Korkusuz

Friday, the 20th of September, 2013

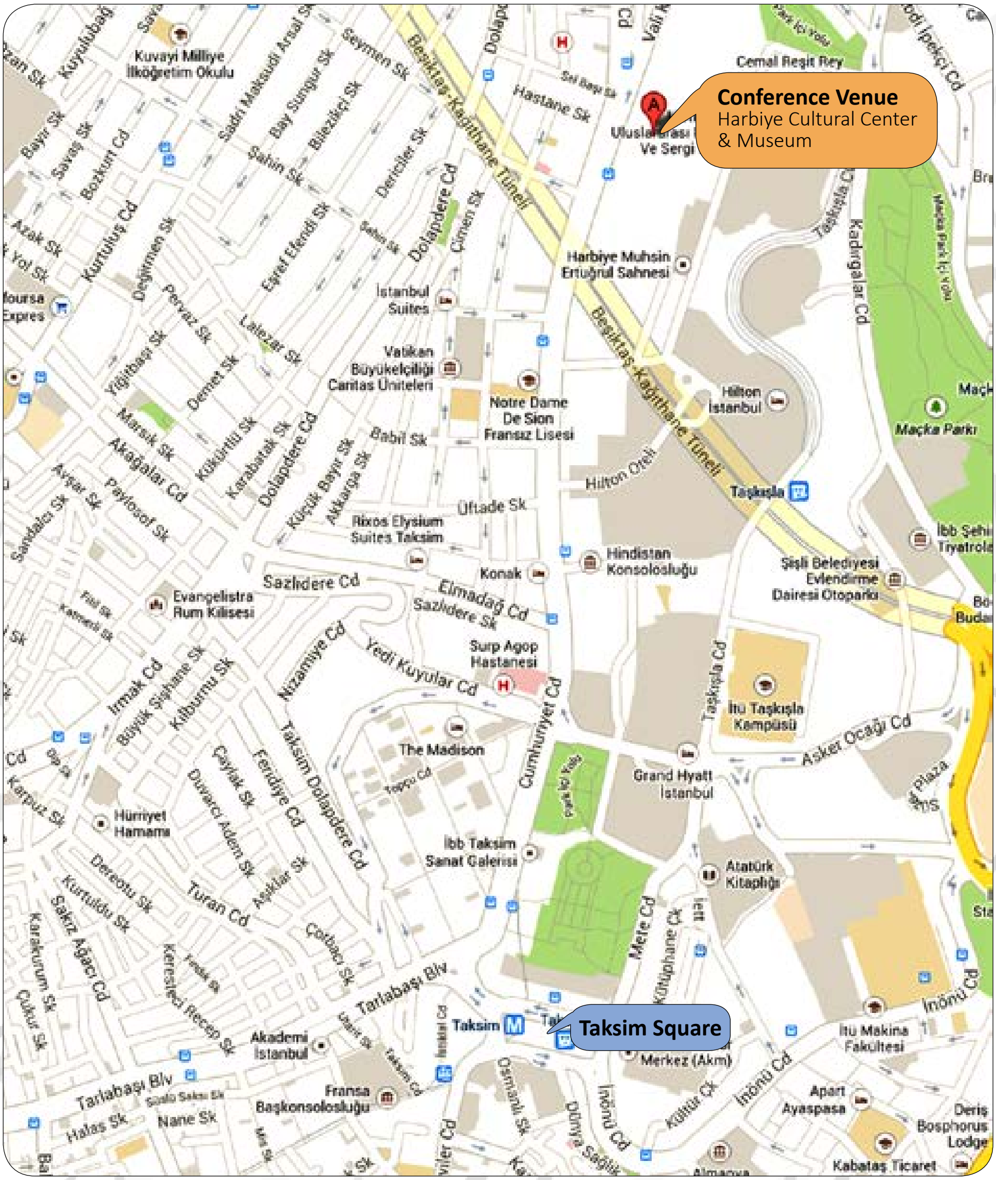
09:00-09:20	**O24 -** Coordinative Interactions between Phthalocyanines and Sc3N@C80 – Switchable Photoinduced Electron Transfer Reactivities ***by Marc Rudolf, Olga Trukhina, Tomas Torres, Dirk Michael Guldi***
09:20-09:40	**O25 -** Electron paramagnetic resonance study of radiation damage in isonipecotic acid single crystal ***by Betül Çalışkan, Ali Cengiz Çalışkan, Rabia Yerli***
09:40-10:00	**O26 -** Distinctive features of push-pull enaminoketones. α-Substitution in β-alkilaminovinyl perfluoromethyl ketones ***by Sergei Ivan Vdovenko, Yuri Zhuk, Igor Gerus, Valery Kukhar***
10:00-10:20	**O27 -** Controlling the defect centers in ZnO nanoparticles by multifrequency and ultra high field EPR spectroscopy ***by Suyan Tu, Stefan Weber, Emre Erdem***
10:20-10:40	Coffee Break
10:40-11:00	**O28 -** Theoretical Studies on Mono-, di-, tri- 2-[(4-Fluorophenly) Imino Methylene] Phenol ***by Güventürk Uğurlu, İsmail Çakmak***
11:00-11:20	**O29 -** Calculation of the Resonant Frequencies in the Vicinity of the Alpha-Beta Transition in Quartz ***by M. Cem Lider, Hamit Yurtseven***
11:20-11:40	**O30 -** Electron paramagnetic resonance of gamma irradiated single crystals of potassium hydroquinone monosulfonate ***by Betül Çalışkan, Ali Cengiz Çalışkan, Emine Er***
11:40-12:00	**O31 -** Molecular structure and EPR spectral studies of trans-Bis(perchlorato-κO) tetrakis(1-vinyl-1H-imidazole-κN3)copper(II) ***by Yunus Çelik, Kamil Küçük, Ramazan Şahin, Bünyamin Karabulut, Ömer Andaç, Necmi Dege***
12:00-12:20	**O32 -** Density Functional Calculations and Experimental Vibrational Spectral Studies of Free m-toluidine and its Copper(II) Chloride Complex ***by Tayyibe Bardakçı, Mustafa Kumru***
12:20-12:40	**O33 -** Investigation of the effects of nitrogen-doped titanate nanotubes by UV-Vis and Raman spectroscopy ***by Balázs Buchholcz, Zoltán Kónya, Zoltán Kónya, Ákos Kukovecz, Ákos Kukovecz***
12:40-13:00	**O34 -** Theoretical Electronic Structure and Spectroscopic investigations of CsRg (Rg=Rare gas) van der Waals Complexes by ***H. Berriche, M. S. Herbane, J. Dhiflaoui, C. Ghanmi, A. G. Al-Sehimi, and M. C. Heaven***

13:00	Closing Ceremony ANNOUNCEMENT OF TURCMOS2015

TURCMOS 2013
International Turkish Congress
on Molecular Spectroscopy

SITE PLANS AND PRACTICAL INFORMATIONS

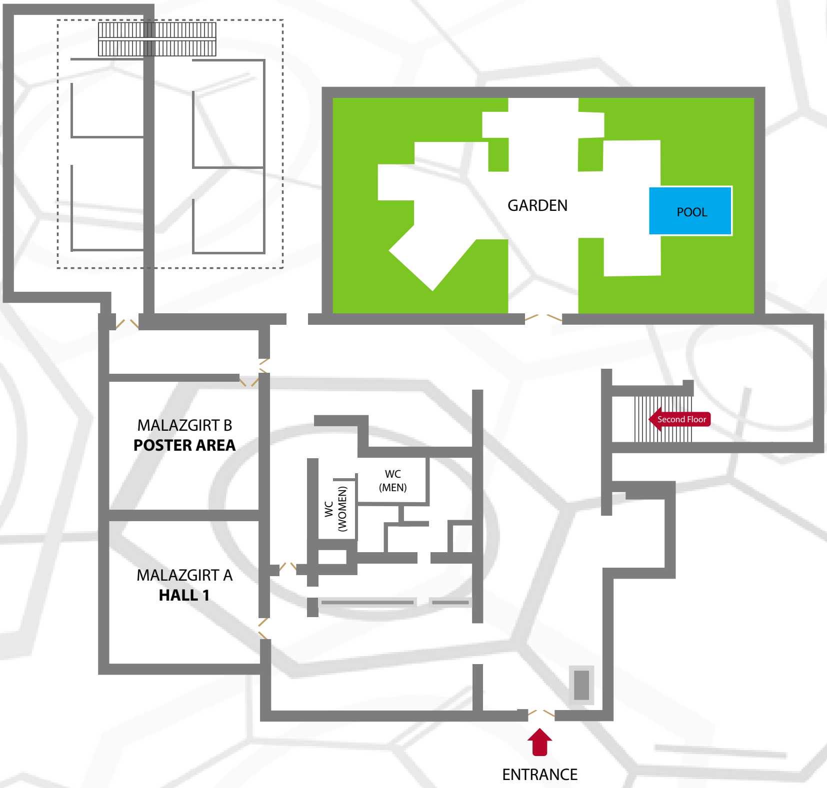
VENUE LOCATION



Conference Venue
Harbiye Cultural Center
& Museum

Taksim Square

FIRST FLOOR PLAN



PRACTICAL INFORMATIONS

Conference Venue

Harbiye Cultural Center & Museum
Valikonagi Caddesi, Harbiye
Istanbul, Turkey- 34298

Official Language:

The official language of the conference is English. No simultaneous translation will be provided.

Conference Venue Facilities

Halls

Congress meeting halls and registration desk located in Harbiye Cultural Center & Museum first level. The Poster Exhibition will take place in the same level.

Registration

Registration Desk (Harbiye Cultural Center & Museum) openning hours

16th of September	08:00-20:30
17th of September	08:00-19:00
18th of September	08:00-11:30
19th of September	08:00-19:00
20th of September	08:00-13:00

Name Badge

All participants should wear their name badge visible at all times in order to guarantee access to the scientific programme sessions, lunch area and to the social events.

Conference Certificate

You are welcome to print your personalized certificate of attendance at the Registration Desk.

Conference Assistants

In addition to the staff at the Conference Information Desk, a number of conference participants available all over the conference area are ready to help participants. They are wearing special T-shirts for easy recognition.

Audiovisual Equipment

All meeting rooms and auditoria are equipped with standard AV – equipment including PC, projector and screen. Conference assistants/volunteers will assist speakers with uploading of presentations. Please note that support for MAC computers will not be available.

Conference Proceedings

Participants will receive the book of the Conference Abstracts.

Poster Sessions

All poster sessions will take place in the Poster Area located in Harbiye Cultural Center & Museum first level.

Internet Access

You will be able to reach free internet access in congress venue.

Accessibility for Wheelchairs

Elevator is available. Personal assistance is provided too.

ATM/Cash Machines

There are branches of major banks very close to the congress venue (Cumhuriyet Street). You can have access to the ATM/Cash Machines there.

Accommodation & Tourist Information Desk

The accommodation and tour information desk is located in Registration Desk.

Language in the country

The official language is Turkish. English is widely spoken in major cities and especially in İstanbul.

Currency

TL (Turkish Lira) 1 Euro approximately equals to 2,50 Turkish Liras.

Sales Tax

Sales tax (VAT) is included in prices quoted. For non E.U. residents, tax free shopping schemes are available in many shops, which give substantial savings to visitors.

Shopping

Fine leather goods, golden and silver jewellery and textiles are considered excellent buys in İstanbul. The pedestrian streets of the city centre, “Taksim Square”, Nişantaşı (just 5 minutes walking distance from the congress venue) and “Grand Bazaar” in the old town Shops are open from 9:00 to 20:00

Monday to Sunday except Grand Bazaar (closed on Sundays). Major shopping malls stay open from 10:00 to 22:00, including weekends. Some of the famous shopping malls are Demirdöken, City's, Kanyon, İstinye Park and Cevahir.

Time Zone

GMT+2; CET +1; and EST (US-East) +7

Business Hours

The workweek in Turkey runs from Monday to Friday. Banks, government offices and majority of corporate offices open at 9 AM and close at 5 PM.

Visas

Visas are easily obtained upon arrival at the airport and are required for citizens of most countries.

Electricity

220V. European standard round two-pin sockets.

Health Services & Requirements

Cities and major touristic towns have a selection of private international and public hospitals with good standards. With the exception of vaccination certificates for persons coming from areas where yellow fever is endemic, at the present there are no special health requirements.

Smoking

The Turkish law, in accordance with the Regulations in force in the majority of European Countries and the USA, does not allow smoking in any public transportation or in any closed public areas.

Food

As with many Mediterranean nations Turkish food is very healthy, fresh and enjoyable.

Water

It is recommended that you consume bottled water, which is readily and cheaply available.

Communications

Turkey has three GSM operators, all of them offering 3G services and almost 95% coverage over the country. Internet service is available all around the country.

International Dial Code

+90

Hotel Check-in/out Policy

Normally check in time at hotels is 14:00. The established check out time is 12:00.

TURCMOS 2013

International Turkish Congress on Molecular Spectroscopy

PLENARY LECTURES

PL1 / 09:30 - 10:20 / Hall 1

Ultrafast QM/MM Simulations of Molecular Spectra: The Conformation of 5 Bromo-Uracil In Aqueous Solution, and Other Applications

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Molecules in solutions are generally treated by quantum mechanics/molecular mechanics (QM/MM) because of the high cost of the full quantum treatment. The solute is treated at QM level and the solvent at the inexpensive MM level. Even QM/MM is too expensive to obtain converged values for free energies in polar solvents (water) because millions of QM calculations are needed in Monte Carlo or Molecular Dynamics simulations. We have developed the Ultrafast QM/MM method [1] which is 104 – 105 times more efficient than traditional QM/MM, and is accurate to ~0.1 kJ/mol. Its essence is that the response of the system to the (irregular) electric field of the solvent is precalculated. No QM calculations are needed in the simulation. We have used this method so far to describe chemical reactions and NMR spectra in aqueous solutions. 5-bromo-uracil is a mutagenic agent. A potential mechanism for mutagenicity postulates that when substituted for thymine in DNA, the enol form binds to guanine instead of adenine, transforming an A-T base pair to G-C [2]. All good quantum calculations predict that the enol forms of 5-Br-U are ~10 kcal/mol more stable than the keto form. The Hobza group [3] carried out high-level calculations on the tautomeric forms, including the 5-Br-U…H2O complex, in vacuo and using a continuum solvation (COSMO) model, and concluded that the mechanism in [2] can be excluded. However, in a recent paper, van Mourik et al. [4] have optimized the geometries of 5-Br-U and its 4 hydroxy enol form with 50 and 100 water molecules using DFT. According to their results, the enol form of 5-Br-U (but not that of U) is lower in energy by 1.5 to 15 kcal/mol in a water nanodroplet, depending on the method and molecular geometry used. However, the large differences between methods, and the neglect of entropy cast doubt on this conclusion.

We have evaluated free energy differences between the keto and the 4-hydroxy enol forms of 5-Br-U using Ultrafast QM/MM at the B3LYP/6-311G(d,p)/TIP4P(2005) level. According to our results, hydration lowers the free energy of the enol significantly more than the keto form, in contrast with the continuum solvent results [3], although the keto form remains more stable, unlike in [4]. However, the presence of a significant enol population cannot be dismissed. A simple resolution of this problem is experiment. We have been able to obtain the solution Raman spectrum of 5-Br-U in water, in spite of its low solubility. Simulating the theoretical spectrum, in vacuum and in a continuous solvation model is a trivial computational task these days. We have used the SQM method with multiple scale factors but this causes only minor changes in the spectrum. The calculated spectra match the predicted spectrum for the keto form, proving that this is the strongly dominant form in aqueous solution, and also in base pairs, and cannot be the cause of mutagenicity.

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Keywords: Ultrafast QM/MM simulations of molecular spectra: The conformation of 5 bromo-uracil in aqueous solution, and other applications

PL2 / 10:20 - 11:10 / Hall 1

Exchange-Correlation Energies from Paring Matrix Fluctuation and Particle-Particle-Random Phase Approximation

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We formulate an adiabatic connection for the exchange-correlation energy in terms of pairing matrix fluctuation. This connection opens new channels for density functional approximations based on pairing interactions. Even the simplest approximation to the pairing matrix fluctuation, the particle-particle Random Phase Approximation (pp-RPA), has some highly desirable properties. It has no delocalization error with a nearly linear energy behavior for systems with fractional charges, describes van der Waals interactions similarly and thermodynamic properties significantly better than particle-hole RPA, and eliminates static correlation error for singly bound systems. Most significantly, the pp-RPA is the first known functional that has an explicit and closed-form dependence on the occupied and unoccupied orbitals and captures the energy derivative discontinuity in strongly correlated systems. These findings illustrate the potential of including pairing interactions within a density functional framework.

Keywords: Exchange-Correlation Energies from Paring Matrix Fluctuation and Particle-Particle-Random Phase Approximation

PL3 / 11:30 - 12:20 / Hall 1

Raman-Based Approaches For Biomedical Diagnosis

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A rapid increase of applications of Raman spectroscopy to address biomedical questions has been observed lately. Here, we report various examples of our latest results concerning the application of linear and nonlinear Raman microspectroscopy for clinical diagnosis. First, the unique potential of Raman microspectroscopy for an online identification of microorganisms is highlighted. The rapid identification of pathogens based in their characteristic Raman fingerprint is of great relevance for an efficient medical diagnosis (e.g. rapid identification of pathogens in urine samples) or air- and soil monitoring (e.g. identification of anthrax endospores embedded in complex matrices). The implementation of Raman spectroscopy and optical traps in a microfluidic chip allows for Raman activated cell sorting which offers large potential for an automated classification of cells like e.g. circulating tumour cells. Besides single cells, the investigation of whole tissue sections like biopsy specimens by means of Raman-microspectroscopy aiming for an early disease diagnosis will be shown. Furthermore, first steps towards in-vivo Raman spectroscopy utilizing novel Raman fiber probes for an intravascular monitoring of the artheriosclerotic plaque in living rabbits will be presented. The rather long acquisition times of Raman imaging can be reduced by utilizing non-linear Raman approaches like CARS (coherent anti-Stokes Raman scattering). In order to improve the diagnostic result CARS microscopy can be easily combined with second harmonic generation (SHG) and two-photon fluorescence (TPF) microscopy. The diagnostics potential of a compact CARS/SHG/TPF multimodal microscope as compared to conventional histopathological images will be shown for the examples of atherosclerosis and cancer.

Acknowledgements

Financial support of the EU, the ”Thüringer Kultusministerium”, the ”Thüringer Aufbaubank”, the Federal Ministryof Education and Research, Germany (BMBF), the German Science Foundation, the Fonds der Chemischen Industrie and the Carl-Zeiss Foundation are greatly acknowledged.

Keywords: Raman-based approaches for biomedical diagnosis

PL4 / 09:00 - 09:50 / Hall 1

Strategies for Conformational Selection in Cryogenic Inert Matrices: Case Studies

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Molecular conformation is a central concept in molecular physics, chemistry and biochemistry. Conformations of molecules determine the physical and chemical properties of substances and their biological functions. Many studies on conformers of small molecules have been performed, and these studies aim to constitute a basis for our understanding of the conformational behavior of more complex chemical systems including biological macromolecules. The molecular conformations of small molecules determine not only the physical properties directly connected with the molecular structure (dipole moment or spectroscopic characteristics) but also properties influenced by intermolecular interactions. Different conformers of a given molecule may show distinct aggregation abilities, with some of them showing greater tendency to interact with other species [1] or promoting specific arrangements of aggregates, which in turn may lead, for example, to polymorphism [2,3]. Conformations are also important in determining the photochemical reactivity [4].

Along the last 10 years we have been using matrix isolation, together with infrared spectroscopy, to promote conformational selection of many different types of organic molecules, thus allowing for the study of these unique forms at leisure. The techniques developed to select a given conformer among all the possible conformers of a molecule include temperature-dependent experimental procedures (e.g., annealing of the matrix of the compound or selection of the appropriate temperature of the substrate during matrix deposition), or experiments where light-induced conformational rearrangements are promoted. These latter techniques take advantage of two main characteristics of the molecular systems: (1) UV-induced conformational selection relies on the fact that the potential energy surfaces of the ground electronic state and of the stimulated excited states are different, so that after promotion to the excited state conformational relaxation can take place leading to a different conformer after return to the ground state; (2) IR-induced conformational selection may occur after selective excitation of a suitable vibrational mode of a given conformer followed by vibrational relaxation to another form, and is a consequence of the intricate processes of vibrational energy redistribution. In many cases, the produced conformers can later relax by tunneling to another form. Combinations of all these procedures led, for example, to the first simultaneous experimental observation of the 5 most stable isomeric forms of cytosine [5].

In this talk, general strategies for conformational selection in cryogenic matrices will be presented and a series of examples provided. These will include the selection of a single conformer in highly conformationally flexible systems exhibiting a large number of conformers in the gas phase (e.g., 1,3-, 2,3-, 1,4- butanediols), controlling of the relative populations of different conformational states by UV-wavelength selection (as in p-anisaldehyde), production of high-energy conformers either by UV or IR selective irradiation of lower energy conformers (e.g., as in hydroxyacetone), creation of novel dimers of simple carboxylic acids containing higher energy units by in situ IR excitation of the most stable conformer followed by thermal mobilization (as for acetic acid), among other illustrative examples.

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Keywords: Strategies for Conformational Selection in Cryogenic Inert Matrices: Case Studies

PL5 / 09:50 - 10:40 / Hall 1

Applications of Mössbauer Spectroscopy with a High Velocity Resolution

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Mössbauer (γ–resonance) spectroscopy is a unique technique which is widely used for study various species containing 57-Fe, 119-Sn, 197-Au, and some other isotopes. This technique is sensitive to nuclear hyperfine interactions and, therefore, provides very precise information about the electronic and magnetic state of the nuclei, chemical bonds, structure of local environment, etc. Mössbauer spectrometer consists of two major parts: velocity driving system which produces a Doppler shift for resonant γ-rays, and system for γ-rays registration and storage of resonant γ-rays intensity synchronized with each velocity step in the first system. Velocity resolution is a term denoted the smallest velocity step in velocity driving system in Mössbauer spectrometer and velocity for the one point in Mössbauer spectrum. Conventional Mössbauer spectrometers use sinusoidal or triangular velocity reference signal which is formed by digital-analog convertor using 256 or 512 bits. The other velocity driving system was developed for Mössbauer spectrometer SM-2201. This system uses saw-tooth shape velocity reference signal which is formed using 4096 bits. Therefore, Mössbauer spectrometers recorded spectra in 256 or 512 channels can be considered as the low velocity resolution spectrometers while those recorded spectra in 4096 channels should be considered as the high velocity resolution spectrometers. Some examples of comparison of the applications of Mössbauer spectroscopy with a low and high velocity resolution in biomedical, pharmaceutical, cosmochemical and nanotechnological research clearly demonstrate advances and new results obtained using Mössbauer spectroscopy with a high velocity resolution.

Keywords: Mössbauer spectroscopy with a high velocity resolution, Biomedical, Pharmaceutical, Cosmochemical and Nanotechnological Applications

PL6 / 11:00 - 13:00 / Hall 1

Electron Paramagnetic Resonance (EPR) Spectroscopy In Biological Sytems

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Since the very beginning of EPR spectroscopy it has been applied to study of biological systems. These applications range from naturally present paramagnetic centers such as transition metal ions to spin labeling or spin trapping. The last two methods enable to receive information from the biological systems when the number of naturally occurring free radicals is insufficient or their lifetimes are too short to perform EPR detection.

EPR studies in biological systems will be summarized and examples related to recent in vivo and in vitro applications on biological systems will be presented.

Keywords: EPR, spin label, spin probe

PL7 / 09:00 - 09:50 / Hall 1

Beyond DFT: Density Matrix Functional Theory For Ground State And Excited State Energy Surfaces

Evert Jan Baerends

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Density functional theory (DFT) owes its success primarily to affording high efficiency in the calculations, combined with quite reasonable accuracy. However, existing functionals show larger errors at geometries further away from the equlibrium geometry, particularly towards bond dissociation. Complete ground state energy surfaces are still a challenge.

Excited state surfaces are even much more problematic: although time-dependent density functional theory (TDDFT) in its adiabatic approximation has enabled vertical excitation energy calculations at equilibrium geometry with quite decent accuracy, it completely fails at elongated bond distances (e.g. twice equilibrium bond distance) in the following cases: 1) single excitation from bonding to corresponding antibonding orbital (erroneously going to zero) [1]; 2) excited states with considerable double excitation character [2] (which is the case in most excited states at long bond distances); 3) charge transfer excitations. Adiabatic TDDFT is not reliable for excited state surfaces and cannot be used for e.g. dynamics on excited state surfaces.

Density MATRIX functional theory, using the one-particle reduced density matrix (1RDM) is in principle able to overcome these deficiencies. We will present the pysical concepts behind 1RDMFT [3], which employs functionals of both the natural orbitals (NOs) and occupation numbers (ONs). We will show that both ground state surfaces and excited state surfaces (with adiabatic TD-1RDMFT) can become nearly perfect if an accurate functional is available [4,5].

Linear response theory applied to the one-particle reduced density matrix (1RDM) affords a formalism, that, within the adiabatic approximation, yields the excitation energies with a single diagonalization of the (inverse) density matrix - density matrix response matrix. [3] We will demonstrate that the size of this diagonalization problem can be reduced to only slightly larger than the one of TDDFT, while still yielding essentially accurate solutions for all the failure cases of TDDFT mentioned above. [4]

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Keywords: Beyond DFT: density matrix functional theory for ground state and excited state energy surfaces

PL8 / 09:50 - 10:40 / Hall 1

Infrared Spectroscopy and Imaging in Diagnosis and Screening

Feride Severcan

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All over the world, scientists working in academia, government and industry are actively engaged in the characterization, screening and diagnosis of different pathological conditions as well as investigating molecular changes associated with interaction of drugs, chemicals and environmental factors on different organisms using an array of analytical techniques. The ideal scenario is to be able to monitor the system of interest, without disturbing the system, in a sensitive, rapid and automated manner with less cost. Infrared spectroscopy together with microspectroscopy is one of the few analytical techniques that meets all of these requirements. This technique monitors vibrational modes of functional groups of macromolecules such as lipids, proteins and nucleic acids in tissues and cells, simultaneously. With the development in technology for recording spectra and in the analysis of data using chemometric methods, infrared spectroscopy has received great attraction from scientists engaged in the study of complex systems such as biomedical and ecotoxicological systems and foodstuff. Unlike traditional techniques, Fourier transform infrared microscopy (FTIRM) can provide information about in situ chemical features from microscopic regions of a tissue section without disrupting the tissue morphology. Using FTIRM, molecular and structural composition can be examined directly in unfixed and unstained tissues, thereby reducing the possibility of introducing artifacts. In recent years, FTIRM has been applied to many kinds of biological tissues, mainly with the aim of structural characterization and diagnosis of pathologies. Moreover, synchrotron-based FTIR microspectroscopy (SR-FTIRM), taking advantage of synchrotron light brightness and small effective source size, is capable of exploring the molecular chemistry within microstructures with high signal-to-noise ratios at high spatial resolutions.

Disease states, drugs, chemicals and environmental factors cause significant alterations in infrared spectral parameters such as signal intensity and/or area which implies a change in the concentration of the related molecules. Such pathological conditions also induce significant shifts on the frequencies of the lipid, protein and nucleic acid bands implying structural changes in these molecules. Furthermore, bandwidth of some specific bands gives fluidity information. All these spectral variations may have diagnostic value [1-8] and also provide early diagnosis [4, 6]. Therefore, FTIR spectroscopy has an important role in the field of pathology and diagnosis of diseases [1-7]. In this presentation, based on macromolecular alterations in concentration, structure and function, the role of FTIR spectroscopy and microspectroscopy in the characterization and diagnosis of different diseases, such as diabetes, epilepsy, cancer from membranes, cells and soft and hard tissues and body fluids, will be presented. These studies are important because they lead to, for example, rapid and automated diagnosis of disease states and monitoring environmental pollutions which will stimulate generation of new treatment and protection strategies.

Keywords: Infrared Spectroscopy And Imaging In Diagnosis And Imaging

PL9 / 09:00 - 09:50 / Hall 1

Conformation Determination By Raman and Infrared Spectra Of Variable Temperatures Of Xenon Solutions

James Durig

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There were a large number of conformational stability studies carried out in the 1960's and 70's which were determined from variable temperature solutions with non-polar solvents or in some cases the pure liquids. Many different techniques were used but infrared and Raman spectroscopy were the most popular. At that time period there were many reasons for obtaining the most stable conformer such as the structure, steric effect, chemical association, to name a few. However the reasons for determining conformational stabilities have drastically increased from the field of biochemistry and nano-chemistry. These areas have caused a great deal of interest in conformational stability due to its effects on binding sites of proteins in biochemistry and the use of conformer interchange to drive molecular motions and shapes in nano-chemistry. Specifically the conformation of organoamines is currently at work in every human alive with this arising from the amino acids in proteins and the substituted bases in DNA and RNA. The importance of conformational stability is further demonstrated in biological systems by enzyme binding where the conformational changes of the protein can change the binding site either enhancing or deactivating the enzyme.

We started with using infrared (IR) spectra of variable temperature rare gas solutions to determine the enthalpy differences of 2 conformer systems. These conformational studies were extremely successful in both the kypton and xenon solutions and gave results which closely matched those from the vapor phase but with much sharper bands. These conformational studies have also progressed to 3-4 conformer systems such as cyclobutylcarboxylic acid chloride where previous vibrational studies had indicated that either there was only a single stable conformer (g-Eq) which is present in the vapor, liquid, and solid phases or that the second conformer (thought to be the t-Eq form) was 490 cm-1 higher in energy giving 4% of the sample at ambient temperature. The infrared spectra of the variable temperature xenon solutions give much sharper band however and fundamentals for the second and third conformer were assigned.

We became interested in the problem of conformational interchange in organoamines where the conformational studies are complicated due to self-association even in the simplest forms so by using analogues of the more complex organoamines such as ethylamine can result in a difficult experiment. Dimer, trimer, and larger complexes are found for many amines even in vibrational spectra of the vapor phase at moderate pressures. The presence of these complexes not only complicate the spectra but will cause any temperature dependent determination of the enthalpy difference value to be significantly higher than is realistic for a conformational interchange. This association may be avoided by utilizing extremely low pressures with very long path lengths or solutions of the organoamine with a solvent that has little to no interaction with the sample. An excellent solvent for this purpose is xenon. However the strong amine bands causes problems for the conformational studies in the infrared spectra where the NH2 modes around 800 cm-1 can obscure a large number of the fundamentals for the different conformers and the infrared spectra can lack the band intensity to allow for a precise enthalpy determination.

Keywords: Conformation determination by Raman and infrared spectra of variable temperatures of xenon solutions

PL10 / 09:50 - 10:40 / Hall 1

Structural and Energetic Stability of Metal Doped Wheel Boron Clusters

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In this talk a series of computational studies on hydrogenated boron [1-3] and metal-doped boron [4,5] clusters will be reviewed. Size dependent effect of the metal-doping on the structural and energetic properties of micro Bn clusters up to n=12 will be discussed for doped Al, Ti, Re, Fe and Cr atoms, respectively. For the computation the B3LYP functional has been used as Density Functional Theory [6]. We have also focused on some spatial structures such as cage and ring form of the considered boron clusters. Especially, wheel structures of Ti centered boron rings will be presented. Their structural changes and energetics will be criticized via comparing valuable findings reported in literature.

Acknowledgement. This work was supported by TUBİTAK (108T466) and Bozok University (BAP-I.F.E./2011-39).

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Keywords: Structural and Energetic Stability of Metal Doped Wheel Boron Clusters

TURCMOS 2013

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ORAL PRESENTATIONS

O1 / 14:00 - 14:20/ Hall 1

Raman Spectrometry Assisting The Investigations Of Pharmaceutical Products And Processes

György Marosi

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The use of Raman spectrometry for non-invasive investigations in the pharmaceutical technology is rapidly increasing. The Raman spectrometer, combined with confocal microscope, was used to perform chemical mapping and extracting a large amount of information regarding each phases of solid state medicaments. Characterization of the samples in terms of qualitative and quantitative composition could be accomplished this way. Furthermore Raman sensor was coupled with fibre optic to perform real time control of crystallization processes of active pharmaceutical ingredients. The spectra of crystalline active pharmaceutical ingredients (API) allowed distinguishing their similar polymorphs from each other and their flat counterparts was used for detecting the amorphous particles. It made suitable not only the monitoring the transformations of polymorphs in a real time manner but also controlling the processes. Understanding of the influence of key process parameters on the quality of the intermediates and the final products allowed us realizing the process analytical technology (P.A.T.) concept of Food and Drug Administration (FDA). Multivariate analysis tools combined with in-line analytical instruments supported the understanding of the mechanism the whole process. Advantages of the integration of the Raman spectrometer into the most advanced pharmaceutical processes was confirmed through critical pharmaceutical compositions (solid solutions, colloidal dispersions and traces of polymorphic impurities) that can be measured only by this analytical tool. Methods have been elaborated to explore structural and chemical content uniformity and stability of solid pharmaceuticals.

Keywords: Chemical imaging, In-line Raman spectroscopy, Pharmaceutical polymorphs

O2 / 14:20 - 14:40 / Hall 1

Bioactivity Of Silver(I) Complexes: Study By Electronic and Vibrational Circular Dichroism Spectroscopy

Iryna Goncharova

Department of Analytical Chemistry,Institute of Chemical Technology, Prague, Czech Republic

The origin of the bioactivity of Ag(I) compounds is currently unknown. The fact that silver compounds do not destroy mammalian cells makes them prospective agents in drug design. It has led to the necessity of investigation of their action mechanism.

In the presented research, the structures of the Ag(I) complexes with amino- (histidine, arginine, aspargine) and hydroxy acids (mandelic acid and its derivatives) were studied by electronic and vibration circular dichroism spectroscopy. The formation of the chiral coordination polymer networks of mentioned Ag(I) complexes was observed in solution and solid state. The couplet oscillator model calculation was performed for interpretation of the obtained VCD spectra.

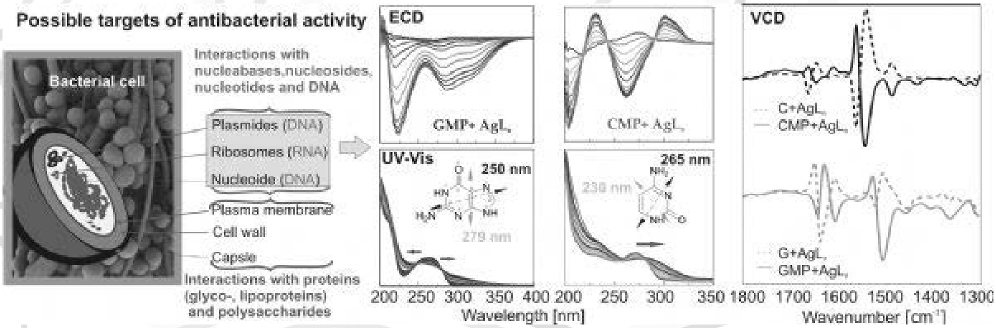
Two ways of the antimicrobial activity of the studied complexes were tested. In the first case, interactions with bacterial cell wall components (peptidoglycans, lyposacharides and proteins) were studied.

In the second case, a systematic chiroptical study on Ag(I) complexes interactions with nucleotides, RNA, and DNA was made. In the case of DNA, strong coordination of Ag(I) to G-C pair was observed. In the case of nucleotides, the formation of the Ag(I)-mediated base pairs and their self-assembles were studied in wide pH range. Based on the obtained data, in the first time, the formation of the Ag(I)-mediated self-assembled species of cytidine with a structure similar to the i-motif structure in DNA was observed. Theoretical interpretation of the obtained VCD spectra of Ag(I)-mediated pairs and their assembles were made using couplet oscillator model calculation

The work was supported by the Grant agency of the Czech Republic (P205/12/P584)

Keywords: circular dichroism, silver,antimicrobial, self-assembling, i-motif, exciton coupling

Possible Targets Of Ag(I) Antimicrobial Activity



O3 / 14:40 - 15:00 / Hall 1

2D Correlation Spectroscopy In Protein Research

***Young Mee Jung*[1], Boguslawa Czarnik Matusewicz[2]**

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Generalized two-dimensional (2D) correlation spectroscopy is now a well-established technique for interpreting spectral data sets obtained during the measurement of spectra with an external perturbation that provides considerable utility and benefit in various spectroscopic studies. In this presentation, example of 2D correlation spectroscopy for protein research will be presented to demonstrate the potential, utility and versatility of this powerful analytical technique that significantly improves information about protein structure gained from infrared spectra. Detailed description of the water-urea-β-lactoglobulin interaction and pH-induced transition of α-lactalbumin from native to molten globule state studied by means of 2D IR correlation spectroscopy will be also discussed.

Acknowledgements

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Keywords: 2D correlation spectroscopy, protein, molten globule state

O4 / 15:20 - 15:40 / Hall 1

Infrared Spectroscopy of HCl and H2O Aggregates at Ultracold Temperatures

Anna Gutberlet[1], Gerhard Schwaab[1], Ozgur Birer[3], Marco Masia[2], Anna Kaczmarek[2], Harald Forbert[2], Martina Havenith[1], Dominik Marx[2]

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Dissociation of acid molecules in confined environments at low temperatures is relevant to atmospheric and interstellar chemistry but remain poorly understood. We performed high-resolution mass-selective infrared laser spectroscopy of HCl and H2O aggregates inside superfluid helium nanodroplets at 0.37 Kelvin. The hydronium ion formed when the aggregate reached HCl(H2O)4 configuration. [1]

The ab initio simulations showed that undissociated clusters assemble by stepwise water molecule addition in electrostatic steering arrangements up to n= 3. Adding a fourth water molecule to the ringlike undissociated HCl(H2O)3 then spontaneously yields the compact dissociated H3O+(H2O)3Cl- ion pair. This aggregation mechanism bypasses deep local energy minima on the n= 4 potential energy surface and offers a general paradigm for reactivity at ultracold temperatures.

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Keywords: helium nanodroplet isolation spectroscopy, laser spectroscopy, mass selective infrared spectroscopy, cryo-chemistry

O5 / 15:40 - 16:00 / Hall 1

Electron Storage In Noval 4H-Imidazol Ruthenium Complexes Assessed With TDDFT Simulations and Resonance Raman Spectroscopy

***Stephan Kupfer*[1], *Linda Zedler*[1], *Inês Rabelo De Moraes*[2], *Sven Krieck*[3], *Rainer Beckert*[4], *Michael Schmitt*[1], *Juergen Popp*[1], *Benjamin Dietzek*[1]**

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In order to deploy regenerative energy sources several propositions have been made. One of those is to use the energy of sun light. In this respect the development of artificial photosynthesis focuses at designing new light-driven catalysts for hydrogen production requiring light-harvesting antennas. This work concentrates on the theoretical analysis of the photophysics of Ruthenium based complexes (see Figure 1) and their electron storage capabilities. First, the photophysical properties of three Ruthenium complexes with functionalized 4H-imidazole bridging-ligands (electron-donating and electron-withdrawing-groups) are investigated with absorption and resonance Raman (RR) spectroscopy.[1-3] The quantum chemical calculations are performed with the density functional theory (DFT) and time-dependent DFT (TDDFT) using the B3LYP functional together with the PCM method, which simulates the acetonitrile solvent. Secondly, the single and double reduced species have been rationalized by means of RR spectroscopy. The exceptional agreement of the spectro-electrical measurements and the quantum chemical simulations allowed us to study structural and electronical alternations during the progressive reduction of the three Ruthenium complexes. It was found that exclusively the complex with the 4H-imidazole bridging-ligand bearing the electron-withdrawing group is capable to store two electrons, which is a preliminary feature for hydrogen-evolving photocatalysts.

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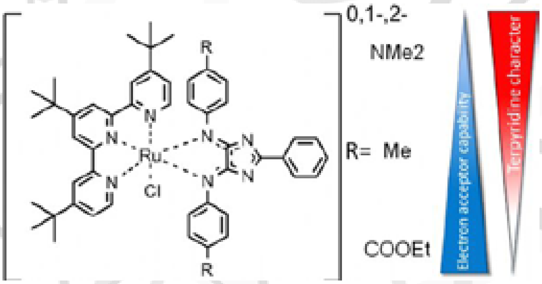
Keywords: TDDFT, resonance Raman, Electron Transfer, Spectro-Electrochemistry, Ruthenium, Photosensitizer

Investigated reduced species of the Ruthenium complexes.



O6 / 16:00 - 16:20 / Hall 1

Investigation Of Trace Amounts Of Drug By Surface Enhanced Raman Chemical Imaging Supported By MCR-ALS Method

***Attila Farkas*[1], *Tamás Firkala*[2], *Balázs Vajna*[1], *György Marosi*[1]**

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Chemical imaging is an emerging technique in vibrational spectroscopy (IR, NIR, Raman) which can be used to extract a large amount of (possibly hidden) information from the investigated object. Using Raman mapping method in the field of pharmaceuticals, a large number of qualitative or quantitative characteristics can be simultaneously determined. In many cases, however, the tablets contain the effective volume of the active pharmaceutical ingredient (API) in a low dose. This low concentration can be detected by a micro-Raman spectrometer, only if the API is concentrated in a small volume. Even in such cases the time of measurement increases significantly as a huge area, where the small amount of API is distributed very homogeneously, must be investigated. These issues are intended to be solved by the surface-enhanced Raman spectroscopy (SERS) technique. We used silver colloid for enhancing the intensities of certain Raman vibrations of SERS-active API-s in the presence of SERS-inactive excipients. Sample tablets with the same qualitative and quantitative composition were prepared in two ways using dry and wet techniques resulting in inhomogeneous and homogeneous API distribution respectively. Due to the various kinds of interactions between the API and the silver colloid particles the SERS Raman mapping resulted in very diverse spectra of the measured points. In order to solve these problems pre-processing and curve resolution of spectra, using MCR-ALS method, was applied successfully for evaluating such Raman maps.

Keywords: Raman chemical imaging, Surface-enhanced Raman spectroscopy, Chemometrics, Multivariate curve resolution, Pharmaceuticals

O7 / 13:00 - 13:20 / Hall 1

Light-Induced Reactions of Matrix-Isolated Heterocycles

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Studies on the reactivity of heterocyclic molecules have been invariably attracting interest of chemists. In this talk, the reactivity of monomeric heterocycles will be addressed and new results obtained over the past few years will be presented.

The studied systems include four-, five-, and six-membered heterocycles, containing oxygen, nitrogen and sulphur heteroatoms. Amongst others, diketene, isoxazoles, tetrazoles, saccharin, and a series of cytosines were investigated. In many cases, the photoinduced reactions were experimentally observed and reported for the first time. The observed reactions included ring-opening, ring-closure, various types of intramolecular hydrogen shifts, and their combinations, resulting in isomerizations or decomposition of the reactant.

Typically, the target molecules were embedded in solid inert matrices (Ar, Xe, N2) and excited in situ using tunable narrow-band UV-light of an optical parametric oscillator. The structures of reactants and photoproducts were characterized experimentally by infrared spectroscopy and theoretically by the computation of vibrational spectra. The results of the photochemical experiments and the underlying reaction mechanisms will be discussed.

Acknowledgments

Contributions of the present and former members of the Laboratory of Molecular Cryospectroscopy and Biospectroscopy (Coimbra), and of our research partners from Portugal, Poland, and Switzerland are acknowledged. This work was supported by the Portuguese “Fundação para a Ciência e a Tecnologia”, Research Project PTDC/QUI QUI/118078/2010, FCOMP-01-0124-FEDER-021082, co-funded by QREN-COMPETE-UE, and bilateral Portuguese-Polish grant (Ficheiro No. 13789). Coimbra LaserLab (http://www.uc.pt/en/uid/laserlab/) supported this work under the Grant Agreement No. 228334, within the European Community’s Seventh Framework Programme.

Keywords: infrared spectroscopy, matrix isolation, photochemistry, heterocyclc compounds

O8 / 13:20 - 13:40 / Hall 1

Matrix Isolation Studies Of Carbonic Acid - The Vapour Phase Above The Two Polymorphs

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Carbonic acid appears as trace compenent in the natural world in solution, e.g., in soda, champagne, blood and rain. Recent work, including ours, suggests carbonic acid to exist even in pure form as a solid in ice clouds, comets, icy moons and polar regions of planets. Twenty years ago, in the lab two different polymorphs of carbonic acid, α- and β-H2CO3, were isolated in pure form as thin, crystalline films. They were characterized by infrared and, lately, by Raman spectroscopy. Recently, we succeeded in sublimating α-H2CO3 and trapping the vapor phase in a noble gas matrix, which was analyzed by infrared spectroscopy. In the same way we have now investigated the β-polymorph. Unlike α-H2CO3, β-H2CO3 was regarded to decompose upon sublimation. Still, we have succeeded in isolation of undecomposed carbonic acid in the matrix and recondensation after removal of the matrix here. This possibility of sublimation and recondensation cycles of β-H2CO3 adds a new aspect to the chemistry of carbonic acid in astrophysical environments, especially because there is a direct way of β-H2CO3 formation in space, but none for α-H2CO3. Assignments of the FTIR spectra of the isolated molecules unambiguously reveal two different carbonic acid monomer conformers (C2v and Cs). By contrast to the earlier study on α-H2CO3 we do not find evidence for centrosymmetric (C2h) carbonic acid dimers here. This suggests that two monomers are entropically favored and might even be detectable in the gas phase, e.g., in the atmosphere of Mars or Venus.

Keywords: Matrix Isolation, FTIR spectroscopy, UV/VIS photolysis, Astrophysics, Atmospheric Chemistry

O9 / 13:40 - 14:00 / Hall 1

Photochemical Transformations Of 5-Methyltetrazole. FT-IR Matrix Isolation and DFT Studies

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Department of Chemistry, Wrocław University, Wrocław, Poland

5-substituted tetrazoles represent an important class of heterocycles which exhibit a large number of practical applications, especially in medicinal chemistry as metabolically stable surrogates for the carboxylic acid group. They are also very stimulating heterocycles from an academic viewpoint due to their tautomeric and conformational properties and very interesting photochemistry.

One of the simplest 5-substituted tetrazoles is 5-methyltetrazole (MT). This compound exists in two tautomeric forms: 1H- and 2H-tautomers.

The X-ray diffraction method revealed the presence of the 1H-tautomer in the MT crystal but according to the theoretical prediction, in the gas phase the 2H-tautomer is the predominate form. The infrared spectrum obtained for MT/Ar matrix shows that both 1H- and 2H-MT tautomers are present in the solid argon with the population of ca. 4% and 96%, respectively in accordance with the performed calculations.

Narrow-band irradiation with OPO laser system of the MT species isolated in argon matrix led to cleavage of the tetrazole ring of the precursor molecule, the N2 elimination and formation of N-methylcarbodiimide (CH3NCNH), methylcyanamide (CH3NHCN) and C-methylnitrilimine (CH3CNNH).

When broad band irradiation was used, the main photoproducts were the same as those observed in the OPO experiment. In addition, after prolonged photolysis with the full output of the high pressure Xe lamp several other species, originating from decomposition of the N-methylcarbodiimide, were identified in the FTIR spectra, especially HCN, HNC and their dimers.

Keywords: matrix-isolation, photochemistry, infrared spectroscopy, tetrazoles

O10 / 14:20 - 14:40 / Hall 1

Melatonin Interactions With Copper (II) Ion: Spectroscopic and DFT Theoretical Studies

Semira Galijasevic*, *Vedran Ljevarevic, Vera Dugandzic

University of Sarajevo, Faculty of Science, Department of Chemistry

Introduction

Melatonin (5-methoxy-N-acetyltryptamine), secreted by the pineal gland is well known strong free radical scavenger and antioxidant. It has been shown to interact with a number of metal ions in a biological milieu, protecting against tissue damage. Copper, essential has been implicated in the promotion of free radicals and development of several diseases. Utilizing experimental and theoretical studies, possible interactions of melatonin with copper have been analyzed in terms of structures and spectroscopic properties.

Methods

IR spectra of copper interactions with melatonin were recorded on a PerkinElmer spectrum BX FTIR System.UV/Vis spectra were recorded on Perkin Elmer lambda 35 spectrophotometer and observed spectra were recorded from 200 to 400 nm. The most stable structure of possible complex of melatonin and copper (II) and vibrational spectra were calculated using density functional theory, with correlation functional B3LYP and the basis set 6-311g for metal ion and 6-31g for other atoms.

Results

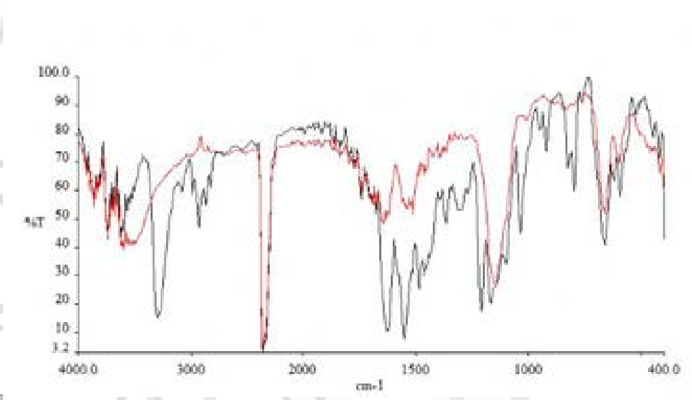
Experimental IR spectra of Cu-melatonin showed a loss of frequency associated with N-H stretching mode at 3562 cm-1. Complex spectra also showed new peak at 510 cm-1 region due to the formation of M-N.. All determined frequencies were compared to theoretically calculated values. Thermodynamical properties and HOMO/LUMO orbital energies were calculated. Small HOMO-LUMO gap is obtained what is characteristic of highly reactive molecules. UV/Visible spectra showed a prominent peak at 235 nm that increased over time.

Conclusion

Experimental and theoretical studies clearly showed a well defined interactions between melatonin and copper (II). Based on this data we proposed structure of Cu(II)-Melatonin.

Keywords: Copper, melatonin, IR spectra, DFT

Copper-Melatonin IR spectra



Black line shows melatonin alone, while red line denotes Copper-melatonin complex

O11 / 14:40 - 15:00 / Hall 1

Determination Of Structural and Vibrational Properties of Quinoline-7-Carboxaldehyde Using Experimental FT-IR, FT-Ra and Dispersive-Ra Techniques and Theoretical HF and DFT Calculations

Mustafa Kumru, Mustafa Kocademir, Levent Sarı

Department of Physics, Fatih Universitesi, Istanbul, Turkey

Experimental part of the study is focused on FT-Raman, dispersive-Raman and FT-infrared spectra of the molecule, while quantum mechanical optimization of the molecule along with harmonic vibrational frequencies, IR intensities, Raman intensities, and potential energy surface analysis around C7-C8-C19=O16 torsion angle have been carried out at the ab initio Hartree-Fock (HF) and density functional (B3LYP) level of theories. Theoretical calculations have been employed with the 6-311++G(d,p) basis set for two possible aldehyde rotamers of Q7C. The FT-IR spectrum (4000-50 cm-1), the FT-Raman spectrum (4000-50 cm-1) and Dispersive-Raman (3500-50 cm-1) spectrum of solid sample of Q7C have been recorded Nicolet 6700 spectrometer.

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We thank the Turkish Scientific and Technical Research Council (TÜBİTAK) for their financial support through National Postdoctoral Research Scholarship Programme and Scientific Research Fund of Fatih University under the project number P50011001_G (1457).

Keywords: DFT, Dispersive-Raman spectra, HF, FT-IR spectra, FT-Raman, quinoline-7-carboxaldehyde, Vibrational Modes, Vibrational Spectroscopy

O12 / 15:00 - 15:20 / Hall 1

Bilirubin-Binding Sites On Serum Albumin: Ligand-Competition Analysis By Circular Dichroism Spectroscopy

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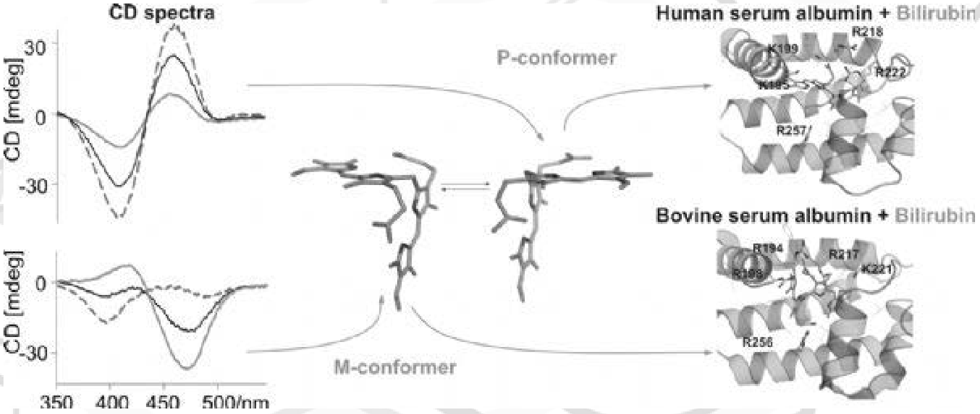
[2]Department of Physics and Measurements,Institute of Chemical Technology, Prague, Czech Republic

Heme and its metabolites bilirubin(BR) and biliverdin(BV) are known as waste products in human body. However, the latest studies accept these pigments exhibit intriguing biological activities as antioxidant agents. The dual physiological role of the BR is a result of its specific chemical properties and spatial chiral structure. The molecule of heme is planar; however BR and BV exist as a racemic mixture of the isoenergetic P- and M- helical conformers fixed by intramolecular H-bonds. In mammalians, BR and BV are bound on serum albumin and this complex plays an important role in their antioxidant properties.

Although serum albumin is among the most studied proteins, the number of pigments binding sites and their location are still under debate. In our work circular dichroism spectroscopy was used for the identification of the number of binding sites and their stereoselectivity in albumins of different mammalian species. Using site-specific ligand-competition experiment with marker ligands for alone subdomains, the binding sites with high and low-affinity were identified. It was found that regardless of the resembling structure, BR and BV high-affinity binding sites are not overlapped. This finding helps to model the antioxidant cycle for these pigments in the human body.

Keywords: binding site, circular dichroism, serum albumin, bilirubin, biliverdin, ligand competition analysis

Stereoselectivity of the binding site on human and bovine serum albumins



O13 / 15:20 - 15:40 / Hall 1

Raman Investigation Of (CdZn)Te, (CdTe)In and (CdTe)Cl Bulk Single Crystals For Gamma-Ray Detectors

Theodore Ganetsos[1]***, Eduard Belas***[2]***, Lukas Cedivy***[2]***, Bill Kotsos***[1]***, Nikolaos Laskaris***[1]

[1]*Department of Electronics, TEI of Lamia, Lamia, Greece*
[2]*Institute of Physics, Charles University, Prague, Czech Republic*

(CdZn)Te bulk single crystals or thin films are widely used in many applications. Room temperature X-ray and Gamma-ray (CdZn)Te detectors, thin-film CdTe/CdS solar cells or electro-optical modulators are already commercially available. The field of applications of these detectors extends from health and medicine to nuclear security and imaging of energetic ions. High collection efficiency of carriers, generated by irradiation at room temperature, represents the main advantage of (CdZn)Te detectors. This ability critically depends upon the high resistivity of this material and good charge transport properties. We studied In-doped CdTe, CdZnTe and CdTeCl after annealing using for investigation the technique of micro-Raman spectroscopy. All samples were grown by the Vertical gradient freeze method directly from the melt. Electrical conductivity – mobility was measured using the Van der Paw method. In this research work, material optical and electrical properties, which are necessary for the production of the high charge collection efficiency detectors, will be discussed and the methods of detector preparation and characterization will be presented.

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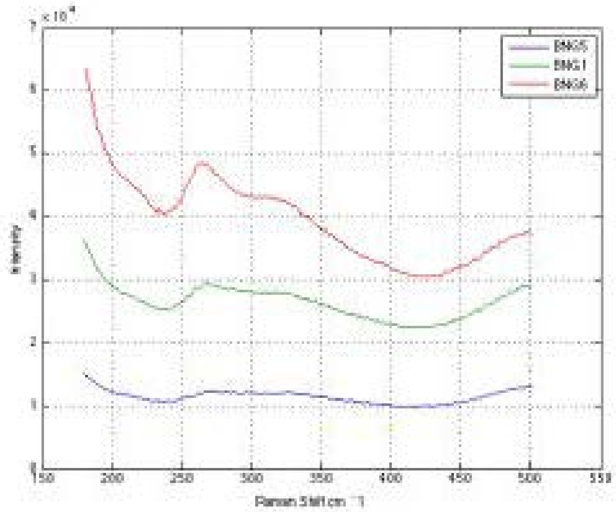
Keywords: Raman, Spectroscopy, detectors, CdTe, conductivity, defects, electrical properties

Figure 1.



A micro-Raman spectrum of CdZnTe 15%Zn in the range 180-500cm-1

Sample BNG5 is undoped and as-grown. Sample BNG1 is undoped, after Cd-rich annealing for 24hrs and sample BNG6 is undoped, after Cd-rich annealing for 48hrs

O14 / 09:00 - 09:50 / Hall 1

Temperature Dependence of the Bragg Peak-Intensity Close to the Alpha-Incommensurate-Beta Transition in Quartz

Hamit Yurtseven*, *Koray Kaymazlar

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Quartz(SiO2) is a mineral in the crystalline form or amorphous with various phases. At room temperature and atmospheric pressure, it has a stable crystalline phase. At low temperatures it is in the alpha phase and when it is heated up, it transforms in to the beta -phase through the intermediate (incommensurate) phase within the temperature interval of nearly 1.3 K at at around 847 K. The order parameter Q occurs due to a tilting of SiO2 tetrahedra around the threefold axis, which can be related to the variation of the peak intensity with the temperature in quartz.

Keywords: Order parameter, Bragg peak-intensity, quartz

O15 / 11:00 - 11:20 / Hall 1

A Possibility to Distinguish Different Microenvironments in the Nanosized Iron Cores in Human Liver Ferritin and its Pharmaceutical Model Ferrum Lek on The Basis of Temperature Dependent Unusual Line Broadening of Mössbauer Spectra

***Michael Oshtrakh*[1], *Irina Alenkina*[1], *Ernö Kuzmann*[2], *Zoltan Klencsár*[3], *Vladimir Semionkin*[1]**

[1]Department of Physical Techniques and Devices for Quality Control and Department of Experimental Physics, Institute of Physics and Technology, Ural Federal University, Ekaterinburg, Russian Federation
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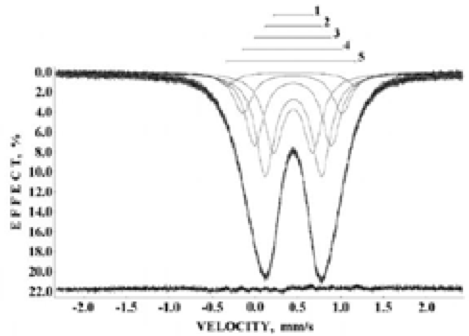
[3]Institute of Molecular Pharmacology, Research Centre for Natural Sciences, Hungarian Academy of Sciences, Budapest, Hungary

Ferritin, an iron storage protein, contains a nanosized ferric hydrous oxide core in the form of ferrihydrite surrounded with 24 protein shell. The size of the cavity for the iron core is about 8 nm which can contain up to 4000 iron atoms. However, ferritin molecule usually contains about 2000–3000 iron atoms. To treat the iron deficiency anemia some pharmaceutically important ferritin models such as Ferrum Lek were developed. In contrast to ferritin the macromolecule of Ferrum Lek consists of nanosized ferric hydrous oxide core in the form of akagenite surrounded with polymaltose shell. Samples of human liver ferritin and Ferrum Lek were studied using Mössbauer spectroscopy with a high and low velocity resolution in the temperature range from 295 to 60 K. In this temperature range all spectra demonstrated two lines shape. An unexpected line broadening was found in the spectra of both samples with temperature decreasing below about 130 K for Ferrum Lek and about 150 K for ferritin. On the basis of the high velocity resolution Mössbauer spectra of both samples the observed anomalous line broadening could be accounted for by a model of five doublets with the common line width, providing a consistent fit at all temperatures. The obtained results enabled elucidation of reasonable variation of other Mössbauer parameters (relative areas, isomer shift, quadrupole splitting) with temperature decrease. These variations were related to possible different microstructures which may be considered as surface and internal layers and internal core.

Keywords: Human liver ferritin, Ferrum Lek, Iron core microenvironments

Fig. 1. Mössbauer spectrum of Ferrum Lek measured with a high velocity resolution (4096 channels) at 170 K. 1-5 are the result of the best fit using consistent heterogeneous model for the iron core. Differential spectrum is shown below



O16 / 11:00 - 11:20 / Hall 1

Study of Chelyabinsk LL5 Ordinary Chondrite Fragments Using Mössbauer Spectroscopy with a High Velocity Resolution

***Michael I. Oshtrakh**, Evgeniya V. Petrova, Victor I. Grokhovsky, Vladimir A. Semionkin*

Department of Physical Techniques and Devices for Quality Control and Department of Experimental Physics, Institute of Physics and Technology, Ural Federal University, Ekaterinburg, 620002, Russian Federation

On February 15, 2013 it was a meteorite rain in Chelyabinsk region of Russian Federation. This meteorite was classified as ordinary chondrite LL5 group and named Chelyabinsk. The Meteoritic expedition of the Ural Federal University immediately started the search and collection of Chelyabinsk meteorite fragments. Some of the first fragments were chosen for the study using metallography, X-ray diffraction, scanning electron microscopy with energy dispersive spectroscopy and Mössbauer spectroscopy with a high velocity resolution. It was observed that Chelyabinsk LL5 chondrite has a breccia structure and it is possible to distinguish bright and dark lithology in meteorite fragments. Two fragments with bright and both bright and dark lithology as well as fusion crust from the second fragment were chosen for this study. The results obtained permitted us to identify iron bearing phases in Chelyabinsk LL5 ordinary chondrite fragments matter and fusion crust composition. Both fragments contain olivine, pyroxene, troilite, and metal phases. However, it was found some differences in the metal and other iron bearing phases content in the studied fragments. Application of the high velocity resolution Mössbauer spectroscopy permitted us to distinguish spectral components related to the 57-Fe in crystallographycally non-equivalent M1 and M2 sites in both olivine and pyroxene. The fusion crust in addition to mentioned iron bearing phases contains magnetite-like phase and ferric compound which were absent in both meteorite fragments. Mössbauer hyperfine parameters of iron bearing phases were evaluated and compared with previously obtained data for other ordinary chondrites.

Keywords: Mössbauer spectroscopy with a high velocity resolution, Chelyabinsk LL5, Ordinary chondrites

O17 / 13:00 - 13:20 / Hall 1

Hyperspectral Scatter Imaging For The Spectral Decomposition Of Multi-Layered Materials

***Mizuki Tsuta*[1], *Kaori Fujita*[1], *Mario Shibata*[1], *Masatoshi Yoshimura*[1], *Mito Kokawa*[2], *Junichi Sugiyama*[1]**

[1]National Food Research Institute, National Agriculture and Food Research Organization, Tsukuba, Japan
[2]The University of Tokyo, Tokyo, Japan

Near-infrared spectroscopy have been widely used for non-destructive monitoring of wide range of materials such as agricultural produce and foods. Methods for decomposition of spectra of materials into that of each layer are demanded because the target of monitoring is in most cases limited to a single layer (e.g. sweetness of the flesh of a fruit, not the skin). Recently, hyperspectral scattering imaging (HSSI) has been introduced for the measurement of light scattering profile, which consists of intensity values at different distances from a spot illumination on a sample surface acquired at different wavelengths. Since the further the distance, light scattered at the deeper in the sample is measured, separation of spectra of different layers would be expected by combining spectral and distance information. The objective of this study was to investigate the potential of HSSI for the spectral decomposition of multi-layered materials. In this study, styrene and ABS sheets were used as model sample. They were accumulated with a bundle of styrene sheets on top. The thickness of the bundle was changed from 0 to 50 sheets. A spot illumination with a diameter of 1.5 mm was casted on the sample surface and the light scattering profile was acquired at different wavelengths from 1200 to 1650 nm with 50 nm intervals. Parallel factor analysis was successfully applied to the HSSI data to decompose the spectra of styrene and ABS as wavelength loadings. In addition, the bundle thickness could be predicted using partial least squares regression.

Keywords: light absorption, light scattering, multivariate analysis, chemometerics

O18 / 13:20 - 13:40 / Hall 1

Observing the Microstructure of Bitumen by Fluorescent Spectroscopy and Microscopy

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Institute of Materials Chemistry, Vienna University of Technology, Vienna, Austria

The definition and improvement of asphalt concrete is the great challenge the ever rising expectations and requirements of roadworks puts in front of the bitumen industry. Thus, the search for techniques allowing an assessment of the adhesive and rheological properties of bitumen is very essential. Confocal Laser Scanning Microscopy (CLSM) is an advanced imaging technique that enables structural analysis of very complex materials due to the combination of highly localized chemical information and improved signal power. Complementary spectroscopic analysis, however, is essential to unravel the sophisticated material behaviour of complex organic composites as bitumen.

CLSM allows the detailed study of the microstructure of bitumen by visualizing fluorescent centres in bitumen. The origin of these fluorescence signals has been the subject of on-going debate. Fluorescence spectroscopy is employed in combination with chromatographic separation techniques to obtain new evidence regarding the composition and ageing behaviour of asphaltene micelles.

The combined results reveal that the aromatic mantle, serving as a stabilizing agent around the micelle, is the source of the fluorescent emissions, which contradicts the concept that the asphaltenes themselves would show fluorescent emissions. These facts serve as the basis for an updated micelle model, capable of describing both the visualized microstructure and explaining the ageing behaviour of asphalt concrete in respect to thermal healing of asphalt.

Keywords: fluorescent microscopy, fluorescent spectroscopy, petrol industry, roadworks

O19 / 13:40 - 14:00 / Hall 1

Fluorescent Properties Of Azacrown-Containing Styryl Derivative Of Naphthopyran: Ion-Binding Response and Photochemical Switching

***Artem Smolentsev**[1]*, ***Evgenii Glebov**[1]*, ***Valerii Korolev**[1]*, ***Olga Fedorova**[2]*

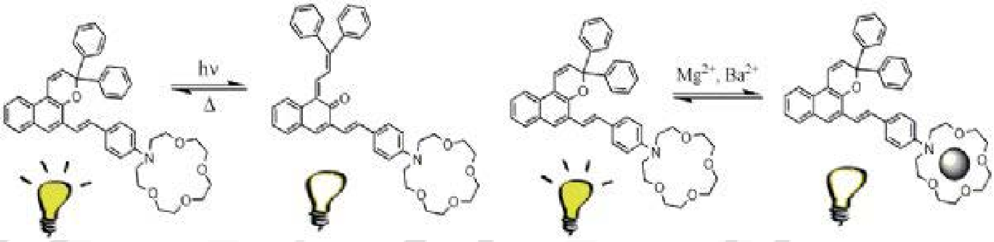
[1]Voevodsky Institute of Chemical Kinetics and Combustion SB RAS, Novosibirsk, Russia
[2]Nesmeyanov Institute of Organoelement Compounds RAS, Moscow, Russia

Macroscopic properties of materials can be modulated by light through switching between the two stable states of a photochromic system. In particular, photochemical transformations associated with photochromic compounds can be exploited to switch the luminescence of molecules under the action of light. Compounds with photocontrolled fluorescence are of interest for 3D optical memory, imaging technologies, visualizing sensors, and characterization of diffusion in polymers and biological systems.

Fluorescent properties of recently synthesized photochromic naphthopyran containing monoaza-15-crown-5 moiety (NP1) and its crownless analogue (NP2) were studied. NP1 emits fluorescence with a maximum at 528 nm, quantum yield 0.1 and characteristic lifetime 2.4 ns (in acetonitrile at room temperature). Its fluorescence could be switched off photochemically in two ways using two parallel photochemical reactions characteristic for this type of naphthopyrans. The first way is the irreversible trans-cis photoisomerzation of a closed form ("stilbene-like reaction"). The second way is the thermally reversible reaction of closed form transition to the open form ("chromene-like reaction", figure 1). The fluorescence of NP1 is quenched by alkali earth metal cations by the mechanism of static quenching. Stability constants for 1:1 complexes of 1b with magnesium and barium cations determined from Stern-Volmer plots are in agreement with that obtained by the UV spectroscopy.

Keywords: Fluorescence, photochromism, cis-trans isomerisation, exciplex, TICT state.

Figure 1



O20 / 14:20 - 14:40 / Hall 1

Investigation Of cis-(Z)-Flupentixol Dihydrochloride (FLU) Interaction With PC Liposomes In Presence And Absence Of Cholesterol By EPR Spin Labeling and DSC Techniques

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Antidepressant drug cis-(Z)-flupentixol dihydrochloride (FLU)-di palmitoyl phosphatidyl choline (DPPC) liposome interactions in presence and absence of cholesterol (CHO) were investigated by Electron Paramagnetic Resonance (EPR) spin labeling and Differential Scanning Calorimetry (DSC) techniques. In the EPR spin labeling studies, 5- and 16- doxyl stearic acid (5-DS and 16-DS) spin labels were used to monitor the head group and alkyl chain region of phospholipids respectively. EPR, DSC and simulation results indicated a shift in the main phase transition towards lower temperature side in the presence of FLU for all liposomes investigated. FLU is an effective drug both in the interfacial and in the acyl chain region of liposomes. In the head group (interfacial) region, FLU changed the order and dynamic of the pure and CHO incorporated liposomes. In the acyl chain region, the addition of FLU increased the dynamic of the nitroxide especially in the liquid crystalline phase for pure liposomes and at almost any temperature for CHO incorporated liposomes. According to the results obtained, it is thought that FLU incorporates into the liposomes with its triple ring parallel to the head group of phospholipids and its chain toward the acyl chain of phospholipids.

Keywords: liposome, antidepressant (cis-(Z)-flupentixol dihydrochloride), EPR, spin label, simulation and DSC

O21 / 14:40 - 15:00 / Hall 1

Ultrafast Time-Resolved Spectroscopy with Supramolecular Assemblies based on Carbon Nanostructures – Insights into Charge Transfer Reactions

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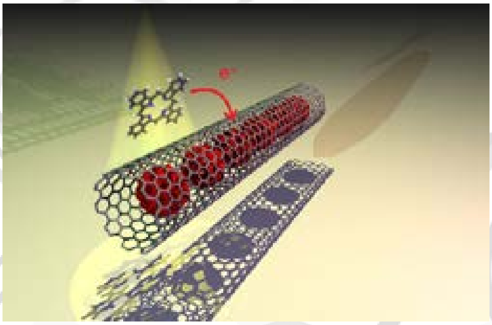
Carbon materials, in general, and sp2 carbon allotropes, bear great potential as building blocks for electronic applications due to their unique electronic properties. It is, however, of importance to retain these properties when implemented into charge transfer systems. In the past, we have focused on designing, devising, synthesizing, and testing novel nanometer scale structures as integrative components for solar energy conversion. Carbon nanostructures, that is, fullerenes, carbon nanotubes, and graphene, were at the forefront of our studies by probing electronic communication between organic and inorganic photosensitizers, on one hand, and carbon nanostructures, on the other hand, in solution, in transparent films, and at electrode surfaces. Here, we present the basic photophysical characterization of Carbon Nanotube Peapods, that is, fullerenes that are encapsulated within single-walled carbon nanotubes (C60@SWCNT), and their electronic interactions with photosensitizing chromophores. The resulting electron donor-acceptor hybrids differ inherently from architectures that are based on empty SWCNTs. To this end, ultrafast time-resolved absorption and emission spectroscopic assays provide insights into the electronic communication in the resulting the carbon nanostructure hybrids. This is further corroborated by steady state absorption and emission spectroscopy, Raman spectroscopy, and high resolution microscopy.

Keywords: Carbon Nanotube Peapods, Ultrafast Laser-Spectroscopy, Supramolecular, Photosensitization, Carbon Nanostructures

peapod photosensitization



Photosensitization of Carbon Nanotube Peapods

O22 / 15:00 - 15:20 / Hall 1

Electronic Structure, Non-Linear Properties and NMR-Structural Analysis of Nicotinic Acid (ortho, meta and para –Hydroxy-Benzylidene)-Hydrazides: Computational Studies

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The present work is aimed at comparing the molecular structural, non-linear and NMR –spectra properties of nicotinic acid (ortho, meta and para –hydroxy-benzylidene)-hydrazides, in gas phase, due to their versatile medical activities and importance. The ground state properties of the title molecules have been calculated employing DFT/B3LYP and HF level of theory using the 6-311++G(d, p) basis set. Potential energy scan for molecules has been performed in dihedral angles C4 C3-C22 H23. The calculated 1H-NMR values compared with the experimental data in the literature. The dipole moment for nicotinic acid (ortho, meta and para –hydroxy-benzylidene)-hydrazides are calculated at 2.2911, 2.3326 and 2.0245 Debye, respectively with DFT/B3LYP level of theory the 6-311++G(d, p) basis set. The dipole moment value of nicotinic acid (para –hydroxy-benzylidene)-hydrazide was seen slightly lower value than others dipole moment values.

Keywords: Nicotinic Acid (ortho, meta and para –Hydroxy-Benzylidene)-Hydrazides, DFT, HF, NMR

O23 / 15:20 - 15:40 / Hall 1

Spectroscopic (Vibrational, NMR and UV-Vis.) and Quantum Chemical Investigations on 4-Hexyloxy-3-methoxybenzaldehyde

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In this study the title molecule as one of the derivatives of vanillin which is a well known flavoring agent, C14H20O3, has been investigated by experimentally and extensively utilizing density functional theory (DFT) at B3LYP/6-311++G(d,p) level. In this context, the optimized geometry, vibrational frequencies, 1H and 13C NMR chemical shifts, UV-Vis. (in gas phase and in methanol solvent) spectra, HOMO-LUMO analysis, molecular electrostatic potensial (MEP), thermodynamic and atomic charges of 4-Hexyloxy-3-methoxybenzaldehyde have been calculated. In addition, theoretically predicted IR, Raman and UV-Vis. (in gas phase and in methanol solvent) spectra of the mentioned molecule have been constructed. The results calculated were compared with the experimental data.

Keywords: Vanillin, DFT, IR, Raman, NMR and UV-Vis. spectroscopies

O24 / 09:00 - 09:20 / Hall 1

Coordinative Interactions between Phthalocyanines and Sc3N@C80 – Switchable Photoinduced Electron Transfer Reactivities

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The mimicry of the complex electron transfer processes occurring within the photosynthetic reaction center is one of the most fascinating fields of contemporary research. In particular, the design of artificial electron donor–acceptor ensembles, that is, covalently linked conjugates and / or non-covalently associated hybrids, is key in solar energy conversion. Without doubt, covalently linked conjugates are quite intriguing. Nevertheless, the use of non-covalent interactions provides a large number of advantages including flexible and easy synthesis, etc.

In recent years, endohedral metallofullerenes have emerged as novel electron acceptors as well as electron donors in a variety of photofunctional ensembles. To this end, we have integrated two different lanthanum metallofullerene derivatives as electron acceptors into electron donor-acceptor hybrids by means of coordinative interactions. Our photophysical assays corroborated that the unique electronic and magnetic properties of endohedral metallofullerenes lead to an outperformance of empty fullerenes in electron transfer reactions. A combination with phthalocyanines, which exhibit remarkable absorptions in the visible, high chemical and thermal stability, and unique optical as well as electrochemical properties, seems particularly promising. In this context, the possibility of tuning the properties of phthalocyanines by introducing different substituents at their periphery is a real asset.

Herein, we report on the coordination of a N-pyridinyl-fulleropyrrolidine derivative of Sc3N@C80 to two different phthalocyanines and on the electronic communication between them. Interestingly, by introducing either tert-butyl or sulfonyl substituents at the phthalocyanine we gain control over the electron transfer events occurring either from the phthalocyanines to the endohedral metallofullerenes or vice versa.

Keywords: donor-acceptor systems, electron transfer, supramolecular chemistry, endohedral metallofullerenes, phthalocyanines

O25 / 09:20 - 09:40 / Hall 1

Electron Paramagnetic Resonance Study Of Radiation Damage In Isonipecotic Acid Single Crystal

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The electron spin resonance spectra of the radical produced by gamma-irradiation of a single crystal of isonipecotic acid (piperidine-4-carboxylic acid) were reported, and the structure of the radical was discussed. Isonipecotic acid single crystals were exposed to 60Co-gamma irradiation at room temperature. The irradiated single crystals were investigated between 125 K and 470 K by Electron Paramagnetic Resonance (EPR) Spectroscopy. The g values of the radiation damage center observed in isonipecotic acid single crystal and the hyperfine structure constants of the free electron with nearby protons were obtained.

Keywords: EPR, Isonipecotic acid, Radiation damage center.

O26 / 09:40 - 10:00 / Hall 1

Distinctive Features Of Push-Pull Enaminoketones. α-Substitution In β-Alkilaminovinyl Perfluoromethyl Ketones

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Institute of bioorganic chemistry and petrochemistry, Natl.Acad.Sci.Ukraine

According to results of 1H, 19F NMR and FT-IR investigations α-substituted β-methylamimovinyl perfluoromethyl ketones exist in solution as equilibrium of three stereoisomeric forms, viz E-s-E(1), E-s-Z(2), and Z-s-Z(3) (for α-fluor substituted derivative designation of appropriate stereoisomers is: Z-s-E(1), Z-s-Z(2), and E-s-Z(3)).

In solution of non-polar solvents β-methylamimovinyl perfluoromethyl ketone exists exclusively as Z-s-Z form, whereas α-substituted derivatives as-solved in non-polar solvents are presented as equilibrium of the (1) and (2) conformer, which spontaneously turn into the (3) isomer. Thermodynamic parameters (-ΔH and -ΔS) of equilibrium between stereoisomeric forms (1) and (3), (2) and (3) of β-methylamimovinyl perfluoromethyl ketone(I), α-methyl β-methylamimovinyl perfluoromethyl ketone (II) and α-fluor β-methylamimovinyl perfluoromethyl ketone (III) increase in following sequence (III)>(II)>(I), whereas for equilibrium between forms (1) and (2) sequence is reversed.

Strong intramolecular resonance-assisted hydrogen bond (RAHB) stabilizes heteroconjugated system (3), lowering its energy in comparison with the (1) and (2).

Keywords: FT-IR spectroscopy, alfa-substituted beta-methylamimovinyl perfluoromethyl ketones

O27 / 10:00 - 10:20 / Hall 1

Controlling The Defect Centers In ZnO Nanoparticles By Multifrequency and Ultra High Field EPR Spectroscopy

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Comprehensive understanding of the defect centers in zinc oxide (ZnO) nanoparticles invokes an important issue of controlling the nanoscopic properties of ZnO compounds. Due to its wide band gap (3.4 eV), ZnO possesses extraordinary electronic and optical properties, which make it a very attractive material for technological applications, particularly for thin film printable electronics. Doping ZnO with transition metal ions, like Fe, Co, or Mn leads to materials with diversified behavior towards magnetic and optical excitation. Even relatively small concentrations of defects and impurities can significantly affect the electronic, magnetic and optical properties of semiconductors. Therefore, 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 bound excitons. Nonetheless, just from the basic principles of defect formation, it is hard to understand or predict what kind of defects will be present in the sample. In order to characterize the ZnO defect structure, both multifrequency and ultra high field EPR has been applied.

Keywords: EPR spectroscopy, ZnO semicondutor, defects

O28 / 10:40 - 11:00 / Hall 1

Theoretical Studies on Mono-, di-, tri- 2-((4-Fluorophenly) Imino Methylene) Phenol

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In this work, the molecular properties for the title molecules have been investigated by ab-initio Hartree-Fock (HF) and also Density Functional Theory (DFT) calculations Becke's three-parameter exchange functional combined with Lee-Young-Parr correlation functional (B3LYP). Molecular structure, dipole moment, polarizability, first static hyper polarizability, 1H-NMR, 13C-NMR and potential energy scan of the molecules have been calculated by using 6-311++G(d,p) basis set for both models. The energy band gap of those molecules have been carried out at different basis sets. The calculated 1H-NMR, the highest occupied molecular orbital (HOMO) energy and the lowest unoccupied molecular orbital (LUMO) energy values of 2-[(4-fluorophenyl) imino methylene] phenol (FPIMP) monomer compared with the experimental data in the literature. The results of DFT calculations with BLYP and LSDA are in good agreement with experimental data in the literature

Keywords: HF, DFT, dipole moment, polarizability

O29 / 11:00 - 11:20 / Hall 1

Calculation of the Resonant Frequencies in the Vicinity of the Alpha-Beta Transition in Quartz

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The alpha-beta transition (573 C) in quartz is investigated using the temperature dependence of the resonant frequency and of the lattice constant correlated by means of the mode Grüneisen parameter. By determining its mode Grüneisen parameter, the resonant frequencies are predicted in the vicinity of the alpha-beta transition in quartz. This calculation is extended to low temperatures (down to about 50 C) and the resonant frequencies are predicted at low temperatures using the lattice parameter data for quartz.

Our predictions indicate that the method of calculating the resonant frequencies using the lattice parameter data is satisfactory and it can be applied to some other crystalline systems.

Keywords: Resonant frequency, Lattice parameter, Quartz

O30 / 11:20 - 11:40 / Hall 1

Electron Paramagnetic Resonance Of Gamma Irradiated Single Crystals Of Potassium Hydroquinone Monosulfonate

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The Electron Paramagnetic Resonance (EPR) spectra of gamma-irradiated Potassium Hydroquinone Monosulfonate (PHM) have been investigation at 125 K. The irradiation of PHM by gamma-rays produces two radicals. The principal values of the hyperfine coupling tensor of the unpaired electron and the principal values of the g-tensor have been determined. The results have been found to be in good agreement with the existing literature data and theoretical predictions.

Keywords: EPR, Potassium hydroquinone monosulfonate, Radiation damage center, Hyperfine coupling constant, Spectroscopic splitting factor.

O31 / 11:40 - 12:00 / Hall 1

Molecular Structure and EPR Spectral Studies Of Trans-Bis(perchlorato-κO)tetrakis(1-vinyl-1H-imidazole-κN3)copper(II)

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A new copper(II) complex of 1-vinylimidazole (1-Vim) and perchlorate has been synthesized and structurally characterized. The molecular structure of the complex exhibits six coordination with a distorted octahedron geometry. The 1-Vim ring is coordinated through the imidazole nitrogen, as expected from earlier spectroscopic studies of related adducts. The complex crystallizes in triclinic system and the space group is P-1. In the title compound, [Cu(ClO4)2(C5H6N2)4], the Cu(II) ion is located on an inversion centre. It features a Jahn–Teller distorted octahedral coordination geometry, defined by four N atoms of four 1-vinylimidazole ligands in the equatorial plane and two nitrate O atoms in the axial positions.

The magnetic environment of the title complex has been identified by electron paramagnetic resonance (EPR) technique. Detailed investigations of the EPR spectra show that the local symmetry of the Cu2+ ions is rhombic. Principal values of g and hyperfine tensors were determined and the ground state wave function of Cu2+ ions was obtained using EPR parameters. The ground state wave function indicates that the ground state of the Cu2+ ion is an admixture of and orbitals.

Keywords: Cu(II) complex; 1-Vinylimidazole; Single crystal; XRD; EPR

O32 / 12:00 - 12:20 / Hall 1

Density Functional Calculations and Experimental Vibrational Spectral Studies of Free m-toluidine and its Copper(II) Chloride Complex

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The FT-IR (including mid and far regions) and dispersive Raman spectra of free m-toluidine and the Copper (II) chloride complex of m-toluidine i.e. Cu(m-tol)2Cl2, have been investigated experimentally. The molecular structure and vibrational assignments of the title molecules have been performed theoretically by DFT/B3LYP calculations using the standard 6-311G+(d,p) basis set. Cu(m-tol)2Cl2 has been optimized as two conformers and the more stable conformer is determined with DFT calculations. The vibrational frequencies have been compared with experimental values, and the normal modes were assigned on the basis of the percent potential energy distribution (PED). The calculated vibrational frequencies of the free and complexed m-toluidine after a scaling procedure agree reasonably well with the corresponding experimental frequencies.

Keywords: DFT; vibrational spectra; Copper(II) chloride complex; m-toluidine.

O33 / 12:20 - 12:40 / Hall 1

Investigation Of The Effects of nitrogen-doped titanate nanotubes by UV-Vis and Raman spectroscopy

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In the past two decades titanate nanotubes have attracted considerable attention from the materials science community because of their simple synthesis and their fascinating properties such as large specific surface area and pore volume and high stability with photocatalytic activity, to name a few.

The doping of the titanate nanotbes with nitrogen can enhance the photocatalytic activity in the visible light region and protect the stability opposite to the transistion metal ion doped ones.

There are several ways to prepare titanate nanotubes and to dope them with nitrogen. The most commonly applied process, after the hydrothermal synthesis, is to mix the titanate with nitrogen containing aqueous solutions. Another popular methods are the heat treatment of the titanate nanostructures in NH3 flow or calcining ammonium trititanate nanotubes. We synthetised titanate nanotubes via hydrothermal method in revolving autoclave followed by nitrogen doping using the thermal decomposition of urea as ammonia gas source. In this study we prepared samples with different synthesis times and we investigated the as-prepared samples by XRD and TEM and they effect with UV-Vis and Raman spectroscopy.

Keywords: titanate nanotube, nitrogen dope, Raman spectroscopy, UV-Vis spectroscopy

O34 / 12:40 - 13:00 / Hall 1

Theoretical Electronic Structure and Spectroscopic investigations of CsRg (Rg=Rare gas) van der Waals Complexes

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Alkali vapor lasers pumped by diode lasers are currently being investigated in several laboratories. This is motivated by their potential to produce high powers with high beam quality, which is desirable for multiple technological applications. A problem with this type of device is the poor matching of the broad linewidth of the pump source with the narrow absorption lines of the alkali atoms. One idea, to overcome this difficulty, is to use far-wing line broadening effects that are associated with alkali metal-rare gas interactions. This concept has recently been demonstrated for optical excitation of Cs-Ar, Rb-Kr and Cs-Kr collision pairs. Accurate potential energy curves for the upper and lower electronic states of M-Rg pairs are needed to evaluate the scaling possibilities for alkali metal rare gas dimer lasers. The potential energy curves of the ground state and many excited states of the CsRg collision complex have been determined using [Cs+] and [e-Rg] pseudopotentials with the inclusion of core polarization operators on atoms. This has reduced the number of active electrons of the CsRg dimer to only one valence electron, permitting the use of large basis sets for the Cs and Xe atoms. Potential energy curves of the ground state and many excited states have been calculated at the SCF level. The core-core interactions for Cs+Rg are included using the accurate CCSD potential of Hickling et al. Spectroscopic constants for the ground and excited states of CsRg are derived and compared with the available theoretical and experimental results.

Experimentally, spectral lineshapes for the alkali atom (Cs) in the presence of various rare gases were investigated and the broadening was verified. The fluorescence signals from the 2P3/2 and the 2P1/2 levels of the alkali atom are detected. Basically, we have a fluorescence spectroscopy experiment in order to evaluate the theoretical results. We excite the blue wings of the Alkali-Rare gas excimers and detect the fluorescence of the alkali atoms. We have examined different cells filled with Argon, Krypton, Xenon, respectively, at a pressure around 500 torr. Three additional cells, filled with the same gases at the same pressure plus ethane at around 100 torr, were also investigated. Each cell wss heated to temperatures ranging from ambient to about 300 °C.

The experimental Setup. 1 : Laser, 2 : Aluminum Mirrors, 3 : Optical Isolator, 4 : Pellicular Beamsplitter, 5 : Spectrometer, 6 : λ/2 plate, 7 : Polarizer, 8 : Chopper, 9 : Pellicular Beamsplitter, 10 : Si Photodiode, 11 : Heating Block, 12 : Cs-Rg Pyrex cell, 13 : Thermocouple, 14 : Cartridge Heater, 15 : XYZ Translation Holding a Lens, a Bandpass Filter and a PIN Photodiode Detector, 16 : Temperature Controller, 17 : Lock-in Amplifier, 18 : Power Meter, 19 : IR Sensor Card.

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TURCMOS 2013

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POSTER PRESENTATIONS

Applied Spectroscopies - P1 / 16:20 - 18:20

Comparison of Thermal and IR Spectroscopy Methods for Determination Amount of Residual Monomer in Dental Composite Materials

***Ceren Koser*[1], Sevi Öz[2], Adil Nalçacı[1], Orhan Atakol[3]**

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Several methods have been reported in literature about determination amount of nonpolymerized monomer after polymerization via light curing of restoration materials which is used in dentistry. These methods are MeOH extraction and HPLC method [1], IR spectroscopy, Differential Scanning Calorimetry (DSC) or Differential Thermal Analysis (DTA) [2].

In general, IR spectroscopy is preferable for acrylate-based composites. Aliphatic C=C bonds of acrilate groups makes IR absorption between 1629-1640 cm-1 and polymerization degree can be calculated of this signal intensity. DTA and DSC methods are used for monomer-based composites like triethyleneglicoldimethylacrilate (TEGDMA) and Silloran that its polymerization reaction is exothermic and polymerization degree can be determined with using this reactions enthalpy value. In this study, amount of residual monomer in the composite which is prepared from different three monomer-based with various irradiation conditions was determined with the help of FTIR and DSC instruments and the results were compared. The commercial names of used composites are silloran, grandio and Z250. Because of the absence C=C bond in silloran, peak intensity was measured at 1255 and 833 cm-1 as literature suggests [3]. Amounts of residual monomer were found 16.4% for sillorane, 16.66% for Grandio and 11.1% for Z250 as average. Polymers were prepared with 1, 2 and 3 mm thickness and as expected the degree of polymerization decreases with increasing thickness.

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1509-1516

Keywords: FTIR, Monomer residue, Nonpolymerized monomer

Applied Spectroscopies - P2 / 16:20 - 18:20

The Use of Vibrational Spectroscopy in Biophysical Characterizations of Novel Non-Viral Lipoplex Gene Delivery Systems

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Department of Pharmaceutical Chemistry

The current work summarizes the utilization of neutral lipids-Mg2+-plasmid DNA ternary complexes as gene carriers, by emphasizing the influence of the physicochemical features of these polyelectrolyte complexes on their functions, such as stability and gene transfer into cells. The major aim of the present study was to follow the DNA compaction with a model plasmid vector using vibrational spectroscopic approaches. The lipoplexes result from the self-assembly of a circular plasmid DNA with multilamellar and unilamellar zwitterionic phosphatidylcholine vesicles, controlled by simple addition of Mg2+ in the medium in a concentration dependent manner. FTIR measurements were employed to follow structural transitions of newly proposed ternary lipoplex complexes as promising gene delivery formulations. Results are described at the levels of carbonyl, phosphate, choline and CH groups and discussed as effects of nucleic acid and phosphatidylcholine moiety on each other in the absence and in the presence of Mg2+. Data suggest that upon recognition of DNA with lipids, the DNA undergoes helical transition. Divalent metal ion effects are interpreted as dehydrations of phosphates and H-bonding inducing effects on carbonyl groups. Conventional Raman and Surface Enhanced Raman Spectroscopy (SERS) were employed to characterize the ternary complexes, monitoring the accessibility of nucleoside residues to silver colloids. The SERS spectra show a decrease of signal intensity when the vector/DNA charge ratio increases. The SERS intensity variations were in agreement with gel electrophoresis and zeta potential experiments. in vitro transfection efficiency of those DNA vectors were also performed and compared to the previously reported control cationic lipoplexes.

Keywords: gene delivery, FTIR, Raman Spectrsocopy, Surface Enhanced Raman Scattering; Mg2+

Applied Spectroscopies - P3 / 16:20 - 18:20

Effects of Thalium Element on Radiation Absorption and Microstructures Properties the Casting Al-Zn Alloy

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In this study, two different types of alloying systems are used as Al-40wt%Zn and Al-40wt%Zn-%5Tl Al-based alloys. The Al-Zn alloy system is commonly used in the building industry for roofing and siding. Therefore, the linear attenuation coefficients of gamma rays for alloys material were measured at 1773 and 1332 keV. The gamma rays were obtained from 60Co sources and the measurement were performed using a gamma spectrometer which contains 3”x3” NaI(Tl) detector connected to 16384 channel Multi-Channel-Analyser (MCA). Then structure of the alloys were defined by scanning electron microscopy (SEM) and weight percentages of the elements in the phases were determined by Energy Dispersive Spectroscopy (EDS) technique. Afterwards, phases of the alloys were investigated by XRD. From XRD and SEM studies obtained phases were identified as α(Al), β(Zn) and mixture regions α+β eutectic phases.

Keywords: Eutectic, Al-Zn Alloys, Scanning Electron Microscopy, Energy-Dispersive Spectrometry, X-Ray Diffraction, Radiation shielding, gamma-ray, NaI(Tl).

Applied Spectroscopies - P4 / 16:20 - 18:20

Experimental Investigations of Linear Attenuation Coefficients at 662, 1173 and 1332 keV Energies in Cu-Mn-Al alloy

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[3]Physics Department, Kırıkkale University, Kırıkkale, TURKEY

The linear attenuation coefficients of gamma rays for Cu-Mn-Al alloy material have been measured at 662, 1773 and 1332 keV. The gamma rays have been obtained from 137Cs and 60Co sources respectively and the measurement have been performed using a gamma spectrometer which contains 3”x3” NaI(Tl) detector connected to 16384 channel Multi-Channel-Analyser (MCA).

Keywords: Radiation shielding, alloy, gamma-ray, Cu-Mn-Al, NaI(Tl).

Applied Spectroscopies - P5 / 16:20 - 18:20

Analytical Studies of The Thracian Tomb Wall Paintings at Alexandrovo

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The ancient Thracian tomb at Alexandrovo, Bulgaria (dated to the fourth century BC) is considered as one of the most important recent discoveries since there are very few sites with mural decoration known from this period. It holds important historical, cultural and scientific information about the life and religion of the ancient Thracians, as well as the construction and painting techniques used back then.

The aim of the current study is to help the preservation work on this site providing important information about of the painting materials and techniques. To understand some phenomena such as the polished semi-glossy surface of the red plinth, the way the ornamental friezes were painted, and the causes for deterioration, Fourier transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM), differential scanning calorimetry (DSC), X-ray fluorescence (XRF), high-resolution transmission electron microscopy (HRTEM) and energy dispersive X-ray (EDX) analyses were carried out. By employing the above techniques, a presence of TiO2, Ce, Zr and Au nanoparticles was established in certain painting components which may enhance the paintings optical effects. The study gave useful information about the paint layers composition and also confirms that the Thracian tomb at Alexandrovo is one of the oldest cultural monuments in the world where beeswax binder had been used in the wall paintings.

Keywords: nano-particles, beeswax, archeology, FTIR, HRTEM

Applied Spectroscopies - P6 / 16:20 - 18:20

Synthesis, Structural Characterization, Thermal and Biological Analyses of (C14H18N2O4)Cu+2(C7H7SO3) Complex

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[3]*Biotechnology Laboratory, Biology Department, KSÜ, Avsar Campus, Kahramanmaras*
[4]*Physics Department, KSÜ, Avsar Campus, Kahramanmaras*

In this study, the metal complex (C14H18N2O4)Cu+2(C7H7SO3) was prepared from the reaction between 4-methylbenzenesulfonic acid and 2-aminobenzamide in the presence of cupper(II) sulfate, and characterized by means of thermal (TG/DTA) and X-ray diffraction methods. The crystallographic analysis shows that the complex crystallizes in the triclinic system, space group. In the complex, the geometry around the cupper ion has distorted octahedral geometry by two N and four O atoms. The C-H...O strong intra- and also N-H...O and O-H...O type weak inter-molecular hydrogen bonding interactions mainly stabilize the crystal structure and form an infinite 3-dimensional network. The thermal decomposition of the complex has been studied and found that the complex is thermally stable up to 98oC. Additionally, some effects of the metal complex on hydrolytic enzymes and antimicrobial activities were carried out and the results are presented.

We would like to thank Dr.Şemistan Karabuğa at Chemistry Department and the Biotechnology Laboratory in Biology Department, KSU, staff for their assistance without which this work could not have been accomplished.

Keywords: Metal Complex, Sulfonic Acid, X-ray Crystallography, Antimicrobial, Enzymatic Activity

Applied Spectroscopies - P7 / 16:20 - 18:20

The Spectroscopic Characterization Of Some Ru(III) Complexes With Schiff Bases Derived From Salicyladehyde And Investigation Of Interaction With CT DNA

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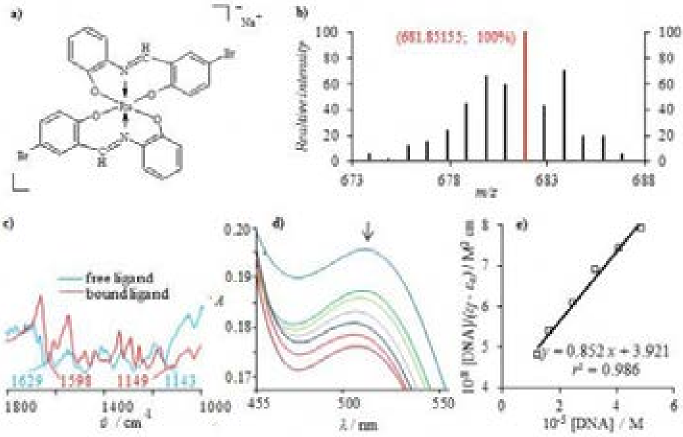
Different spectroscopic techniques are very useful in the field of design and development of new compounds. Numerous Ru(III) compounds are reasonably synthesized as potential anticancer agents whose key target is thought to be DNA. While very accessible infrared spectroscopy provide an easy way to identify the modes of ligand binding and environment of central atom, the interaction of the compounds with DNA can be followed by spectrophotometric titration in UV/visible region. A number of anionic and cationic Ru(III) compounds with Schiff bases derived from salicyladehyde were prepared for possible biological evaluation. The compositions of compounds Na[RuCl2(N-R-Salim-X)2], Na[Ru(N-R-Salim-X)2], [RuB2(N-R-Salim-X)2]Cl, where R = C4H9, C6H5, C6H4O, X - represents 5-subsituting atom group (H, Cl, Br, NO2) on salicyladehyde, B = indazole, pyrazole and pyridine, were confirmed by MALDI - TOF mass spectra. Infrared spectra of complexes showed typical shifts of azomethine group toward lower wavenumbers (10 - 34 cm-1) and phenolic C-O(Ru) toward higher frequencies (6-25 cm-1) compared to free ligands, clearly demonstrating ON, O2N or ON2 mode of binding. Interaction of synthesized complexes with CT DNA has been followed by spectrophotometric titration. The µL – amounts of stock solution DNA were being added into Ru(III) solution by keeping the concentration of complexes unchanged. The decrease of absorption of complex compounds in the region of LMCT bands after DNA adding suggests an intercalative mode of binding, as confirmed by electrochemical measurements. Kb is slightly varying from 1.81 x 104 – 4.90 x 104 M-1 for DNA / compounds ratio 1.54 - 5.51.

Keywords: Spectroscopy, Ruthenium, Schiff base, DNA intercalation

Spectroscopic investigation of Na[Ru(N-C6H4O-Salim-Br)2]



Applied Spectroscopies - P8 / 16:20 - 18:20

Optical Luminescence Studies Of The Ethyl Xanthate Adsorption Layer On The Surface Of Sphalerite Minerals

Radu Todoran**, **Daniela Todoran, Zsolt Szakacs

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We propose optical luminescence as a method for the evaluation of the kinetics for adsorption processes, to determine the time to achieve dynamic balance for the thin layers formed at the mineral-xanthate solution interface. The method is based on the determination of the intensity for the integral optical radiation, obtained from the mineral-xanthate thin layer, stimulated with a monochromatic pulsating optical signal, as a function of time. The luminescence was studied for sphalerite with sodium ethyl xanthate, for different xanthate-solution concentrations and diverse values of the pH at constant temperature. Using this method one gained information on the kinetics for the adsorption of xanthates. A better determination of the time to achieve equilibrium of formation for the adsorption layer was obtained.

Keywords: Sphalerite; Ethyl xanthate; Adsorption; Kinetics

Applied Spectroscopies - P9 / 16:20 - 18:20

Nonionic and Zwitterionic Forms of Glycylglycylarginine Part of Spider Silk Protein: Structural and Vibrational Spectroscopic Search

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Spider silk have gained growing interest during the last ten years because of their remarkable properties. In order to understand these remarkable characteristics, the structural properties of these silk proteins must be investigated [1]. All types of silk share four types of amino acid motifs comprising of GPGXaXb (XaXb= GA, GS, GY, or QQ), GGX (X: A, L, R, Q and Y), polyalanine and polyglycylalanine [2]. GGX motifs have 310-helix structure and provide silk with elasticity [3]. Amino acids are present nonionic and zwitterionic forms in gas and liquid states, respectively. In this study, nonionic and zwitterionic forms of Glycylglycylarginine (non-GGR and zwt-GGR) parts of the spider silk chain have been examined from theoretical and spectroscopic aspects.

The calculations including conformer analysis, geometry optimization and vibrational analysis of non-GGR and zwt-GGR have been performed in the ground state by using the DFT/B3LYP with 6-31G(d) basis set. Non-GGR was calculated in the gas phase. Zwt-GGR was calculated in the aqueous media using the IEFPCM. All computational studies have been performed with the Gaussian 09 program package [4]. Potential Energy Distributions of normal modes have been calculated using the VEDA4 program [5].

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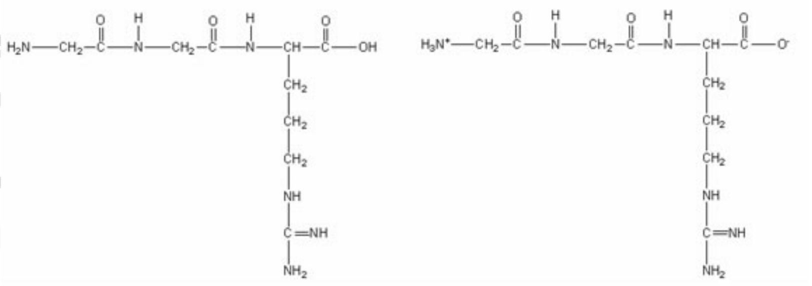
This study was supported by Erciyes Üniversity Scientific Research Project (Project no: FDK-2013-4543)

Keywords: Spider silk, Glycylglycylglutamine, Structural - Vibrational Study, DFT.

Figure 1. non-GGR and zwt-GGR



Applied Spectroscopies - P10 / 16:20 - 18:20

Structural and Vibrational Studies on Nonionic and Zwitterionic Forms of Glycylglycylglutamine Part of Spider Silk Protein

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Spider silk is a secretion produced by the abdominal glands that transforms a viscous and concentrated protein aqueous solution into an insoluble solid fiber at ambient temperature. These proteins are high-molecular-weight biopolymers composed of a repetition of numerous consecutive sequence units. Repeat units are often composed of small submotifs, such as An, (AG)n, GGX, or GPGXaXb, that are considered the hallmark of silk proteins [1]. GGX (X=L, Q, R, or Y) and GPGXaXb (XaXb=GA, GS, GY, or QQ) modules adopt less ordered conformations, most likely 310-helices and turns, and are important for fiber extensibility [2]. Nonionic and zwitterionic forms of Glycylglycylglutamine (non-GGQ and zwt-GGQ) part of the spider silk chain have been calculated by using the DFT/B3LYP with 6-31G(d) basis set. Conformer analysis, geometry optimization and vibrational analysis have been carried out in gas and in solution phase for Non-GGQ and Zwt-GGQ, respectively. Zwt-GGQ was calculated in the aqueous media using the SCRF method and the IEFPCM model. All the calculations have been made using Gaussian 09 program package [4]. The potential energy distributions of the normal modes have been calculated using the VEDA4 program [5]. Theoretical results were compared with observed spectra to discuss structural details.

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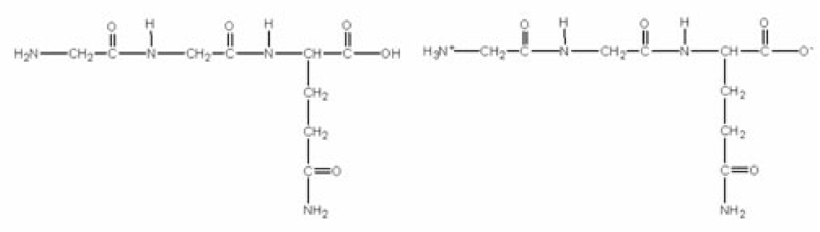
4. M.H. Jamroz, Vibrational Energy Distribution Analysis:VEDA 4 program, Warsaw, (2004).

This study was supported by Erciyes Üniversity Scientific Research Project (Project no: FDK-2013-4543)

Keywords: Spider silk, Glycylglycylglutamine, Structural-Vibrational Study, DFT

Figure 1: non-GGQ and zwt-GGQ



Applied Spectroscopies - P11 / 16:20 - 18:20

Spectroscopic analysis of the impact of oxidative stress on the structure of human serum albumin (HSA) in terms of its binding properties

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Oxygen metabolism plays an important role in the pathogenesis of rheumatoid arthritis (RA). The excessive production of ROS can damage protein, lipids, nucleic acids, and matrix components. It results in oxidation of serum albumin, which causes a number of structural changes in the spatial structure, that may influence its binding and affect significantly drug interactions, particularly in polytherapy. The aim of the study was to estimate the influence of oxidative stress on human serum albumin (HSA) structure and evaluate a disorder in the binding of drug to oxidized human serum albumin (oHSA). Changes of albumin conformation due to its oxidation were examined by comparison of modified (oHSA) and non-modified human serum albumin (HSA) absorption spectra, emission spectra, red-edge shift (REES) and synchronic spectroscopy. Studies of absorption spectra indicated that changes in the value of absorbance associated with spectral changes in the region of 200 to 250 nm involve structural alterations in peptide backbone conformation. Synchronic fluorescence spectroscopy technique confirmed changes of position of tryptophanyl and tyrosyl residues fluorescent band caused by CT. Moreover analysis of REES effect allowed to observe structural changes by CT in the region of the hydrophobic pocket containing the tryptophanyl residue.

Effect of oxidative stress on binding of anti-rheumatic drugs, sulfasalazine (SSZ) and sulindac (SLD) was investigated by spectrofluorescence and 1HNMR spectroscopy. Both SSZ and SLD caused the fluorescence quenching of modified (oHSA) and nonmodified (HSA) albumin molecule.

Acknowledgement: This work was supported by grants from Medical University of Silesia KNW-1-001/K/3/0 and KNW-2-001/N/3/K.

Keywords: REES effect, synchronic spectroscopy, 1H NMR, oxidative stress

Applied Spectroscopies - P12 / 16:20 - 18:20

Determination of Natural Radionuclide Concentration of Some Metamorphic Rock in Turkey

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There are various amounts of radioactivity substances in the underground and the earth was irradiated by this substances. These radioisotopes are found naturally in the earth and their decay products constitute the natural radiation in the environment. Thus humans are exposed to various kind of radiation from these sources.

The main goal of this study is to determine 40K, 226Ra and 232Th activities on metamorphic rocks. The measurements have been carried out using a NaI(Tl) gamma-ray spectrometer. Activity of 40K was measured from its intensive line at 1460 keV, for 226Ra activity peak from 214Bi at 1760 keV and 232Th activity, peak from 208Tl at energy of 2615 keV was used.

Keywords: Radioactivity, Metamorphic Rock, Gamma-Ray Spectrometer

Applied Spectroscopies - P13 / 16:20 - 18:20

The Photon Attenuation Coefficients Of Self Compacting Concrete (SCC

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People spend most of their time (80%) indoors so the photon attenuation coefficients in buildings are important in the assessment of possible radiation exposure. The concrete is one of the basic building materials and there are different types of concrete. In this study, the photon attenuation coefficients of Self Compacting Concrete (SCC) have been measured using a gamma spectroscopy with NaI(Tl) detector. The SCC is the a concrete with the ability to compact itself only by means of its own weight without the requirement of vibration. The measurements have been performed using 60Co source which gives 1173 and 1332 keV energies gamma rays and 137Cs source which gives 662 keV energy gamma rays.

Keywords: Photon Attenuation Coefficient, Self Compacting Concrete, Gamma Spectrometer

Applied Spectroscopies - P14 / 16:20 - 18:20

FTIR-Chemometric Methodology For The Prediction Of The Heat Stability Of Extra Virgin Olive Oil

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The aim of this work was studying the heat stability of extra virgin olive oil (EVOO). Fourier-transform infrared (FTIR) followed by multivariate treatment of spectral data was used to predict heating of EVOO.

The wavelength scale of FTIR spectra of the samples was divided in 28 regions. The normalized absorbances of these regions were used as predictors.

Two multivariate calibrations, namely multiple linear regression (MLR) and partial square (PLS) were optimized for constructing the calibration models.

An MLR model constructed using four predictors was able to predict the heating temperature with coefficient of determination (R2) of 0.9938.

PLS models were used for predicting the heating temperature of EVOO with a coefficient of determination (R2) of 0.9775. These models were validated by the leave-one-out procedure

The main wavelength region affected by heating selected to construct this model corresponded to: -CH (CH3, bending asym), - CH (CH2, bending scissoring), O-H (bending in plane), =C-H (trans and cis) and –C=O (ester stretching).

The proposed methodology based on FTIR spectroscopy in conjunction with multivariate analysis was very suitable for the prediction of heating temperature of EVOO.

Keywords: Extra virgin olive oil; heat stability; FTIR-Chemometric methodology

Applied Spectroscopies - P15 / 16:20 - 18:20

Mineralogic Characterization Of Limestone, Jebel Kellel, North-East Constantine

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The importance of the complexity of the geological context situated in the north-east of Constantine encourages us to further investigation and characterization of limestone of this region.

The improvement that require road infrastructure in the composition of asphalt (bitumen and aggregate) is an important element in the objective of this study.

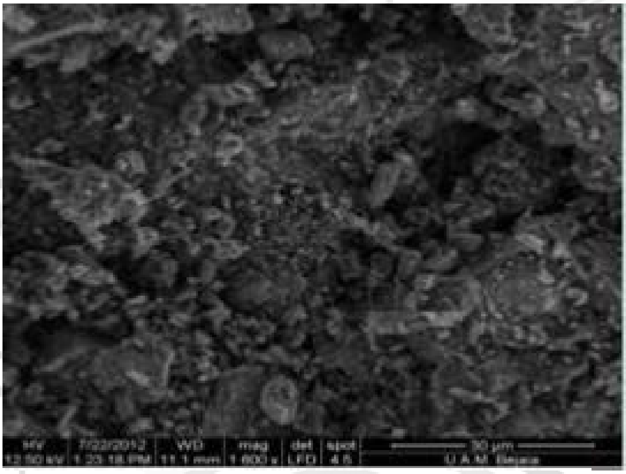
The X- ray diffraction (XRD) analysis, SEM/EDS, FTIR spectroscopy of limestone are required for qualitative and quantitative analysis of the existing phases.

In addition, chemical analysis of the same samples (gray and white limestone) is required to confirm the XRD, EDS and FTIR results.

The results of this multidisciplinary study (obtained by various analytical techniques) show good agreement on the existing phases.

Keywords: Limestone, XRD, SEM/EDS, FTIR

SEM morphology of white limestone (X 1600)



Applied Spectroscopies - P16 / 16:20 - 18:20

Mineralogic Characterization Of Sandstone And Clay, Jebel Kellel, North-East Constantine

Mounia Benguedouar, Samia Kherfi, Merzoug Bouchear

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The north-east area of Constantine has a very complex geological setting.

The variety of sedimentary rocks such as sandstone clay and in abundance, represent a big importance in the industry and road infrastructure.

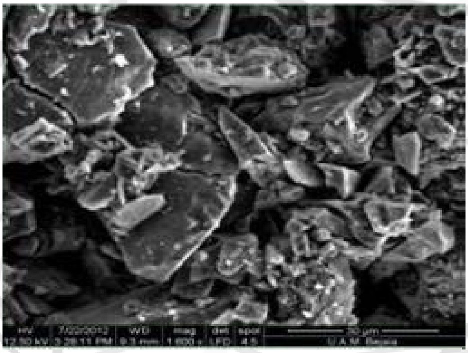
The X- ray diffraction (XRD) analysis, SEM/EDS, FTIR spectroscopy of sandstone and clay are required for qualitative and quantitative analysis of the existing phases.

In addition, chemical analysis of the same samples is required to confirm the XRD, EDS and FTIR spectroscopy results.

The results of this multidisciplinary study (obtained by various analytical techniques) show good agreement on the existing phases.

Keywords: Sandstone, Clay, XRD, SEM/EDS, FTIR.

SEM morphology of sandstone (X 1600)



Applied Spectroscopies - P17 / 16:20 - 18:20

Explanation Of 3D Ions Behavior In The Aqueous Solution Of MgSO3.6H2O: M (M = Cr, Co or Cr+Co)

<u>Ivaylo Parushev</u>*[1]*, Petya Petkova*[1]*, Petko Vasilev*[1]*, Veselin Nedkov*[1]*, Jordanka Tacheva*[1]*,
***Mohamed Toufik Soltani*[2]*, Youri Tzukrovski*[3]**

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In this work, the absorption of the complexes [Cr(H2O)6]2+, [Co(H2O)6]2+ and [Cr+Co(H2O)6]2+ is measured in the spectral region 400 – 800 nm. The aqueous solutions of MgSO3.6H2O: M (M = Cr, Co or Cr+Co) are prepared with the concentration 2%. The energies of the electron transitions in M are calculated. The role of the spin-orbit interaction and Jahn-Teller effect is evaluated also. Zeeman splitting which is characteristic for M is determined and discussed.

Keywords: spin-orbit interaction, Jahn-Teller effect, Zeeman splitting

Applied Spectroscopies - P18 / 16:20 - 18:20

Temperature Effect on the Recovery Process of Stretched Bombyx Mori Silk Fibers

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Bombyx Mori silk fibers being natural biological macromolecules were stretched in the extension range from 3 to 14% at room conditions for 10 min during which stress-relaxation process occurs. Following stress-relaxation process, the strain recovery processes of stretched silk filaments were investigated after being heated at different temperatures for long term up to several days. The FT-IR/ATR spectra of the silk filaments were obtained at different time intervals during recovery process. The dependence of the recovery process of silk filaments on the temperature was examined on the basis of observed decrease in the present state of the sample length during recovery process and structural changes were discussed by using FT-IR/ATR spectroscopy method. It was observed that the strain recovery process was very slow at room conditions; however, increasing temperature accelerated the recovery process. Hence, it enhanced the recovered part of the each applied strain, that is, reversibility property of the stretched silk filaments and it left lower residual deformation (strain) on the sample.

Keywords: Silk fibers, recovery process, residual deformation, temperature

Applied Spectroscopies - P19 / 16:20 - 18:20

Pollutant Identification On The Walls Of "Valence Aqueduct" (Bozdoğan Kemeri, İstanbul) By Portable Handheld Raman, SEM-EDX, Far-Infrared And Mid-Infrared Techniques

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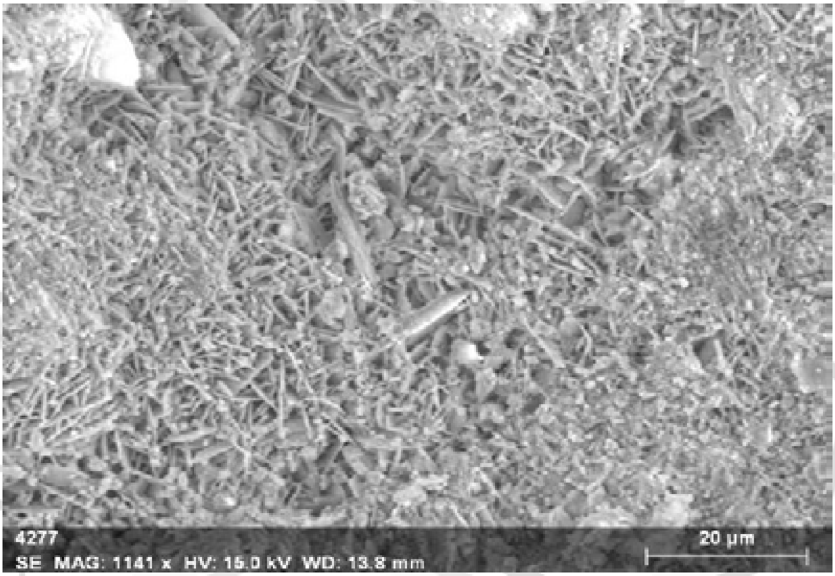
[3]University of Istanbul, Faculty of Letters, Department of Conservation and Restoration of Artifacts, Fatih, Istanbul, Turkey

This study represents the first Far infrared, Mid infrared, Raman spectroscopic and SEM-EDX studies of the pollutants from the walls of Valence Aqueduct (Bozdoğan Kemeri), İstanbul, Turkey. Provided that enough amount of sample is available, Far infrared spectroscopy is a useful analytical method particularly in characterisation of inorganic compounds such as painting materials and corrosion products, which are not active in the mid-infrared. Furthermore, far-infrared spectroscopy is a complementary technique to Raman spectroscopy in particular in the presence of fluorescence.

Keywords: Valence Aqueduct, Bozdoğan Kemeri, Risk Analysis, Cultural Heritage, pollutant, Raman, MIR, FIR, SEM-EDX

SEM image of the pollutants from the surface of the column of Valence Aqueduct, İstanbul



Applied Spectroscopies - P20 / 16:20 - 18:20

Far-infrared, Mid-infrared, Raman and SEM-EDX Investigations On Pigments From Pallette Of Old Paintings By Feyhaman Duran and Comparison With Organic Pigments

***Ozan Unsalan**[1]*, ***Gülder Emre**[2]*, ***Ayberk Yılmaz**[1]*, ***Alpaslan Kuzucuoğlu**[3]*, ***Gözem Yaşayan**[2]*

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[3]Yeniyüzyıl University, İstanbul, Turkey

This study mainly represents the first Far infrared spectroscopic investigation of the inorganic pigments found in the paints from the palette of Feyhaman Duran, a famous painter in Turkey. On the other hand, provided that enough amount of sample is available, Far infrared spectroscopy is a useful analytical method particularly in characterisation of inorganic compounds such as painting materials and corrosion products, which are not active in the mid-infrared. Furthermore, far-infrared spectroscopy is a complementary technique to Raman spectroscopy in particular in the presence of fluorescence. Besides, the Raman spectra and Mid infrared spectra were recorded for investigation of the pigments (white, red, yellow and black) employed in art. We also built a small Far-infrared spectral library for the pigments used in the pallete of the artist in order to use our further Far-infrared studies of any other artists.

Keywords: Cultural Heritage, Pigments, Far infrared, Mid infrared, Raman

Applied Spectroscopies - P21 / 16:20 - 18:20

FT-IR Spectroscopic Investigation Of Bipolar Patients' Blood Samples

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In this study, Fourier-transform infrared spectroscopic analysis is used to find spectral parameters for the blood plasma samples in order to use as biomarkers for the classification of bipolar patients. 30 samples were obtained from each bipolar patients and healthy control group. The spectral analysis shows that in certain spectral regions the intensity of the bands of bipolar patients' samples significantly increased compared to healthy ones. These obtained spectral parameters can be used as a diagnostic tool in detection of bipolar disease.

Keywords: FTIR, Bipolar, Blood Plasma

Electron Spin Resonance (ESR) Spectroscopy - P22 / 16:20 - 18:20

The EPR Study Of Mn2+ Ion Alloyed KBr and VO2+ Ion Alloyed KH2PO4 Single Crystals Under High Pressure

***Ümit Ceylan*, Recep Tapramaz**

Department of Physics, Ondokuz Mayıs University, Samsun, Turkey

EPR study of Mn2+ ion alloyed KBr single crystal study was performed under 100 bar pressure, 70 0C temperature and argon gas with constant pressure. The VO2+ ion alloyed KH2PO4 single crystal study was performed in Autoclave and O2 atmosphere under 100 bar pressure and 51 0C temperature. The spectrums of the obtained single crystals are recorded in room temperature. The measured hyperfine and g values of the spectrums and the transitions of UV-VIS spectrums were determined.

Keywords: Autoclave, EPR, UV-VIS

Electron Spin Resonance (ESR) Spectroscopy - P23 / 16:20 - 18:20

The EPR Study Of Mn2+ Ion Alloyed DADT Single Crystal Under High Pressure

***Ümit Ceylan*, Recep Tapramaz**

Ondokuz Mayıs University, Department of Physics, Samsun, Turkey

EPR study of Mn2+ ion alloyed di ammonium d tartrat, DADT, [(NH4)2C4H4O6] single crystal was performed in Autoclave under 70 bar pressure, 94 0C temperature and N2 gas. The transitions were determined by the obtained optical absorption spectrum from single crystal. Also the hyperfine splitting of Mn2+ ion and experimental g value errors were determined by the obtained single crystal spectrum. The splitting values or the D and E values which are the zero field splitting parameters due to the spin-spin interactions were found by the simulation techniques. The Spin-Hamiltonian matrix of Mn2+ ion alloyed, DADT crystal was represented in |m_I; S,m_S basis.

Keywords: Autoclave, EPR, Zero Field Splitting Parameters

Electron Spin Resonance (ESR) Spectroscopy - P24 / 16:20 - 18:20

EPR Study Of Cu2+ Ion Doped Orotato(nicotinamid)Cobalt(II) Single Crystal

***Ilkay Yildirim*, Bünyamin Karabulut, Orhan Büyükgüngör**

Department of physics, OMÜ, Samsun, Turkey

The title complex has been prepared and characterized by EPR spectroscopy and X-ray diffraction. The single crystal is triclinic with the space group P-1. The unit cell dimensions of the crystal are a=7.2785(4) Å, b=10.2349(5)Å, c=12.7372(6)Å, α=69.297(4)°, β=74.791(4)° and γ=76.995(4)°, with Z=2. EPR spectra of the single crystal and the powder have been studied at room temperature. EPR analysis indicates the presence of only one Cu2+ site. The spin Hamiltonian parameters obtained from single cyrstal data for Cu2+ complex. The spin Hamiltonian parameters are gx=2.032, gy=2.116, gz=2.319, Ax=66 G, Ay=28 G, Az=126 G. These have indicated that the paramagnetic center is rhombic symmetric. The ground state wave function of Cu2+ ion is constructed.

Keywords: EPR, orotato, Cu2+

Fluorescence Spectroscopy - P25 / 16:20 - 18:20

Diffusion Energies and Oxygen Diffusion Coefficients of Porous Silicon

***Önder Yargı*[1], Süreyya Aydın Yüksel[1], Ali Gelir[2], Kenan Koç[1]**

[1]Department of Physics, Yildiz Technical University, Istanbul, Turkey
[2]Department of Physics, Istanbul Technical University, Istanbul, Turkey

Fluorescence technique was employed for the measurement of the diffusion coefficient of oxygen into porous silicon (PS). In this work, the PS layers on n-type Si substrates were prepared by anodic etching in the mixture of hydrofluoric acid and ethanol (50%) solution at a dc current under white light illumination. In order to determine the diffusivity of oxygen, diffusion measurements were performed over the temperature range of 25-65 0C. It is shown that quenching is influenced by the temperature. Using the well-known Stern–Volmer relation for fluorescence quenching, diffusion of oxygen into porous silicon was modeled using Fick's law and the Stern-Volmer equation for fluorescence quenching, to extract diffusion and permeation coefficients. The average oxygen concentration change in the porous silicon was monitored by studying the average intensity change of the fluorophore using a steady state fluorescence (SSF) technique. The results showed that D values are strongly dependent on temperature in the porous silicon. It was also observed that D coefficients obey Arrhenius behavior.

Keywords: Fluorescence, temperature, diffusion, oxygen, porous silicon

Fluorescence Spectroscopy - P26 / 16:20 - 18:20

FRET Study And G-quadruplex Folding Ability Of Fluorescent Oligonucleotide Probes At The Langmuir Monolayer Interface

***Bernard Juskowiak**, Angelika Swiatkowska*

Adam Mickiewicz University, Faculty of Chemistry, Poznan, Poland

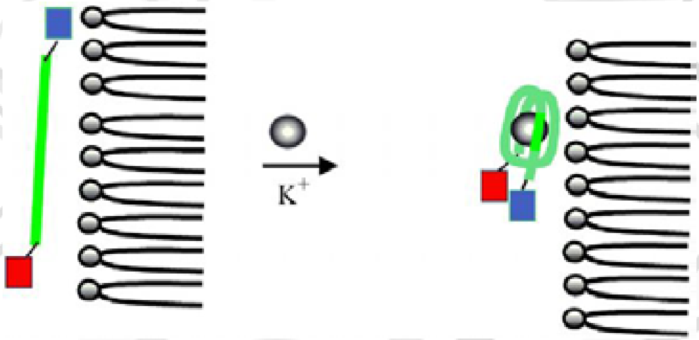
In this contribution we report an attempt to characterize spectral properties and G-quadruplex folding ability of fluorescent oligonucleotide probes at the cationic Langmuir monolayer interface. Two oligonucleotides, 19- and 21-meric guanine-rich sequences, were end-labeled with reporter fluorescent groups (FAM and TAMRA). The probes exhibited abilities to fold into a quadruplex structure and to bind metal cations (e.g., Na+ and K+). Scheme of G-quadruplex formation is shown below.

In an unbound state, both termini of oligonucleotide are separated, thus fluorophores do not interact with each other and probe exhibits unperturbed fluorescence spectrum. In the presence of K+, the quadruplex structure is developed that enables fluorophores to be arranged in a close proximity causing generation of different fluorescence spectrum (FRET signal). Investigations of FRET probes at the monolayer interface included film balance measurements (p-A isotherms) and fluorescence spectra recording using a fiber optic accessory interfaced with a spectrofluorometer. The effect of the presence of monolayer, metal cations and surface pressure of monolayer on spectral behavior of probes was examined. Interaction (adsorption) of probe with cationic monolayer induced FRET signal generation even in the absence of metal cation. Fluorescence energy transfer efficiency increased with increase in concentration of sodium or potassium ion in aqueous subphase, which indicated that the probes retained their cation-binding properties when adsorbed on the monolayer interface. The variation in the monolayer surface pressure exerted rather modest effect on spectral properties of probes.

Acknowledgements This work was supported by the National Science Centre (NCN) of Poland (Grant NCN No. 2011/01/B/ST4/01188)

Keywords: air-water interface, G-quadruplex, fluorescence, FRET probes, Langmuir monolayer

Figure. Scheme of G-quadruplex formation in the presence of monolayer.



Fluorescence Spectroscopy - P27 / 16:20 - 18:20

Transport Of Gliclazide By Serum Albumin Altered In Diabetes: Spectroscopic Analysis

Agnieszka Szkudlarek Hasnik, Joanna Równicka Zubik, Malgorzata Maciazek Jurczyk, Anna Sulkowska

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Human serum albumin (HSA), transporting protein, is exposed during its life to numerous factors that cause its functions become impaired.One of the basic factors - glycation of HSA – occurs in diabetes and may affect HSA-drug binding. Accumulation of advanced glycation end-products (AGEs) leads to diseases e.g. diabetic and non-diabetic cartdiovascular diseases, Alzheimer disease, renal disfunction. Gliclazide (GLZ) is used for control of hyperglycemia in gliclazide-responsive diabetes. It is used when insulin therapy is not appropriate.

The effect of glycation on the interaction of gliclazide (GLZ) was studied by using fluorescence technique.

Based on the emission fluorescence spectra of non-modified HSA and HSA (gHSAFRC) glycated with fructose the quenching effect of gliclazide on their fluorescence was studied.

Piracetam (PIR) is used in addition to standard treatment in diabetes.

Quenching curves, Stern-Volmer dependence, Scatchard depencence allows for conclusions that (1) the complexes GLZ-HSA, GLZ-gHSAFRC and GLZ-(gHSAFRC +PIR) are formed at molar ration 20:1, (2) Ka and Ks-v values are higher for GLZ-gHSAFRC complex than GLZ-HSA and show that glycation leads to an increase of an extent of the binding of GLZ to HSA. This causes the free fraction of drug in serum decreases, the therapy may be less effective in diabetes. Piracetamcauses Ka and Ks-v values are also lower than those of gHSAFRC. The inhibiting effect of PIR on HSA glycation process was proved.

The binding of GLZ to HSA and gHSAFRC was confirmed by using 1H NMR spectroscopy.

Acknowledgement: This work was supported by grants KNW-1-001/K/3/0 and KNW-2-001/N/3/K.

Keywords: fluorescence, 1H NMR, gliclazide binding

Fluorescence Spectroscopy - P28 / 16:20 - 18:20

Elucidation of the Porous Size Dependence of the Oxygen Diffusion into Porous Silicon by Using Fluorescence Technique

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[1]*Department of Physics, Yildiz Technical University, Istanbul, Turkey*
[2]*Department of Physics, Istanbul Technical University, Istanbul, Turkey*

Steady state fluorescence (SSF) technique is proposed for the measurement of the diffusion coefficient of oxygen into porous silicon (PS). In this work, the PS layers on n-type Si substrates were prepared by anodic etching in Hydrofluoric (HF) acidic solution at a dc current under white light illumination. Oxygen diffusion into porous silicon was monitored with SSF measurements. The measurements were performed at room temperature for PS samples etched using the different HF concentration in ethanol (from 33% to 67%) to evaluate the effect of porous size on oxygen diffusion. The diffusion coefficients, D, of oxygen were determined by the fluorescence quenching method by assuming Fickian transport and were found to be increased with increasing porous size. SSF technique showed that the rate of emission intensity decay when oxygen diffuses into a porous silicon structure is much faster than the rate of emission intensity enhancement when oxygen diffuses out of the same film. The results showed that the D values are strongly dependent on porous size in the silicon. This increase in the D values can be explained with formation of microvoids in the film. These voids are large enough to contribute to the penetration of oxygen molecules into the structure.

Keywords: Fluorescence, quenching, porous silicon, oxygen

Fluorescence Spectroscopy - P29 / 16:20 - 18:20

New Fluorogenic Substrate For DNAzyme With Peroxidase-Like Activity

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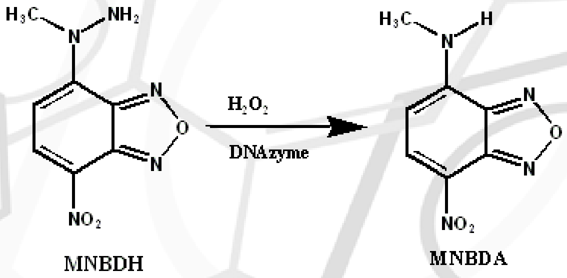
DNAzymes – catalytically active DNA oligonucleotides with peroxidase activity have proved their great potential in development of bioassays. The enzymatic activity of peroxidase-like DNAzyme is connected with its G-quadruplex structure and formation of the hemin/G-quadruplex complex. Commonly used substrates such as ABTS (2,2'-azino-bis(3-ethylbenzthiazoline-6-sulphonic acid) are oxidized by H2O2 into colored products (ABTS) allowing facile colorimetric monitoring of the reaction progress. Such substrates were successfully used in development of many DNAzyme-based assays but colorimetric approach suffers from rather low sensitivity. Application of a fluorogenic substrate in the indicator reaction and subsequent fluorescence measurements present very attractive alternative to colorimetric methods.

Here we report new fluorogenic substrate N-methyl-4-hydrazino-7-nitrobenzofurazan (MNBDH), the compound that has been proposed before as a substrate for an HRP-based assay. MNBDH oxidation product exhibits much stronger fluorescence when reaction is catalyzed by DNAzyme comparing with that in the absence of DNAzyme. Two G-quadruplex-based DNAzyme systems were tested: first formed by PS2.M sequence (5'-GTGGGTAGGGCGGGTTGG-3'), and second, created by human telomeric sequence of (5'-AGGGTTAGGGTTAGGG TTAGGG-3'). The system based on PS2.M oligonucleotide appeared to catalyze MNBDH oxidation effectively and produced high level of fluorescence. In order to use this reaction in bioassays development we optimize the reaction conditions. The influence of pH, H2O2 concentration, type of cation, type and concentration of surfactant were investigated. As a result we developed DNAzyme system, which produced a high level of fluorescence. Obtained results demonstrate that MNBDH is a potential substrate, which oxidized in the presence of DNAzyme allows for the quantitative adetection of DNA target.

Keywords: DNAzyme, G-quadruplex, fluorescence, fluorogenic substrate, MNBDH, peroxidase activity

Fig. Oxidation of MNBDH into fluorescent MNBDA catalyzed by DNAzyme with peroxidase activity



Fluorescence Spectroscopy - P30 / 16:20 - 18:20

Spectrofluorimetric Determination Of Nateglinide In Pure And Pharmaceutical Preparations Through Derivatization With 4-Chloro-7-Nitrobenzo-2-Oxa-1,3-Diazole

Ayça Karasakal[1]***, Sevgi Tatar Ulu***[2]

[1]Department of Chemistry, Faculty of Science and Letters, Namik Kemal University, Tekirdag, Turkey
[2]Department of Analytical Chemistry, Faculty of Pharmacy, Istanbul University, Istanbul, Turkey

A sensitive method was developed for the determination of nateglinide in pure and pharmaceutical preparations. The proposed method is based on the derivatization reaction between nateglinide and 4-chloro-7-nitrobenzo-2-oxa-1,3-diazole in borate buffer of pH 10 highly fluorescent derivative this is measured at 464 nm using an excitation wavelength of 537 nm. The described method was validated and the analytical parameters of linearity, limit of detection (LOD), limit of quantification (LOQ), accuracy, precision (intra- and inter-day) and recovery were evaluated. The assay was linear over the concentration range of 50-500 ng/mL. The proposed method was applied to study of nateglinide in pure and pharmaceutical preparations.

Keywords: Derivatization, Spectrofluorimetry, Validation, NBD-Cl,Nateglinide

Fluorescence Spectroscopy - P31 / 16:20 - 18:20

New Spectrofluorimetric Method for the Determination of Nizatidine In Bulk Form And In Pharmaceutical Preparations

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[2]*Department of Analytical Chemistry, Faculty of Pharmacy, Istanbul University, Istanbul, Turkey*

A simple, accurate and highly sensitive spectrofluorimetric method has been developed for determination of nizatidine in pure form and in pharmaceutical dosage forms. The method is based on the reaction between nizatidine and 1-dimethylaminonaphthalene-5-sulphonyl chloride in carbonate buffer, pH 9.5, to yield a highly fluorescent derivative peaking at 513 nm after excitation at 367 nm. Various factors affecting the fluorescence intensity of nizatidin- dansyl derivative were studied and conditions were optimized. The method was validated as per ICH guidelines. The fluorescence concentration plot was rectilinear over the range of 25-300 ng/mL. Limit of detection and limit of quantification were calculated as 11.71 and 35.73 ng/mL, respectively. The proposed method was successfully applied to pharmaceutical preparations.

Keywords: Derivatization, Spectrofluorimetry, Dansyl chloride, Nizatidine.

Matrix Isolation Infrared Spectroscopy and Low Temperature Spectroscopy - P32 / 16:20 - 18:20

FTIR Matrix Isolation And DFT Studies Of Thermal Decomposition And Photochemistry Of (tetrazol-5-yl)Acetic Acid

***Magdalena Pagacz Kostrzewa,* Justyna Krupa, Maria Wierzejewska**

Department of Chemistry, Wroclaw University, Wroclaw, Poland

There is a significant interest in the tetrazole derivatives due to their diverse applications as high energy materials and medicinal agents. The (tetrazol-5-yl)acetic acid (TA), is an interesting example of the 5-substituted tetrazole derivative that possesses a free N-H group and the –CH2COOH moiety attached to the tetrazole C atom.

A conformational analysis of monomeric TA was performed at the B3LYP/6-311++G(2d,2p) level in the aim to locate both minima and transition states on the potential energy surface and to identify those isomers that are present in low temperature matrices. The performed calculations revealed the presence nine stable structures of TA and the three most stable of them were identified in the experimental TA/Ar spectra.

During preparation of the matrices containing TA species a partial, thermal decomposition of the compound was observed leading to the 5-methyltetrazole and carbon dioxide formation. In order to get further details on the thermal decomposition pathway detected experimentally, the theoretical calculations were carried out on the mechanism and energetics of the reaction. The results clearly indicate the role of water traces in the decarboxylation process.

When the spectra of the TA species isolated in solid argon was obtained at conditions that avoided the thermal decomposition of the sample, the UV photolysis experiment was performed. The obtained results indicate that the tetrazole ring cleavage and nitrogen elimination take place in the matrices leading to the carbodiimidyl acetic acid formation that may further photolyse to N-methylcarbodiimide.

Keywords: Matrix isolation, FTIR spectroscopy, DFT calculations, tetrazoles, photochemistry, conformational analysis

Matrix Isolation Infrared Spectroscopy and Low Temperature Spectroscopy - P33 / 16:20 - 18:20

Ultraviolet-Tunable Laser Induced Transformations of Matrix Isolated Safrole. The First Example of the Allyl Group Photorotamerization

Justyna Krupa, Maria Wierzejewska

Department of Chemistry, Wrocław University, Wroclaw, Poland

Safrole (SF) is an abundant natural product usually extracted from sassafras oil or other essential oils. This compound contains the 1,3-dioxolane ring (methylenedioxy unit) and possesses interesting chemical functionality and reactivity suggesting its use as an versatile drug component.

Although regarded itself as weak carcinogen, safrole was found to display antitumor activity when conjugated with amino acid residues or small peptides. Safrole is also used to manufacture pesticides, fragrances, and other chemicals.

Phototransformations of the monomeric safrole (5-(2-propenyl)-1,3-benzodioxole) isolated in low temperature xenon matrices were induced by narrow-band UV radiation from the OPO laser system. The narrow band tunable UV laser radiation in the 300 – 298 nm range allowed for the conformational changes as manifested by the growth or decrease of the infrared bands associated with the population of three safrole conformers. The experiment allowed, for the first time, unequivocal observation of the allyl group rotation in low temperature matrices. The progress of the reactions was followed by FTIR spectroscopy.

Photolysis of the studied compound was also observed, with the 1,3-oxolane ring breaking, decarbonylation reaction and formation of long-chain conjugated ketenes. These species are characterized by very intense absorption due to the C=C=O stretching mode appearing in the 2160-2080 cm-1 region. Interpretation of the occurring processes was supported by the B3LYP/6-311++G(2d,2p) calculations.

Keywords: photoisomerization, photolysis, 5-(2-propenyl)-1,3-benzodioxole, methylenedioxy unit, xenon matrix

Matrix Isolation Infrared Spectroscopy and Low Temperature Spectroscopy - P34 / 16:20 - 18:20

Ultraviolet-tunable Laser Induced Phototransformations of Matrix Isolated Isoeugenol and Eugenol

Justyna Krupa[1], ***Adriana Olbert Majkut***[1], ***Igor Reva***[2], ***Rui Fausto***[2], ***Maria Wierzejewska***[1]

[1]*Department of Chemistry, Wroclaw University, Wroclaw, Poland*
[2]*Department of Chemistry, Coimbra University, Coimbra, Portugal*

The most known plant phenols, including the propenylphenols (such as isoeugenol, anol) and the allylphenols (eugenol, chavicol) as well as their derivatives, are aromatic constituents of essential oils. Given their unique properties as antioxidants and free radical scavengers, plant phenols have garnered the attention of scientists interested in the elucidation of many aspects of their biological activity. More recently, plant phenols have also gained increasing interest as multi-purpose functional agents.

In situ photochemical transformations of monomers of 2-methoxy-4-(prop-1-enyl)phenol (isoeugenol) and 2-methoxy-4-(prop-2-enyl)phenol (eugenol) isolated in low temperature matrices were induced by tunable UV laser light, and the progress of the reactions was followed by FTIR spectroscopy.

Conformer-selective E↔Z geometrical isomerizations could be successfully induced by irradiation at different wavelengths from the 310-298 nm range in the isoeugenol molecule that contains asymmetrically substituted exocyclic C=C bond. Photolysis of both studied compounds was also observed, with H-atom shift from the OH group and formation of two types of long-chain conjugated ketenes. The photoproduced ketenes were found to undergo subsequent photo-decarbonylation. Interpretation of the observed photoprocesses was supported by quantum chemical calculations undertaken at different levels of theory (DFT, MP2, QCISD).

Keywords: Matrix-isolation; FTIR Spectroscopy; UV-Induced E-Z photorotamerization; Photolysis; DFT and MP2 calculations

Matrix Isolation Infrared Spectroscopy and Low Temperature Spectroscopy - P35 / 16:20 - 18:20

Conformational Properties And Photochemistry Of Allyl Tetrazoles In Low-Temperature Matrices

Magdalena Pagacz Kostrzewa, ***Malgorzata Mucha, Marek Weselski, Maria Wierzejewska***

Department of Chemistry, Wroclaw University, Wroclaw, Poland

Azole derivatives containing unsaturated substituents such as vinyl or allyl groups receive increasing attention due to their unusual and valuable properties. They have potential applications in various fields such as polymer chemistry, metal ions chelation or pharmacology. Allyl tetrazoles are also interesting from the fundamental point of view since they exhibit conformational isomerism as well as they are expected to show an interesting photochemistry. [1]

The molecular structure and photochemistry of 1-allyltetrazole (1-ALT) and 2-allyltetrazole (2-ALT) were studied in argon matrices by infrared spectroscopy and B3LYP/6-311++G(2d,2p) calculations.

Both allyltetrazoles were found to possess three stable conformers (1-ALT1, 1-ALT2, 1-ALT3 and 2-ALT1, 2-ALT2, 2-ALT3) differing in the orientation of the allyl group relative to the ring. Matrix isolation technique together with the annealing experiments allowed for detection of all 1-ALT and 2-ALT conformers. A conformational cooling phenomenon was observed for the 1-ALT3→1-ALT1 process in agreement with the predicted low energy barrier of 4.84 kJ mol-1 for this reaction.

The broad band UV irradiation of 1-ALT/Ar and 2-ALT/Ar matrices led to the same photoproducts. The main product N-allylcarbodiimide and two minor photoproducts allylcyanamide and C-allylnitrilimine are formed through the tetrazole ring cleavage and N2 elimination.

[1] M. Pagacz-Kostrzewa, M. Mucha, M. Weselski, M. Wierzejewska, J. Photochem. Photobiol. A: Chemistry 251 (2013) 118-127.

Keywords: FTIR spectroscopy, photochemistry, allylcarbodiimide, DFT, conformational cooling, C-N rearrangement

Matrix Isolation Infrared Spectroscopy and Low Temperature Spectroscopy - P36 / 16:20 - 18:20

Low Temperature Matrix-Isolation of Methyl Paraben: FTIR, DFT and Photochemistry Studies

Nihal Kuş[1]***, Sevgi Haman Bayarı***[3]***, Rui Fausto***[2]

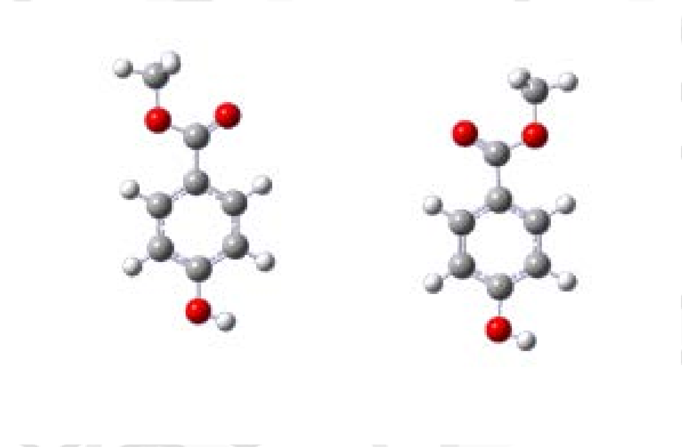
[1]Anadolu University
[2]Coimbra University
[3]Hacettepe University

Methylparaben (MP) is the methyl ester of p-hydroxybenzoic acid which shows antimicrobial activity. It has been widely used in food, pharmaceutical and cosmetics industries because of past reports on their effectiveness as preservative, low cost and rapid excretion from the body. Nevertheless, the generalized use of MP has become controversial, with many reports of dangerous side effects. For example, the presence of parabens (including MP) in human breast tumors has been reported recently [1]. MP seems also to have harmful effects on human skin when exposed to the Sun's UV light [2].

In the present study, the infrared spectrum of MP isolated in a cryogenic argon matrix (T= 15 K) was obtained and interpreted with help of theoretical calculations performed at the DFT(B3LYP)/6-311++G(d,p) level of theory. The potential energy surface (PES) of the molecule was investigated, revealing the existence of two almost isoenergetic low-energy conformers (Fig. 1; ΔE= 0.31 kJ mol-1), with predicted populations in gas phase at room temperature (~298 K) of 54% (I) and 46% (II) (I:II population ratio of ca. 0.85). Besides, two high-energy forms were also located on the PES of the molecule, with the ester group assuming the s-trans configuration, which however have relative energies above 50 kJ mol-1 and are not relevant in experimental terms. The infrared spectrum of MP isolated in solid argon was found to be in good agreement with the theoretical predictions.

Keywords: Low Temperature Matrix-Isolation, Methylparaben, Photochemistry, UV irradiation, DFT calculation

Low-energy s-cis ester conformers of methylparaben. Form I corresponds to the conformational ground state, being only slightly more stable than form II by 0.31 kJ mol-1 (as predicted by the B3LYP calculations).



Matrix Isolation Infrared Spectroscopy and Low Temperature Spectroscopy - P37 / 16:20 - 18:20

Matrix Isolation Infrared Spectra and Photochemistry of Hydantoin

***Gulce Ogruc Ildiz**[1,2], Claudio M. Nunes[1], Rui Fausto[1]*

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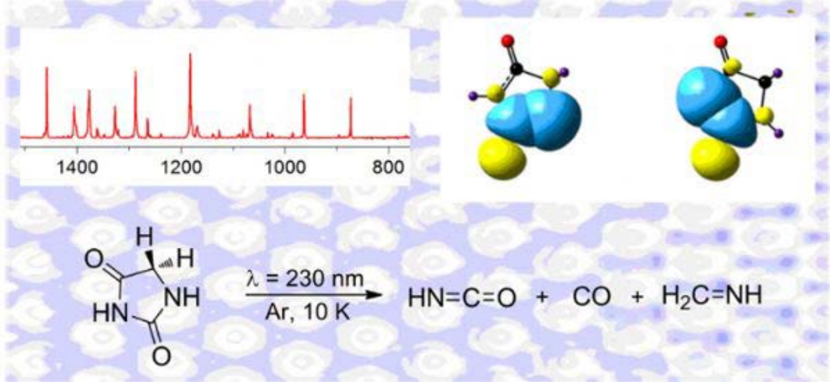
[2]Faculty of Science and Letters, Department of Physics, Istanbul Kultur University, Atakoy Campus, Bakirkoy 34156, Istanbul, Turkey

Methylparaben (MP) is the methyl ester of p-hydroxybenzoic acid which shows antimicrobial activity. It has been widely used in food, pharmaceutical and cosmetics industries because of past reports on their effectiveness as preservative, low cost and rapid excretion from the body. Nevertheless, the generalized use of MP has become controversial, with many reports of dangerous side effects. For example, the presence of parabens (including MP) in human breast tumors has been reported recently [1]. MP seems also to have harmful effects on human skin when exposed to the Sun's UV light [2].

In the present study, the infrared spectrum of MP isolated in a cryogenic argon matrix (T= 15 K) was obtained and interpreted with help of theoretical calculations performed at the DFT(B3LYP)/6-311++G(d,p) level of theory. The potential energy surface (PES) of the molecule was investigated, revealing the existence of two almost isoenergetic low-energy conformers (Fig. 1; ΔE= 0.31 kJ mol-1), with predicted populations in gas phase at room temperature (~298 K) of 54% (I) and 46% (II) (I:II population ratio of ca. 0.85). Besides, two high-energy forms were also located on the PES of the molecule, with the ester group assuming the s-trans configuration, which however have relative energies above 50 kJ mol-1 and are not relevant in experimental terms. The infrared spectrum of MP isolated in solid argon was found to be in good agreement with the theoretical predictions.

Keywords: Low Temperature Matrix-Isolation, Methylparaben, Photochemistry, UV irradiation, DFT calculation



Microwave Spectroscopy - P38 / 16:20 - 18:20

Some Projects At The Infrared Microspectroscopy Beamline D7 At The MAX IV Laboratory

Anders Engdahl

MAX IV laboratory, Lund University, P. O. Box 118, SE 22100, Sweden

1. Assessment of bone quality during fracture repair.

Fracture repair is a highly complex biological and mechanical process. Fracture healing is especially complicated in elderly patients with osteoporosis. The numbers of osteoporotic patients with complicated fractures are expected to increase with the increasing age of the population.

(Hanna Isaksson)

2. Use of synchrotron-radiation-based FTIR imaging for characterizing changes in cell contents. (Cyril Petibois)

3. Conformational studies on myelin proteins from the vertebrate nervous system - links

between structure and function

This overall project aims to provide structural information in the crystal state and in solution on

proteins of the nervous system and the complexes that they form. (Petri Kursula)

4. Compositional and structural changes of human articular cartilage and subchondral bone during early osteoarthritis. (Simo Saarakkala)

Objective of this research project is to obtain accurate and specific chemical information of composition and structure of articular cartilage and subchondral bone at tissue level and at cellular level during the development of osteoarthritis.

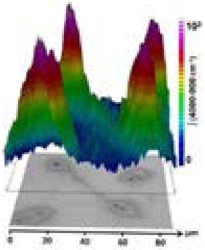
5. Molecular preservation of the pigment melanin in fossil melanosomes.

Using IR-microscopy at MAX-lab, among several other techniques, we show that melanonsomes in a 54 million years old fish eye contain high concentrations of melanin, having a molecular structure very similar to melanin found in modern melanosomes

(J. Lindgren, P. Uvdal, A. Engdahl et. al.) Nature Comm., DOI 10.1038/ncomms1819, 2012.)

Keywords: MAX IV laboratory, syncrotron, infrared, microspectroscopy

FTIR Image of cell cultures.



FTIR image of cells cultures on Si_3N_4 substrate. The image shows an example of overlay of visible views of two hCMEC/D3 cells connected by a filopode. FTIR image rendering shows absorption intensity for the full spectral region (4000–900 cm^{-1})

Mössbauer Spectroscopy - P39 / 16:20 - 18:20

Study of Ferritin Iron Cores in the Rhizobacterium Azospirillum Brasilense Sp245 Using Mössbauer Spectroscopy with a High Velocity Resolution

***Alexander Kamnev*[1]*, Irina Alenkina*[2]*, Michael Oshtrakh*[2]*, Anna Tugarova*[1]*, Borbála Biró*[3]*, Vladimir Semionkin*[2]**

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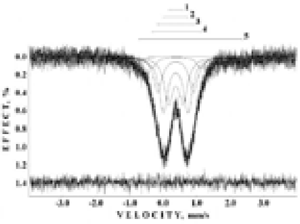
Ferritin is the main iron storage protein in various living systems from mammals to bacteria. This protein consists of nanosized ferric hydrous oxide core surrounded with 24 protein subunits. It is well known that ferritin molecules from different organisms have different amino acid sequences and variations in the iron core structure. In the present work we studied bacterial ferritin using Mössbauer spectroscopy with a high velocity resolution. Bacteria of the genus Azospirillum, particularly the species A. brasilense, belong to the most widely studied plant-growth-promoting rhizobacteria. They can form associations with roots of various higher plants, promoting their growth and development via phytohormone excretion, N2 fixation, and other mechanisms. Cells of A. brasilense (strain Sp245) were grown in a standard salt medium supplemented with 57Fe(III)-NTA complex as a sole Fe source. Two samples were prepared in lyophilized form: sample 1 was made from cells washed from the medium after 18 h of growth, and sample 2 was made from the same cells after additional 3 days of storage at ambient temperature in aqueous saline suspension. Mössbauer spectra were measured at room temperature and fitted using two models: homogeneous iron core (a rough model using one quadrupole doublet) and heterogeneous iron core (four quadrupole doublets). It was shown that in both cases Mössbauer parameters for samples 1 and 2 appeared to be different indicating different processes of the iron core formation. Moreover, the best fit of Mössbauer spectra with four quadrupole doublets supports the heterogeneous iron core model in ferritin.

Keywords: Azospirillum brasilense, Bacterial ferritin, Iron core structure

Fig. 1. Mössbauer spectrum of Azospirillum brasilense cells (sample 1) measured with a high velocity resolution (presented in 2048 channels) at 295 K.



Mössbauer Spectroscopy - P40 / 16:20 - 18:20

A Comparative Study of Troilite Extracted from Sikhote-Alin Iron Meteorite and in Some Bulk Ordinary Chondrites Using Mössbauer Spectroscopy with a High Velocity Resolution

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Troilite (FeS) is a magnetic compound at room temperature which is very rare in terrestrial minerals while it is often found in meteorites. For instance, ordinary chondrites contain 4–6 wt.% of troilite. Mössbauer spectroscopy is one of the useful probes for the study of iron-bearing phases in meteorites. A long experience in the study of iron containing minerals in ordinary chondrites using Mössbauer spectroscopy demonstrates that the spectral component related to FeS (magnetic sextet) cannot be fitted satisfactorily when the quadrupole interaction is treated as a perturbation to the first order (PFO) on the nuclear Zeeman levels. To establish a more accurate model, we have studied troilite extracted from the Sikhote-Alin iron meteorite using Mössbauer spectroscopy with a high velocity resolution, and evaluated the spectrum with the MossWinn program applying numerical diagonalisation of the full static Hamiltonian of the hyperfine interaction (magnetic + quadrupole) for the excited and ground nuclear states. This approach resulted in a clearly superior fit, indicating that it is the mixing of excited-state nuclear sublevels of 57-Fe nuclei that prevents accurate fitting of troilite spectra when the usual PFO method is used. The same approach was also successfully applied to account for the contribution of troilite to the Mössbauer spectra of ordinary chondrites Farmington L5, Tzarev L5 and Chelyabinsk LL5 measured with a high velocity resolution. The results obtained for meteoritic troilite showed some similarities in Mössbauer parameters indicating similar conditions of troilite formation.

Keywords: Mössbauer spectroscopy with a high velocity resolution, Troilite, Iron meteorite, Ordinary chondrites

New Materials - P41 / 16:20 - 18:20

Structural and Optical Properties of Si3N4 Thin Films Deposited by RF Magnetron Sputtering

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The material Silicon nitride plays an important role in optoelectronics applications due to its unique properties such as its excellent thermal shock resistance, high-temperature strength and high transmission ratio in the visible light range. Silicon nitride layers are especially used as anti-reflective coating and passivation layers for industrial solar cells. In this study, thin silicon nitride films were deposited on Silicon substrate through the use of the RF magnetron sputtering tecnique and were labeled I, II, III, and IV. Sample I was deposited at 100°C, and samples II, III, and IV at 200°C. The film thickness of the samples were 750, 750, 1500 and 2000 Å, respectively. The structural characterization of the films was performed using the X-ray diffraction technique. The results of the aforementioned characterization have been depicted in Figure 1. The crystal structures were determined and different phase formations were observed according to the XRD patterns of the samples. The chemical bonding structure of the samples was analyzed by evaluating the absorbance spectra obtained by an FT-IR spectrophotometer. In addition, optical characterizations of the deposited films were carried out by using photoluminescence (PL) system and UV-VIS spectrometer at room temperature. Band gap of the films was determined by evaluation of the PL spectra, as shown in Figure 2. The reflectance of the films was measured in the range of 200-1100nm and presented in Figure 3. Using the Kubelka Munk Theory, due to the fact that the samples were opaque, the absorbtion energy capacity of the samples was calculated.

Keywords: FT-IR, RF Magnetron Sputtering, Silicon Nitride, UV-VIS Reflectance, XRD

Figure 1

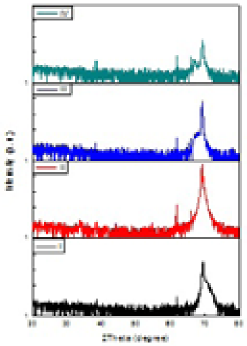


Figure 2

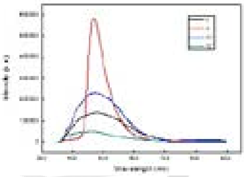
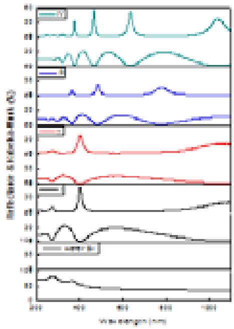


Figure 3



New Materials - P42 / 16:20 - 18:20

Structural Characterization, Spectroscopic, Magnetic, And Electrochemical Studies Of Monomer N-Substituted-Sulfanilamide Copper(II) Complex With 2,2'-Bipyridine

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New copper(II) complex of sulfamethazine (4-amino-N-[4,6-dimethyl-2-pyrimidinyl]benzene sulfonamide, Hsmz) ([Cu(smz)2bipy]·0.8H2O; bipy: 2,2'-bipyridine) has been synthesized and characterized by elemental analyses, IR, EPR, single crystal X-ray diffraction and electrochemical methods. The compound crystallizes in the monoclinic space group P21/c with Z=4. The central copper(II) ion, which rides on a crystallographic center of symmetry, is coordinated by bidentate from nitrogen atoms of two deprotaned sulfamethazine and 2,2'-bipyridine ligands.

Keywords: Cu(II); sulfamethazine; X-ray crystal structure; EPR; IR

New Materials - P43 / 16:20 - 18:20

Phonon and magnetic properties of Ni(II) and Fe(III) doped CoCr2O4

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CoCr2O4 is well known spinel-type structure compound, but a few years ago it was rediscovered in view of unique magnetoelectric properties. This spinel exhibits onset of collinear ferrimagnetic ordering below 98K and undergoes another magnetic phase transition to spiral magnetic structure below 26K, which becomes “lock-in” magnetic phase at 13K. The spiral magnetic component induces ferroelectric polarization. The magnetoelectric coupling manifests itself in many physicochemical properties and offers potential applications due to controlling of the magnetoelectric coupling by external electric or magnetic field.

A series of CoCr2-xFexO4 (where x = 0, 0.5, 1 and 2) and Co0.9Ni0.1Cr2O4 were synthesized using solid state reaction method. XRD patterns proove that Fe(III) and Ni(II) cations built in the structure and only single phase of spinel-type is observed. Here we report the effect of substitution of the A and B positions in the CoCr2O4 spinel structure on its phonon and magnetic properties. Magnetization as a function of temperature clearly shows that Curie temperature dramatically increases when bigger fraction of Fe(III) is introduced into the structure. As a result, the compound with composition x = 0.5 exhibits ferrimagnetic ordering close to the room temperature. Infrared and Raman spectra show significant changes such as broadening and shifts of bands. Those effects were attributed to disorder induced by incorporation of the Fe(III) ions and fact that CoFe2O4 crystallizes in a partially inverted spinel structure with very high degree of inversion. The temperature-dependent infrared spectra down to liquid helium were also measured and discussed.

Keywords: spinel, multiferroic

New Materials - P44 / 16:20 - 18:20

Optic Absorption of GaSe<B,Dy> Thin Films

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Boron and dysprosium doped GaSe thin films have been grown for the first time by Modified Chemical Bath Deposition (M-CBD) on glass, GaSe crystalline substrates. The optic absorption spectra of undoped and doped GaSe films, and van der Waals junctions obtained on GaSe substrates were studied in the UV-VIS region. The absorption intensity was observed to increase with B and Dy doping. The absorption tail started at 1.94 eV and long wavelength tail was found to vary exponentially with incident photon energy according to the Urbach-Martiensen's theory. The Urbach energies were determined from the experimental spectra to be in the 0.80-0.90 eV range. The analysis of optic absorption spectra showed that the GaSe<B,Dy> films have direct band gaps as the absorption varies with photon energy as (αhν)2~ hν. The surface and structure of the films were investigated by the AFM and XRD which indicated that the films consist of nano regions. The exponential absorption tail observed is believed to be due to the defects and nanosized regions that exist in these films.

Keywords: GaSe thin films, Optical absorption, M-CBD

New Materials - P45 / 16:20 - 18:20

Effect Of Uv-Light On The Uniaxial Tensile Properties Of Tio2 Coated Bombyx Mori Silk Fibers By Sol-Gel Method

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The Bombyx Mori Silk Fibers were coated with TiO2 by using sol-gel Method. From the comparison of the uniaxial tensile properties of the uncoated Silk fibers with those of uncoated silk fibers, it was observed that the rigidity of the silk fibers increased after being coated with TiO2. The uncoated and TiO2 coated silk filaments were exposed to UV-light at 760 W/m2 for different time intervals in a Chamber equipped with UV-bulb source. The changes in the tensile properties of TiO2 coated silk fibers after being exposed to UV-light were compared with those of uncoated silk fibers. The results showed that the characteristic shape of the stress-strain curve of the silk fibers did not change. While the exposure time increased, the tendency of the change in the tensile properties of TiO2 coated silk fibers became similar to that of uncoated silk fibers. However, the decreasing tendency of the TiO2 coated silk fibers became lower than that of uncoated silk fibers. The structural changes in the TiO2 coated silk fibers after different exposure time were examined by using FT-IR/ATR spectroscopy method and compared with those of uncoated silk fibers.

Keywords: silk fibers, Titanium dioxide, UV-light, Uniaxial Tensile Properties, Rigidity, FT-IR/ATR spectroscopy

New Materials - P46 / 16:20 - 18:20

Structural And Energetic nalysis of Aethyl 2-(3-Benzoylthioureido)-Acetate: A DFT Study

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The molecular structures, vibrational frequencies, and corresponding vibrational assignments of ethyl 2-(3-benzoylthioureido)-acetate (Figure 1) have been determined and its energetic values have been calculated by using Density Functional Theory (DFT) [1]. Various suitable basis sets have been used with selected B3LYP theory. The comparisons of the findings show that B3LYP/DGDZVP2 level of theory is superior for both the vibrational frequencies and the geometric parameters. With this theory the calculated frequencies, bond lengths and bond angles are in well agreement with the experimental data [2].

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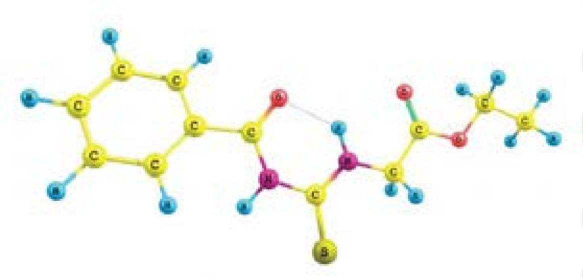
Keywords: Structural and energetic analysis of ethyl 2-(3-benzoylthioureido)-acetate: a DFT study

Figure 1



Optimized geometry of ethyl 2-(3-benzoylthioureido)-acetate.

New Materials - P47 / 16:20 - 18:20

Synthesis and Characterization of Halogen Containing Aryl Amide Polymer-Clay Composites

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Polymer composite materials are used widely in diverse applications such as transportation vehicles, construction materials, electronics and sporting goods and consumer products. The properties of polymer composites are affected greatly by the dimensions and microstructure of the dispersed phase. Polymer nanocomposites are a new class of materials with at least one ultrafine phase dimension, typically a few nanometers. Nanocomposites possess unique properties that are not shared by conventional composites primarily because of large interfacial area per unit volume. Polymer–clay nanocomposites can improve dramatically the mechanical reinforcement and high temperature durability, provide enhanced barrier properties and reduce flammability [1,2].

In this study, synthesized N-(4-bromophenyl)-2-methacrylamide (BrPMAAm) and N-(4-fluorophenyl)-2-methacrylamide (FPMAAm) monomers are polymerized via free radical polymerization. Montmorillonite-containing raw clay (NaMT), pure clay (SMT) and synthesized organoclay (OSMT) interlayer distances for the structure elucidation FT-IR and X-Ray Diffraction (XRD) analyze were determined. Later, composites of N-(4-bromophenyl)-2-methacrylamide (BrPMAAm) and N-(4-fluorophenyl)-2-methacrylamide (FPMAAm) monomers were obtained using 2,4,6, and 10% organoclay by mass with place (in-situ) polymerization. The synthesized polymer-clay composites were characterized by FT-IR, XRD and scanning electron microscopy (SEM) analysis. Homopolymer and 10% organoclay doped polymers molecular weight to were determined using Gel Permeation Chromatography (GPC). Thermal properties of polymers were performed using thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC). The exfoliated structure has been found for the low organoclay content, the increase of clay content resulted the intercalated structure for nanocomposites. Thermal properties of the polymer were also developed.

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Keywords: Synthesis and Characterization of Halogen Containing Aryl Amide Polymer-Clay Composites

New Materials - P48 / 16:20 - 18:20

Rutherford Backscattering Spectroscopy Study Of Antimony Electrical Activation In Si(111) Samples

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In this work, we studied the electrical activation of antimony atoms by means of Rutherford backscattering spectroscopy (RBS). The dopant (i.e. antimony) was introduced in Si(111) substrates by ion implantation process which was performed at an energy of 120 keV. The dose was selected to be 1e15 or 1.6e15 Sb+cm-2. Afterwards, an annealing treatment was applied at 900°C during 30 min. under high vacuum. The specimens were principally analyzed by Rutherford backscattering spectroscopy, in channeling mode, using a beam of 2 MeV He+ particles. In parallel, we measured the samples resistivity by four probes resistivity method.

Several results were obtained. In non annealed samples, no electrical activation has been noticed. The antimony migration to substitutional silicon lattice was observed for annealed specimens only. The fraction of that substituted atoms (fs) was computed with a good accuracy. Moreover, it was found that the fraction fs increased while the resistivity samples decreased.

Keywords: Rutherford backscattering spectroscopy, electrical activation, antimony, silicon.

New Materials - P49 / 16:20 - 18:20

An open three-dimensional Paul trap for the separation of the calcium isotopes at King Khalid University

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The analysis of the calcium 41 isotope at very low concentration has applications in multiple domains of science [1]. In the medical sciences for example, 41Ca with concentrations of the order of 10-11, is used as a tracer for the study of the calcium metabolism in the human body [2]. To detect the 41Ca at such a low concentration, very sensitive techniques are used [3]. Recently a method based on the ion trapping and laser cooling has been investigated [4]. At King Khalid University in Abha, Saudi Arabia, we are developing a similar method.

Our ion trap, is an open three-dimensional Paul trap. It is made of six rings and is similar to the trap of the Laboratoire de Physique Corpusculaire in Caen, France (LPC Caen) [5]. Our first goal is to trap the isotopes of natural calcium and study the effect of the trapping potential on them. We plan to use the laser cooling technique to separate between the isotopes according to the scheme shown in figure 1.

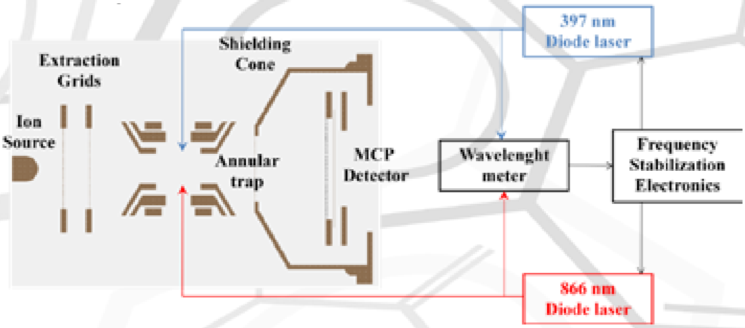

Figure 1 General scheme of the Calcium Paul trap experiment at King Khalid University

The Paul trap has been developed in collaboration with the LPC Caen. It is shown in figure 2. The calcium ions are produced by a surface ion source and are injected into the trap using 2 high transmission metallic grids. The trap is loaded periodically. At the end of every trapping cycle, the radiofrequency field, necessary for the ion trapping, is switched off and the ions fly freely in the high vacuum. Those reaching the microchannel plate (MCP) detector are counted. That allows to realize a preliminary study of the trapping without using the lasers.

In this poster, we will describe in details the actual status of our experiment and show the first results of the trapping.

Figure 2 The Paul trap

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Surface Enhanced Raman Spectroscopy (SERS) - P50 / 16:20 - 18:20

Detection of DNA Mutations Using Novel Surface-Enhanced Raman Spectroscopy (SERS) Diagnostic Platform

***Agnieszka Michota Kaminska*[1], *Evelin Witkowska*[1], *Arumugam Sivanesan*[1], *Janusz Weyher*[2], *Igor Dziecielewski*[2], *Jakub G.*, *Dominika Nowis*[3]**

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Development of simple, reliable and high-throughput methods for DNA mutation detection is of paramount importance for both research and medical diagnostics of genetic diseases. Detection of particular mutations in patients greatly affects the prediction of cancer risk and helps to refine therapeutics aims. Development of a SERS-based method to detect DNA and RNA qualitatively and quantitatively still remains a challenge. A standard application of SERS in biological and biomedical tests does not exist despite almost 40 years of studies. One major obstacle in transferring this technique into industry has been the challenge of fabricating low cost, stable, reproducible and sensitive SERS substrates.

This work describes the detection of DNA mutations using novel Au-Ag coated GaN substrate as surface-enhanced Raman spectroscopy (SERS) diagnostic platform. Especially reliable reproducibility and good time stability of SERS substrates are highly important properties for fabrication DNA hybridization assay. In our laboratory, we have developed a novel SERS active substrates based onto Au or Ag coated porous GaN. The resultant SERS platforms exhibited very strong surface-enhancement effects (up to 107), high stability (up to three month under ambient conditions) and high reproducibility which could be used in the design of efficient SERS-active platform for analytical applications. We have used this platform for the detection of BCR/ABL mutants associated with chronic myelogenous leukemia using SERS combined with either thermal or electrochemical cycling.

Keywords: SERS, DNA mutations, DNA hybridization

Surface Enhanced Raman Spectroscopy (SERS) - P51 / 16:20 - 18:20

Detection And Identification Of Bacterial Cells In Blood Samples On Gold-Silver Hybrid SERS Substrate

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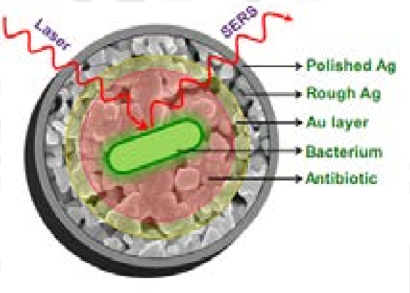
There are a lot of bacteria species that are still unknown. For this reason our knowledge about bacterial ecology and possibilities of using them in technology and other branches of science is poor. Therefore it is not surprising that in many laboratories researchers are working on new techniques which enables bacteria identification. Consequently nowadays there are many advanced methods that make the taxonomic affiliation of many bacteria species possible. Those methods are based on differences such as morphology, chemical composition of the cell wall, nutrition requirements, genomic DNA sequences and many more. The most popular techniques currently used in laboratories are DNA sequencing fallowed by PCR (polymerase chain reaction), biochemical and immunochemical tests. Despite the fact that all mentioned methods used for identification of bacteria are very efficient and acurate, they have one major drawback which is time consumption. This is a very serious problem when it comes to detecting fast progressing diseases. Due to this fact, in recent years researchers have shown that it is possible to detect and identify bacteria with the help of interaction between bacterial cell and electromagnetic wave. One of spectroscopic methods used for this purpose is surface enhanced Raman spectroscopy (SERS). This spectroscopic method enables detection and classification of microorganisms in a fast and highly specific manner by using only a roughened metal surface and the laser beam. In our experimental work we have developed a novel SERS substrate which offers a high enhancement and makes the taxonomic affiliation of many bacteria species possible.

Keywords: bacteria, SERS, gold-silver hybrid substrate

Scheme of SERS substrate with bacterial cell placed on it



Terahertz Spectroscopy - P52 / 16:20 - 18:20

Concentration Based Measurement Studies of L-Tryptophan Using THz-Time Domain Spectroscopy

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L-trytophan is an extremely important amino acid for a variety of biological functions in living organisms. In this study we were able to measure changes in the concentration of L-trytophan when incorporated into pellets with polyethylene as a host. The changes were not only measured through the characteristic absorption bands of the C11 and C12 bonds in the low terahertz frequency range, but were also measured by changes in the refractive index where pellets with higher concentrations of L-trytophan showed higher refractive indices. Using a simple model that explains the contribution to the complex refractive index for the resultant sample due to the two constituent materials the volumetric concentration of L-tryptophan in the polyethylene pellet was accurately determined. These measurements show that THz time-domain techniques can be applied to detect variation in concentration of certain amino acids rapidly by examining the relative phase delay and amplitude change of the THz transients.

Keywords: THz-TDS, L-trytophan, CRI Model, Biological Screening

Theoretical and Computational Methods - P53 / 16:20 - 18:20

The DFT and Vibrational Studies of Sudan Red G

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Sudan azo-dyes which are the most widely used class of dyes are non-ionic fat-soluble dyes used in various fields such as the dyeing of textile fibers, the coloring of different materials, colored plastics and polymers, biological-medical studies and advanced applications in organic synthesis [1]. The optimize molecular structure, electronic properties, molecular electrostatic potential, NBO analysis and vibrational studies of the Sudan Red G (SRG) [1-(2-methoxyphenylazo)-2-naphthol] have been investigated by performing B3LYP level with 6-311++G(d,p) basis set for the azo (OH) and hydrazo (NH) forms of the title compound. The vibrational studies of SRG have been performed by FT-IR and FT-Raman spectroscopy. The observed FT-IR, FT-Raman wavenumbers were have calculated at B3LYP/6-311++G(d,p). The scaled theoretical wavenumbers showed very good agreement with the experimental values.

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Keywords: Sudan Red G, DFT, FT-IR, FT-Raman

Theoretical and Computational Methods - P54 / 16:20 - 18:20

Theoretical and Experimental IR Studies on a Series of Azophenols and their Respective Ester Molecules Serving in Nonlinear Optics

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A theoretical investigation on a series of nonlinear optical molecules, which have been synthetized in addition to their respective experimental IR spectra [1] is established in the present work.

The concerned systems studied are a series of azophenols, as well as their respective esters generated from these azophenols as shown in Figure 1.

A full geometry optimisation at B3LYP/6-31G(d,p) level of theory and static first-order hyperpolarizabilities β(0) [2] with MP2/6-31+G(d) have been performed.

Subsequently IR vibrational modes calculations have been achieved with several DFT functionals and different basis sets. Thus, a comparison has been established between the experimental and the theoretical IR frequencies.

The best result has been attributed to HCTH functional associated to cc-PVTZ basis set.

The energy gap HOMO/LUMO has been found in a good correlation with β(0) magnitudes for all the systems studied. An approach has been established between the experimental IR frequencies, the bond lengths N=N and their respective β(0) values.

Keywords: Nonlinear optics, first hyperpolarizability, IR frequency, MP2

Theoretical and Computational Methods - P55 / 16:20 - 18:20

Molecular Structure And Vibrational And Chemical Shift Assignments Of 3’-Chloro-4-Dimethlamino Azobenzene By DFT Calculations

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[2]*Department of Physics,Faculty of Arts and Sciences, Amasya University, İpekköy, Amasya, Turkey.*

The vibrational frequencies and gauge including atomic orbital (GIAO) 1H and 13C chemical shift values and several thermodynamic parameters of 3’-chloro-4-dimethlamino azobenzene in the ground state have been calculated by using the density functional method (B3LYP) with 6-311++G(d,p) basis set. The vibrational spectral data obtained from solid phase FT-IR spectra are assigned based on the results of the theoretical calculations. The calculated results show that the theoretical vibrational frequencies and chemical shift values show good agreement with experimental values. Using the TD-DFT method, electronic absorption spectra of the title compound have been predicted, and a good agreement is determined with the experimental ones. In addition, molecular electrostatic potential, frontier molecular orbitals and NLO properties of the title compound were investigated by theoretical calculations.

Keywords: Azobenzene, Vibrational frequencies, GIAO, TD-DFT, MEP, NLO

Theoretical and Computational Methods - P56 / 16:20 - 18:20

Theoretical Investigation Of 2’-Chloro-4-Dimethlamino Azobenzene: MEP, FMO And NLO Analysis, FT-IR, UV-Vis And NMR Spectra

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[2]*Department of Physics,Faculty of Arts and Sciences, Amasya University, İpekköy, Amasya, Turkey.*

The molecular geometry, vibrational frequencies, gauge including atomic orbital (GIAO) 1H and 13C chemical shift values and several thermodynamic parameters of 2’-chloro-4-dimethlamino azobenzene in the ground state have been calculated by using the density functional method (B3LYP) with 6-311++G(d,p) basis set. The calculated results show that the theoretical vibrational frequencies and chemical shift values show good agreement with experimental values. Using the TD-DFT method, electronic absorption spectra of the title compound have been predicted, and a good agreement is determined with the experimental ones. In addition, molecular electrostatic potential, frontier molecular orbitals and NLO properties of the title compound were investigated by theoretical calculations.

Keywords: Azobenzene, Vibrational frequencies, Visible spectra, TD-DFT, MEP, NLO

Theoretical and Computational Methods - 057 / 16:20 - 18:20

Spectrocopic Investigations (FT-IR, NMR and UV-Vis) And Quantum Chemical Studies Of 4’-Chloro-4-Dimethlamino Azobenzene

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The molecular geometry, vibrational frequencies, gauge including atomic orbital (GIAO) 1H and 13C chemical shift values of 4’-chloro-4-dimethlamino azobenzene in the ground state have been calculated by using the density functional method (B3LYP) with 6-311++G(d,p) basis set. The energetic behavior of the title compound in solvent media has been examined by applying the Onsager and the polarizable continuum model. To investigate second order nonlinear optical properties of the title compound, the electric dipole, linear polarizability and first-order hyperpolarizability were computed using the density functional B3LYP method with the 6-31+G(d) basis set. According to our calculations, the title compound exhibits nonzero hyperpolarizability value revealing second order NLO behavior. In addition, DFT calculations of the title compound, molecular electrostatic potential (MEP), frontier molecular orbitals, and thermodynamic properties were performed at B3LYP/6-311++G(d,p) level of theory.

Keywords: Azobenzene, FT-IR, GIAO, TDDFT, NLO, MEP

Theoretical and Computational Methods - P58 / 16:20 - 18:20

Molecular Structure And Vibrational Assignment Of 1-(N-(2-pyridyl) Aminomethylidene}-2(1H)-Naphtalenone By Density Functional Theory (DFT) And Ab Initio Hartree-Fock (HF) Calculations

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The molecular geometry and vibrational frequencies of 1-[N-(2-pyridyl)aminomethylidene}-2(1H)-Naphtalenone in the ground state have been calculated by using the Hartree–Fock (HF) and density functional method (B3LYP) with 6-311++G(d,p) basis set. The results of the optimized molecular structure are presented and compared with the experimental X-ray diffraction. The computed vibrational frequencies were used to determine the types of molecular motions associated with each of the experimental bands observed. In addition, calculated results are related to the linear correlation plot of computed data versus experimental geometric parameters and IR data. From the results it was concluded that the B3LYP method is superior to the HF method for the vibrational frequencies. Using the time-dependent density functional theory (TD-DFT) and Hartree-Fock (TD-HF) methods, electronic absorption spectra of the title compound have been predicted and a good agreement with the TD-DFT method and experimental ones is determined.

Keywords: Schiff base, IR, electronic absorption spectra, DFT, HF

Theoretical and Computational Methods - P59 / 15:50 - 17:50

Laser Flash Photolysis- Time Resolved Infrared Spectroscopy on the Photooxidation of Triarylphosphines Combined with DFT Computations

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The mechanism of the photooxidation of triarylphosphines Ar3P was explored by laser flash photolysis (LFP) time-resolved infrared spectroscopy (TRIR) with the aid of DFT computations.

Results and Discussion

Steady-state photolysis of Ar3P under air results in the oxidation of Ar3P to phosphine oxide Ar3P=O. Likely, Ar3P is excited to 1Ar3P*, which undergoes electron transfer to O2 to generate a radical ion pair, Ar3P•+ and O2•-. The radical cation Ar3P•+ would undergo the reaction with O2 under the conditions, giving peroxidic radical cation Ar3P+OO• (1). Alternatively, if the radical ion pair, Ar3P•+ and O2•-, couples with each other before each component diffuses into the solvent bulk, then the transient intermediate would be phosphadioxirane (2). To determine which intermediate is formed during the reaction, LFP experiment was conducted in an acetonitrile solution of Ar3P (Ar = Ph, o-Tol, m-Tol, p-Tol, p-An, p-Cl-Ph, p-F-Ph, Mes; 1 ~ 6 mM) under air at 266 nm using Nd:YAG laser. The reaction was monitored by TRIR, which showed appearance of a transient spectrum consisting of several absorption bands at the region of 1050 ~ 1300 cm-1 with a microsecond time-scale (Figure 1). The IR spectra of possible intermediates, 1 and 2, were simulated by theoretical computations with the DFT B3LYP/6-31G(d). In each derivative, the absorption bands in IR spectrum simulated for 1 are in good agreement with the absorption bands in the transient spectrum observed by LFP-TRIR. Meanwhile, the simulation of the IR spectrum for 2 did not reproduce the observed spectrum.

Keywords: triarylphosphine, radical cation, time-resolved infrared spectroscopy, laser flash photolysis, DFT computation

Figure 1

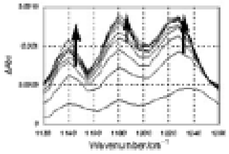

Figure 1. Changes in IR spectra after the LFP at 266 nm on o-Tol$_3$P recorded with time-interval of 4 μs.

Theoretical and Computational Methods - P60 / 15:50 - 17:50

Validity of HOMO/LUMO Approach Calculations: DFT study Of Chemical Reactivity Of Melatonin And Its Metabolites: N1-acetyl-N2-formyl-5-methoxy Kynuramine And N1-Acetyl-5-Methoxykynuramine

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[2]University of Bihac, Biotechnical Faculty, Bihac, Bosnia and Herzegovina

INTRODUCTION: Melatonin is a neurohormone synthesized from the amino acid tryptophan and secreted by the pineal gland in the brain. It has been found to be involved in numerous aspects of biological and physiological regulation. Recent data showed that melatonin inhibits myeloperoxidase, an enzyme that has been used as a marker for indentifying inflammation in the walls of coronary arteries, and its downstream inflammatory byproducts. The oxidized form of melatonin, N1-acetyl-N2-formyl-5-methoxynuramine (AFMK) has no effect on myeloperoxidase catalytic activity, but functions as a potent antioxidant due to its ability to serve as free radical scavenger.

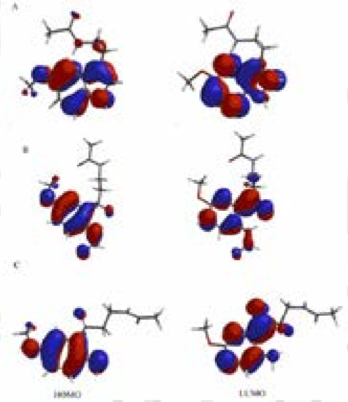
METHODS:.Initially, conformer analysis was performed at HF ab initio level. The seven conformers with the lowest energy were analysed and ones with the lowest energy selected for further optimisation using density functional theory (DFT) method with B3LYP nonlocal exchange functionals with 6-31G* basis set as implemented in Spartan without restrictions. Additionally, vibrational frequencies were calculated and analyzed. Reactivity descriptors such as HOMO-LUMO orbitals density, HOMO-LUMO gap, MEP surfaces, minimum and maximum electrostatic potentials, global reactivity and electronegativity values were calculated at the same level of theory.

RESULTS: Melatonin electrostatic map showing most notable region prone to electrophilic attack was in a good agreement with several proposed mechanistic pathways of melatonin oxidation. The values for HOMO-LUMO gap are used do denote the order of activity: AFMK>AMK>melatonin.

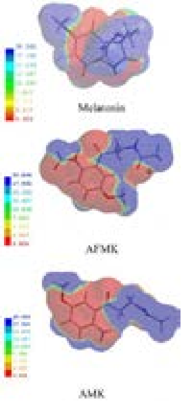
CONCLUSION: These results showed the use and pitfalls of theoretical approach in predicating reactivity of antioxidant molecules normally existing in complex reaction environment.

Keywords: Melatonin, DFT, HOMO-LUMO, AFMK, AMK

HOMO LUMO orbitals



MEP surfaces



Theoretical and Computational Methods - P61 / 15:50 - 17:50

Computational Investigation of Interactions Between Some Polyaromatic Hydrocarbons and Porphyrin

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[2]*Ege University Faculty of Science, Chemistry Department*

One of the significant reasons of the atmosphere pollution PAH (polyaromatic hydrocarbons) can damage the metabolism by entering the metabolism over respiratory tract. Porphyrin and its derivates are the molecule groups which have too important functions for all living organisms. Nitrogen containing porphyrin molecules and PAH can constitute donor-acceptor complexes as a result of their π-electronic systems.

In this study, the charge-transfer complexes between donor-acceptor molecules are investigated by using of quantum chemical methods. Molecules and their all possible conformers were investigated to determine minimum energy geometries by using Density Functional Theory (DFT/ωB97X-D). Time-Dependent Density Functional Theory (TD-DFT/ωB97X-D) has been used to investigate electronic transitions in the studied systems.

Calculations showed that interactions between donor-acceptor molecules are van der Waals type interactions. Additionally, dipole moments and HOMO-LUMO energy levels related to donor-acceptor complexes were calculated.

Keywords: Polyaromatic Hydrocarbons,Computational,Donor-acceptor Complexes

Theoretical and Computational Methods - P62 / 15:50 - 17:50

Vibrational and Theoretical Investigation of (6,7-bis(2-methoxy-ethoxy)quinazoline-4-Yl)-(3-ethynylphenyl)amine (erlotinib)

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The epidermal growth factor receptor (EGFR) is a transmembrane receptor tyrosine kinase of the ErbB family that is abnormally activated in many epithelial tumors [1]. 4-anilinoquinazoline derivatives are potent and highly selective inhibitors of EGFR. These small molecules competitively bind to the ATP binding pocket of intracellular kinase domain and block induction of downstream signaling network mediated by tyrosine kinase. Erlotinib is one of 4-anilinoquinazoline derivatives used for the treatment of non-small cell lung cancer and inhibit tyrosine kinase (TK) activity [2]. Many studies were carried out on bioactivity and clinical use, however there is not enough study related to the illumination of molecular structure and vibrational characteristics. Conformer analysis has been carried out in isolated and in solvated form. The most stable conformers have been found for both of the two forms and the Potential Energy Distribution (PED) have been calculated by VEDA4 program [3]. The calculations have been performed with Gaussian 09 program package [4] using several hybrid functionals of Density Functional Theory (DFT/6-31G*). Molecular bonds have been characterized by NBO analysis. The results have been discussed.

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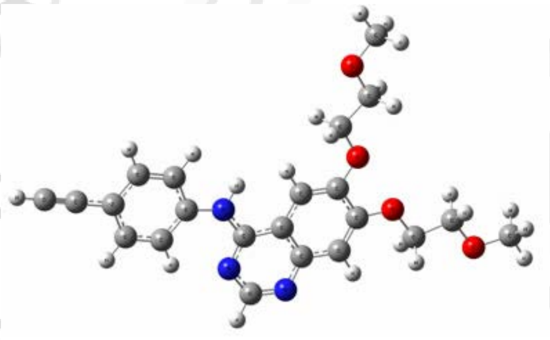
This study was supported by Erciyes Üniversity Scientific Research Project (Project no: FDK-2013-4586)

Keywords: Erlotinib, 4-anilinoquinazoline derivatives, theoretical - vibrational analysis, DFT

Figure 1. Geometry of ERLOTINIB



Theoretical and Computational Methods - P63 / 15:50 - 17:50

Conformational Analysis and Vibrational Study of n-(3-chloro-4fluoro-phenyl)-7-methoxy-6-(3-morpholin-4-ylpropoxy)-quinazolin-4-amine (gefitinib)

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[2]Institute of Science, Erciyes University, Kayseri, Turkey

Quinazolines and their derivatives are compounds which play an important role in medicinal chemistry due to their wide biological-pharmacological activities [1]. GEFITINIB is one of quinalizoline derivatives, as a new anti-cancer agent, is designed to target activity of epidermal growth factor receptor(EGFR) which promotes the growth, division and spread of cancer cells. It is highly expected that better compounds based on gefitinib will be designed in the future drug developments [2]. The vibrational and theoretical analysis of this compound have not been studied yet. In this study, conformer analysis of the molecule has been carried out both in gas and solvent form respectively. The most stable conformer has been found for each form. The differences between their geometrical structures have been discussed. NBO analysis has been performed to characterize intra-molecular interactions and possible H bondings. All the calculations have been performed with Gaussian 09 program package [3] using several hybrid functionals of Density Functional Theory(DFT/6-31G*). Vibrational analysis of the minimum energetic conformer has been calculated by VEDA4 program [4] and Potential Energy Distribution(PED) has been obtained for each form to be discussed.

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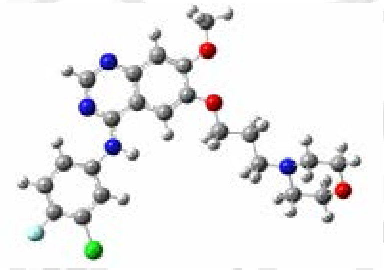
This study was supported by Erciyes Üniversity Scientific Research Project (Project no: FDK-2013-4586)

Keywords: gefitinib, morpholin-4-quinazolin derivatives, theoretical - vibrational analysis, DFT

Figure 1. Geometry of GEFITINIB



Theoretical and Computational Methods - P64 / 15:50 - 17:50

Intermolecular hydrogen bonding interactions of dimethyl sulfoxide, ethylene and pyrrole with water

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Water being the most abundant and essential for life, the contact with the molecules is unavoidable. Water has the strongest hydrogen bonding and the highest surface tension. To gain an insight into the structure of different species of hydrogen bonds between dimethyl sulfoxide, ethylene, pyrrole and water, the equilibrium geometry and the vibrational frequencies are computed. Hydrogen bonding plays an important role in determining the structure and physical properties of many compounds. Hydrogen bonds occur between molecules that have a permanent net dipole resulting from hydrogen being covalently bonded to either fluorine, oxygen or nitrogen. Intermolecular hydrogen bonding between dimethyl sulfoxide, ethylene, pyrrole, and water has been analysed using theoretical methods. Ab initio and DFT methods have been employed to optimize the adducts of molecules (dimethyl sulfoxide, ethylene and pyrrole) with water molecule. The important distances and angles that are indicative of hydrogen bonding are recorded. Hydrogen bonding induced slight changes in geometry of molecules. The results show that the some stretching vibrations and charges (NBO) on atoms, involved in hydrogen bonding are changed.

Keywords: Intermolecular Hydrogen Bonds, Water, Ab initio and DFT calculations, Molecule-water interactions, Vibrational spectroscopy, NBO.

Theoretical and Computational Methods - P65 / 15:50 - 17:50

Theoretical Studies on 1-(2,6-Dimethylphenylamino) Propone-1,2-dione Dioxime

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The name oxime is a contraction of oxy-imine, C=NOH [1]. Because of their wide application in medicine, industry and analytical chemistry, oximes are interesting compounds. These are used as analytical reagents for the detection and determination of some metal ions [2].

In this study, we compared theoretically 1-(2,6-Dimethylphenylamino) propone-1,2-dione dioxime, whose molecular geometry obtained from X-Ray crystal structure has been previously reported [3], by using the Hartree-Fock (HF) and Density Functional Theory (DFT) with 6-31G(d) basis set in the ground state. In addition, theoretical methods were applied to the compound, and its accordance with IR, UV-Visible analysis [4] was investigated. The energetic behavior of the title compound in solvent media has been examined by using B3LYP method with the 6-31G(d) basis set by applying the Onsager Method and the Isodensity Polarized Continuum Model (IPCM). Besides DFT calculations of the title compound, molecular electrostatic potential (MEP), natural bond orbital (NBO), frontier molecular orbitals (FMO) analysis and thermodynamic properties were carried out at the B3LYP/6-31G(d) level of theory.

References

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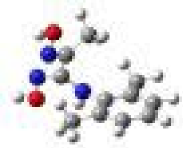
Keywords: Oximes, Density Functional Theory, Hartree-Fock, Molecular Electrostatic Potential, Electronic Absorption Spectra, Vibrational Assignments

Figure 1. Optimized structure of the title compound (DFT/B3LYP/6-31G(d))



Theoretical and Computational Methods - P66 / 15:50 - 17:50

Synthesis, Characterization and Theoretical Calculations of Bicylic Monoterpens α- pinene and Nitrile Oxide Compounds 1,3-Dipolar Cycloaddition Reaction

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1,3-dipolar cycloaddition reactions, both in the field of theoretical and applied chemistry as well as the key compound used in the synthesis of the basic compounds [1]. Currently, 1,3-DC is an important route to the regio- and stereoselective synthesis of five-membered heterocycles and their ring-opened acyclic derivatives. As well as pharmaceutical and agricultural industry Dipolar cycloaddition chemistry, including asymmetric synthesis of high importance, especially newly formed chiral centers are known as a useful method of synthesizing [2]. Several theoretical works have been devoted to the study of one 1,3 DC reactions; however, this cycloaddition form has not received the same amount of attention as its counterpart, Diels-Alder reaction.

In this study, new bicylic monoterpens α- pinene and nitrile oxide compounds 1,3-DC has been synthesized and characterized with spectroscopic methods by using FT-IR, GS-MS, 1H-NMR and 13C-NMR and X-ray techniques. The molecular geometry of structure was optimized applying Hartree-Fock (HF) and Density Functional Theory (DFT/B3LYP) with 6-31G(d,p) basis set in the ground state. Furthermore molecular electrostatic potential (MEP), natural bond orbital (NBO), frontier molecular orbitals (FMOs) analysis have been calculated at the B3LYP/6-31G(d,p) level. The computational methods employed in this study were rigorously tested by performing model calculations on well-established experimental observations.

We gratefully acknowledge financial support of this work by the Amasya University Scientific Research Projects Coordination Department (FMB-BAP 13-035)

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Keywords: 1,3-Dipolar Cycloaddition Reaction, Density Functional Theory, Hartree-Fock

Theoretical and Computational Methods - P67 / 15:50 - 17:50

Experimental and DFT Computational Studies on Bis(1-(2,6-dimethylanilino)propane-1,2-dionedioximato)nickel(II)

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The synthesis, structures and solution chemistry of vicinial dioximes and their transition metal complex have been extensively studied [1-3]. The complexes prepared by vicinal dioximes have received considerable attention as model compounds to mimic biofunction such as reduction of vitamin B12[3,4].

In recent years, theoritical studies on been applied and oxime and their complexes are more popular. Theoretical calculations can be aply to these compunds and this allow to compare the experimentel and theoretical results.

The X-ray crystal structure of Bis[1-(2,6-dimethylanilino)propane-1,2-dionedioximato]nickel(II) complex has been previuosly reported by our working group [5]. On the other hand, theoretical calculation on this compound hasn't yet been published.

In this study, molecular structure, vibrational assignments, chemical shifts, frontier molecular orbital (FMO) analysis, and molecular electrostatic potential (MEP)of this complex in the ground state were investigated by using density functional theory (DFT/B3LYP) with LANL2DZ basis set. The optimized geometric bond lengths and bond angles correspond with the experimental data. The basic aim of the study is to understand the crystal and molecular structures of this complex by using X-ray analysis and quantum chemical method, comparing experimental and theoretical results.

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Keywords: vic-Dioxime; Ni(II) complex; Density Functional Theory

Theoretical and Computational Methods - P68 / 15:50 - 17:50 / Hall 1

Density functional theory studies and vibrational spectra of Tribromomesitylene

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Halogenomethylbenzenes in particular trihalogenomesitylenes are considered as prototype systems for studying the quantum-rotational tunneling of methyl groups [1]. So, it is interesting to study their internal vibrations. In addition, they own interesting properties of phase transitions due to dynamic reorientation of the molecules in their plane. The fundamental vibrational frequencies and intensity of vibrational bands were evaluated by density functional theory (DFT) by using the MPW1PW91 functional with the lanL2DZ(d,p) basis set and assuming C3h symmetry. The solid phase IR and Raman spectra of Tribromomesitylene have been recorded in the regions 400-3500 cm-1 and 100-3500 cm-1 respectively. The agreement between the calculated and experimental frequencies is very good.

Keywords: Trihalogenomesitylene, IR, Raman spectra, DFT

Theoretical and Computational Methods - P69 / 15:50 - 17:50

Computational Characterization Of Aromatic Hydrocarbons Involved In Non-Bonded Interactions

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Pi-pi interactions play an outstanding role in chemistry, however their accurate description is a challenging task for theoretical methods. Ab initio correlated methods, such as CCSD(T) combined with large basis sets, provide a good level of accuracy, however they are prohibitively expensive for large systems. Cheaper methods, such as MP2, remain unfeasible for large systems and, moreover, tend to overestimate the binding energy, especially for dispersive pi-pi interactions.

As an alternative having a very accessible computational cost, density functional theory (DFT) has become a common tool for first principles quantum chemical calculations. B3LYP is by far the most popular density functional in chemistry, but there is growing evidence showing that B3LYP degrades as the system becomes larger and fails to bind van-der-Waals systems. The last years have been marked by an intense research of new DFT variants accounting for the dispersive effects.

The performance of the currently available density functionals has been benchmarked in several recent publications. From these comparative studies, emerge the M06-2X, wB97X-D, B97-D, and BLYP-D functionals, which significantly outdo B3LYP for such chemical property as interaction energy in all kinds of pi-pi complexes.

The above mentioned hybrid functionals accounting for dispersion were used in the present study to characterize the structural preferences of selected aromatic hydrocarbons. The mechanistic proposals resulting from these calculations will be discussed.

Acknowledgments

This work was supported by the Portuguese “Fundação para a Ciência e a Tecnologia”, Research Project PTDC/QUI QUI/118078/2010, FCOMP-01-0124-FEDER-021082, co-funded by QREN-COMPETE-UE.

Keywords: DFT calculations, conformers, aromatic hydrocarbons, non-bonding interactions

Theoretical and Computational Methods - P70 / 15:50 - 17:50

The Redox Behavior of Uranium Metallocene Complexes. A Relativistic DFT/ZORA Study

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Electron affinities (EAs) of a series of metallocene uranium(IV) complexes Cp*2ULL’2 (LL’ sigma or pi donor; Cp* = C5Me5) [1] related to the U(III)/U(IV) and U(V)/U(IV) redox systems were calculated using relativistic Density Functional Theory (DFT) based methods coupled with COSMO-RS (Conductor-like Screening Model - Real Solvents) approach and spin-orbit coupling. Experimental measurements of half-wave potentials E1/2 (V) in solution (THF) were carried out for all these compounds under the same rigorous conditions. A good correlation (R2= 0.98) is obtained between the calculated EA values, at the ZORA/BP86 level and the redox potentials. Our study brings to light the importance of spin-orbit coupling and solvent effect in order to achieve such a good agreement between theory and experiment.

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

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

Cp2ULL’

Structure of the Cp2ULL’ metallocene complexes were the co-ligand LL’ can be ether sigma or pi donors.

Theoretical and Computational Methods - P71 / 15:50 - 17:50

Theoretical Analysis of Phenolic Components from the Extracts of Walnut (Juglans regia) Leaves

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Many plants can be used in the food industry for nutritional qualities, as sources of antioxidants to preserve food quality and also for medicinal purposes. Walnut leaf (Juglans regia L.) has been widely used in folk medicine for treatment of venous insufficiency and haemorrhoidal symptomatology, depurative, antihelmintic and astringent properties. Antifungal, hypoglycaemic, hypotensive, keratolytic, anti-scrofulous and sedative activities have also been described[1,2]. Essential extracted compound of Juglans regia L. was reported as quercetin-3-galactoside(Fig.1.) and calculated IR spectrum(Fig.2.) [3].

In this study, we carried out theoretical and vibrational analysis of this component. The conformational analysis of its structure has been performed to find the most stable form. Natural Bond Orbital (NBO) analysis was performed to examine possible hydrogen bondings using Gaussian 09 programme [4] for both conformer and NBO analysis employing DFT/B3LYP method with 6-31G (d,p) basis set. The vibrational band assignments have been performed through normal co-ordinate analysis. The vibrational analysis was performed through VEDA4 programme [5].

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Keywords: Walnut Leaves, Phenolic compounds, Vibrational Analysis, DFT

Fig. 1. Structure of quercetin 3-galactoside

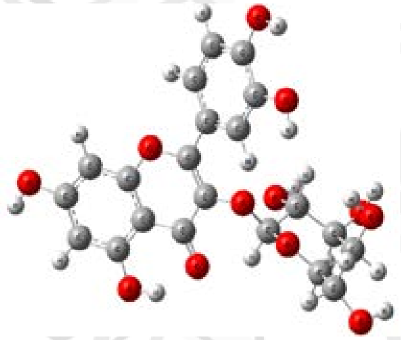
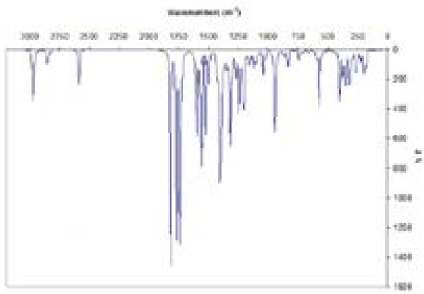


Fig. 2. IR spectrum of quercetin 3-galactoside



Theoretical and Computational Methods - P72 / 15:50 - 17:50

Electronic Properties Of II-VI Semiconductor Nanocrystals

Bariza Ellagoune

Department of material science, Guelma university, Algeria

We were interested for the II-VI semiconductors because of their promising applications especially in optoelectronics, and wide energy gap.In this work, we studied the effect of confinement on the electronic properties of II-VI semiconductor nanocrystals. To access to the electronic levels of nanomaterials, the effective mass model was used which required the knowledge of the structural properties and the band structure of the solid compound.

Based on the density functional method, we used plane waves increased with a total potential (FP-LAPW). The exchange-correlation effects are treated by the local density approximation (LDA) and the generalized gradient approximation (GGA). We calculated the lattice parameter, the compressibility modulus and the total energy equilibrium of semiconductor CdX (X = S, Se and Te)

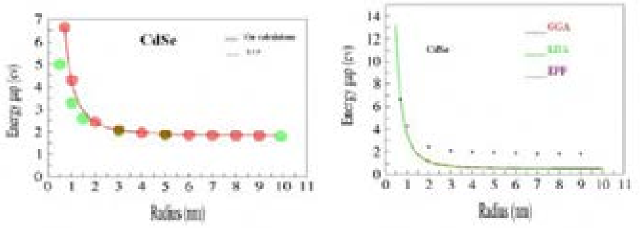
The calculation of the band structure shows that CdX compounds (X = S, Se and Te) are semiconductors that have a direct energy gap Γ point, maintaining their basic structure of zinc-blende or wurtsite.

These results are included in the model of the effective mass reveal a significant effect of quantum confinement. Our results are in good agreement with those found by the method of pseudo-potential for studied nanoparticles.

Then, we can obtain an important parameter: the Bohr radius of the exciton for each compound, this allowed us to estimate the energy of the exciton in each confinement regime.

Keywords: nanomaterials of II -VI semiconductors,local density approximation, FPLAPW,electronic properties.

Energy gap of CdSe from diffirent calculation



Theoretical and Computational Methods - P73 / 15:50 - 17:50

FTIR and DFT Quantum Chemical Studies on Aurin

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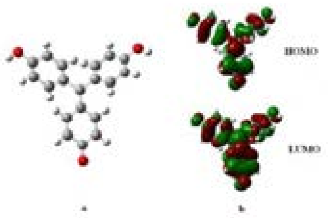
Aurin (4-[Bis(4-hydroxyphenyl)methylene]-2,5-cyclohexadien-1-one or p-rosolic acid) used as a pH indicator and as an intermediate in manufacturing of dyes. It is also used to help differentiate tubercle bacilli from other acid-fast microorganisms. The possible stable conformers of aurin were searched by potential energy surface scan at DFT/B3LYP-6311++G(d,p) level of theory. Calculations were used to identify the lowest energy conformer (Figure 1a). Fourier transform infrared (FTIR) spectrum of the solid phase aurin was recorded in the range 4000-400 cm-1. The experimental vibrational frequencies were compared with those obtained theoretically from DFT calculation. Vibrational assignments were made for normal modes on the basis of scaled quantum mechanical force field (SQM) method.

The frontier molecular (HOMO and LUMO) orbitals (Figure 1b), HOMO-LUMO energy gap, electronegativity and thermodynamic properties of the most stable conformer were also calculated and discussed.

Keywords: Aurin, DFT, FTIR

Figure 1 Aurin: (a) DFT optimized geometry (b) Frontier orbitals



Theoretical and Computational Methods - P74 / 15:50 - 17:50

Structural Study of 4-(2-morpholinoethanoylamino)-benzenesulfonamide by X-Ray Diffraction Experiment and DFT Calculations

Erol Eroğlu[1]***, Mustafa Durgun***[2]***, Hasan Türkmen***[2]***, Şerife Pınar Yalçın***[3]***, Mehmet Akkurt***[4]

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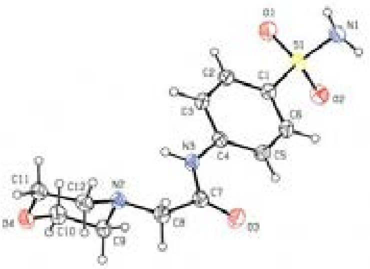
This work presents a combined experimental and computational DFT study of 4-(2-morpholinoethanoylamino)-benzenesulfonamide. The crystal structure of the title compound was determined by single crystal X-ray diffractometry (XRD), forms inversion dimers linked by pairs of intermolecular N—H...O hydrogen bonds. The molecular geometry was also optimized by using density functional theory (DFT/B3LYP) method with the 6-31G and 6-31+G (d) basis sets in ground state and compared with the experimental XRD data. The degree of conformity of the obtained structural parameters between the XRD experiment and DFT calculations were given by two statistical formulas namely R2, squared correlation coefficient and RMSD, root mean square deviation. Further rise in conformity of the bond lengths was achieved by introducing a bigger, 6-31++G (3df, 3pd) extra basis set on Sulfur atom. Obtained results clearly showed that of the size of used basis set influences the conformity of the structural parameters. DFT optimized structure is in excellent agreement with the XRD crystal structure of the title compound.

Keywords: benzenesulfonamide, DFT, X-Ray

4-(2-morpholinoethanoylamino)-benzenesulfonamide



Theoretical and Computational Methods - P75 / 15:50 - 17:50

Vibrational Spectral Analysis And Theoretical Investigation On The Molecular Structure Of Isopropyltriphenylphosphonium Iodide

T Raci Sertbakan

Ahi Evran University, Art and Science Faculty, Department of Physics, Kirsehir, TURKEY

In this work, conformational search of the Isopropyltriphenylphosphonium iodide ((1-Methylethyl) triphenylphosphonium iodide – (CH3)2CHP(C6H5)3I) has been performed. The FT-IR spectrum of this compound was recorded in the region 4000–400 cm-1. The FT-Raman spectrum was also recorded in the region 3500–50 cm-1. Vibrational frequencies of the title compound have been calculated by B3LYP with lanl2dz and SDD basis sets. The calculations were performed at DFT levels by using Gaussian 09 program package, invoking gradient geometry optimization [1-2]. The calculated geometric parameters and vibrational frequencies were analyzed and compared with obtained experimental results.

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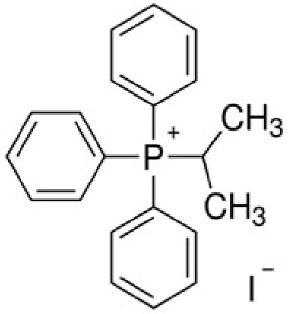
Keywords: Vibrational Spectral Analysis, Theoretical Investigation, Molecular Structure, Isopropyltriphenylphosphonium Iodide

Fig 1



Isopropyltriphenylphosphonium iodide ((1-Methylethyl)triphenylphosphonium iodide)

Theoretical and Computational Methods - P76 / 15:50 - 17:50

Molecular Geometry, Vibrational Spectra (FT-IR, Raman, and NMR), Vibrational Assignments and Density Functional Theory (DFT) Calculations for 2,2/- Ethylenedianiline Molecule

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2,2/-Ethylenedianiline molecule(2EDA) of possible stable forms were studied theoretically and experimentally using FT-IR, Raman and NMR spectroscopic methods. FT-IR and Raman spectra were recorded in the region of 4000–50cm-1 and the isotropic chemical shifts computed by 1H and 13C NMR analysis. The optimized geometric structures concerning to the minimum on the potential energy surface was investigated the DFT method B3LYP with 6-311++G(d,p), cc-pVDZ and cc-pVTZ basis sets were used for the computation of molecular structure, vibrational frequencies, HOMO, LUMO energies and molecular electrostatic potential map. It carried out that the optimized geometric bond lengths have been obtained by DFT shows the best agreement with the experimental values. The vibrational modes were assigned on the basis of total energy distribution (TED) calculated for 6-311++G(d,p) basis set, on the basis of with scaled quantum mechanical (SQM) method.

Keywords: 2,2/-Ethylenedianiline molecule(2EDA), DFT, TED, SQM method, FT-IR, FT-Raman, and NMR spectra.

Theoretical and Computational Methods - P77 / 15:50 - 17:50

Time-Dependent Density Functional Study on Variation of UV-Visible Spectrum of Poly(phospolo(3,4b)phosphole) as a Function of Substituent

***Zeki Büyükmumcu*, Ilknur Koçyiğit**

Department of Chemistry, Erciyes University, Kayseri, Turkey

Polyphosphole is one of the heterocyclic conducting polymers which has not been studied in detail. In a theoretical study [1], band gap of polyphosphole has been estimated to be lower comparing to polypyrrole and polythiophene. In another study [2], polyphosphole has been synthesized and it is concluded that polyphosphole has extremely low band gap and has a high level electron-accepting ability. Considering these results, it can be said that polyphospoles may be good candidate for some applications of conducting polymers. To best of our knowledge, polyphospolo[3,4b]phosphole has not been synthesized and it can be considered as a material that has appropriate properties for some special applications. In this study, substituent effect on UV-visible spectrum of polyphospolo[3,4b] phosphole has been examined. Unsubstituted and substituted phospolo[3,4b]phosphole oligomers have been optimized employing hybrid functional B3LYP [3,4]. Optimized geometry of -NO2 substituted phospholo[3,4b]phosphole monomer is shown in Figure 1. Then, TD-DFT calculations have been performed on these optimized structures to obtain excitation energies. Gaussian program suite [5] has been used for all the calculations. Excitation energies and HOMO-LUMO gaps have been analyzed through the results obtained. As a result, it is concluded that not only the type of substituent but also substituent position has an influence on the excitation energies. These two parameters may be used to tune excitation energies and band gap of conducting polymers. This lets us to design conducting polymers with properties that would fit to special applications.

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This study was supported by TUBITAK Scientific Research Project (Project no: 212T051)

Keywords: phospholo[3,4b]phosphole, B3LYP, TD-DFT, substituent effect, conducting polymer.

Figure 1

Optimized geometry of -NO2 substituted phospholo[3,4b]phosphole monomer.

Theoretical and Computational Methods - P78 / 15:50 - 17:50

Theoretical Analysis of Substituent Effect on UV-Visible Spectrum of Poly(pyrrolo(3,4b)pyrrole)

Ilknur Koçyiğit*, *Zeki Büyükmumcu

Department of Chemistry, Erciyes University, Kayseri, Turkey

Different forms of polypyrrole have been studied extensively and used for several purposes [1]. Polypyrrolo[3,4b]pyrrole which has not been synthesized yet is a good candidate as a conducting polymer for multiple applications including solar cells. UV-visible spectrum of the polymer is an important tool in terms of determining whether material can be used as a solar cell or not since absorbance wavelengths of the material should fit the high intensity regions of solar spectrum for high yield usage. In one of the studies [2] substituent effect on the electronic properties of thiophene–pyrrole-based pi-conjugated oligomers has been studied. HOMO-LUMO gaps and excitation energies as function of substituent and its substitution position were examined. In this study, the substituted oligomers of pyrrolo[3,4b]pyrrole with functional groups in several positions have been optimized and the time dependent density functional theory calculations have been carried out on the optimized structures to obtain UV-visible absorption spectrum of them. All the calculations have been done using B3LYP functional [3,4] within Gaussian program package[5]. Through the results, the effect of electron donating and withdrawing groups on electronic properties and UV-visible spectrum has been analyzed. The possible applicability of the polymer with several functional groups to some areas has been discussed on the basis of the results.

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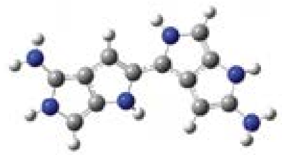
This study was supported by TUBITAK Scientific Research Project (Project no: 212T051)

Keywords: pyrrolo[3,4b]pyrrole, TD-DFT, substituent effect, UV-Visible Spectrum, B3LYP

Figure 1.



Optimized geometry of -NH2 substituted pyrrolo[3,4b]pyrrole dimer.

Theoretical and Computational Methods - P79 / 15:50 - 17:50

Investigation Of Structural And Electronic Properties Of Ternary Co-Pt-B Clusters

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[3]*Çankaya University, Elec. and Communication Engineering Dept., TR-06530 Ankara, Turkey*

A series of computational study by using Density Functional Theory (B3LYP/LANL2DZ) has been improved to investigate the structural and energetic properties of small ternary CoxPtyBz (x+y+z=4) nano alloy clusters [1]. We attempt to predict various stable structural isomers and the lowest-lying energy geometries for each size within them through following a systematical search for one, two and three dimensional (1D, 2D and 3D) configurations. The findings are compared with any similar studies [2,3]. Our results indicate that the most stable isomers have three-dimensional structures (tetrahedron) for x+y+z=4. Their total and average binding energies per atom have been calculated with respect to the cluster size. Energies for the highest occupied and the lowest unoccupied molecular orbitals (HOMO and LUMO) have been computed and the HOMO-LUMO energy gaps have been determined. Moreover, the charge distributions have been analyzed for the Co, Pt and B atoms in each cluster.

Acknowledgement. This work is supported by Bozok University (with project no: BAP-I.F.E./2011-39).

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Keywords: Investigation of Structural and electronic properties of ternary Co-Pt-B clusters

Theoretical and Computational Methods - P80 / 15:50 - 17:50

Gaussian Calculations Of 3-Methyl-4-(3-Sinnamoyloxybenzylidenamino)-4,5-Dihydro-1H-1,2,4-Triazol-5-One Molecule

Haydar Yüksek, Murat Beytur

Kafkas Üniversitesi Fen-Edebiyat Fakültesi Kimya Bölümü 36100-Kars

In this study, 3-methyl-4-(3-sinnamoyloxybenzylidenamino)-4,5-dihydro-1H-1,2,4-triazol-5-one molecule was optimized by using the B3LYP/631G (d) and HF/631G (d) basis sets [1,2]. Afterwards, 1H-NMR and 13C-NMR isotropic shift values were calculated by the method of GIAO using the program package Gaussian G09 [2]. Experimental and theoretical values were inserted into the grafic according to equatation of δ exp=a+b. δ calc. The standard error values were found via SigmaPlot program with regression coefficient of a and b constants. IR absorption frequencies of analysed molecule were calculated by two methods. Then, they were compared with experimental data, which are shown to be accurate. Infrared spectrum were composed by using the data obtained from both methods. The veda4f program, was used in defining IR data, which were calculated theoretically [3].

References:

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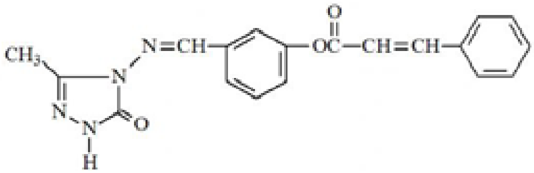
Keywords: Gaussian Calculations Of 3-Methyl-4-(3-Sinnamoyloxybenzylidenamino)-4,5-Dihydro-1h-1,2,4-Triazol-5-One Molecule

Figure 1



Theoretical and Computational Methods - P81 / 15:50 - 17:50

The Investigation Of Spectroscopic Properties Of 3-Ethyl-4-(4-Sinnamoyloxybenzylidenamino)-4,5-Dihydro-1H-1,2,4-Triazol-5-One Compound Using B3LYP And Hf Basis Sets

Murat Beytur[1]***, Haydar Yüksek***[1]***, Murat Tolga Kayalar***[2]

[1]*Kafkas Üniversitesi Fen-Edebiyat Fakültesi Kimya Bölümü 36100-Kars*
[2]*Kafkas Üniversitesi Eğitim Fakültesi İlköğretim Bölümü 36100-Kars*

The study, 3-ethyl-4-(4-sinnamoyloxybenzylidenamino)-4,5-dihydro-1H-1,2,4-triazol-5-one compound was optimized by using the B3LYP/631G (d) and HF/631G (d) basis sets [1,2]. 1H-NMR and 13C-NMR spectral data were obtained theoratically by using this optimizing structure. The experimental and the obtained theoretical values were compared and found by regression analysis that are accurete. Furthermore, molecule's theoretical bond lengths, bond angles, UV-Vis values, dipole moments, formal charges, HOMO-LUMO energies and total energy of the molecule for both methods were calculated

References

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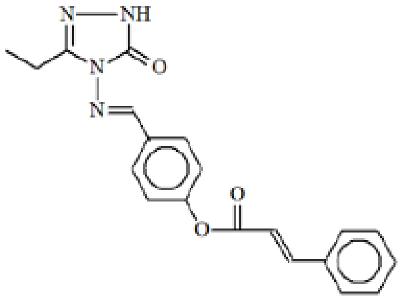
[2] K. Wolinski, J.F. Hilton, P. Pulay, J. Am. Chem. Soc., 112, 512, (1990).

Keywords: The Investigation Of Spectroscopic Properties Of 3-Ethyl-4-(4-Sinnamoyloxybenzylidenamino)-4,5-Dihydro-1H-1,2,4-Triazol-5-One Compound Using B3LYP And Hf Basis Sets

Figure 1



Theoretical and Computational Methods - P82 / 15:50 - 17:50

Computation of Antimony Atoms Transmission Through Nanometric Foils

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Laboratoire Physique Mathématique et subatomique, Département de Physique, Université Constantine1, Route de Ain El Bey, 25000 Constantine, Algérie

In this work, the antimony transmission through several ion implantation materials or foils (Al, SiO_2 or Si_3N_4) was computed. The study was mainly performed by simulation using the program SRIM-2006, and then a comparison with literature was provided. Several parameters were taken into account: the foil thickness, the beam energy and the beam orientation with respect to the foil.

In particular, the antimony ions transmission, beyond the different materials, was studied. The phenomenon was investigated in the case corresponding to a thickness equal to dmin. According to the literature approximation, the minimum thickness (dmin) is supposed to be the value sufficient to stop 99,99% of the incident ions. The simulation, which was run for this particular value, showed a different result. In other words, the percentage of the stopped incident ions was lower than 99,99% which means a higher rate of ions transmission beyond the foil. The noticed difference could not be neglected especially for the applications performed in nanometric scales (i.e. inferior than 100 nm).

Finally, the preferable geometry (i.e. orientation of the ions with respect to the specimen), corresponding to a minimum ions transmission beyond the foil, was obtained for an angle of 10°.

Keywords: antimony, silicon, transmission, nanometric foils

Vibrational (IR and Raman) and Electronic Spectroscopies - P83 / 15:50 - 17:50

Hydrogen Bonds In Sucrose Crystal And Its Contribution To Optical Nonlinearity Studied By IR, Polarized Raman, IINS And NMR Spectroscopy

Katarzyna Piela[1]**, **Magdalena M. Szostak[1], Ireneusz Natkaniec[2], Krystyna Holderna Natkaniec[3]

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[2]Joint Institute for Nuclear Research, Dubna, Russia
[3]Faculty of Physics, Adam Mickiewicz University, Poznań, Poland

It is well known that sucrose crystal reveals second harmonic generation (SHG) process [1]. However, the origin of this phenomenon has not paid much attention. SHG requires a non–centric crystal lattice and the additional factors that affect this process are intermolecular charge transfer via hydrogen bonds (HBs), molecular motions and helical formation which leads to chirality [2,3].

The IR, polarized Raman spectra of sucrose single crystal and IINS spectra of sucrose powder were measured to reinvestigate and complete the already known assignments of vibrations [4,5], especially those connected with HBs in normal and lattice spectral ranges. We aimed to get knowledge about motions executed in sucrose crystal by the studies of 1H-NMR second moment line. Additionally, the hyperpolarizability of sucrose monomer, dimer and trimer along the polar axis which form helix in crystal structure were computed by the DFT method to better understand the NLO properties. In this work we discuss the positive influence of HB, proton transfer and molecular motions on SHG response.

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Keywords: second harmonic generation, 1H NMR line second moment, DFT calculations, hyperpolarizability

Vibrational (IR and Raman) and Electronic Spectroscopies - P84 / 15:50 - 17:50

Conformational And Structural Studies of N-Propylamine From Temperature Dependent Raman And Far Infrared Spectra Of Xenon Solutions And Ab Initio Calculations

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The Raman and infrared spectra (4000 to 50 cm-1) of the gas, liquid or solution, and solid have been recorded of n-propylamine. Variable temperature (-60 to -100oC) studies of the Raman (1175 to 625 cm-1) and far infrared (600 to 10 cm-1) spectra dissolved in liquid xenon have been carried out. The five possible conformers have been identified and their relative stabilities obtained with enthalpy difference relative to Tt of 79 ± 9 cm-1 (0.9 ± 0.1 kJ/mol) for Tg >= 91 ± 26 cm-1 (1.08 ± 0.3 kJ/mol) for Gg > 135 ± 21 cm-1 (1.61 ± 0.2 kJ/mol) for Gg’ >= 143 ± 11 cm-1 (1.71 ± 0.1 kJ/mol) for Gt. The percentage of the five conformers is estimated to be 18 % for the Tt, 24 ± 1 % for Tg, 23 ± 1 % for Gg, 18 ± 1 % for Gg’ and 18 ± 1 % for Gt at ambient temperature. The conformational stabilities have been predicted from ab initio calculations utilizing several different basis sets up to aug-cc-pVTZ from both MP2(full) and density functional theory calculations. Vibrational assignments have been provided for all five conformers which are supported by MP2(full)/6-31G(d) ab initio calculations to predict harmonic force constants, wavenumbers, infrared intensities, Raman activities and depolarization ratios. Estimated r0 structural parameters have been obtained from adjusted MP2(full)/6-311+G(d,p) calculations.

Keywords: N-propylamine, Xenon, Structural parameters, Vibrational assignments, Raman, Far infrared

Vibrational (IR and Raman) and Electronic Spectroscopies - P85 / 15:50 - 17:50

FT-IR And Computational Study Of Raffinose And Melezitose

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The melezitose and raffinose, are trisaccharides built from 2 mols glucose and 1 mol fructose, and from 1 mol each of D-galactose, D-glucose, and D-fructose respectively.

Recently, a vibrational analysis (Infrared absorption and spectrum of the Raman diffusion) and

Ab-initio methods as particularly well suited to investigate the physical properties (geometry, vibrational frequencies, and force constants). The density functional theory (DFT) was used for the molecules.

In this work, we have determined the parameters of the potential energy function, using the force field a modified Urey-Bradely-Shimanouchi force field (mUBSFF) involving non-redundant symmetry coordinates, combined with a complete intermolecular potential energy function taking into account the Van-der-Waals and the electrostatic interactions and also a contribution of the hydrogen bonds.

The infrared spectra of raffinose and melezitose were recorded and analyzed. These spectra constitute the experimental support that allows reproducing the vibrational frequencies theoretically and establishing a force field for this molecule through a normal coordinate analysis.

The data obtained from vibrational wavenumber calculations were used to assign vibrational bands obtained in IR spectrum of the studied molecules.

Keywords: IR and Raman Spectra, Normal Coordinate Analysis

Vibrational (IR and Raman) and Electronic Spectroscopies - P86 / 15:50 - 17:50

Study Of The Solvent Effect On The Molecular Structure And C=O Stretching Vibrations Of Michlers' Ketone

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Carbonyl group is known to be a good probe of local environment. Michler's ketone (MK) as a representative of carbonyl – containing and at the same time highly positive solvatochromic compound has been used as our subject of investigation. Its photochemical and photophysical properties were widely studied, mostly using UV-Vis spectroscopy. There also are several works investigating MK using vibrational spectroscopy in it's excited state.

The significant change of position, intensity or/and shape of the absorption shift is called solvatochromism. Its vibrational analogue is known as vibrational slovatochromism. Using IR spectroscopy we examined solvatochromism of Michler's ketone dissolved in carbon tetrachloride, cyclohexane, chloroform, 2-butanone, acetone, DMSO, acetonitrile and methanol solvents. It has been observed that change of solvent polarity has an ambiguous influence on MK's IR band shifts and molecular geometry. We have observed that not only vibrations of carbonyl group (>C=O) are affected by the solvent polarity, there are other vibrations (of Carom-N and C-Carom) that behave in similar way.

Experimental investigations have been supported by the quantum-mechanical computations to gain more insight into the solvatochromic behavior of Michler's ketone. Calculations have been carried using Kohn-Sham formulation of Density Functional Theory and the Polarizable Continuum Model was employed to account for solute-solvent interactions.

The work was financed by a statuory activity subsidy from the Polish Ministry of Science and Higher Education for the Faculty of Chemistry of Wrocław Univeristy of Technology.

Keywords: solvent effect, solvatochromism, infrared, IR, Michler's ketone, vibrational spectroscopy

Vibrational (IR and Raman) and Electronic Spectroscopies - P87 / 15:50 - 17:50

Structural and Vibrational Properties, Quantum Chemical Calculation of 2-(Triphenylphosphoranylidene)butyraldehyde

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Triphenylphosphonium compounds and their various derivatives are key reagents in the wittig reactions and they are used to convert aldehydes and ketones into alkene, specifically in applications ranging from the synthesis of simple alkenes to the construction of complex biologically active molecules in the pharmaceutical researches. They are also important class of isoaromatic compounds and have widespread applications in antimicrobial and anticancer activity. In addition, phosphonium compounds enhance flame retardancy mainly in textile industry [1].

In order to establish the stable possible conformations, the conformational space of the title molecule was scanned with molecular mechanic simulations. This calculation was performed with the Spartan 10 program [2]. Then, Gaussian 09 quantum chemical software was used in all calculations [3]. The optimized structural parameters and vibrational wavenumbers for the title molecule were calculated by using B3LYP functional with 6-311++G(d,p), cc-pVDZ and cc-pVTZ as basis set. The vibrational modes were assigned on the basis of TED analysis using SQM program [4]. The calculated vibrational wavenumbers were scaled for all of level of theory in order to figure out how the calculated data were in agreement with those of the experimental ones [5].

References

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Keywords: Structural Properties, Vibrational Properties, Quantum Chemical Calculation, 2-(Triphenylphosphoranylidene)butyraldehyde

Vibrational (IR and Raman) and Electronic Spectroscopies - P88 / 15:50 - 17:50

Infrared, Raman and NMR spectra, conformational stability and vibrational assignment of 7-Hydroxy-4-(Trifluoromethyl) coumarin

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Coumarin is a chemical compound which is found naturally in some plants. Coumarin is found in a variety of plants such as tonka bean, vanilla grass, woodruff, mullein, sweet grass, lavender, sweet clover grass, and licorice, and also occurs in food plants such as strawberries, apricots, cherries, and cinnamon. It is thought to work by serving as a pesticide for the plants that produce it. It can be synthetically produced as well. It has a distinctive odor, which has led people to use it as a food additive and ingredient in perfume. Due to concerns about coumarin as a potential liver and kidney toxin, its use as a food additive is heavily restricted, although it is perfectly safe to eat foods which naturally contain coumarin.

To the best of our literature survey, there is no complete vibrational and conformational analysis data on 7H4TFC molecule in the literature. In the present paper, an exhaustive conformational search of the 7H4TFC has been performed by molecular mechanic calculations. Geometry parameters and vibrational frequencies of the title compound have been calculated by B3LYP method using 6-311++G(d,p), cc-pVDZ and cc-pVTZ basis sets. The calculated geometric parameters, NMR Chemical shifts and vibrational frequencies were analyzed and compared with obtained experimental results.

Keywords: Infrared, Raman and NMR spectra, conformational stability,vibrational assignment, 7-Hydroxy-4-(Trifluoromethyl)coumarin

Vibrational (IR and Raman) and Electronic Spectroscopies - P89 / 15:50 - 17:50

Combined experimental-theoretical characterization of chelidamate nickel complex with 4-methylpyrimidine

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Chelidamic acid, is commonly used inorganic and coordination chemistry, biochemistry, medical chemistry and even in HIV investigation [1]. The multifunctional ligands containing N and O-donors have attracted attention, since they may cause diversity in the coordination modes and interesting properties such as luminescent probe, radical adsorption and ferromagnetic interaction [2]. A new chelidamate complex of nickel(II) ion, [Ni(chel)2H2O(mpd)]·2H2O [chel: chelidamate, mpd: 4-methylpyrimidine] was synthesized and characterized by single-crystal X-ray diffraction, UV-Vis and FT-IR spectroscopy. Theoretical calculations have been carried out by using the density functional theory (DFT) [3] and Hartree-Fock (HF) [4] with 6-31G (d) basis set. Molecular geometry from X-ray experiment of Ni(II) complex in the ground state was compared using unrestricted hybrid density functional B3LYP. HOMO-LUMO energies, absorption wavelengths and excitation energy were computed by time dependent DFT (TD-DFT) method with polarizable continuum model. The observed FT-IR vibrational frequencies are analyzed and compared with theoretically predicted vibrational frequencies. The natural charges on the atoms and second-order interaction energies were derived from natural bond orbital analysis (NBO).

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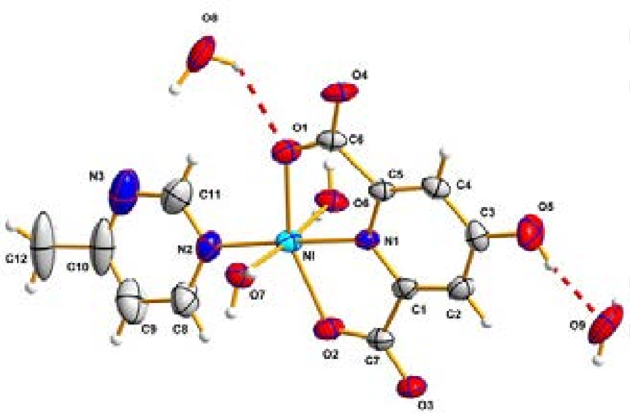
Keywords: chelidamic acid, X-ray diffraction, IR, UV-vis, DFT, NBO

Figure



A view of Ni(II) complex showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and hydrogen atoms are shown as small spheres of arbitrary radii.

Vibrational (IR and Raman) and Electronic Spectroscopies - P90 / 15:50 - 17:50

Synthesis, Spectroscopic, Thermal And Structural Properties Of (M(3-Aminopyridine)2Ni(µ-CN)4)n (M = Co and Cu) Heteropolynuclear Cyano-Bridged Complexes

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Two novel cyano-bridged heteropolynuclear complexes, {[Co(3-Aminopyridine)2Ni(µ-CN)4]n and [Cu(3-Aminopyridine)2Ni(µ-CN)4]n (3-Aminopyridine = 3AP)} have been synthesized in the powdered form and characterized by FT-IR spectroscopy, thermal analysis, powder XRD analysis method and elemental analysis. Their FT-IR spectra have been reported in the range of (4000-400) cm-1. General information was acquired about structural properties of these complexes from IR spectra by considering changes at characteristic peaks of the cyano group and 3AP. It was understood that the cyano group acts as a bridge because the ν(C≡N) stretching vibration of cyano groups split into two peaks in the all complexes. The thermal behaviors of these complexes have been also investigated in the range of (25-750) oC. Thermal behaviors of these complexes were studied using TG and DTG methods. Structural and crystal properties of these complexes were studied using powder XRD analysis in the range of (4-70) o. The powder XRD analyses showed that these complexes were in crystalline form.

Keywords: 3-Aminopyridine complexes, Co and Cu complexes, cyano-bridged complexes, Heteronuclear coordination polymeric complexes, powder XRD analysis, thermal analysis

Vibrational (IR and Raman) and Electronic Spectroscopies - P91 / 15:50 - 17:50

Comparing The Effects Of Valdecoxib, Rofecoxib And Celecoxib Drugs On The Model Membrane Properties Using Infrared Spectroscopy, DSC And Turbidity Techniques

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Celecoxib (CLX), Rofecoxib (RFX) and Valdecoxib (VLX) drugs belong to a family of NSAIDs which are selective COX-2 inhibitors. While these drugs are established analgesics, they also have a number of pleiotropic effects such as cancer chemoprevention, occasionally in a COX-2 independent manner. As these drugs are highly hydrophobic, studies are underway on how the drugs can alter membrane properties such as fluidity, phase transition temperature and others. We have previously shown that CLX decreases the fluidity of the membrane and induces phase separation of the lipids.

The current study compares the effects of RFX and VLX on DSPC model membrane properties and compares it with effects of CLX previously reported by our group. Differential scanning calorimetry, turbidity measurements and Fourier transform infrared (FTIR) spectroscopy techniques are employed.

We have observed that VLX can alter the properties of DSPC model membranes very similarly to CLX: it decreases the phase transition temperature (Tm) and fluidity in a concentration-dependent manner. FTIR and calorimetry studies show that increasing drug concentration enhances these effects. Interestingly, RFX appears to have no significant effect on membrane fluidity and Tm.

Given the fact that Celecoxib and Valdecoxib have a common sulfoneamide group while Rofecoxib lacks it and only has sulfone group, we suggest that the sulfoneamide group may be responsible for specific interactions with the lipid bilayers altering the biophysical properties of model membranes.

Keywords: FTIR, DSC, Celecoxib, Rofecoxib, Valdecoxib, colon cancer, model membranes.

Vibrational (IR and Raman) and Electronic Spectroscopies - P92 / 15:50 - 17:50

Characterization Of The Effect Of Selective COX-2 Inhibitor Valdecoxib On The Colon Cancer Cell Lines Using ATR-FTIR Spectroscopys

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Cyclooxygenases (COX-1 and COX-2) are the major enzymes of eicosanoid reactions, converting arachidonic acid to prostaglandins. COX-2 enzymes are expressed in the early stage of colon cancer and by altering membrane fluidity they lead to structural and cellular changes in the tissue.

That's why COX-2 inhibitors play a role in colon cancer treatment. Valdecoxib, which is selective COX-2 inhibitor, was used in this study. The cancer chemopreventive ability of VLX, particularly in colorectal cancer, has been shown in epidemiological studies.

The Attenuated Total Reflectance Fourier Transform Infrared Spectroscopy (ATR-FTIR) was used in order to study the effect of VLX on colon cancer cell lines at the molecular level. We have examined the biophysical effects of VLX on the cellular membranes of COX-2 expressing (HT29) and COX-2 non-expressing (SW620) cells lines using ATR-FTIR. The bands originating from saturated and unsaturated lipids, such as CH2 symmetric and assymetric stretching or olefinic bands in the 3050-2800 cm-1 region of the obtained spectra were analysed and provided valuable information on lipid concentration and lipid order. Our data show that VLX treatment decreased lipid fluidity in the cancer cell lines. As metastatic cells have higher membrane fluidity, we examined the effect of VLX on the metastatic potential of these cells. VLX treatment efficiently decreased the proliferation of the cells. We propose that one of the ways by which VLX exerts its antitumorigenic effects is via alterations in the cellular membrane fluidity which has a notable impact on the cell's metastatic potential.

Keywords: ATR-FTIR, Valdecoxib, COX-2, fluidity, colon cancer

Vibrational (IR and Raman) and Electronic Spectroscopies - P93 / 15:50 - 17:50

Raman Characterization Of "Yannis Papadellis" Colour's Collection

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[2]*TEI of Lamia Department of Electronics, Material Analysis and Research Laboratory*
[3]*Athens School of Fine Arts, Technical University of Athens*

Yannis Papadellis (1926-2006) was a painter and iconographer. He was nephew of the painter Fotis Kontoglu (1895–1965) and his collaborator. During a period of two decades spend his energy to make a complete collection with all the referred materials in the book of Dionysius of Fourna (1670-1744) who was an Eastern Orthodox author of a manual of iconography and painting in the 18th century. The treatise of Dionysius of Fournas is also called Mount Athos Painter's Guide and is in three parts. The first part of the work gives recipes for colors, gesso, and instructions on body proportions for human figure painting. The samples of Yannis Papadellis collection have been saved in the laboratory of traditional painting techniques of the School of Fine Arts in Athens. In accordance to a document the sale of the collection was dated in 1973. We have identified cinnabar, orpiment, verdigris, lead white, red and yellow iron ochre, lapis lazuli, calcite, red lead. For characterization of the mineral pigments we use also the Romanian Raman Library. All the analytical results shall be given in a databank in Byzantine and Christian Museum useful for study of Post-Byzantine Iconography.

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Keywords: Raman, colour's collection, data base

Vibrational (IR and Raman) and Electronic Spectroscopies - P94 / 15:50 - 17:50

FT-IR, FT-Raman and Molecular Structure Studies of Mirtazapine and its Comparison of Mianserin

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Kocaeli University

Mirtazapine(±)-1,2,3,4,10,14b-hexahydro-2-[11C]methylpyrazino(2,1-a)pyrido(2,3-c)(2) benzazepine (Remeron) is a compound with antidepressant therapeutic effects. It is the 6-aza derivative of the tetracyclic antidepressant mianserin (Tovol) (±)-2-methyl-1,2,3,4,10,14b-hexahydrodibenzo[c,f] pyrazino[1,2-a]azepine. The FT-IR and FT-Raman spectra of mirtazapine have been recorded in 4000–400 cm-1 and 3500–10 cm-1, respectively. The optimized geometry and vibrational frequencies of mirtazapine have been determined using the density functional theory (DFT/B3LYP) method. A comparison of the experimental and theoretical results of mirtazapine indicates that the density-functional B3LYP method is able to provide satisfactory results for predicting vibrational properties. The experimental and calculated results for mirtazapine have also been compared with mianserin.

Keywords: Mirtazapine, Mianserin, Vibrational spectra, DFT

Vibrational (IR and Raman) and Electronic Spectroscopies - P95 / 15:50 - 17:50

Synthesis, FT-IR Spectroscopic, Thermal And Structural Properties Of M(4-Pyridinecarboxaldehyde)Ni(CN)4 complexes (M = Mn, Co, Ni, Cu and Cd)

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Department of Physics, Dumlupinar University, Kütahya, Türkiye

In this study, complexes of 4-Pyridinecarboxaldehyde-tetracyanonickel given by the formula M(4-Pyridinecarboxaldehyde)Ni(CN)4 (M = Mn, Co, Ni, Cu and Cd; 4-Pyridinecarboxaldehyde = 4PCA) have been synthesized in the powdered form and characterized by FT-IR spectroscopy, thermal analysis, powder XRD analysis method and elemental analysis. Their FT-IR spectra have been reported in the range of (4000-400) cm-1. General information was acquired about structural properties of these complexes from IR spectra by considering changes at characteristic peaks of the cyano group and 4PCA. The thermal behaviors of these complexes have been also investigated in the range of (25-750) oC. Thermal behaviors of these complexes were studied using TG and DTG methods. Structural and crystal properties of these complexes were studied using powder XRD analysis in the range of (4-70) o. The powder XRD analyses showed that these complexes were in crystalline form.

The similarities of the observed spectra indicate that the obtained complexes of M(4PCA)Ni(CN)4 (M = Mn, Co, Ni, Cu and Cd) are new examples of the Hofmann-type complexes.

Keywords: 4-Pyridinecarboxaldehyde (4PCA); Hofmann-type complexes, Infrared Spectroscopy (IR), powder XRD analysis, Tetracyanonickelate, thermal analysis.

Vibrational (IR and Raman) and Electronic Spectroscopies - P96 / 15:50 - 17:50

Molecular Structure And Vibrational Spectra Of 7-Methylcoumarin By Density Functional Method

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In the present study, structural and conformational analysis of 7-Methylcoumarin were performed. The FT-IR and Raman spectra were recorded in the region 4000-400 cm-1 and 3500-50 cm-1, respectively. Vibrational frequences of the title compound were calculated by B3LYP method. The ground state energies and dipole moments have also been computed. The calculated and scaled frequencies were compared with experimental values and on the basis of this comparison and TED data assignments of fundamental vibrational modes were examined.

Keywords: 7-Methylcoumarin, molecular structure, FT-IR, FT-Raman, DFT, vibrational spectra

Vibrational (IR and Raman) and Electronic Spectroscopies - P97 / 15:50 - 17:50

Vibrational Spectral Investigations Of Glyoxime

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[2]Department of Medicinal Laboratory, Vacational School of Health Services of Selcuk University, Selcuklu, Konya, Turkey

The FT-IR and Raman spectra were recorded in the region 4000-400 cm-1 and 3500-50 cm-1, respectively. Vibrational frequences of the title compound were calculated by B3LYP method. The calculated and scaled frequencies were compared with experimental values and on the basis of this comparison and TED data assignments of fundamental vibrational modes were examined.

Keywords: Glyoxime, molecular structure, FT-IR, FT-Raman, DFT, vibrational spectra

Vibrational (IR and Raman) and Electronic Spectroscopies - P98 / 15:50 - 17:50

Molecular Structure And Spectral Investigations Of 3-Aminocoumarin

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In the present study, structural and conformational analysis of 3-Aminocoumarin were performed. The FT-IR and Raman spectra were recorded in the region 4000-400 cm-1 and 3500-50 cm-1, respectively. Vibrational frequences of the title compound were calculated by B3LYP method. The ground state energies and dipole moments have also been computed. The calculated and scaled frequencies were compared with experimental values and on the basis of this comparison and TED data assignments of fundamental vibrational modes were examined.

Keywords: 3-Aminocoumarin; molecular structure; FT-IR; FT-Raman; DFT; vibrational spectra

Vibrational (IR and Raman) and Electronic Spectroscopies - P99 / 15:50 - 17:50

Comparison of Experimental and Theoretical IR and UV Spectra of Some Benzimidazole Derivatives

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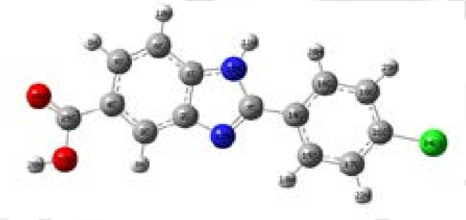
Benzimidazoles are known for biological and commercial importance as pharmaceuticals, veterinary anthelmintics and fungicides. It is also of a considerable interest as a ligand towards transition metal ions with a variety of biological molecules including ionheme systems, Vitamin B12 and its derivatives and several metallo-proteins. The complexes of transistion metal salts with benzimidazole derivatives have been extensively studied as models of some important biological molecules.

In this study, we carried out experimental and theoretical study on molecular and vibrational structure of 2-(4-chlorophenyl)-1H-benzimidazole-5(6)-carboxylic acid which synthesized by Göker H. et.al. The Fourier transform infrared spectra of this benzimidazole derivative were recorded in the solid phase. The harmonic vibrational wavenumbers and UV spectra were calculated by Gaussian 09 program package. In addition we compared experimental and theoretical UV spectra. The theoretical bands for FT-IR spectra of the title molecule have been constructed.

Keywords: Benzimidazole, FT-IR spectra, UV

Structure of 2-(4-chlorophenyl)-1H-benzimidazole-5(6)-carboxylic acid



Vibrational (IR and Raman) and Electronic Spectroscopies - P100 / 15:50 - 17:50

Near-Infrared Spectroscopy For Co Doped (80-x)Sb2O3-20Na2O-xWO3

***Petya Petkova*[1]*, *<u>*Ivaylo Parushev*</u>[1]*, Petko Vasilev*[1]*, Mohamed Toufik Soltani*[2]**

[1]Shumen University "Konstantin Preslavsky", Shumen, Bulgaria
[2]Department of Physics, Faculty of Sciences and Engineering sciences, University "Mohamed Khider", Biskra, Algeria

In this work, the absorption spectra of the undoped and doped with 0.1% Co2O3 glasses with the composition (80-x)Sb2O3-20Na2O-xWO3 are measured in the spectral region 1238-1362 nm. The optical structure of Co2+ is investigated and the energies of the electron transitions in this metal cation are determined. The influence of W5+ on the cobalt structure is also established. The role of the spin-orbit interaction and Jahn-Teller effect is evaluated also. Zeeman splitting which is characteristic for Co2+ is determined and discussed.

Keywords: glasses, absorption, 3d electron transitions

Vibrational (IR and Raman) and Electronic Spectroscopies - P101 / 15:50 - 17:50

An Experimental and DFT Study on 1,3-Bis(2-(2-hydroxybenzylideneamino)phenoxy)propane: Vibrational Analysis and Solvent Effect on Prototropic Tautomerism

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[4]Department of Primary School Teaching, Faculty of Education, Akdeniz University, 07058, Antalya, Turkey.

IR and Raman spectra of a salicylaldimine compound, namely 1,3-Bis[2-(2-hydroxy benzylideneamino) phenoxy]propane have been recorded and vibrational bands of the these spectra have been assigned based on the results from PED (Potential Energy Distribution) calculation using VEDA4 [1]. All calculations have been performed at the DFT level together with the B3LYP functional and 6-311+G(d,p) basis set. The influences of the solvents with different polarity on the prototropic tautomerism of the title compound were also investigated theoretically. Potential barriers of the between keto-amine and phenol-imine forms were calculated by PES (Potential Energy Scan) in vacuo and the different solvent media. Results show that the phenol-imine form of the compound is energetically more favorable than the keto-amine form in vacuo and solvent media. Calculated results are in accordance with the experimental results which is published elsewhere [2,3].

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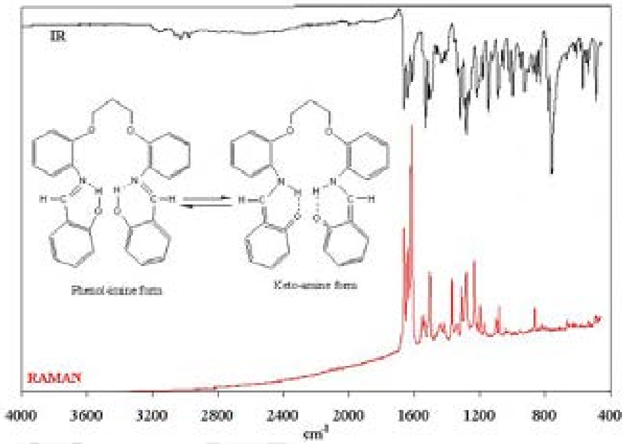
Keywords: 1,3-Bis[2-(2-hydroxybenzylideneamino)phenoxy]propane, DFT, IR, Raman, Vibrational Analysis.

IR&Raman Spectra of 1,3-Bis[2-(2-hydroxybenzylideneamino)phenoxy]propane



Vibrational (IR and Raman) and Electronic Spectroscopies - P102 / 15:50 - 17:50

Molecular Structure and Vibrational FT-IR, FT-Raman, FT-NMR spectra Investigatıons of (2-hydroxyel)triphenylpphosphonium chloride

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Theoretical and experimental carried out vibrational spectra and electronic properties of (2-hydroxyel) triphenylpphosphonium chloride(2HTPHCl). The FT-IR(4000–400 cm-1), FT-Raman (3500–50 cm-1) and FT-NMR spectra have been recorded and analyzed. The molecular geometry, harmonic vibrational frequencies, chemical shifts, HOMO, LUMO energies and molecular electrostatic potential map of 2HTPHCl have been calculated by using DFT method at either both (B3LYP) with 6-311G++(d,p) and cc-pVDZ basis sets. Total energy distributions of vibrational modes are calculated by using SQM method.

Keywords: (2-hydroxyel)triphenylpphosphonium chloride, SQM method, DFT, FT-IR, FT-Raman and FT-NMR.

Vibrational (IR and Raman) and Electronic Spectroscopies - P103 / 15:50 - 17:50

Experimental (FT-IR, FT-Raman, UV, 1H and 13C NMR) And Computational (Density functional theory) Studies On 3-Bromophenylboronic Acid

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Structurally, boronic acids are trivalent boron-containing organic compounds that possess one alkyl substituent (i.e., a C–F bond) and two hydroxyl groups to fill the remaining valences on the boron atom. We studied 3-bromophenylboronic acid (3BrPBA); the derivative of boronic acid. The paper includes the experimental (FT-IR, FT-Raman UV-Vis, 1H and 13C NMR) techniques and theoretical (DFT-Density Functional Theory) calculations. The experimental data were recorded, FT-IR (4000–400 cm–1) and FT-Raman spectra (3500–0 cm–1) in the solid phase the UV-Vis spectrum that dissolved in water and ethanol was recorded in the range of 200-800 nm for each solution and 1H and 13C NMR spectra were recorded in DMSO solution, respectively. The theoretical calculations were computed DFT (B3LYP) with 6-311++G(d,p) basis set calculations. The optimum geometry was also obtained from inside for possible four conformers using according to position of hydrogen atoms after the scan coordinate of this structure. The fundamental vibrations were assigned on the basis of the total energy distribution (TED) of the vibrational modes, calculated with scaled quantum mechanics (SQM) method and PQS program. 13C and 1H NMR chemical shifts were racked on by using the gauge-invariant atomic orbital (GIAO) method. The time-dependent density functional theory (TD-DFT) was used to find HOMO and LUMO energies, excitation energies, oscillator strength. The density of state of the molecule was also investigated as Total (TDOS) and partial (PDOS) density of state and also overlap population density of state (OPDOS) diagrams have been demonstrated. Besides, frontier molecular orbitals (FMO), molecular electrostatic potential (MEP) and thermodynamic properties were performed. At the end of this work, the results were ensured beneficial for the literature contribution.

Keywords: 3-Bromophenylboronic acid, DFT, FT-IR and Raman, UV, NMR; HOMO–LUMO.

Vibrational (IR and Raman) and Electronic Spectroscopies - P104 / 15:50 - 17:50

Molecular Structure, Spectroscopic Characterization (FT-IR, FT-Raman, UV and NMR), HOMO And LUMO Analysis Of 3,3Diaminobenzidene With DFT Quantum Chemical Calculations

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In this work, Infrared, Raman, UV and NMR spectra of 3,3Diaminobenzidene(3,3-DAB) were carried out by using density functional theory DFT/B3LYP method with the 6-311++G(d,p) basis set. FT-IR and FT-Raman spectra were recorded in the regions of 4000-400 cm-1 and 4000-50 cm-1, respectively. The geometrical parameters, energies and wavenumbers were obtained and the complete assignments of fundamental vibrations were performed on the basis of the total energy distribution (TED) of the vibrational modes, calculated with scaled quantum mechanics (SQM) method and PQS program. The 1H and 13C NMR spectra were recorded and calculated. The UV spectrum of investigated compound was recorded in the region of 200–400 nm in ethanol solution. The electronic properties, such as excitation energies, absorption wavelengths, HOMO and LUMO energies were performed by DFT/B3LYP approach and the results were compared with experimental observations. The thermodynamic properties such zero-point vibrational energy, thermal energy, specific heat capacity, rotational constants, entropy, and dipole moment of the studied compound were calculated. Mulliken atomic charges and molecular electrostatic potential (MEP) were calculated by the DFT/B3LYP for title molecule. As a result, the calculated results were compared with the observed values and generally found to be in good agreement.

Keywords: 3,3Diaminobenzidene, DFT, FT-IR and FT-Raman, NMR, UV-vis.

Vibrational (IR and Raman) and Electronic Spectroscopies - P105 / 15:50 - 17:50

Differentation of Different Inbreed Obese Mouse Lines at Adipose Tissues By ATR- FTIR Spectroscopy With Chemometric Tools

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Obesity is a metabolic disorder resulting in elevated levels of free fatty acids and triglycerides in the blood circulation together with accumulation of lipids within various tissues. The Berlin fat mouse inbreed line (BFMI) is an important new model for obesity which has a complex genetic background and generates spontaneous obesity while they are fed with a rodent standard breeding diet (SBD). These lines are not generated by knock-out mutations as a causative effect for the generation of spontaneous obesity phenotype. That is why, according to their polygenic nature underlying obesity phenotypes, the BFMI lines are excellent models for the study of obesity induced changes in humans. This current study aims to characterize BFMI male and female mice having gonadal and inguinal adipose tissue. For this purpose, attenuated total reflectance- Fourier transform infrared (ATR-FTIR) spectroscopy was used to differentiate male and female control (DBA/2J) and BFMI lines; namely BFMI856, BFMI860 and BFMI861. These lines contain two different adipose tissues; inguinal fat (IF) which is SCAT (Subcutenous adipose tissue), gonadal fat (GF) which is VAT (Visceral adipose tissue). FTIR spectroscopy is a rapid and effective technique to monitor of molecular alterations induced by different conditions such as disease, chemicals and environmental in biological tissue components. Principal Component Analyses (PCA) is a widely used technique to determine relationship between biological samples and to interpret similarities and differences between these samples. Also, hierarchical clustering is a multivariant technique that group the samples in terms of their characteristics. Chemometric results based on FTIR data showed that BFMI856 line is succesfully differentiated from BFMI860 and BFMI861 lines. Line BFMI856 is resistant to high fat diet, while the lines BFMI860 and BFMI861 responded to high fat diet by additional fat deposition. These findings reveal that ATR-FTIR spectroscopy together with chemometric tools allowed us to differentiate these inbreed obese mouse models.

Keywords: Dıfferentatıon Of Dıfferent Inbreed Obese Mouse Lınes At Adıpose Tıssues By Atr- Ftır Spectroscopy Wıth Chemometrıc Tools

Vibrational (IR and Raman) and Electronic Spectroscopies - P106 / 15:50 - 17:50

FT-IR, FT-Raman, surface enhanced Raman scattering and computational study of 2-(p-fluorobenzyl)-6-nitrobenzoxazole

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The epidermal growth factor receptor (EGFR) is a transmembrane receptor tyrosine kinase of the ErbB family that is abnormally activated in many epithelial tumors [1]. 4-anilinoquinazoline derivatives are potent and highly selective inhibitors of EGFR. These small molecules competitively bind to the ATP binding pocket of intracellular kinase domain and block induction of downstream signaling network mediated by tyrosine kinase. Erlotinib is one of 4-anilinoquinazoline derivatives used for the treatment of non-small cell lung cancer and inhibit tyrosine kinase (TK) activity [2]. Many studies were carried out on bioactivity and clinical use, however there is not enough study related to the illumination of molecular structure and vibrational characteristics. Conformer analysis has been carried out in isolated and in solvated form. The most stable conformers have been found for both of the two forms and the Potential Energy Distribution (PED) have been calculated by VEDA4 program [3]. The calculations have been performed with Gaussian 09 program package [4] using several hybrid functionals of Density Functional Theory (DFT/6-31G*). Molecular bonds have been characterized by NBO analysis. The results have been discussed. FT-IR and FT-Raman spectra of 2-(p-fluorobenzyl)-6-nitrobenzoxazole [1] were recorded and analyzed. A surface enhanced Raman scattering spectrum (SERS) was recorded in silver colloid. Using Gaussian03 [2] set of quantum chemistry codes, the vibrational wavenumbers and corresponding vibrational assignments were examined theoretically. The presence of CH_2 and NO_2 bands in the SERS spectrum indicates the nearness of these groups to the metal surface, which affects the orientation and metal molecule interaction. From the SERS study, it is inferred that the para substituted phenyl ring is more tilted while the tri-substituted phenyl ring assumes a nearly perpendicular orientation with respect to the metal surface. The results indicate that the B3LYP method is able to provide satisfactory results for predicting vibrational wavenumbers and structural parameters. The calculated first hyperpolarizability is comparable with the reported values of similar derivatives. The geometrical parameters of the title compound are in agreement with that of similar derivatives [3].

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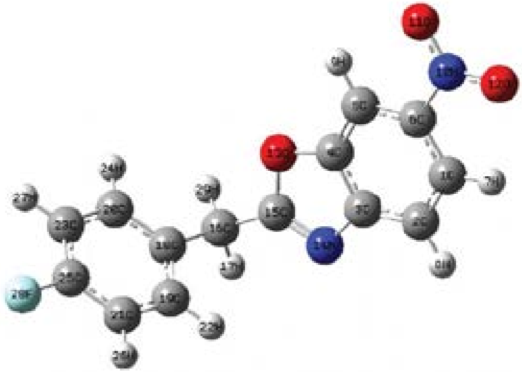
Keywords: FT-IR, FT-Raman, surface enhanced Raman scattering and computational study of 2-(p-fluorobenzyl)-6-nitrobenzoxazole

Figure


11O
10N
12O
9H
5C
6C
13O
4C
1C
7H
24H
29H
27H
26C
23C
16C
15C
3C
2C
18C
14N
17H
8H
28F
25C
19C
21C
22H
20H

Vibrational (IR and Raman) and Electronic Spectroscopies - P107 / 15:50 - 17:50

FT-IR, NMR, UV And Structural İnvestigations of 4-(2,5-Dİ(THİOPHEN-2-YL)-1H-PYRROL-1-YL)Aniline By Usıng Ab-Inıtıo Calculatıons

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Design and syntesis of new conjugated polymers play significant role in the conducting polymer research. Among conducting polymers, polythiophene and its derivatives have drawn much attention due to their high conductivity, good redox reversibility, swift change of color with potential and stability in environment [1]. Therefore, these important properties cause them to have important applications, such as, electrical conductors, nonlinear optical devices [2], polymer light-emitting diodes [3], sensors [4], batteries [5], artificial noses and muscles [6], transistors [7] and electrochromic devices [8]. In this study, we focus on the spectroscopic properties of 4-(2,5-di(thiophen-2yl)-1H-pyrrol-1-yl)aniline (Compound) by carriying out ab-initio calculations based on Hartree-Fock (HF) method and Density Functional Theory (DFT). All calculations are performed by using Gaussian 09 program with B3LYP/6-31G(d,p) type Exchange correlation function basis set and GaussView 5.0.8 is used visualization of the structure and simulated vibrational spectra and energies of optimized structure. Bond length, bond angle and dihedral angles are calculated as a structural properties. Vibrational modes (FTIR), 1H and 13C NMR chemical shifts and UV-Vis spectra of Compound1 are investigated and compared with experimental result. The vibrational modes are assigned on the basis of PED analysis using VEDA4 program. Our calculated results are consistent with the experimental data. To the best of our knowledge, the spectral properties (Compound) are calculated the first time in this study.

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Keywords: FT-IR, NMR, UV And Structural İnvestigations OF 4-(2,5-Dİ(THİOPHEN-2-YL)-1H-PYRROL-1-YL)Aniline By Usıng Ab-Inıtıo Calculatıons

Vibrational (IR and Raman) and Electronic Spectroscopies - P108 / 15:50 - 17:50

Crystallographic, Spectroscopic and Computational Studies on (E)-2-(((3-bromophenyl)imino)methyl)-5-(diethylamino)phenol

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Schiff base and its complexes use in many fields of chemistry and biochemistry. Herein, we have determined crystal structure of (E)-2-(((3-bromophenyl)imino)methyl)-5-(diethylamino)phenol by X-ray diffraction and spectroscopic methods. The unit cell parameters of the crystal structure are a=6.6456 (5), b=15.4880(17), c=15.4473 (16) and Z=4 with in orthorhombic space group P212121. The molecule has (E) configuration with respect to central C=N double bond. The nitrogen atom of this central C=N with hydroxyl group establishes intramolecular O—H•••N hydrogen bond. In addition to these hydrogen bonds, weak π···π interactions present in the crystal structure.

The ground state geometry of the molecule has been calculated using the density functional theory (DFT) method with B3LYP 6-31G (d,p) and Hartree Fock (HF) with 6-31G (d,p) basis sets and the theoretical results have been compared with the experimental results. Besides, the infrared spectrum of the molecule was recorded at 500-4000 cm-1 region.

Keywords: (E)-2-(((3-bromophenyl)imino)methyl)-5-(diethylamino)phenol, XRD, DFT, HF, Hydrogen bonding, Schiff base

Vibrational (IR and Raman) and Electronic Spectroscopies - P109 / 15:50 - 17:50

A First Look into Phenylephrine's Conformational Landscape

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Phenylephrine, (R)-3-[-1-hydroxy-2-(methylamine)ethyl]phenol - also known as neosynephrine - is a sympathomimetic amine that acts as a direct-acting α1-receptor agonist, and thus, as an agonist of norepinephrine1, differing solely from the latter by lacking a p-OH group. It is reckoned as a potent vasoconstrictor – although less potent than epinephrine and norepinephrine – much used in medicine2. There are a great number of studies, focusing on the neurological aspects of phenylephrine; however, as far as we could find in literature, no work focusing on the conformational preferences of phenylephrine, either theoretical or experimental, in gas-phase or other, has been done until now, making the present work pioneer in the unravelling of the conformational landscape of phenylephrine. All experiments were performed using a laser ablation molecular beam Fourier-transform microwave (LA-MB-FTMW)3 spectrometer, in the 5 - 6 GHz frequency region. Two conformers of phenylephrine (Figure 1) have been successfully ascribed - through the comparison of the experimental rotational and quadrupole coupling constants with those calculated ab initio4 - to the two lowest-energy forms calculated. The experimental determination of the 14N quadrupole coupling constants constitutes an exceptional tool that allows the unequivocal establishment of the orientation of the side chain -NH2 group with respect to the molecular frame. Those constants can be used to deduce the nature of the intramolecular interactions in which this functional group is involved.

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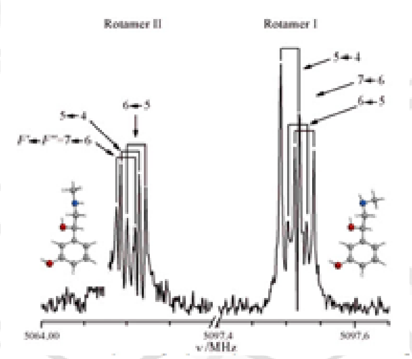
[4] For the ab initio calculations, the MP2 level of theory with the 6-311++G(d,p) basis set was used consistently in both conformational search and molecular properties prediction.

Keywords: Fourier-Transform; Microwave; Conformers; Laser ablation; Rotational transition

Fig. 1



A section of the microwave spectrum of phenylephrine depicting the 616←515 rotational transition for the two detected rotamers.

Vibrational (IR and Raman) and Electronic Spectroscopies - P110 / 15:50 - 17:50

Infrared Reflection Absorption Spectroscopy for Characterization of Monolayers on Ceramic Surfaces

Xia Stammer

Bruker Optics, Ettlingen, Germany

Infrared reflection absorption spectroscopy (IRRAS) is a well-established technique for the characterization of surfaces and adsorbate films, which provides specific information on the chemical composition and structure of thin surface layers and adsorbed molecules. Most of the investigations have been carried out on metal substrates due to the high reflectivity and the ease of the spectra interpretation. Only since the 1980s the method has also been used for dielectric substrates with high refractive index, weakly reflection and vanishingly small absorption in the mid-IR region [1].

In this work, we used IRRAS to determine the film quality of self-assembled monolayers formed on antireflective ceramic substrates for state-of-the-art applications in the industry. We first prepared organic thin films on silicon and silicon nitride surfaces using n-alkylsilanes with different chain length. IRRA spectra were then taken under polarized light with a Bruker Vertex 80 FT-IR in combination with an optimized reflection optical system and a special sample table. With the help of the resulting IRRA spectra we could make a statement for the ordering, the density and even for the orientation of the adsorbed molecules on the substrate surface. In our new application of the IRRAS method, monolayer sensitivity in combination with detailed structural information also on weakly reflecting, nonmetal surfaces was demonstrated.

Keywords: Infrared, Reflection, Absorption, Spectroscopy, Monolayers, ceramic

Vibrational (IR and Raman) and Electronic Spectroscopies - P111 / 16:20 - 18:20

Experimental and Quantum Chemical Study on 1-Methylindole

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Quantum chemical calculations of energies, geometrical structure and vibrational wavenumbers of 1-Methylindole (1MI) were carried out by using density functional (DFT/B3LYP) method with 6-311++G(d,p) basis set.The fundamental vibrations were assigned on the basis of the total energy distribution (TED) calculated with scaled quantum mechanics (SQM) method and PQS program. Total and partial density of state (TDOS and PDOS) and also overlap population density of state (OPDOS) diagrams analysis were given. The energy and oscillator strength of each excitation were calculated by time-dependent density functional theory (TD-DFT).The UV absorption spectra of monomers were observed in the range of 200–800 nm in ethanol.Isotropic chemical shift of hydrogen and carbon nuclei were investigated via observed 1H and 13C NMR spectra in DMSO solution and predicted data applied with gauge–invariant atomic orbitals (GIAO) method. A detailed description of spectroscopic behaviors of compound was given based on the comparison of experimental measurements and theoretical computations.

Keywords: 1-Methylindole, DFT; NMR, UV, Infrared spectra; HOMO–LUMO, DOS.

Vibrational (IR and Raman) and Electronic Spectroscopies - P112 / 15:50 - 17:50

Oxidative Effect Of Algerian Olive Oil Using Derivatives FTIR Spectroscopy and Chemometrics methods

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A study of the influence of external parameters such as temperature, light and storage medium and a better understanding of the influence of endogenous parameters on the aging and deterioration of olive oil were studied. Thermal effect on six different samples of virgin olive oil, in order to determine oxidative stability, was realized. Classical methods of analysis were used for a preliminary characterization of olive oil. Fourier transform infrared (FTIR) spectra and gas chromatography were employed for differentiation and classification of olive oils from several producing regions of Algeria. The samples were subjected to heating treatment at 50°C and also 60°C evaluated after 0 up to 90 days. The investigation is conducted by exploiting as well the specters IR of samples as well as resorting first and second derivation. Considerable differences were observed also by analytical methods and FTIR spectroscopy. The combination of spectroscopic and chemometrics methods as MLR and PLS lead to reliable models to certify the quality of olive oil as well as on the phenomenon of aging.

Keywords: Virgin olive oil, Thermal effect, Oxidative stability, FTIR, Chemometrics methods

Vibrational (IR and Raman) and Electronic Spectroscopies - P113 / 15:50 - 17:50

Experimental and Theoretical Study of Novel Pyrrolo(1,2-α) perimidin-10-one dyes

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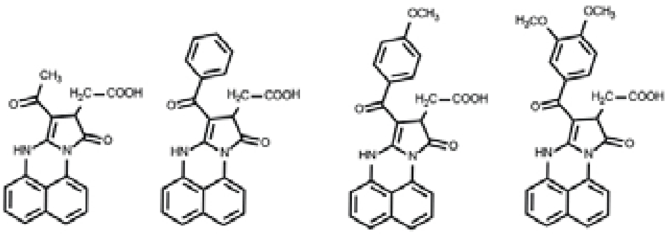
In this work, a complementary investigation has been realized via both experimental and theoretical analysis of four pyrrolo[1,2-a]perimidin-10-one derivatives (Figure 1). Pyrrolo[1,2αa]perimidin-10-one framework is an integral part of the structure of some patented dyes and pigments, which are useful for organic sensors and industrial plastics [1-3]. Hence, they are interesting compounds due to their reaction and application properties. These derivatives here have been synthesized by reaction of maleic anhydride with heterocyclic ketene aminals (HKAs) containing perimidine moiety. The structures of synthesized compounds were confirmed by IR, 1H-, 13C-NMR and elemental analyses. These compounds have been optimized by HF and DFT/B3LYP methods via using 6-311++G(d,p) basis set [4]. Various physical and chemical quantities are in good agreement with both experimental and theoretical findings.



1a 1b 1c 1d

Figure 1. Pyrrolo[1,2-a]perimidin-10-one derivatives

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Keywords: Experimental and Theoretical Study of Novel Pyrrolo[1,2-a]perimidin-10-one dyess

Vibrational (IR and Raman) and Electronic Spectroscopies - P114 / 15:50 - 17:50

Investigation of N,N' –'-Bis(salisiliden)-1,9-diamino nonane Schiff Base Complexes with different Ions by 1H-NMR Relaxation Time Measurements and Computional Studies

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In this study, the spin-lattice relaxation time (T1) and the spin-spin relaxation time (T2) of Schiff base[1,2] derivative N,N' – ethylenebis (salicylideneimine)-1,9-diamino nonane in DMSO-d6 solvent were studied in terms of the temperature in the range of 20 – 50 °C by a 400 MHz 1H - NMR spectrometer. Furthermore, T1M relaxation times of the complexes formed by adding different Ni(II), Zn(II) and Co(II) ions were measured and these derivatives were measured in the range of 25 – 40 °C. Hence, their binding constants (Kf), free energy exchange (ΔG), molecular dynamics and ion-dipole interactions were investigated for OH and N=CH proton. Based on activation energy (Ea) and correlation time (τc) values it was suggested that Schiff base derivatives do molecular tumbling motion [3,4]. It was postulated that the dipole-dipole interaction is the dominant interaction type for ligands and complexes due to the increase in the relaxation times with the increasing temperature [5-7]. Additionally, the structural stabilities of the considered systems have been confirmed through the electronic structure analysis realized by using Hartree-Fock (HF) and density functional theory (DFT) B3LYP methods with 6-311++g (d,p) basis set [8].

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Keywords: Investigation of N,N' –'-Bis(salisiliden)-1,9-diamino nonane Schiff Base Complexes with different Ions by 1H-NMR Relaxation Time Measurements and Computional Studies

Vibrational (IR and Raman) and Electronic Spectroscopies - P115 / 15:50 - 17:50

Molecular Structure Investigation And Spectroscopic Studies On 5-Bromo-2-Chlorotoluene: A Combined Experimental And Theoretical Analysis

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This work presents the characterization of 5-bromo-2-chlorotoluene (5Br2ClT) by density functional theory DFT/B3LYP method with 6-311++G(d,p) basis set and spectral techniques. The spectroscopic properties were investigated by FT-IR, FT-Raman, UV–vis., 1H and 13C NMR techniques. The FT-IR spectrum (4000–400 cm–1) and the FT-Raman spectrum (4000-50 cm–1) were recorded for 5Br2ClT molecule. The geometrical parameters, energy and wavenumbers were obtained and the complete assignments were performed on the basis of the total energy distribution (TED) of the vibrational modes, calculated with scaled quantum mechanics (SQM) method, and PQS program. The 1H and 13C NMR spectra were recorded in chloroform (CDCl3) and calculated by (GIAO) method. The UV–Vis absorption spectra of title molecule were recorded in the range of 200–400 nm in ethanol solution. The electronic properties, such as excitation energies, absorption wavelengths, HOMO and LUMO energies, were performed by DFT/B3LYP approach. Molecular electrostatic potential (MEP) and thermodynamic properties such zero-point vibrational energy, thermal energy, specific heat capacity, entropy, and dipole moment of the studied compound were performed. Mulliken and natural charges of the title molecule were also calculated and interpreted. Finally the calculation results were analyzed to simulate infrared, Raman, NMR and UV spectra of the studied compound which show good agreement with observed spectra.

Keywords: 5-Bromo-2-chlorotoluene, DFT, Vibrational spectra, NMR, UV-vis.

Applied Spectroscopies - P116 / 16:20 - 18:20

The natural radioactivity of some soil sample of Pamukkale region by using gamma spectroscopy

İskender Akkurt[1], Kadir Günoğlu[2], Feride Kulalı[1]

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[2]Technical Sciences Vocational School, Süleyman Demirel University, Isparta, Turkey

Since the beginning of the universe, the radiation due to the radionuclide which are in the depths of the earth contribute to daily natural background radiation. Those are generally occurs in the land-sources materials (stone, soil, rocks, etc.) in different rate. The most important part of those radiations are due to the uranium, thorium and potassium in the material. In this study, the activity of naturally occurring radionuclides 40K, 226Ra, 232Th have been measured to determine natural radioactivity level in collected soil samples in different places of Pamukkale region in Denizli (TURKEY).

Keywords: Natural Radioactivity, Gamma Spectroscopy, Soil, Pamukkale

Applied Spectroscopies - P117 / 16:20 - 18:20

Investigation of Gamma-Ray Shielding Properties of Plasters Containing Different Boron Compounds

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In this study linear attenuation coefficient for gypsum containing ulexite and colemanite boron compounds has been investigated. The measurements have been performed by using gamma spectrometer system. This system contains NaI(Tl) detector and Multi-Channel-Analyser (MCA). In measurements, 137Cs and 60Co radioactive sources, emitted 662, 1173 and 1332 keV gamma energies, were used. The measured results were compared with the calculation obtained using computer code of XCOM.

Keywords: Gamma-Ray Shielding, gamma spectrometry, boron, XCom

New Materials - P118 / 15:50 - 17:50

Study of Interaction Metal Ion With Carbohydrates

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University Of Tlemcen

We particulary interest on the properties for chemical systems occuring in the oral cavity, to understand and resolve corrosion problems related to dental restorations in systems where such data are not currently available. We have been studying interactions of various metal ions such as copper with carbohydrates.

The classification approach metal ion with ligand interactions is based on the

concept of acid and basic hard and soft and has called HSAB from this approach we used fukui indices that provide information on the reactivity and sites privileged attacks in the ligand and subsequently optimised these complexes by molecular modeling.

Keywords: fukui indices, hard and soft ion, carbohydrate, complex, molecular modeling

New Materials - P119 / 15:50 - 17:50

Interpretation of acoustics properties of Tellurite-based glasses

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Interest in glass, due to its diverse applications has been observed from time immemorial. Glass as a material comparatively cheap, relatively easy to produce as well as for synthesis in wide range of compositions. For these, we are intrested to Tellurite-based glasses whitch have been the subject of high interest in recent years due to their interesting electrical, optical and magnetic properties. In this paper, we present acoustic properties of Lithium borate glasses containing TeO2 as Li0.6 TexB1.4_2xO2.4_x glasses of the composition: x= 0–0.35 mol%, and Niobium-containing tellurite glass with starting composition of (90-x)TeO2–10Nb2O5–(x)ZnO (x=0–15 mol%). Using simulation conditions of scanning acoustic microscopy we put into evidence Rayleigh velocity variation with TeO2 and ZnO contents. Moreover, linear dependences were found and quantified via the determination of analytical relations that are important in properties prediction.

Keywords: Glass system, elastic properties, SAW velocities, Tellurite glass.

Applied Spectroscopies - P120 / 15:50 - 17:50

Effect of nitrogen addition on the acoustical properties and the structure of oxynitride bioglasses

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[2]Laboratoire des semi-conducteurs, Département de physique, Faculté des sciences, Université Badji-Mokhtar-Annaba

Bioactive glasses are seen with alacrity for their excellent potential in the repair and regeneration of bone defects, because of their ability to support the growth of bone cells. The rate of development of the bond to bone and its strength vary with the composition of the bio-glasses. The objective of this work is to investigate the acoustic properties of oxynitride bioglasses. These are silicate-type glasses in which bridging and non-bridging oxygens are replaced by nitrogens and their molar composition is (55-3x) SiO2 –13.5CaO–31.5Na2 O–xSi3N4 (x is the number of moles of Si3N4). The methodology consists of several steps: calculation of acoustic materials signatures from angular spectrum model and determination of Rayleigh velocity via fast Fourier transform treatment of such signatures. It was found that the change of the quantity of nitrogen of 0 wt% to 2.16 wt% involves a variation of the space period varies from 36.2µm to 48.5µm, which generated a shifting of Rayleigh velocity from 2886 m/s to 3308m/s. Thus, incorporation of nitrogen into silicate glasses can result in stiffer, harder and stronger glasses. Also, the characterization of these oxynitride bioglasses using solid state nuclear magnetic resonance and infrared spectroscopy have shown firstly that all the N atoms are bonded to Si atoms and secondly that this increase in rigidity of the glass network can be explained by the formation of SiO3N, SiO2 N2 tetrahedra.

Keywords: Bioactive glass, acoustical parameters, Rayleigh velocity

New Materials - P121 / 15:50 - 17:50

Optoelectronic properties of SrxCd1-xO mixed crystals: FP-LAPW investigations

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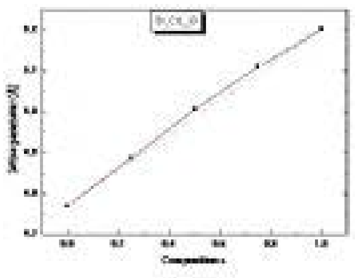
Using first-principle method, we investigate the structural, electronic and optical properties of the strontium semiconductors SrxCd1-xO with 25%, 50% and 75% of Sr. The calculations are performed by using the full potential linearized augmented plane wave (FP-LAPW) method within the framework of the density functional theory (DFT) as implemented in theWien2k code. As exchange-correlation potential we used the generalized gradient approximation (GGA) of Perdew et al. The variation of the calculated equilibrium lattice constant versus concentration shows that a small deviation from Vegard's law is clearly visible with upward bowing parameter equal to -0.072 Å. The bulk modulus as a function of x for SrxCd1-xO alloy shows a significant deviation from the linear concentration dependence (LCD) with downward bowing equal to 38.51 GPa. The different roles of structural and chemical effects on the gap bowing and its variation with composition are identified and discussed. In addition, densities of electron states and charge densities are also determined for both the binary and their related ternary alloys.

Keywords: SrxCd1-xO, Vegard's law, band structure, dielectric constants

Composition dependence of the calculated lattice constant (solid squares) of SrxCd1-xO ternary alloy compared with Vegard'law (dashed line).



Theoretical and Computational Methods - P122 / 15:50 - 17:50

Density functional theory investigation of energy gaps and optical properties of SrTe1-xOx

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Biofilms and Biocontamination of Materials Laboratory, Faculty of Sciences, Badji Mokhtar University,
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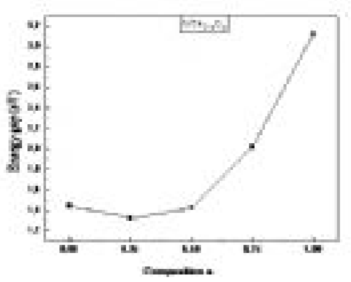
The band structure and optical properties of the SrTe1-xOx ternary mixed crystals have have been studied using the ab initio full potential linearized augmented plane wave (FP-LAPW) method within density functional theory. Quantities such as, energy gaps, band-gap bowing parameters, charge density, total and partial density of states and dielectric constants are calculated. Our results agree well with the available data in the literature. The composition dependence of all studied quantities has been expressed by quadratic polynomial forms

Keywords: FP-LAPW; DFT; alloys; band structure; optical properties

Band-gap energies of the SrTe1-xOx alloy as a function of O concentrations using GGA approximation



New Materials - P123 / 15:50 - 17:50

The effect of strontium concentration upon optical and dielectric properties of Pb1-xSrxS

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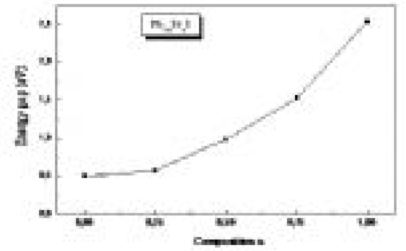
Theoretical investigations of the optical and dielectric properties of Pb1-xSrxS with rocksalt crystal structure are reported. The calculations are mainly based on the full potential linearized augmented plane wave (FP-LAPW) method within the density functional theory (DFT) the generalized gradient approximation (GGA) of Perdew et al.

A meaningful agreement with the experimental optical band-gap bowing parameter is only obtained when the disorder effect is included in the calculation.The strontium concentration dependence of the selected features of Pb1-xSrxS, such as energy band-gaps, refractive index and dielectric constants has been examined. All studied quantities are found to vary monotonically with strontium concentration x. The high-frequency and static dielectric constants have been scaled with the fundamental band gap energy (Eg). Such scaling showed that the variation of the dielectric constants versus Eg exhibits a non-linear behavior.

Keywords: Pb1-x SrxS alloy, DFT, FP-LAPW, GGA, static dielectric constants

Band-gap energies versus Sr compositions for the Pb1-xSrxS ternary alloys.



Theoretical and Computational Methods - P124 / 15:50 - 17:50

Calculation of structural, electronic, optical and thermodynamic properties of PbS, PbSe and their ternary alloy PbS1-xSex

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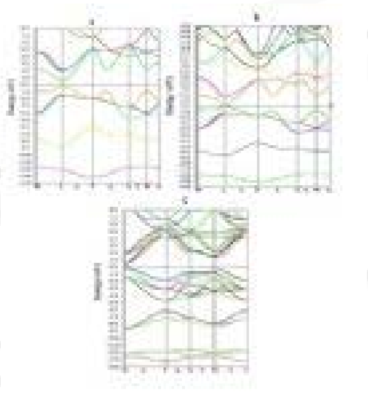
On the basis of ab initio calculations employing density functional theory (DFT) we investigate the structural, electronic and optical properties of two binaries: PbS and PbSe in rock-salt structures. In addition several compositions with various ordered structures of PbS1-xSex alloys were studied. The calculations are performed using the full potential linearized augmented plane wave (FP-LAPW) method within the generalized gradient approximation (GGA) and the new form of GGA (WC) which is an improved form of the most popular Perdew-Burke-Ernzerhof (PBE). The ground state properties, equilibrium lattice constants, bulk modulus and band structures for all Se-concentrations are presented. Furthermore, in order to understand the optical properties of PbS1-xSex alloy, the dielectric function, refractive index, and extinction coefficient are calculated for radiation up to 30 eV. In addition, the thermodynamic stability of this alloy was investigated by calculating the excess enthalpy of mixing as well as the phase diagram.

Keywords: FP-LAPW, PbS1-xSex, electronic properties, dielectric function

Band structures of (a) PbS, (b) PbSe and (c) PbS0.75Se0.25 along high symmetry directions in the Brillouin zone. The Fermi energy is at zero.



New Materials - P125 / 15:50 - 17:50

Single Cristal Materials Growth for Scintillation Applications

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During recent years, the field of the production of scintillators materials has become more active and gravitational due to the strong demand for the manufacturing of powerful detectors intended for very diverse applications: as well in physics (in particular in the field of the high-energy physics) but also in the medical imagery. By its remarkable fluorescence properties the Lu2SiO5 compound doped cerium known as LSO: Ce takes more interested in the world of the scintillators. Its characteristics such as, (high stopping power, intensity of emission relative to 75% of NaI, fast decline about 40ns under excitation γ and of 30ns under excitation UV, etc…), give it a potential advantage in the various applications and especially in the applications of PET Scan. Indeed, currently it is one of best materials known for application PET Scan application.

In this work, the growth of LSO in the form of single-crystal fiber will be studied. The technique of the growth Laser Heated Pedestal Growth (LHPG) was applied. The fibers obtained by this technique were transparent with a stable diameter and of crystalline good quality. The conditions of growth and the results got will be also discussed.

Keywords: Fiber, LHPG, Scintillators, LSO

New Materials - P126 / 15:50 - 17:50

Impact of higher order effects on soliton pulse dynamics in optical fiber systems

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Optical soliton studies have recently attracted a lot of attention due to their potential applications in long distance communications. Solitons pulses are localized electromagnetic waves that propagate in nonlinear media with dispersion and/or diffraction without any change in shape or intensity. From a mathematical point of view, a solitary waves or solitons are exact propagative solutions of a certain class of nonlinear partial differential equations (e.g., Korteweg de-Vries equation, the nonlinear Schrödinger equation, Sine-Gordon equation, Ginzburg-Landau equation, etc.) The existence of soliton pulses implies perfect balance between nonlinearity and dispersion effects which usually requires specific conditions. It should be noted that nonlinear optics is the field, where all soliton features are exhibited to a great extent.

In this work, we present a systematic analysis of the soliton pulse propagation within the framework of some nonlinear wave equations with distributed coefficients. The models under consideration apply to the description of ultrashort optical pulse propagation in highly-nonlinear media. The stability analysis as well as the interaction process between solitons will be also presented. These results are useful to understand the mechanism of the complicated nonlinear physical phenomena which are related to wave propagation in higher-order nonlinear and dispersive physical systems.

Keywords: soliton, nonlinear equations, nonlinearity effect, dispersion effect

Theoretical and Computational Methods - P127 / 15:50 - 17:50

Inhibition of the phosphathase Cdc25 by methods of molecular modeling

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University of Tlemcen Laboratory of Naturals Products and Bio actives-LASNABIO

Cdc25 phosphatase have been regarded as attractive drug targets for anticancer therapies due to the correlation of their over expression with a wide variety of cancers. Cdc25 phosphatases play a significant role in the regulation of the progression of eukaryotic cell cycle by activating cyclin Cdk that serve as central regulators of cell cycle with the lead role of each state of cell division. Due to a major contribution to cell cycle phosphatase Cdc25 have been implicated in oncogenic transformation and human cancers. The role of Cdc25s in cancer has become increasingly evident in recent years. Phosphatase Cdc25 heavily involved in the regulation of cell division could be potential oncogenes. Their crucial role in cell cycle Cdc25A and B are the targets for the development of new anticancer. Until now, quinone derivatives are among the most efficient inhibitors of Cdc25 phosphatase activity.

Our work consists with a study of molecular interaction between Phosphatase Cdc25and the substrates, the various molecular numerical models are used to conclude this work (mechanical molecular, dynamic molecular and docking molecular) or the docking makes it possible to envisage how a small molecule (drug) can bind to a receiver (protein) of which the structure 3D is known.

Keywords: Cdc25phosphatase (code PDB 1QB0)/ naphtoquinone/ molecular modeling (MM, DM, and Docking).

Balance of energies (kcal / mol)

Inhibitors	Etotal. pot of the complex E-I (Kcal/mol)	Etotal. Pot of the inhibitor I (Kcal/mol)	Evdw (complex-inhibitor) (Kcal/mol)	EVdw (inhibitor) (Kcal/mol)	Einterc. de Vdw (Kcal/mol)	E inter totale (Kcal/mol)
Inhibitor_1 (Cpd 5)	420.967	19.80	-549.137	12.49	-224.228	6490.802
Inhibitor_2 (NSC 95397)	3020.926	25.93	-561.354	13.76	-578.317	1434.173

Theoretical and Computational Methods - P128 / 15:50 - 17:50

The role of the trifluoromethyl group in reactivity and selectivity in polar cycloaddition reactions. A DFT study

<u>Sobhi Sobhi Chafia</u>[1]***, Djerouorou Abdelhafid***[2]

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The role of the trifluoromethyl group in reactivity, regio-, and stereoselectivity in cycloaddition reactions has been analyzed by studying the 1,3-dipolar cycloaddition (13DC) reactions of nitrone 4 with 3,3,3-trifluoro-1-nitropropene 7b and 3,3,3-trifluoro-2-nitropropene 14 using density functional theory (DFT) methods at the B3LYP/6-311G(d) level. The recent M06-2X functional has also been evaluated but, although the thermodynamic performance is improved, the kinetic data are not necessarily better than those obtained by the popular B3LYP functional for cycloaddition reactions. Four reactive channels associated with the meta and ortho regio- and endo and exo stereoselective approach modes of the nitro group of these disubstituted ethylenes relative to nitrone 4 have been explored and characterized. Unlike other electron-withdrawing groups, the trifluoromethyl group increases the reactivity of the nitroethylene, but it does not modify the meta and endoselectivities when it is located at the b conjugated position of nitroethylene. Analysis of the global and local electrophilicity indices allows for an explanation of the role of the trifluoromethyl group in reactivity and regioselectivity of electrophilically activated ethylenes.

Keywords: 1,3-Dipolar cycloaddition, Trifluoromethyl group, Regioselectivity, Stereoselectivity, DFT calculations.

New Materials - P129 / 15:50 - 17:50

TEM diffraction study of T1 phase precipitated in an Al-Li-Cu-Mg (Zr)

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Department of Physics, Ment University, Constantine 1

Transmission electron diffraction patterns made in the selected area (TEM SAD) of 8090 alloy (Al-2, 7% Li-1, 4% Cu-1% Mg (wt.%)), aged at 190 ° C, have been carried out. To index the diffraction spots of the different precipitated phases appearing on [(100)]α* and [(112)]α* diagrams of the aluminum matrix α, the crystallographic orientation relationships of these phases with this matrix, have been used. In addition to the diffraction of matrix α, δ ‘, β’ and S ‘/ S, indexed in a previous work, we are interested especially to the diffraction of T1 (Al2LiCu) which has a hexagonal structure and the following orientation relationships:

(0001)T1//[(111)]α;[(101̄0)]T1//[(1̄1̄0)]α;(112̄0)T1//[(21̄1̄)]α

Theoretically, the superposition of stereographic projections of hexagonal systems (T1 phase) and cubic (α matrix), taking into account the orientation relationships between these two phases, leads to twelve variants of the T1 phase. Each of these variants gives very specific permitted reflections on the diagrams [(100)]_α^* and [(112)]_α^*. Identification of T1 reflections on experimental patterns is carried out by comparison with the theoretical diagrams. The obtained results seem to be in very good agreement.

Keywords: 8090 alloy, Precipitation, T1 phase, TEM SAD.

New Materials - P130 / 15:50 - 17:50

The study of the order-disorder transition and hardening behavior in AuCuAg alloy

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Order-disorder transition takes a very important place because of its influence on the physical and mechanical characteristics of metals. The Cu-Au system provides a classical example of such type of transition The. The presence of silver additions to the AuCu alloys leads to the changes in the ordering process and hardening behavior in AuCu system. Therefore, we paid our attention to the study of the different phase transitions in the Au-35% wt. Ag-15% wt. Cu alloy using differential scanning calorimetry (DSC) and dilatometry (DT1000). In addition, the hardening behavior was investigated in this alloy by hardness testing at different transition temperature.

The obtained results show that the silver additions make increase the hardness of AuCu alloy with the **occurring of Ag-rich α1 and AuCu3 ordered phases.**

Keywords: order disorder transition, Au-Ag-Cu system, superlattice, dilatometry, differential scanning calorimetry.

New Materials - P131 / 15:50 - 17:50

Radiative transport in a high pressure discharge using discrete ordinates method on a line-by-line basis

Elloumi Hatem, Ghrib Basma, Bouaoun Mohamed

LaTICE Lab ESSTT, Sfax University, Tunisia

This work deals with radiation transfer of a high pressure mercury discharge doped with thallium iodide additive. We assume that the local thermodynamic equilibrium (LTE) conditions are valid for the total arc cross section. A S-N discrete ordinates method is used to solve the radiative transfer equation on a line-by-line basis. It is a numerical technique that solves the radiative equation of transfer along a number of discrete directions.

The equation that describes the transfer of radiant energy through a participating medium is the radiative equation of transfer. The line-by-line solution is an exact method of handling the spectral characteristics of thermal radiation. A chemical equilibrium model is employed to study the plasma composition using a parabolic temperature profile and a constant Mercury/Thallium ratio throughout the discharge tube. The influence of the thallium in HgTℓI discharges on the spectroscopic parameters such as the spectral intensity, the radiative flux and the net emission coefficient are studied.

Once the spectral intensity, as a function of position and direction is known, all the other interesting quantities, namely the radial flux, the local net emission coefficient and the radiative source term can be calculated for any required wavelength interval.

To validate this model, we have carried out a comparative study between the computed and the measured values of the spectral absolute side-on intensities relating to the principal thallium and mercury lines.

Keywords: Radiative transport, discrete ordinates method, high pressure discharge, spectral intensity

New Materials - P132 / 15:50 - 17:50

Fabrication and characterization of the Polystyrene / CdS nanocomposite

Harieche Barkahoum, Ouili Zeineddine, Boudjada Fahima, Boudine Boubekeur, Halimi Ouahiba, Sebais Miloud

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The synthesis and characterization of large gap semiconductors nanocristalline entrapped in a polymer matrice arouse special interest. This research effort is stimulated by the interesting properties that appear as size decreases. Indeed, confinement of excitations to a narrow space is then observed. Intensive research is conducted in order to fabricate nanocrystals having a desired size and shape [3], and to understand the influence of the fabrication conditions and the host matrix on the properties of the nanocrystals.

The present work consists on the fabrication and the characterization of the nanocomposite based polystyrene-CdS (PS/CdS). The fabrication process was carried out using the soft chemistry. The PS/CdS nanocomposite was deposited on glass substrates using a spin coating method. The X-ray diffraction (XRD) revealed the incorporation of the CdS semiconductor nanocristallites in the polystyrene matrix with a texture along the (110) line. The appearance of the band at 300 cm-1 on the Raman spectrum of the PS/CdS nanocomposite confirmed the XRD result. The X ray photoelectron spectroscopy (XPS) showed peaks corresponding to Cd3d, S2p and C1s which proves the existence of the two materials on the surface of the PS/CdS nanocomposite. The UV-visible spectroscopy displays the blue shift of the CdS gap. The photoluminescence spectrum presents an emission band in the visible area.

Keywords: CdS, Polystyren, nanocomposite, XRD, XPS, Raman, Photolumionescence

Vibrational (IR and Raman) and Electronic Spectroscopies - P133 / 15:50 - 17:50

Analysis of Eucalyptus Essential Oils by Capillary Gas Chromatography / Fourier Transform Infrared Spectroscopy (GC / FTIR)

***Yazid Foudil Cherif*[1], Noureddine Yassaa[2], Brahim Youcef Meklati[3]**

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The leaf oils of the following Algerian Eucalyptus species: E.leucoxylon F.Muell; E.cladocalyx F.Muell; and E.globulus Labill have been studied. The extracted oils obtained by steam distillation extraction procedure have been analysed by GC/FTIR. The information obtained with this technique is complementary to this obtained by GC/MS technique. Moreover this technique allowed us to assist the differentiation between some compounds (homologues or isomers) which have been very difficult by GC/MS coupling when used separately. The GC/FTIR technique allowed the detection more than 40 compounds in each oil, the main compounds were 1,8 cineol and benzaldehyde. Combined with GC/MS and linear retention indices (RI) of the volatiles compounds, the reliability of qualitative analysis is greatly enhanced.

In addition, the emission of volatile organic compounds from E. globulus Labil into the atmosphere has also been studied by employing cartridge sampling and thermal desorption GC-MS. 1,8 cineole was also the predominant compound in the atmospheric emission of E. globulus Labill.

Keywords: GC/FTIR; Eucalyptus leucoxylon;; Eucalyptus cladocalyx; Eucalyptus globulus; Essential oils; 1,8 cineole; benzaldehyde, volatile organic compounds

Vibrational (IR and Raman) and Electronic Spectroscopies - P134 / 15:50 - 17:50

Detection and Characterization of Antioxydants from Artemisia herba-alba growing in Algeria

Nacéra Dahmani Hamzaoui[1], Sofia Salido[2], Pablo Linares Palomino[2],
Aoumeur Baaliouamer[3], Joaquin Altarejos[2]

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[2]Department of Org. Chem, Jaèn University, Jaèn, Spain
[3]Department of Org. Chem, Houari Boumediene University, Bab Ezzouar, Algeria

Many pathologies are associated with the damaging effects of uncontrolled free radicals in living organisms. Natural antioxidants, mainly contained in fruits and vegetables, should be an important part in human diets, since they have the ability to scavenge free radicals. So, there is an increasing interest in finding new sources of natural antioxidants to provide safe antioxidant additives.

Artemisia herba-alba Asso is a prominent plant of the Irano-Turanien steppes of North Africa, Spain and the Middle East. In Algeria, it abounds over large areas of the steppes and Sahara desert. A survey carried out among the South Algerian population showed that A.herba-alba is the most recognized aromatic and medicinal plant.

The present study deals with the detection and subsequent isolation and characterization of the antioxidants present in Algerian A. herba-alba, using the on-line HPLC-DAD-radical scavenging detection technique.

The natural antioxidants were detected in the most active extracts using the on-line HPLC-DAD-DPPH scavenging assay. The isolation of phytochemicals was carried out by column chromatography and further preparative RP-HPLC purifications. The identification of pure compounds was based on the information deduced from UV, IR, MS, HRMS, 1H NMR, 13C NMR and 2D NMR data.

Four caffeoylquinic acid derivatives, 5-O-caffeoylquinic acid (1), 3,5-di-O-caffeoylquinic acid (3), 4,5-di-O-caffeoylquinic acid (4) and 3,4,5-tri-O-caffeoylquinic acid (5), have been isolated and characterized showing a fair good antioxidant activity determined by the DPPH• scavenging assay. In the course of the purification work a non-frequent glucosylmethoxycinnamic acid (2) has also been isolated.

Keywords: Artemisia herba-Alba, antioxydant activity, on line HPLC-DAD-DPPH, spectroscopic methods, caffeoylquinic acids derivatives

Vibrational (IR and Raman) and Electronic Spectroscopies - P135 / 15:50 - 17:50

Study of surface chemistry of an oxidized activated carbon by spectroscopy FTIR, Boehm titration and methylene blue adsorption

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This work deals with the effect of the concentration of nitric acid solution on the chemicals properties of activated carbon obtained by oxidation of parent activated carbon under reflux. The change in surface chemical properties, resulting from this treatment, was studied by FTIR spectroscopy, Boehm titration and methylene blue adsorption. The results obtained from FTIR and selective titration show that more concentrated nitric acid solutions introduce large amount of chemical groups at the carbon surface. Adsorption capacity of methylene blue mainly depends on the porosity of samples and pH of solution, i.e., the total number of acid sites.

Keywords: Activated carbon, FTIR, Chemical treatment

New Materials - P136 / 16:20 - 18:20

Theoretical self-broadening and self-shifting coefficients of 12C2H2 transitions in the 3v5, (2v4+v5)I and (2v4+v5)II bands

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The self-broadening and self-shifting coefficients of 12C2H2 have been calculated for transitions belonging to the P, Q and R branches of the 3v5, (2v4+v5)I and (2v4+v5)II cold bands near the 5µm region using a semi-classical model based upon the Robert and Bonamy formalism. The intermolecular potential used in this work includes, in addition to the overwhelming electrostatic interactions, a Tipping-Herman potential. Such a calculation leads to satisfactory agreement with measurements from literature.

For the studied bands, the theoretical results reproduce the experimental rotational dependence of the self-broadening and self-shift coefficients. These coefficients decrease with J quantum number.

The self-broadening coefficients show the predominance of the quadrupole-quadrupole contributions, especially for middle J values.

In contrast to the theoretical self-broadening coefficients, the shifting coefficients vary with the type of branch but without systematic rotational trends.

Keywords: C2H2, self-broadening coefficients, self-shift coefficients, semi-classical formalism.

New Materials - P137 / 15:50 - 17:50

Analytical transfer by rapid liquid chromatography method for quality control of a series of pharmaceuticals

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This work focuses on the use of liquid chromatography to ultra-high performance (UPLC) with which it is possible to significantly reduce analysis time without loss of efficiency. This technology uses stationary phases of small particle size (1.7 µm) with a system to work at high pressures (up to 1000 bar) and reach high speeds.

The main of the developed methods in pharmaceutical analysis are available on conventional columns. This study concerns the transfer of existing methods to the new analytical methods.

The objectives of this study is in a first step to evaluate the performance offered by UPLC through various pharmaceutical applications (diclofenac diethylamine, sodium citrate and hydrochlorothiazide). Qualitative and quantitative performance were evaluated and proove the reduced analysis time, where it is an important advantage of this approach compared to conventional LC. The efficiency is significant in UPLC (ratio equal 10 compared to the conventional LC).

The second step was the transfer of methods developed on conventional columns with geometries (4.6 × 250 mm, 5 microns) in pharmaceutical analysis to UPLC. The work was done on pharmaceutical formulations mentioned above, in isocratic mode. It has been shown that the chromatographic performance was very satisfactory (resolution, sensitivity, selectivity).

Finally, the validation methods transferred to UPLC was performed according to ICH criteria used in the pharmaceutical field. The results show similar quantitative results for all methods tested, with an efficiency in analysis time more significative with UPLC.

Keywords: UPLC, HPLC, pharmaceutical formulations, chromatographic performance

New Materials - P138 / 15:50 - 17:50

An X-ray Absorption Study of Two GeCl3-Modified Silicas

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In this work, the structure and stability of the grafted sites created by the vapor phase reaction of GeCl4 with silica that is partially dehydroxylated at two different temperatures, 200 °C and 500 °C have been investigated. The product was studied by elemental and gas-phase analysis, in situ IR, 1H solid-state NMR, and X-ray absorption spectroscopy. The germanium product has the empirical formula ≡SiOGeCl3. The XANES and EXAFS analysis at the Ge K-edge reveal that the sites have a uniform first coordination sphere regardless of the origin or the extent of hydroxylation of the silica support (controlled by thermal treatment in vacuo at 200 and 500 °C). EXAFS curve-fitting confirmed that the sites are ≡SiOGeCl3.

Keywords: X-ray Absorption; dehydroxylated silica; XANES; EXAFS

New Materials - P139 / 15:50 - 17:50

Synthesys, Antimicrobial Activities And Spectroscopic Properties Of New Lanthanides Complexes With Furan hydrazone ligand Based

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Novel Ln(III) complexes with N'-[(furan-2-yl)methylene]isonicotinohydrazide (L) have been synthesized. The ligand and complexes were characterized based on elemental analyses, molar conductance, IR, 1H and 13C-NMR, UV-vis., and TGA studies. The conductivity data show a 1:2 electrolytic nature with a general formula [LnL2(NO3)2]NO3. The IR spectra reveal the coordination of the ligand through the azomethine nitrogen and the furane O-atom in addition to the carbonyl oxygen to the lanthanide ion. The coordinated nitrate ions behave in a bidentate fashion. Under the excitation, the luminescence emission properties for Sm, Tb, Eu and Dy complexes are observed. These observations show that the ligand favor energy transfers to the emitting energy level of these lanthanide ions. Furthermore, the antimicrobial activities of all complexes were studied against different types of bacteria. It was observed from the results that most of the synthesized complexes of the tested series possessed good antibacterial activity against bacteria and the microbial activities of the complexes in most cases are higher than that of the corresponding ligand.

Keywords: Schiff base ligand; Lanthanides Complexes; Luminescence properties; antibacterial activity.

Vibrational (IR and Raman) and Electronic Spectroscopies - P140 / 15:50 - 17:50

Spectroscopic studies on N-((2-hydroxynaphthalen-1-yl) metylene)nicctinohydrazide (L) Lanthanide complexes in solid and solution

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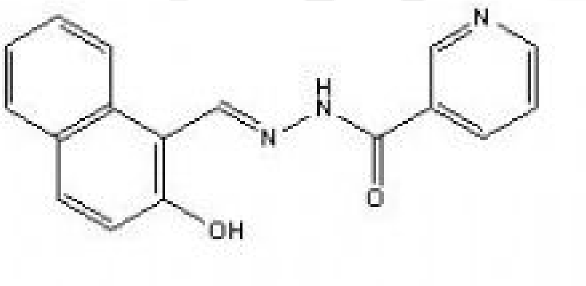
An aryl amide ligand L, and its lanthanide complexes, [Ln (L)2 (NO3)3], [Ln = Sm(III), Er(III), Tb(III), Dy(III), La(III), Gd(III), Nd(III), and Pr(III)] were synthesized. All the complexes were characterized based on elemental analysis, TGA, molar conductance, U.V., IR, 1H and 13C-NMR spectroscopic techniques. Preparing a single crystal is in progress. The spectroscopic data show the 2:1 electrolytic nature of the complexes with a general chemical formula of [Ln (L)2 (NO3)3]. The IR spectra reveal the coordination from the nitrogen and the hydroxyl group of the ligand to the central lanthanide ions. This fact is also supported by the 1H and 13C-NMR data. The fluorescence properties of complexes were studied in detail.

Keywords: Ligand, Lanthanides, electrolytic structure, flourescence

N-((2-hydroxynaphthalen-1-yl)metylene)nicctinohydrazide



Fluorescence Spectroscopy - P141 / 15:50 - 17:50

Fluorescence spectra of discharged obelin in the presence of exogenous compounds

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Discharged photoprotein obelin, the enzyme-substrate complex of polypeptide with coelenteramide, is a fluorescent protein. Discharged obelin is stable and non-toxic; it can be used as fluorescent marker in biological and medical investigations, for example, in cytology, histology, and cryology. It is very important to know how exogenous compounds influence the fluorescent characteristics of the discharged obelin. We chose glycerin, ethanol, dimethyl sulfoxide and polyethylene glycol as widely used accompanying compounds.

Fluorescent spectra of discharged obelin were analysed under addition of glycerin (C = 0.06 – 0.36 M), ethanol (C = 0.01 – 1.18 M), dimethyl sulfoxide (C = 0.002 – 2.65 M) and polyethylene glycol (C = 17 µM – 17 mM). The compounds effected destructively on the discharged obelin: they decreased its fluorescence intensity and changed emission spectrum. As the changes resulted from variation of spectral component contributions in the presence of exogenous compounds, the spectra were deconvolved into Gauss components and analyzed [1]. The spectral changes were explained with reduction of efficiency of energy and proton transfers in the active center of the photoprotein. Red peak (λmax= 660 nm) was newly discovered in the discharged obelin emission in the presence of the exogenous compounds. It was hypothetically attributed to indole-coelenteramide complex. The expansion of the known group of colors (from violet to yellow) by adding the red color increases the potential of obelin as a colored biomarker for monitoring biochemical processes.

[1] Belogurova N.V., Kudryasheva N.S., Alieva R.R., Sizykh A.G. // J.Photochem. Photobiol.B, 2008, V.92, P. 117–122.

Keywords: photoprotein, fluorescent protein, spectral components

Vibrational (IR and Raman) and Electronic Spectroscopies - P142 / 15:50 - 17:50

A comparative study on synthesized tricyclic pyrrolidinyl alcohol ligands: Determination of absolute configuration, spectroscopic and chiroptic properties

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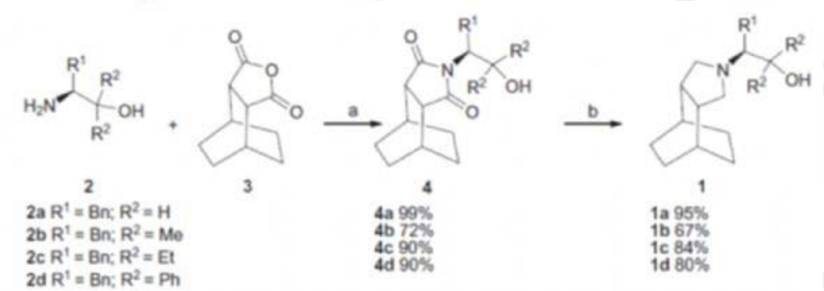
In the present work, a computational study was carried out on the structural, spectroscopic and chiroptic properties of a series of chiral stericallyconstrained tricyclic pyrrolidinyl alcohol ligands 1a–d which were derived from (S)-β-amino alcohols 2a-d, as shown in Scheme 1 [1]. The ground state equilibrium structures, vibrational spectra (IR, Raman and VCD) and optical rotations of studied compounds were obtained DFT(B3LYP) method applied with 6-311++G(d,p) basis set. The magnetic properties were pointed out via 1H and 13C NMR calculations using with GIAO method. TD-DFT/6-311++G(d,p) approach was used to predict the electronic features along with the UV-Vis and ECD spectra. All calculations were done for both (S) and (R) enantiomers of mentioned compounds, and results were compared with available previously reported experimental data [1].

References

[1] E. Sahin, H. Kilic, Tetrahedron: Asymmetry 22 (2011) 277–282.

Keywords: A comparative study on synthesized tricyclic pyrrolidinyl alcohol ligands: Determination of absolute configuration, spectroscopic and chiroptic properties

Figure 1



Vibrational (IR and Raman) and Electronic Spectroscopies - P143 / 15:50 - 17:50

The spectroscopic characterization of 5-methoxyindole-2-carboxylic acid: A combined density functional and experimental (NMR, UV, FT-Raman and FT-IR) study

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In the present work, a combined experimental and quantum chemical study on ground state equilibrium structure and spectroscopic properties of 5-methoxyindole-2-carboxylic acid are reported. The equilibrium structure was identified by using density functional calculations (B3LYP/6-311++G(d,p)), and results were compared with previously reported experimental crystallin structure. The electronic properties were defined via UV absorption spectroscopy and TD-DFT method. The 1H, 13C and DEPT NMR spectra were recorded in DMSO solution, andgauge-invariant atomic orbitals (GIAO) method was used to predict the isotropic chemicalshifts.The vibrational spectra of title compound were recorded insolid state by FT-IR and FT-Raman in the range of 4000-400 cm-1 and 4000-10 cm-1,respectively. The fundamental assignments were done on the basis of the total energydistribution (TED) of the vibrational modes, calculated with scaled quantum mechanical(SQM) method. A detailed description of ground state structural and spectroscopic behaviors of investigated compound was reported with the help of comparison of experimental measurements and theoretical calculations.

Keywords: The spectroscopic characterization of 5-methoxyindole-2-carboxylic acid: A combined density functional and experimental (NMR, UV, FT-Raman and FT-IR) study

New Materials - P144 / 15:50 - 17:50

Synthesis, characterization of nanostructured iron and manganese mesoporous molecular sieves catalysts

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The syntheses of highly ordered mesoporous molecular sieves have attracted much attention in recent years. In 1994, a new pathway was proposed by Tanev et al. to prepare mesoporous silicas at room temperature by a neutral templating route (S°I°). In this case, the organic surfactant is not quaternary ammonium cation but a primary amine, and the assembly involves hydrogen-bonding interactions between neutral primary amines and neutral inorganic precursors. These materials denoted HMS (hexagonal mesoporous silica) exhibit excellent catalytic ability for macromolecular reactions and offer new opportunities for transition metal incorporation into silica frameworks. In the present study, we report the results of preparation and characterization of iron-HMS-n and manganese-HMS-n (n=50, 25, 15) catalysts. The catalysts were prepared using a protocol reported by Tanev et al. and the resulting precursors were dried at 100°C and calcined in air. The solids were characterized by their atomic absorption spectroscopy, BET specific area, XRDiffraction and IRFT spectroscopy.

Keywords: HMS, iron, manganese, ordered molecular sieve

Vibrational (IR and Raman) and Electronic Spectroscopies - P145 / 15:50 - 17:50

Study of the stability of polymeric membrane by FTIR spectroscopy characterization

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In this work, the stability of polymeric membrane under different experimental conditions has been examined using FTIR spectroscopy characterization. Two kinds of membranes were synthesized by solvent evaporation technique. Both membranes contain cellulose triacetate (CTA) as support and polyvinylpyrrolidone (PVP) in the matrix. In the composition of membrane polyethyleneglycole (PEG) and polysorbate (PS) have been added respectively in the first and second membrane. It has been shown according examination of spectrum in the whole range of 4000 to 400cm-1 that all characteristic band of each compounds appear in the membrane material. The application of membrane in the transport process at different temperature may cause a little shift of band between 1650 and 1690 cm-1 at temperature higher than 140°C in the case of PEG membrane. The polysorbate membrane show a good stability until 140°C and then an important deformation of the spectrum was observed.

Keywords: Polymer Membrane, FTIR characterization, stability

Vibrational (IR and Raman) and Electronic Spectroscopies - P146 / 15:50 - 17:50

Quantum-chemical, spectroscopic and X-ray diffraction studies on Diethyl (5-(4-methylbenzoyl)-4-(4-methylphenyl)-2-oxo-pyrimidin-1(2H)-yl)dithiocarbonimidate

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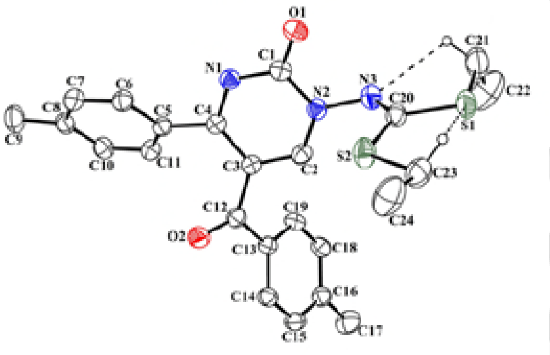
Pyrimidine derivatives have occupied a unique position in medicinal chemistry. N,N-disubstituted dithiocarbamate and dithiocarbonimidate derivatives have showed antibacterial, antiviral and antifungal activites. The majority of the reaction between carbon disulfide and N-nucleophiles involve addition of carbon disulfide to N-H bond. In our work, highly efficient and simple synthesis of dithiocarbonimidates are based on the one-pot reaction of aromatic amine with carbon disulfide and ethyl iodide, in DMF and basic conditions without using a catalyst.

The experimental geometry obtained from single-crystal X-ray diffraction was compared with those obtained from quantum chemical calculations in the gas phase. Vibrational frequencies and gauge-independent atomic orbital (GIAO) 1H and 13C NMR chemical shift values of the title compound in the ground state have been calculated using Hartree-Fock (HF) and Density Functional Theory (DFT/B3LYP)

methods with the 6-31G(d,p) basis set and compared with the experimental data. Also, molecular electrostatic potential (MEP) distribution, non-linear optical properties, frontier molecular orbitals (FMOs) and thermodynamic properties of the title compound were performed at B3LYP/6-31G(d,p) level.

Keywords: Dithiocarbonimidates, HF and DFT calculations, IR and NMR spectroscopy, X-ray structure determination

A view of the dithiocarbonimidate derivative showing the atom-numbering scheme.



Displacement ellipsoids are drawn at the 40% probability level. For clarity, only H atoms involved in hydrogen bonding have been included. Hydrogen bonds are indicated by broken lines.

Vibrational (IR and Raman) and Electronic Spectroscopies - P147 / 16:20 - 18:20

Micro-Raman, Mid-IR, Far-IR and DFT studies on 2-(4-(4-Fluorobenzamido)phenyl)benzothiazole

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Molecular structure of 2-[4-(4-Fluorobenzamido)phenyl]benzothiazole was identified by Fourier Transform Infrared (with KBr and ATR techniques), Far Infrared (ATR technique), Raman spectroscopies and quantum chemical calculations. MidIR and FarIR spectra were recorded at room temperature, with 4 cm-1 resolution in the 4000-400 cm-1 and 700-30 cm-1 regions, respectively for the first time. Raman spectrum was recorded in the 4000-100 cm-1 range. Optimized molecular structure and vibrational wavenumbers of the compound in its ground state have been calculated by using Density Functional Theory using UB3LYP functional with 6-311++G(d,p) basis set. All calculations were performed with Gaussian09 software. Vibrational wavenumbers and optimized geometric parameters were seen to be in good agreement with the experimental data. Furthermore, assignments of each vibrational mode were interpreted in terms of potential energy distributions in detail.

Keywords: 2-[4-(4-Fluorobenzamido)phenyl]benzothiazole, Micro-Raman, Far-infrared, Mid-infrared, DFT, PED

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