



# TURCMOS 2022

# ABSTRACT BOOK

5<sup>th</sup> International  
Turkish Congress on Molecular Spectroscopy  
26-27 March 2022 | Online via Zoom

## Chair's Message

We cordially invite you to 5<sup>th</sup> TURCMOS which will be held online (via ZOOM) between 26-27 March 2022 (Saturday & Sunday). 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 TURCMOS 2022, all aspects of spectroscopic methods as well as related computational and theoretical approaches will be considered. Our participants will also benefit from a broad range of spectroscopy applications. Contacts between young researchers (M.Sc. and Ph.D.) and prominent experts will be particularly stimulated, aiming at the development of future collaborations. We are sure that the congress will provide a stimulating environment for many interesting scientific discussions. This time, we are looking forward to hosting you online where the globe meets.

Ozan Unsalan

Chair

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## Scientific Program

Time UTC+3		26 March 2022 - Saturday		27 March 2022 - Sunday	
Start	End	Zoom Main Conference Room		Zoom Main Conference Room	
09:00	09:20				
09:20	09:40	PREPERATIONS AND LOBBY ENTRANCE		PREPERATIONS AND LOBBY ENTRANCE	
09:40	10:00				
10:00	10:20	Opening Ceremony by Congress President			
10:20	10:40	Session 1	Invited Speaker - Juergen POPP	Session 6	Invited Speaker - Parvez HARIS
10:40	11:00		ID - 191 M.I. Oshtrakh		ID - 180 Dogan Kazan
11:00	11:20	Coffee Break (11:20-11:40)		Coffee Break (11:20-11:40)	
11:20	11:40				
11:40	12:00	Session 2	ID - 185 Áron K. Bekel	Session 7	Invited Speaker - Ramazan AKCAN
12:00	12:20		ID - 189 D.V. Belyaev		ID - 197 Carla M. Magalhães
12:20	12:40		ID - 186 Kadriye I.B. Cetin		ID - 190 D.V. Belyaev
12:40	13:00	Lunch Break (12:40-13:40)		Lunch Break (12:40-13:40)	
13:00	13:20				
13:20	13:40				
13:40	14:00	Session 3	Invited Speaker - Philippe COLOMBAN	Session 8	Invited Speaker - Joaquín BARROSO
14:00	14:20		ID - 183 Marco Consumi (Not attended)		ID - 206 Berguzar Yilmaz
14:20	14:40	Coffee Break (14:40-15:00)		Coffee Break (14:40-15:00)	
14:40	15:00	Session 4	ID - 199 Eylem Celik	ID - 193 Ulviya Abilova	
15:00	15:20		ID - 194 Dilay Kahvecioglu	ID - 200 Gözde B. Sekitmen	
15:20	15:40	Coffee Break (15:40-16:00)		Coffee Break (15:40-16:00)	
15:40	16:00				
16:00	16:20	Session 5	Invited Speaker - Weitao YANG	Session 9	ID - 202 Fehmi Bardak
16:20	16:40		ID - 187 Emine Nakilcioglu		ID - 203 Dilek Yonar
16:40	17:00		ID - 188 E. Nakilcioğlu		ID - 204 Sergey Katsyuba
17:00	17:20		ID - 198 Igor Reva		ID - 201 Omer Faruk Cug
17:20	17:40	ID - 205 Ozan Unsalan	ID - 207 Zeki Buyukmumcu	Closing Ceremony by Congress President	
17:40	18:00	END of DAY 1		END of DAY 2	

ID-180	Conformation Analysis of 6-Amino-1,3-Dipropyluracil Molecule	Dogan Kazan, Ersin Durgut, Ebru Karakas Sarikaya, Omer Dereli, Ulfet Atav
ID-182	The Effect of Radiation on Omeprol Drug: An Overview of its Use as an EPR Dosimeter	Nazrin Babayeva, Emel Ece, Recep Biyik, Ayhan Ozmen, Ulku Sayin
ID-183 (N.A.)	Quantification of Water Content in Polysaccharides by FTIR	Marco Consumi, Gemma Leone, Gabriella Tamasi, Agnese Magnani
ID-185	Digital Twin Development of Continuous Powder Blending with Artificial Neural Networks and Residence Time	Áron K. Bekel, Martin Gyürkés, Attila Farkas, Zsombor Kristóf Nagy, György Marosi
ID-186	Modifications of Fe (III)-Based Antioxidant Capacity Methods	Kadriye Işıl Berker Cetin
ID-187	Determination of Vitamin C in Foodstuffs by UV-Vis Spectrophotometer	Emine Nakilcioglu
ID-188	Comparison of Color Characteristics of Red and White Grape Juice by UV-Vis Spectrophotometer	Emine Nakilcioglu
ID-189	Mössbauer Spectroscopy of Ferrum Lek: Further Development of the Heterogeneous Iron Core Model	D.V. Belyaev, I.V. Alenkina, M.I. Oshtrakh
ID-190	The Iron State in Some Iron -Containing Vitamins and Dietary Supplements Analyzed by Mössbauer Spectroscopy	D.V. Belyaev, V.S. Moskvitin, I.V. Alenkina, M.I. Oshtrakh
ID-191	Structural and Spectroscopic Study of the Iron - Bearing Phases in Bursa L6 Meteorite	A.A. Maksimova, E.V. Petrova, A.V. Chukin, O. Unsalan, C. Altunayar-Unsalan, M.I. Oshtrakh
ID-193	Concentration of Palladium Which Chelate Sorbent on The Basis of Maleic Anhydride Styrene Copolymer	Ulviya Abilova, Esmira Hashimova, Sevinj Hajiyeva, Famil Chiragov
ID-194	Molecular Docking Analysis for Bace1 Inhibition of Novel Thiosemicarbazide Derivatives	Dilay Kahvecioglu, Gozde Yenice Cakmak, Serap Yilmaz, Bedia Kocyigit Kaymakcioglu
ID-196	Ab-Initio Study on Structural, Spectroscopic and Electronic Properties of (E)-1-(4-Methoxyanthracen-1-Yl)-2phenyldiazene Azodyes Molecule	Arini Qurrata Ayun, Pinar Tunay Tasli, Sevgi Ozdemir Kart
ID-197	Chemiluminescent Self-Activating Photosensitizers for a Selective Anticancer Therapy	Carla M. Magalhães, Patricia Berdullas, Joaquim Esteves da Silva, Luís Pinto da Silva
ID-198	UV-Induced Photochemistry of Monomeric Benzoxazole and its Isomers	Igor Reva
ID-199	Ab-Initio Study Aiming Some Spectroscopic and Electronic Properties of 2-[(1H-Benzimidazol-1-Yl)-Methyl]Benzoic Acid	Eylem Celik, Pinar Tunay Tasli, Sevgi Ozdemir Kart

ID-200	Sterilization Studies of Hydrogel Nanocomposites Designed for Biomedical Applications Before in vivo Research	Gozde Bayazit Sekitmen, Esra Su, Sinem Diken Gur, Semra Ide, Oguz Okay
ID-201	Synthesis, Characterization, Experimental and Theoretical Investigation of Spectroscopic Properties of Schiff Base Molecules	Omer Faruk Cug, Yunus Kaya
ID-202	Electronic Structure and Nonlinear Optical Properties of 1-Butyl-3-Methylimidazolium Dicyanamide Ionic Liquid	Fehmi Bardak
ID-203	Non-Invasive Spectroscopic Profiling of Spent Embryo Culture for Predicting the Cell Free DNA Content of Embryos in Women Undergoing in vitro Fertilization	Dilek Yonar, Leyla Ozer
ID-204	What We Can Learn from Infrared Spectra about the Structurally Flexible Molecules in Liquids and Solutions with Quantum Chemical Computations	Sergey Katsyuba, Tatiana Gerasimova
ID-205	A Contribution to AH-B Sweetness Theory: Theoretical Infrared and Raman Spectroscopic Investigation on Artificial Sweetener Alitame	Ozan Unsalan, Cisem Altunayar-Unsalan, Berguzar Yilmaz
ID-206	Computed Vibrational Spectra of Hexamethylenetetramine and its Derivatives	Berguzar Yilmaz, Ozan Unsalan



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Invited Speakers' Abstracts



## Clinically Applicable Multi-Contrast Spectroscopy for an Aging Society

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We will introduce various clinically applicable multi-contrast spectroscopy approaches to reliably assess tumor tissue. We will present a multimodal scanning microscope, combining optical coherence tomography, fluorescence lifetime imaging microscopy, and Raman spectroscopy together with the possibility for co-registering H&E information. Furthermore, we introduce a computer-based tracking system in conjunction with augmented and mixed reality, enabling molecular Raman imaging with a fiber optical probe of three-dimensional surfaces and real-time data visualization. Last but not least it will be shown that multi-contrast nonlinear imaging, utilizing different innovative endospectroscopic concepts represents a powerful tool to reliably assess the success of an operation.

<b>Presentation Method: Invited Speaker</b>
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## Tracing Innovations and Technology Exchanges Between Europe and China. Enamelled objects at the 17<sup>th</sup>-18<sup>th</sup> Century Turn

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Enamelling, i.e. coating of a substrate with a layer of glass by firing, is one of the most sophisticated technologies developed to decorate artefacts. China has a long expertise in the production of ceramics and glass but for technical and aesthetic reasons, 17th century (Ming Dynasty and then part of Kangxi reign) Chinese decors were rather similar to those obtained on paper with lavish or watercolour techniques. These productions did not permit to represent a 'realistic' decor, as prepared on majolica, (soft-paste)porcelain and metal wares by European craftsmen who were capable of making enamelled copies of famous paintings. Actually, much information about the ingredients and production process remains imprinted in the matter accessible by advanced spectroscopical methods. The rareness and high value of artefacts, particularly those made at the Imperial Palace under the guidance of Jesuits, require the use of non-invasive mobile instruments. We present here an overview of the on-site non-invasive Raman and pXRF study of French (enamelled watches, Limoges wares, soft-paste porcelain, etc.) and Chinese (wucai, fengcai, falangcai, huafalang, cloisonné etc.) artefacts prepared during the 17th and first part of the 18th century (Qing Dynasty). We are able to identify the first use of European ingredients (blue As-rich cobalt, white cassiterite) and recipes (purple-red Perrot' gold nanoparticles, Naples yellow lead pyrochlore type pigments) for the preparation of 'realistic' decors on Chinese porcelains and metalwares, which shed light on the technological exchange between Europe and China. The results are significant in terms of comparison with the written records analyzed by historians.

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- [5] Colomban, P.; Gironde, M.; Vangu, D.; Kirmizi, B.; Zhao, B.; Cochet, V. The Technology Transfer from Europe to China in the 17th–18th Centuries: Non-Invasive On-Site XRF and Raman Analyses of Chinese Qing Dynasty Enamelled Masterpieces Made Using European Ingredients/Recipes. *Materials* 2021, 14, 7434. <https://doi.org/10.3390/ma14237434>

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**Presentation Method: Invited Speaker**

## Photoemission and Photoexcitation Spectroscopy from Ground State DFT Calculations

Weitao YANG

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For a universal elimination of systematic delocalization and static correlation errors in DFT, we developed a localized orbital scaling correction (LOSC): it is capable of correcting system energy, energy derivative and electron density in a size-consistent manner. The LOSC–DFAs lead to systematically improved results, including the dissociation of ionic species, single bonds, multiple bonds without breaking the space or spin symmetry, the band gaps of molecules and polymer chains, the energy and density changes upon electron addition and removal, and photoemission spectra, and energy-level alignments for interfaces. The LOSC DFA orbital energies are excellent approximations to quasiparticle energies, comparable to or better than GW. This also leads to the QE-DFT (quasiparticle energies from DFT) approach: the calculations of excitation energies of the  $N$ -electron systems from the ground state DFA calculations of the  $(N - 1)$ -electron systems. Results show good performance with accuracy similar to TDDFT for valence excitations with commonly used DFAs with or without LOSC. For charge transfer and Rydberg states, good accuracy was obtained only with the use of LOSC DFA. The QE-DFT method has been further developed to describe excited-state potential energy surfaces (PESs), conical intersections, and the analytical gradients of excited-state PESs.

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<b>Presentation Method: Invited Speaker</b>
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## **A Novel Hypothesis for Prevention of Alzheimer's Disease and Other Diseases: A Daily Cycle of Hydration and "Dehydration", Induced by Sleep, Physical Activity and Diet Triggers Cell Swelling and Cell Shrinking that Improves Circulation and Drives Clearance of Toxic Wastes and Prevents Disease**

Parvez I. HARIS

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A study using real-time assessments of tetramethylammonium diffusion and two-photon imaging in live mice revealed that natural sleep or anesthesia is associated with a 60% increase in the interstitial space [1]. This causes an increase in convective exchange of cerebrospinal fluid with interstitial fluid. This was suggested to be responsible for increased clearance of  $\beta$ -amyloid peptide, the accumulation of which in the brain is linked to the development of Alzheimer's disease and other forms of dementia. This was used to explain the beneficial role of good quality sleep for the prevention of neurodegenerative disease. The authors suggested that the brain sleep-awake dependent changes of the interstitial space volume are unlikely to be due the circadian rhythm as anesthesia also increased glymphatic influx and efflux [1]. However, this explanation is at best incomplete since the authors did not consider the hydration status of the animals during awake, sleep and anesthetized states. Information regarding water consumption, food intake and hydration was absent from the discussion and was absent in the methodology [1]. Under sleeping and anesthetized conditions, the mice will not be drinking or eating and therefore they will be more "dehydrated". "Dehydrated" refers to lower water status during sleep compared to the awake state where the animals will have access to water and foods. It is well known that both body weight decreases during sleep and Magnetic Resonance Imaging studies have shown that brain volume also decreases during sleep. The change in body weight and brain volume during sleep can be attributed to lower water status due to insensible water loss, sweating and of course the absence of water ingestion and food intake. This makes the sleeping state more dehydrated leading to an increase in osmolality of extracellular fluids, such as in the interstitial space, which cause the cells to shrink increasing the volume of the interstitial space. This "dehydration"/reduction in water status will induce cell shrinking and increase in interstitial volume enhancing convective exchange of cerebrospinal fluid with interstitial fluid leading to removal of the toxic wastes from the brain. During the awake state, drinking to quench thirst and eating to quell hunger leads to a more hydrated state that causes cell swelling therefore a reduction in interstitial space. This prevents greater clearance of waste during the awake state compared to the sleeping state. The theory presented here is more comprehensive since it provides a scientifically sound mechanism for protection against Alzheimer's disease, dementia and indeed other types of diseases where accumulation of toxic wastes and their inefficient clearance triggers disease. In contrast, to the theory provided Nedergaard and colleagues [1], the novel theory presented here does not restrict enhanced waste clearance to the sleep state only as enhanced waste clearance during the day can be achieved through physical exercise, diet and fasting that creates opportunity for hydration-"dehydration" or higher water-lower water status induced swelling and shrinking of cells and changes in the volume of the interstitial space. Thus, for example, physical exercise leads to higher loss of water due to deep breathing and sweating. This causes "dehydration" or reduction in water status leading to cell shrinking which in turn will increase the volume of the interstitial space leading to greater clearance of wastes [see Figure 1].

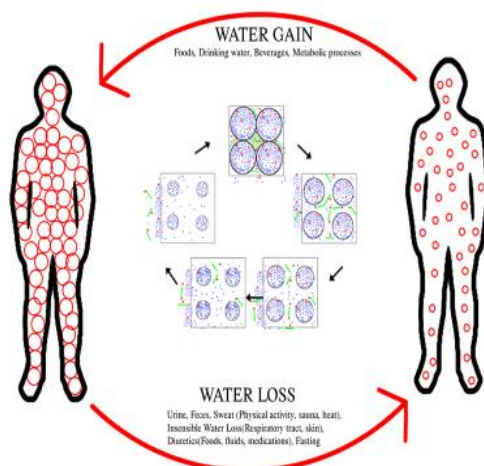


Figure 1: Water loss and water gain leads to changes in the water status within the body that causes cell swelling and cell shrinking that helps improve circulation and clearance of wastes from the brain and other organs and tissues. The body, including the brain contain less water during sleep and physical exercise due to abstinence from fluid and food intake and sweating, respectively.

The hypothesis presented here suggests that not only good sleep but a daily pattern of physical exercise as well as consumption of water-rich foods and diuretic foods/fluids, along with drinking water, is good for triggering a cycle of hydration- “dehydration” induced cell swelling and cell shrinking. This will act as a “pump”, working in synchrony with the beating of the heart, to clear wastes, improve circulation and thereby prevent accumulation of harmful toxins preventing or delaying the development of disease. The theory presented also suggests that one of the most important reasons for the beneficial effects of sleep, exercise, fasting is due to these conditions creating a temporary dehydrated state that enables shrinking of cells for removal of wastes. The theory has been inspired by observation of plants where loss of water through the stomata in the leaves not only cools the plant but provides the necessary force to drive the movement water from the roots, embedded in the ground, to the top of the trees. This follows a circadian rhythm. Likewise in humans and indeed in other animals, water loss through the skin, such as through sweating, is suggested to not only serve in cooling the human body it also acts to drive water circulation, nutrient delivery and waste clearance. These are novel ideas and the theory presented provides a realistic public health guidance for prevention of neurovegetative disease and other diseases through maintaining a healthy water cycle in the body through a rhythmic pattern of hydration- “dehydration” induced by sleep, exercise, fasting and diet.

**Keywords:** hydration, “dehydration”, water, sleep, amyloid, Alzheimer’s

## References

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**Presentation Method: Invited Speaker**

## Use of Raman Spectroscopy in Forensics Toxicology

Ramazan AKCAN

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Raman Spectroscopy gains more popularity in forensic toxicological analyses since it is a fast, accurate and reliable that could be utilized in laboratory and in the field. Raman spectroscopy, with its different types, has potential to be modified for any specific conditions. Different laser sources, Raman-active surfaces and application of various nanoparticles increase the efficiency of Raman spectroscopy and its enhanced capacity creates surface enhanced Raman spectroscopy, which widens its analytical spectrum. The literature revealed that Raman spectroscopy took its place in the analysis of street samples, seized drugs, simulated samples, contraband productions and pure stable materials. However, it still needs more researchers dealing with biological samples, mixed liquids, and complex media. The number of studies performing quantitative analysis from real samples should increase and the need for establishing large libraries of toxic materials should be met for achieving Raman spectroscopy's journey into forensic toxicological routine. This presentation aims to emphasize technical needs for the field of forensic toxicology and discuss use of Raman spectroscopy in forensic toxicological analyses, based on past and current researches.

**Keywords:** Raman spectroscopy, SERS, forensic sciences, forensic toxicology, illicit drugs, therapeutic drugs.

**Presentation Method: Invited Speaker**



## New Perspectives on Excitonic Energy Transference Mechanisms in Photosynthesis

Joaquín BARROSO-FLORES

*Institute of Chemistry from the National Autonomous University of Mexico*

Photosynthesis is the central chemical process that sustains life on Earth, as well as one of the most closely related to its origin. Despite all the acquired knowledge on the various stages of photosynthesis, from solar energy capture to the synthesis of carbohydrates, there are still some gaps in the knowledge of excitonic transfer energy upon photon capture. With the use of computational chemistry tools, we explore the possibility of alternative excitonic transfer mechanisms between photosynthetic pigments such as Singlet Fission. Additionally, we've assessed the electronic structure effects behind a remarkable, red-shifted absorption exhibited by the organism *Blastochloris viridis* whose main absorption is observed in the near IR region (1015 nm) despite the Light Harvesting Complex-1 being made up of Bacteriochlorophyll—b molecules, whose main absorption is observed at 795 nm. The modified Redfield theory is used to assess the dynamics of excitonic transfer between constituting pigments.

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## Oral Abstracts

## Conformation Analysis of 6-Amino-1,3-Dipropyluracil Molecule

Dogan Kazan<sup>1</sup>, Ersin Durgut<sup>2</sup>, Ebru Karakas Sarikaya<sup>3</sup>, Omer Dereli<sup>4</sup>, Ulfet Atav<sup>5</sup>

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In this study, conformational analysis calculations were made in order to determine the structure of the 6-Amino-1,3-dipropyluracil molecule. 6-Amino-1,3-dipropyluracil (C<sub>10</sub>H<sub>17</sub>N<sub>3</sub>O<sub>2</sub>) is a chemical compound used in pesticides and insecticides in Europe. Pesticides: besides providing benefits such as growing vegetables and fruits in nature without being damaged and purification of our living spaces from harmful microorganisms, can also pose a great threat to human health due to incorrect use. It is important to reveal the stable structure of this molecule because of its effects on human health. While performing conformational analysis on this molecule; molecular mechanics methods were used. The conformers of the molecular structure of the title compound were determined. The energy of the most stable conformer and the main geometric parameters of this stable conformer (bond lengths, bond angles and dihedral angles) were calculated. Gaussian 03 (Frisch et al., 2003) and Spartan 08 (Irvine, 2008) package programs were used in the calculations made within the scope of this study. First, the conformational surface of 6-Amino-1,3-dipropyluracil was scanned by Merck Molecular Force Field (MMFF) method in Spartan 08 (Irvine, 2008). Then, the geometry optimization calculations of these conformers were made using the Gaussian 03 (Frisch et al., 2003) Program. After these calculations 17 conformers were determined by applying the B3LYP method and the 6-311 ++ G (d, p) basis set. The conformational domain of the 6-Amino-1,3-dipropyluracil molecule was scanned with molecular mechanical calculations to investigate possible conformers, and the dihedral angles that enable the 6-Amino-1,3-dipropyluracil molecule to rotate around single bonds were determined during this process. By rotating these dihedral angles at intervals of 10 degrees, their energies were calculated. Thus, the conformer, which has the lowest energy level and is the most probable structure of the molecule according to the Boltzmann distribution, was determined. The energy of conformer 1, which has the lowest energy level, was calculated as -706,26451 Hartree.

**Keywords:** Conformational Analysis, 6-Amino-1,3-dipropyluracil, energy level, structure of the molecule.

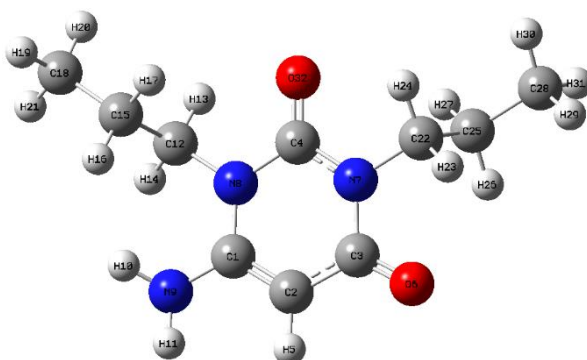


Fig. 1. The most stable conformer of 6-Amino-1,3-dipropyluracil

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**Presentation Method: Oral**

## The Effect of Radiation on Omeprazole Drug: An Overview of Its Use as an EPR Dosimeter

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Especially in recent years, the widespread use of nuclear technology in the field of health and energy is an important issue, and new developments in technology and different applications have strengthened the presence of radiation in human life. However, the fact that ionizing radiation has the energy to remove electrons from atoms and molecules makes it vitally important to know the dose absorbed by living things [1]. Especially in radiological/nuclear emergencies, when victims are not wearing a personal dosimeter, there is a need for appropriate methods to measure the absorbed dose retrospectively. If the radiation-induced paramagnetic centers in any material are sensitive to the absorbed dose and stable enough, it can be used as an EPR dosimeter [2]. Investigating the dosimetric properties of the materials (natural materials, drugs etc.) present on and around the individual is extremely valuable for radiation measurement after accidental exposure. It is important to determine the effects of radiation on drugs for both radiosterilization and dosimetric purposes [3].

In this study, by using EPR spectroscopic technique we investigated the radiation effect on Omeprazole drug which contains active component Omeprazole and its possible usability as an emergency/accident dosimeter for retrospectively dose measurement. The powdered drug samples were irradiated with a gamma source of <sup>60</sup>Co in the dose range of 10-800 Gy for EPR method-based dose-response studies that proves the dose sensitivity of the radiation-produced radical(s). The behavior of the radical(s) at both room and high temperatures were examined by the experiments fading and isochronal, isothermal annealing, respectively. Omeprazole, a frequently used medication for gastroenterological diseases, might be considered a promising dosimeter for nuclear accidents due to the radiation dependent stable radical induced in its structure, and its low cost and portability.

**Keywords:** Electron Paramagnetic Resonance (EPR), gastroenterological drugs, Omeprazole, EPR dosimeter, irradiation

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**Presentation Method: Oral**

## Quantification of Water Content in Polysaccharides by FTIR

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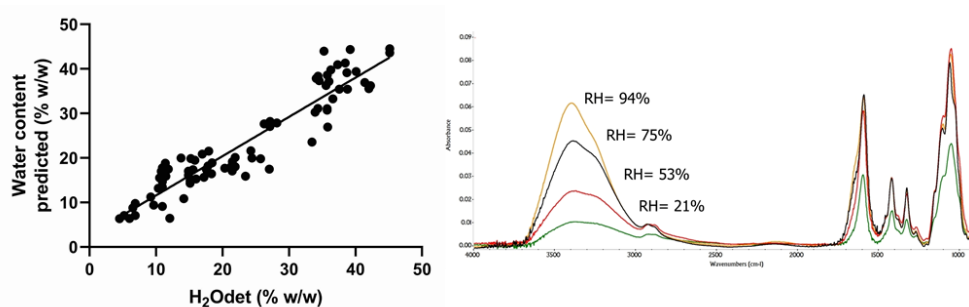
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Water content quantification on raw polysaccharide materials for food processing is generally performed by gravimetric analysis or titrimetric methods, which are time and energy consuming, non-eco-friendly and sample destructive. The present study develops and validates a new approach, based on the use of Fourier transform infrared (FTIR) spectroscopy, resulting in a model on the water content of polysaccharides. Samples were exposed to different relative humidity conditions. Water content was determined standard gravimetric methods (OIV-Oeno 404-2010) and compared with the area of FTIR absorption in the range 3700 - 2800 cm<sup>-1</sup>, attributed to the stretching of OH groups. The strong correlation between gravimetric results and FTIR area ( $R^2 = 0.88$ ) showed no signs of bias across the water content range. A cross validation technique to predict the water content by band area was performed obtaining a general equation:  $y = 2.12x + 2.80$  with a high repetitively and good prediction of the tested models. There were no significant differences ( $p < 0.05$ ) between samples measured using gravimetric and spectrophotometric methods. According to the cross-validation test, the good performance of the prediction was tested, demonstrating the consistency and effectiveness of the obtained linear equation to predict the water content of the samples. The variation coefficient of the data between both methods was lower than 5 % for all the cases.

In addition, since the method was independent by the chemical nature of the investigated polymer, this allows the analysis of polysaccharides, that cannot be easily dissolved in the Karl Fischer titration or that are thermosensitive.

**Keywords:** Polysaccharides; water content; ATR-FTIR; cross-validation; ANOVA



*Figure:* Water content determined by gravimetric method compared to the value forecasted by the prediction model (left) and example of ATR-FTIR spectra of carboxymethyl cellulose at different relative humidity (right)

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**Presentation Method: Oral**

## Digital Twin Development of Continuous Powder Blending with Artificial Neural Networks and Residence Time Distribution Models

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A paradigm shift has taken place in the pharmaceutical industry during the last decade, which led to rise of continuous manufacturing (CM) technologies [1]. The rapid spread of CM is promoted by the higher efficiency and flexibility of the processes, better product homogeneity, and a more complete quality assurance thanks to the Process Analytical Technology (PAT) framework initialized by the FDA in 2004 [2]. We present a thorough description of the digital twin development for a continuous pharmaceutical powder blending process in accordance with PAT and Quality by Design (QbD) guidelines (Fig. 1) [3]. A low-dosage system of caffeine active pharmaceutical ingredient (API) and dextrose excipient was examined via continuous blending experiments. Near infrared (NIR) spectroscopy-based process analytics were applied; the quantitative evaluation of spectra was achieved using multivariate partial least squares (PLS) data analysis. The blending process was represented with mechanistic residence time distribution (RTD) models and two types of recurrent artificial neural networks (ANN). We used experimental datasets for model training, fitting and validation. Detailed comparison of the two modelling approaches, the optimization of the model-based digital twin, and efficiency of the soft sensor-based process monitoring is presented through several validating simulations. Both RTD models and nonlinear autoregressive neural networks demonstrated excellent predictive power for the low dosage blending process. RTD models can prove to be more advantageous in industrial development as they are less resource-intensive to develop and prediction accuracy on low concentration levels lacks dependency from the precision of chemometric calibration. Reduced material costs and limited development timeframe render the digital twin an efficient tool in technological development.

**Keywords:** Digital twin; Process analytical technologies; Soft sensor; Continuous powder blending; Machine learning

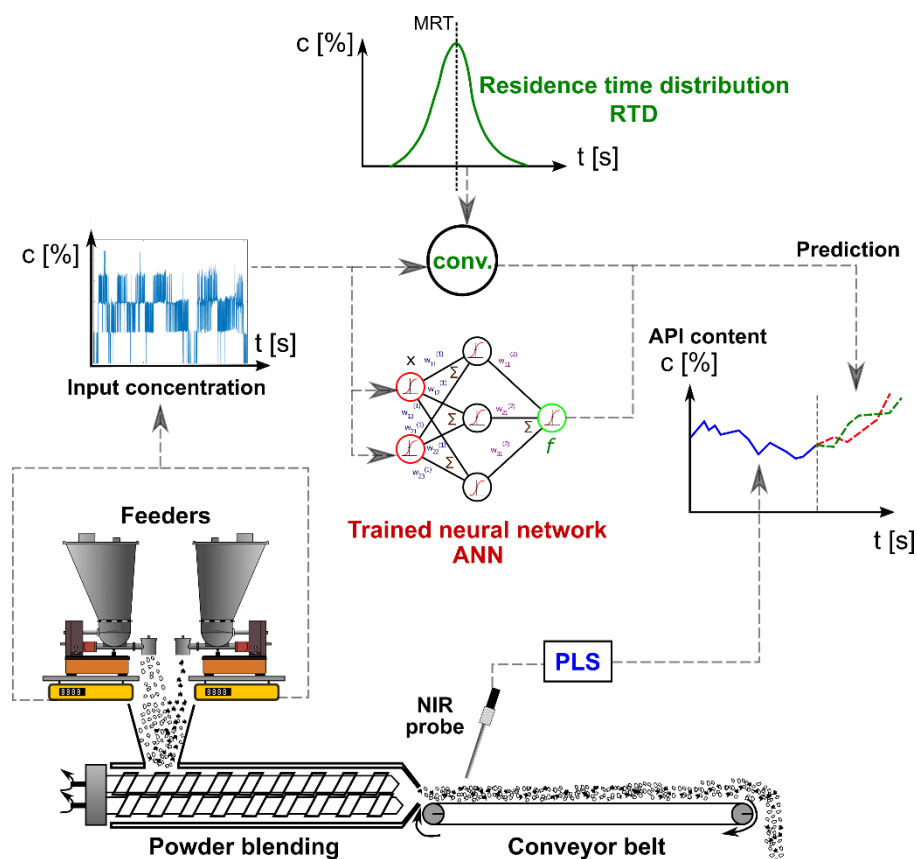


Figure 1

## Acknowledgements

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<b>Presentation Method: Oral</b>
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## Modifications of Fe(III)-Based Antioxidant Capacity Methods

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In the spectrophotometric antioxidant capacity assays, many chromogenic ligands have been used up till now. Some of these radicals comprise unstable radicals under laboratory conditions.

On the other hand, the use and modification of Fe(III)-based antioxidant determination methods are not common in the literature. The Ferricyanide/Prussian blue assay of reducing capacity measurement was optimized so as to obtain a more reproducible, linear and additive response from antioxidants. Synthetic antioxidant mixtures gave the theoretically expected total antioxidant capacities conforming Beer's law. The assays were responsive to biologically important thiols which are not oxidized by other Fe(III)-based assays.

Developed Fe(III)-based antioxidant capacity methods merely requiring a colorimeter can be widely used in conventional laboratories of food and agricultural chemistry not equipped with highly sophisticated instruments for antioxidant measurement. This work has focused on the total antioxidant capacity assay of ascorbic acid, flavonoids, and phenolic acids individually or in mixtures-using the reagent of Fe(III)-TPTZ, Fe(III)-Ferrozine, Ferricyanide, Fe(III)-o-phenantroline, and Fe(III)-bathophenantroline. In these comparative assays existing methods were modified and improved so as to measure antioxidant capacity. Various modifications have been made on the conventional methods in order to drive the chromogenic redox reactions to completion. The disadvantage of precipitate formation in the ferricyanide method was overcome by the use of sodium dodecyl sulfate (Na-SDS). The developed methods had a high sensitivity for antioxidants e.g., for quercetin, the molar absorptivities achieved by use of 1,10-phenanthroline, bathophenanthroline, original FRAP, modified FRAP, and modified ferricyanide methods were  $8.00 \times 10^4$ ,  $1.59 \times 10^5$ ,  $1.34 \times 10^5$ ,  $1.99 \times 10^5$ , and  $8.73 \times 10^4$  L mol<sup>-1</sup> cm<sup>-1</sup>, respectively. The molar absorptivity, linear concentration range and TEAC (Trolox equivalent antioxidant capacity) values of the studied antioxidants were found using these Fe(III)-based assays.

**Keywords:** Antioxidants, FRAP, TPTZ, Ferrozine, TEAC

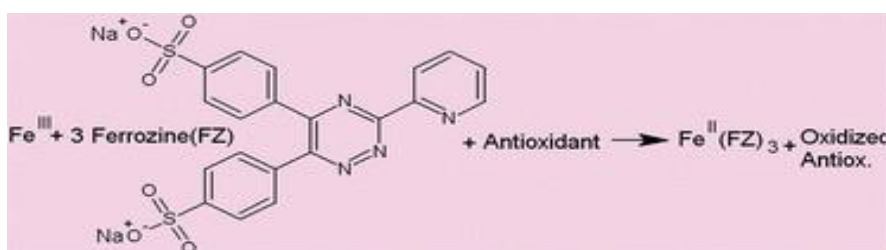


Fig. 1 The reaction of oxidation of ascorbic acid and reduction of the iron(III).

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**Presentation Method: Oral**

## Determination of Vitamin C In Foodstuffs by UV-Vis Spectrophotometer

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Vitamin C is known as L-ascorbic acid which is one of the most important water-soluble vitamins in the human diet. It assists the body in forming connective tissue, teeth, bone, blood vessel walls, and absorbing iron and amino acids. Vitamin C deficiency can cause scurvy. Consumption of vitamin C reduces the incidence of mortality from cardiovascular disease and cancer [1]. It has anti-allergic properties and prevents colds and infections by strengthening the immune system [2]. Although plants and some animals produce their own vitamin C, people do not make it. Therefore, people need to get it into their bodies from other sources [1]. The daily intake of vitamin C is 60 mg/day, and its high intake results in its excretion from the body in the urine [3]. Fruits and vegetables are the main sources of vitamin C. The fruits richest in vitamin C are acerola, guava, cashew, strawberry, orange, and lemon, while yellow pepper, broccoli, cabbage, spinach, peas are some vegetables containing high levels of vitamin C [2]. Several techniques have been used for the analysis of vitamin C in foods such as titrimetric, spectrophotometric, voltametric, fluorometric, flow injection analysis, and potentiometric methods [1]. In addition, liquid chromatography, capillary electrophoresis, and gas chromatography are among the alternative methods used to analyze this vitamin [3]. UV-vis spectrophotometry is widely used to quantitatively determine vitamin C because it is a simple and speed method and vitamin C can absorb UV rays [1,3]. The method is suitable for use in fresh or packaged fruit juices, vitamin C tablets, and fruits and vegetables [3]. Most of the spectrophotometric methods are based on the reducing effect of vitamin C. In many of these, Fe (III) is reduced to Fe (II) in the presence of AA and the reduced Fe (II) is complexed with different reagents such as 1,10-phenanthroline, 2-(5-bromo-2-pyridylazo)-5 diethylaminophenol (Br-PADAP), ferrozine, and 4-(2 pyridylazo) resorcinol (PAR). Cu (II) is another reducible agent. It is also used for the determination of ascorbic acid. The reaction occurs by reducing Cu (II) to Cu (I) with ascorbic acid and complexing the reduced Cu(I) with different reagents such as 5-(4-hydroxy-3-methoxybenzilidene) rhodanine (HMBR), and 2,9-dimethyl-1,10-phenanthroline (neocuproine (Nc)) [1]. At the same time, ascorbic acid is oxidized to dehydroascorbic acid. Then, the absorbance value of mixture is determined by UV-Vis spectrophotometer. The vitamin C content of the analyzed sample is calculated using the calibration curve plotted from the ascorbic acid standards.

Vitamin C has limited stability. It can be added into the foods as an antioxidant. It can be lost from foods during food processing such as storage, preparation, and cooking [1]. It is important to determine the vitamin C content in the quality control of foodstuffs and for this purpose, the spectrophotometric method is often preferred.

**Keywords:** Ascorbic acid; uv-vis spectrophotometer; vitamin C.

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**Presentation Method: Oral**

## Comparison of Color Characteristics of Red and White Grape Juice by Uv-Vis Spectrophotometer

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Grape juice and products obtained from grape such as wine, jam and raisins are widely consumed today. Grape juices are known as important sources of phytochemicals. Phytochemicals found in grape juice, such as flavonoids and anthocyanins, shows antioxidant, platelet inhibitory, and anti-inflammatory effects both in vitro and animal studies [1]. While flavonoids (quercetin and five other aglycones, catechin, epicatechin, and procyanidins) in grapes are found to be especially high amounts in white grape juice, anthocyanins such as malvidin 3,5-diglucosides, peonidin, petunidin, cyanidin, and delphinidin are predominant in red grape juice [2,3]. Anthocyanins and flavonoids are responsible for the characteristic juice color, as well as exhibit antimicrobial properties [1]. One of the most important quality factors of grape juice is color [4]. All people are sensitive to the color of foods. Appetite is stimulated or suppressed almost directly in relation to the reaction of the observer to food color, while the color we see can indicate the flavor. In addition, color may indicate to the consumer that the quality of product is high, while a washed out or artificially bright product may show that the product is of such low quality to be rejected by the consumer [3]. Color is a characteristic of grape juice that can be determined both by instrumental and sensory analysis. The color of grape juice is due to some color components such as tannins, polyphenols, and anthocyanins and is affected by the pH, and total acidity of grape juice, grape variety, the degree of maturity of the grapes, process conditions of grape juice production etc. [5]. In this study, the differences between chromatic indicators, which are known to affect consumer preference closely, were revealed with the help of uv-vis spectrophotometer for white grape juice and red grape juice. The absorbances of the samples were measured at 420, 520, and 620 nm wavelengths, and their chromatic parameters (color intensity, color hue, and chromatic structure of grape juices) were calculated. The color intensity (IC) values of white and red grape juices were 0.58 and 1.31, while the color hue values of white and red grape juices were 3.50 and 1.82, respectively. The chromatic structure shows the ratios of the colors in terms of percent of yellow, red, and blues pigments for the grape juice samples. While the rate of yellow pigment in white grape juice (72.59%) was found to be higher than that of red grape juice (58.67%), the rate of red and blue pigment was found to be higher in red grape juice (32.25% and 9.09%) compared to the other (20.74% and 6.67%) ( $p < 0.05$ ). The color parameters of white and red grape juice determined by the spectrophotometric method are statistically different from each other ( $p < 0.05$ ). These results indicate that the spectrophotometric method can be used quickly and effectively in determining the color of the product, which has the first effect on the consumer's choice. In addition, the use of uv-vis spectrophotometer can be preferred to determine the color changes in fruit juice during processing and storage.

**Keywords:** Color characteristics; red grape juice; UV-Vis spectrophotometer; white grape juice.

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**Presentation Method: Oral**

## Mössbauer Spectroscopy of Ferrum Lek: Further Development of The Heterogeneous Iron Core Model

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Study of the iron cores in ferritin and its pharmaceutical analogues which are used for treatment of the iron deficiency anemia is very important for further analysis of the nanosized ferric hydroxide core structure. It is possible that ferritin functions as well as iron bioavailability in pharmaceutical analogues in the body may be related to the iron core peculiarities. Earlier, the heterogeneous iron core model was suggested to fit the Mössbauer spectra of ferritin and its analogues measured with a high velocity resolution, i.e., in 4096 channels (see [1, 2]). This model implies the presence of different areas/layers in the iron cores, therefore, the Mössbauer spectra of these samples measured in the temperature range 295–90 K can be better fitted using a superposition of five quadrupole doublets with equal line widths. Quadrupole doublet with the smallest quadrupole splitting was assigned to the most close-packed FeOOH areas/layers while that with the largest quadrupole splitting was associated with the less close-packed FeOOH areas/layers in the core. Recently, we have measured the 295 K Mössbauer spectrum of Ferrum Lek, an iron-polymaltose ferritin analogue, with much higher signal-to-noise ratio (S/N) and compared the results of the fits of the intermediate spectrum with S/N = 101 and the final one with S/N = 240 (Fig. 1). It was found that the latter spectrum should be better fitted using 6 quadrupole doublets while 5 quadrupole doublets were not enough. The same fits of the spectrum with S/N = 101 showed similar differential spectrum and  $\chi^2$  decrease on  $1.8\sigma$  only. In contrast, two fits of the spectrum with S/N = 240 demonstrated improving the misfits at the differential spectrum and decreasing of  $\chi^2$  on  $9.6\sigma$ . This fact indicates that increasing of S/N may help to extract more details in the complex Mössbauer spectra of ferritin and its analogues.

**Keywords:** Mössbauer spectroscopy; Ferrum Lek; the iron core structure.

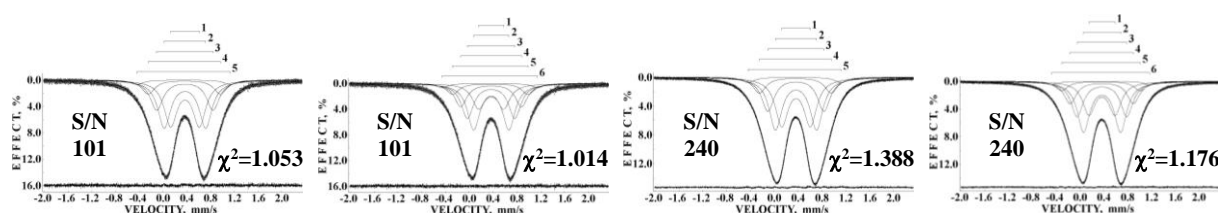


Fig. 1. Mössbauer spectra of Ferrum Lek measured with signal-to-noise ratios (S/N) 101 and 240 and fitted using 5 and 6 quadrupole doublets within the heterogeneous iron core model. T = 295 K.

### Acknowledgements

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**Presentation Method: Oral**

## The Iron State in Some Iron-Containing Vitamins and Dietary Supplements Analyzed by Mössbauer Spectroscopy

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Iron is essential metal for live. Iron ions are in the active sites of hemoglobin, myoglobin, cytochromes, catalases and other iron-containing enzymes. Therefore, to keep iron status in the body the iron-containing vitamins and dietary supplements are used. These pharmaceuticals contain iron in different forms, namely, ferrous fumarate ( $\text{FeC}_4\text{H}_2\text{O}_4$ ), ferrous sulfate ( $\text{FeSO}_4$ ), iron chelates and some other iron compounds. The most suitable iron salts for oral administration are ferrous compounds. In this case,  $^{57}\text{Fe}$  Mössbauer spectroscopy is the most sensitive tool for the control of the iron state(s) in these products including aging effect (see, e.g., [1–3]). We have studied tablets of some fresh and outdated vitamins and dietary supplements containing iron salts and iron chelates by Mössbauer spectroscopy with a high velocity resolution in order to analyze the iron states and formation of iron impurities with aging. Selected room temperature Mössbauer spectra of outdated Feosol® (SmithKline Beecham Corporation, USA), containing ferrous sulfate and measured in 2007 and 2021, and fresh PreNatal (21st Century HealthCare, Inc., USA), containing ferrous fumarate and measured in 2021, are shown in Fig. 1. The differences between the spectra of Feosol® measured in 2007 and 2021 are clearly seen. In the first case the spectrum shows the presence of the main component 1 associated with ferrous sulfate and the minor component 2 (~1.7%) related to ferric compound. In the spectrum of Feosol® measured in 2021 the main component 1 corresponds to ferrous sulfate with the relative area of ~65.5% while components 2 and 3 belong to other ferrous compounds. In the spectrum of PreNatal two main spectral components 1 and 2 with close parameters may be associated with two slightly different forms of ferrous fumarate while the minor component 3 (4.5%) has the  $^{57}\text{Fe}$  hyperfine parameters corresponding to ferric compound. This content exceeds 2% limitation of ferric compound in ferrous fumarate announced by the Food and Drug Administration (USA).

**Keywords:** Mössbauer spectroscopy; iron-containing vitamins and dietary supplements; control of the iron state.

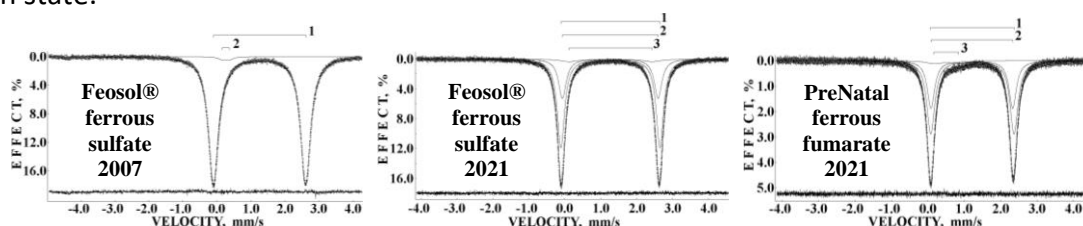


Fig. 1. Mössbauer spectra of Feosol® measured in 2007 and in 2021 and fresh PreNatal measured in 2021.

### Acknowledgements

This work was supported by the Ministry of Science and Higher Education of the Russian Federation, project № FEUZ-2020-0060.

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## Structural and Spectroscopic Study of The Iron-Bearing Phases in Bursa L6 Meteorite

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Study of various extraterrestrial materials by structural and spectroscopic techniques is very important for excavating new information about formation and evolution of the Solar System. In this work we present an example of such studies using Bursa L6 ordinary chondrite which fell in 1946 in Turkey and analyzed in [1, 2]. Fragments of Bursa L6 were studied by X-ray diffraction (XRD), Raman spectroscopy, Mössbauer spectroscopy with a high velocity resolution and some other techniques described in [1, 2] while here we consider the results of the first three structural and spectroscopic methods applied for analysis of the iron-bearing phases. XRD demonstrated the phase composition of Bursa, the unit cell parameters for olivine, orthopyroxene and clinopyroxene as well as Fe<sup>2+</sup> and Mg<sup>2+</sup> occupancies of the M1 and M2 sites in these silicates. The Raman spectrum of olivine and the Mössbauer spectrum of the bulk Bursa L6 sample are shown in Fig. 1. The results obtained from these spectra showed Fa and Fs values for olivine and orthopyroxene, the relative Fe contents in iron-bearing phases, the Fe<sup>2+</sup> distributions among the M1 and M2 sites and the temperatures of equilibrium cation distribution in silicates as well as confirmed Bursa classification as L ordinary chondrite in spite of the relatively larger content of Fe alloy.

**Keywords:** Bursa L6; XRD; Raman spectroscopy; Mössbauer spectroscopy.

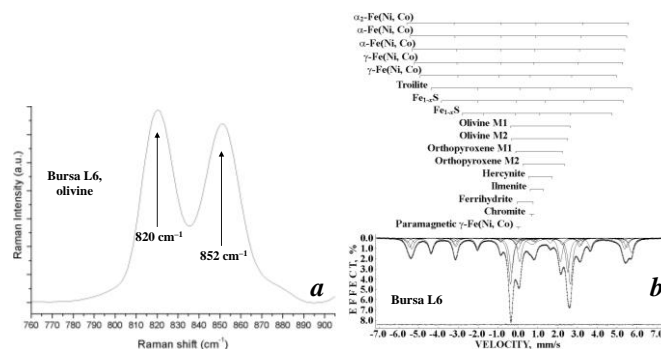


Fig. 1. Raman spectrum of olivine from Bursa L6 (a) and Mössbauer spectrum of the bulk Bursa L6 (b).

### Acknowledgements

The authors acknowledge Prof. Emin Ozel for supplying the Bursa meteorite sample. This work was supported by (1) the Ministry of Science and Higher Education of the Russian Federation, Project № FEUZ-2020-0060 and Project № AAAA-A19-119071090011-6 (A.A.M.), (2) the Ege University Scientific Research Projects Coordination Unit, Project № 17-FEN-050 and (3) MFAG/113F035 by The Scientific and Technological Research Council of Turkey (TUBITAK).

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## Concentration of Palladium Which Chelate Sorbent on The Basis of Maleic Anhydride Styrene Copolymer

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New chelating polymeric sorbent on the basis of maleic anhydride styrene copolymer by the chemically modification with streptocide has been synthesized. Sorbent has showed complexing properties. The synthesized sorbent has been investigated by IR spectroscopy. It's sorption characteristics toward palladium(II) ions has been studied.

**Keywords:** Chelating sorbent, sorption, streptocide, palladium

### Introduction

Over the last years the considerable success is achieved in using of different organic and inorganic sorbents for the selective concentration of elements. From this point of view high efficiency shows polymeric chelating sorbents. Polymeric chelating sorbents differs for their stability and consist of functionally active groups which can interact with metal ions palladium [1].

Establishing brand new sorption decontamination technologies of industrial and domestic drain is one of the most important fields of chemical investigation. Wastewater of companies, fabrics contains toxic metal ions, which can cause harm to humanity. Thus, they need to be cleaned before using. Removal of toxic metal ions from different natural sources is a matter of serious concern due to their high toxicity. Toxic metal drains entering the environment negatively impacts ecological system [2-3]. Therefore, synthesis of different adsorbents which can selectively absorb these metal ions is very important. One of the most priority pollutants are Pd<sup>2+</sup> ions. In this case polymeric chelating sorbents show high effectiveness. Current work is dedicated to studying Pd<sup>2+</sup> sorption ions from its salt solutions. To determine the character of interaction between the heavy metal ion and sorbent dependence of sorption capacity on pH value, initial metal concentration, ionic strength, time, and desorption process have been studied.

### Material and method

All the chemicals and reagents used in this work are of analytical grade and standard solution of palladium(II) ion was prepared by dissolving palladium(II)chloride. Pd(II) solution with concentration  $1,0 \times 10^{-2} \text{ mg} \cdot \text{l}^{-1}$  is used in this work. Equilibrium concentration of metal ions were determined in the liquid phase by photometric method using 2,2', 3,4 tetrahydroxy sulfo chloro azobenzene as a reagent with concentration  $1,0 \times 10^{-3} \text{ mg} \cdot \text{l}^{-1}$  [4].

Different pH buffers from 3 to 8 have been used to study the effect of pH to the sorbent's sorption capacity over Pd<sup>2+</sup> ions. Buffer solutions were prepared using acetic acid and ammonium hydroxide solutions respectively. Sorbent synthesis was carried out using maleic anhydride styrene copolymer as matrix and streptocide as a linkable amine.

## Results and discussion

To determine the amount of synthesized sorbent over the Pd<sup>2+</sup> ions, pH values from 3 to 8 were used. It is found that the cation of Pd(II) ions is observed at pH 5.0. Investigation have shown that time impacts the process of sorption of Pd<sup>2+</sup> ions by synthesized sorbent and reaches its maximum level when the adsorption time is 90 minutes. This work includes studying of influence of KCl ions as a parameter, which prevents sorption of Pd(II) ions. Results have shown that at the  $\mu = 0,8 \text{ mol}\cdot\text{L}^{-1}$  value of ionic strength KCl verily impacts sorption of Pd(II) ions. The effect of initial Pd (II) ions concentration on adsorption was studied at the range of  $0.2\times 10^{-3} \text{ mol}\cdot\text{L}^{-1}$  to  $8.0\times 10^{-3} \text{ mol}\cdot\text{L}^{-1}$ . The percentage adsorption of Pd(II) ions increased with increasing of Pd(II) concentration. Investigation have shown that the maximum adsorption is observed when the metal ion concentration is  $8.0\times 10^{-3} \text{ mol}\cdot\text{L}^{-1}$ . Results are illustrated on the diagram and table below (Table 1).

Table 1. Removal efficiency percentage of Pd(II) ions by the investigated sorbent

$C_{Me} \times 10^{-3}, \text{ mol}\cdot\text{L}^{-1}$	0.2	0.4	0.8	1.0	2.0	4.0	6.0	8.0
Sc mg/g	8,61	22,8	54,618	66,204	136,428	258,197	335,514	354,666

### Sc- sorption capacity

Table 1 shows that removal percentage of Pd(II) sorption reaches its maximal value when the metal ion concentration is  $8.0\times 10^{-3} \text{ mol}\cdot\text{L}^{-1}$ . As we see at the range of concentration  $0.2\times 10^{-3} - 0.8\times 10^{-3} \text{ mol}\cdot\text{L}^{-1}$  full sorption of Pd(II) ions by investigated sorbent is observed. Therefore, to determine sorption capacity volume of metal ion solution should be increased. Desorption of Pd<sup>2+</sup> ions was carried out by using different acids with  $0.5 \text{ mol}\cdot\text{L}^{-1}$  of concentration: HNO<sub>3</sub>, HClO<sub>4</sub>, HCl and H<sub>2</sub>SO<sub>4</sub>. Investigations have shown that the highest effect on palladium(II) desorption have shown  $0.5 \text{ mol}\cdot\text{L}^{-1}$  solution of HClO<sub>4</sub>. Results of research are shown on the table below (Table 2):

Table 2. Desorption of Pd(II) ions with different acids

Acid, $\text{mol}\cdot\text{L}^{-1}$	HNO <sub>3</sub>	HClO <sub>4</sub>	HCl	H <sub>2</sub> SO <sub>4</sub>
Sc, mg/g	701	742	651	704
R%	93.6	99	86.9	94

## Conclusion

The present study has shown that maleic anhydride styrene copolymer-based sorbents can be used for removal of Pd<sup>2+</sup> ions from natural and industrial objects. Moreover, the functionally active groups of amine streptacide show high selectivity over Pd<sup>2+</sup> ions.

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**Presentation Method: Oral**

## Molecular Docking Analysis for Bace1 Inhibition of Novel Thiosemicarbazide Derivatives

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Neurodegenerative diseases are characterized by progressive degeneration of neurons in the central and peripheral nervous system. Diseases such as Alzheimer's disease (AD), Parkinson's disease (PD), Amyotrophic lateral sclerosis (ALS) are common neurodegenerative diseases (1). Pathologically, the presence of extracellular amyloid plaques (APs) and intracellular neurofibrillary plaques (NFTs) in the brain are an indicator of AD. While amyloid plaques are formed by the aggregation of  $\beta$ -amyloid peptides ( $A\beta$ ), neurofibrillary plaques are formed by intracellular abnormal phosphorylation and aggregation of tau proteins (2). Recent research has shown that there is a robust connection between AD and BACE1 ( $\beta$ -site APP cleaving enzyme 1 or  $\beta$ secretase). BACE1 is a new face of Alzheimer's disease (AD) research because this is responsible for the abnormal production of  $\beta$  amyloid plaques ( $A\beta$ ), the character of its pathophysiology. As such, inhibition of  $A\beta$  in the brain should prove supporting for AD treatment.  $A\beta$ , the product of the large type1 trans-membrane protein amyloid precursor protein (APP), is made in a two-stage proteolytic way initiated by BACE1 ( $\beta$ -secretase) and pursued by  $\gamma$ -secretase. Due to its obvious grade limiting function, BACE1 emerges to be an efficient target to prevent  $A\beta$  generation in AD (3). Thiosemicarbazide ligands containing of nitrogen and sulfur are considered useful targets for drug design and development. Thiosemicarbazide ligands today use like variety of compounds with potent neuroprotectant, antioxidant, radical scavenging, antibacterial, antifungal, anticancer, antiHIV, antiviral, insecticidal, and antiparasitic activity (5). Also due to NH-NH-C(S)-NH structural motif, 1,4-disubstituted thiosemicarbazides are suitable precursors for the synthesis of heterocyclic analogs with 1,3,4-thiadiazole or 1,2,4-triazole cores (4). We performed docking studies of new designed compounds with BACE1 enzyme (pdb: 1W51) by using CDocker approach in Discovery Studio 3.5 to understand the binding features of compounds and design more potent and selective compounds as the lead BACE1 inhibitors. Our study focuses on enlightening the role of some novel thiosemicarbazide derivatives as BACE1 inhibitors to open new perspective for drug development in the treatment of AD.

**Keywords:** BACE1 enzyme; thiosemicarbazide derivatives; neurodegenerative diseases.

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**Presentation Method: Oral**

## Ab-initio Study on Structural, Spectroscopic and Electronic Properties of (E)-1-(4-methoxyanthracen-1-yl)-2-phenyldiazene Azodyes Molecule

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(E)-1-(4-Methoxyanthracen-1-yl)-2-phenyldiazene or  $C_{21}H_{16}N_2O$  is one of tautomer azodyes which is the most usable compound in a number of industries as a sensing molecule, nowadays. As we know, more than 90% of the existing commercial azodyes are tautomeric ones [1]. Quantum chemistry calculations can clarify the relationship between structure and electrochemical properties of azodyes compounds for futuristic applications. A comparison of the experimental and theoretical calculations can be very useful in making correct assignment and understanding the relation between molecular structure and the properties of the compounds.

In this study, our main aim is to characterize the structural geometries, spectroscopic and electronic properties of  $C_{21}H_{16}N_2O$  azodyes compound by utilizing *ab-initio* method based on density functional theory (DFT) [2]. The molecular geometry and vibrational spectroscopy of the molecule, in the ground state, have been computed by applying DFT/B3LYP method with the basis set of 6-31G (d,p). Our results of structural properties of bond length, bond angle and dihedral angle are in excellent agreement with those of available experiment data [3]. 114 vibrational modes of the title molecule have been specified with stretching, in-plane-bending, out-of-plane-bending, and torsion vibrations. UV's absorption spectra and, <sup>1</sup>H and <sup>13</sup>C NMR chemical shifts within dimethyl sulfoxide (DMSO) solvent have been predicted by using time dependent density functional theory (TD-DFT). Furthermore, the electronic properties of the title molecule have been also attained by using the Frontier Molecular Orbital Theory (FMO) enable to determine the Lowest Unoccupied Molecular Orbital - Highest Occupied Molecular Orbital (HOMO-LUMO) interaction. It can be reported that this molecule has gap ( $E_g$ ) bigger than 1.5 eV which indicates thermodynamically stable and durable, low ionization potential energy ( $IP$ ) which tends to be reducing agents because it is easily losing its electron, about 2.43 eV electron affinity ( $EA$ ) which denotes that it has good conductive properties, high electronegativity ( $\chi$ ) which shows that the molecule is polar, low value of chemical hardness ( $\eta$ ) and global electrophilicity index. To the best of our knowledge, this work presents the theoretical characterization of the  $C_{21}H_{16}N_2O$  azodyes molecule for the first time.

**Keywords:** DFT, UV's absorption, chemical shifts, electronic properties, azo dyes.

### Acknowledgements

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**Presentation Method: Oral**

## Chemiluminescent self-activating photosensitizers for selective anticancer therapy

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Cancer is a very challenging disease to treat, in terms of treatment efficiency and side-effects. To overcome these problems, there have been extensive studies exploring therapeutic modalities with reduced side-effects, such as photodynamic therapy (PDT) [1]. PDT has significant advantages over conventional cancer therapies, however its dependence on light has limited it to treating tumors on just under the skin or on the outer lining of organs/cavities [2].

Herein, we have developed new photosensitizers capable of intracellular self-activation with potential tumor-selectivity based on chemiluminescent reactions involving only a cancer marker. The photosensitizer is directly chemiexcited to a triplet excited state generating singlet oxygen, without requiring a light source. So, in this work we aimed to develop self-activating photosensitizers which can be used for light-free photodynamic therapy, eliminating light-related restrictions presented by this therapy [3,4].

Cytotoxicity assays with breast and prostate cell lines showed that the novel photosensitizers possess significant toxicity toward tumor cells, while not affecting normal cells. Besides we compared the activity of these compounds with standard treatments, finding a higher cytotoxicity than the reference drugs [4,5].

**Keywords:** Chemiluminescence; Self-illuminating; Tumor-selective; Anticancer.

### Acknowledgements

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**Presentation Method: Oral**

## UV-induced Photochemistry of Monomeric Benzoxazole and Its Isomers

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Monomers of 1,3-benzoxazole were isolated in a cryogenic argon matrix and characterized by infrared (IR) spectroscopy. The photochemistry of 1,3-benzoxazole, induced by excitations with narrowband UV light of different wavelengths, was investigated [1]. Irradiation at 233 nm resulted in a quantitative conversion of 1,3-benzoxazole into 2-isocyanophenol (see Fig.1). The individual photochemical behavior of the *in situ* produced 2-isocyanophenol was studied upon excitations at 290 nm, where 1,3-benzoxazole does not react. The photochemistry of isomeric matrix-isolated 2-cyanophenol was also studied in a separate experiment [2]. The photoreactions of 2-substituted (cyano- or isocyano-) phenols were found to have many similarities: (i) OH bond cleavage, yielding a 2-substituted (cyano- or isocyano-) phenoxy radical and an H-atom, (ii) recombination of the detached H-atom, resulting in an oxo tautomer, and (iii) decomposition leading to fulvenone, together with HCN and HNC (Fig. 1). All photoproducts were identified by comparing their observed IR spectra with those computed at the B3LYP/6-311++G(d,p) level. The mechanistic analysis of the photochemistry occurring in the family of the title compounds will be discussed.

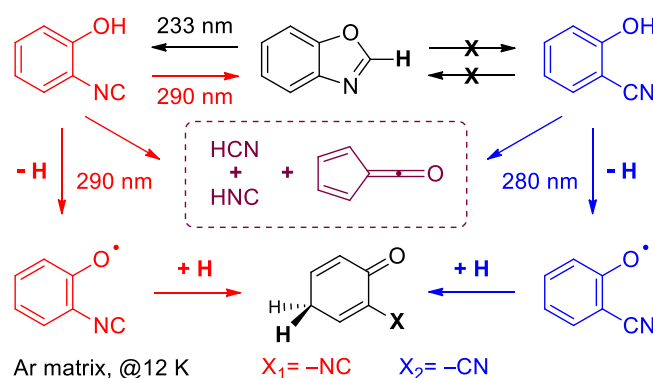


Fig. 1. UV-induced photochemistry of monomeric 2-isocyanophenol (top-left, red), 1,3-benzoxazole (top-centre, black), and 2-cyanophenol (top-right, blue) isolated in cryogenic argon matrix.

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Presentation Method: Oral

## Ab-Initio Study Aiming Some Spectroscopic and Electronic Properties of 2-[(1H-Benzimidazol-1-yl)- Methyl]Benzoic Acid

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Benzimidazole and its derivatives, which have a unique place in heterocyclic chemistry, have attracted great attention in recent years, due to its versatile properties in chemistry and pharmacology. Especially, they are found in the structure of many drugs which have contain a therapeutic effect in many cases, such as antifungal, antimicrobial, anti-inflammatory, anticancer, antiviral, antidiabetic, etc. They can be synthesized from benzoic acid which is the simplest aromatic carboxylic acid. These compounds, consisting of benzoic acid as a functional group, can provide the formation of a metal-organic structure leading to create supramolecular networks. More recently, in order to be candidates for forming coordination polymers with different metal ions, 2-[(1H-benzimidazol-1-yl)methyl]benzoic acid compound (C<sub>15</sub>H<sub>12</sub>N<sub>2</sub>O<sub>2</sub>) has been synthesized by a condensation reaction of benzimidazole and 2-(bromomethyl) benzonitrile in acetonitrile followed by hydrolysis process [1]. In this study, our main aim to characterize the title molecule of C<sub>15</sub>H<sub>12</sub>N<sub>2</sub>O<sub>2</sub> by using quantum chemistry computational method. We have performed *ab-initio* simulations to determine the quantized energy levels of molecules, ions or nuclei, which enable to obtain its structural parameters and, some spectroscopic, electronic and thermal properties. The compound is optimized by using *ab-initio* method based on the density functional theory (DFT)/B3LYP with 6-31G(d,p) basis set [2] implemented in Gaussian 09W subprogram [3]. The geometric parameters of bond length, bond angle and dihedral angle computed are in good agreement with those of available experiment [1]. The same basis set and computational method have been utilized for the vibrational spectra of the title compound by using the optimized structure. The marking of the vibrational frequencies of the molecule have been carried out via the VEDA4 program (Vibrational Energy Distribution Analysis) [4]. The title molecule has 31 atoms and 87 fundamental vibrational modes, with the most bending vibrations. Since experimental chemical shifts are generally obtained in DMSO (Dimethyl Sulfoxide) and Acetonitrile solutions, the <sup>1</sup>H and <sup>13</sup>C NMR chemical shifts of the molecule in the same solutions are computed by using the Gauge-Independent Atomic Orbital (GIAO) approach applying DFT/B3LYP method with the basis set of 6-31G (d,p). Moreover, UV-Vis spectral analyzes of the studied molecule have been investigated in both of the DMSO and Acetonitrile solvents. The maximum absorption peaks of compound have been evaluated by the Time Dependent Self-Consistent Field (TD-SCF)/DFT/B3LYP/6-31G(d,p) method. A single absorbance without any shoulder at 257 nm in both solvents have been observed. At last, electronic properties such as chemical hardness/softness, ionization potential, highest occupied molecular orbital (HOMO)-lowest unoccupied molecular orbital (LUMO) energy levels, electronegativity and energy bandgap have been predicted. The calculated value of the energy bandgap is nearly consistent with the value of experiment measured from absorption spectra as 4.6 eV. This large band gap may arise due to the high  $\pi$ -conjugated polarization of this molecule. Our results from DFT calculations not only aid in the interpretation of available experimental data, but also illuminate the spectroscopic and electronic properties of the title molecule in detail. In the future, our theoretical study may lead to performing experimental studies aiming to characterize the molecule.

**Keywords:** Benzoic acid, DFT, vibrational spectroscopy, UV-Vis and NMR spectral analyzes,

## Acknowledgements

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<b>Presentation Method: Oral</b>
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## Sterilization Studies of Hydrogel Nanocomposites Designed for Biomedical Applications Before *in vivo* Research

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As it is known, mechanically strong hydrogels with anisotropic orientation and bioactive properties can be used as implants or scaffolds for many biological tissues such as skin, muscle, and cartilage [1]. It is necessary to determine the most suitable sterilization method before *in vivo* studies for such hydrogels whose original syntheses have been made, structure characterizations have been completed, and their 3D properties have been examined in detail.

In this study, a series of (N=1-6 coded) hydrogel nanocomposites have been focused on, whose pioneering research has been completed [2]. For these novel composites to be used in *in vivo* studies, it was determined, which of the physical sterilization methods met the expected biophysical functions without damaging the structure of the material.

UV, X-Ray, and Gamma Rays were used in physical sterilization methods. The use of these electromagnetic waves, which have three different energies, brings different advantages and disadvantages. While it is possible that energetic rays can penetrate deeply into the structure, it is also aimed not to cause damage to the material at the atomic and molecular level. In addition, it is previewed that during the irradiation process, the emergence of new nano-formations in the structure and the new structure arrangements formed during the irradiation process may positively change the properties of the material. Nanoscopic analyzes of the materials used before and after irradiation were investigated by SAXS-WAXS (X-ray Small and Wide Angle Scattering) and SEM methods. The 3D *ab-initio* electron density morphologies DAMMIN[3] obtained by Indirect Moore's Method were given in Fig.1 in comparison with the real structure model (for composite sample N:3).

As a result, it was determined that in the nano-scale structure; the closest structural change to the control group occurred with UV sterilization, deterioration in the structure occurred due to the effect of gamma rays, and in X-rays applications. Crystallite morphologies formed more compact structures that would increase the mechanical properties of the material.

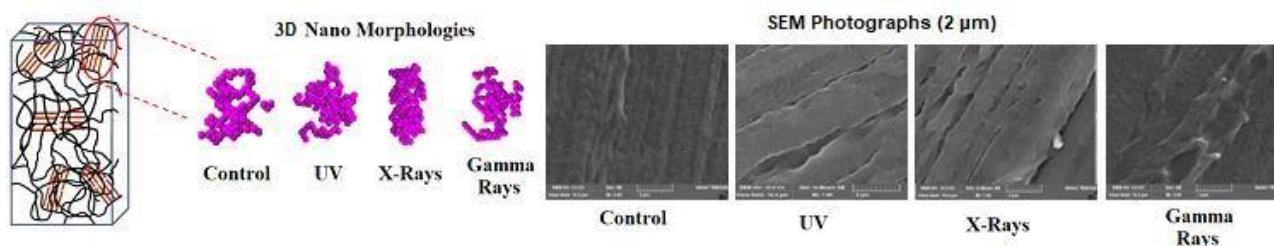


Fig. 1. Comparison the effects of different sterilization processes (N:3 composite) on nano-microstructure

**Keywords:** Hydrogels, sterilizations, nanostructures, X-ray Studies, Biofilm formations

**Acknowledgements** This study was supported within the scope of Hacettepe University, BABK project (FHD-202018669) and G.B. Sekitmen's doctoral work is also related to gaining experience in nanoscopic analysis.

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<b>Presentation Method: Oral</b>
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## Synthesis, Characterization, Experimental and Theoretical Investigation of Spectroscopic Properties of Schiff Base Molecules

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Schiff bases are a group of chemical compounds that were first synthesized by H. Schiff[1] and attracted attention in fields such as chemistry, biology, pharmacy, and medicine. Due to the ligand properties of Schiff bases and the high number of coordination they can make with metal, studies have been on them for many years and their widespread use and activity still keep the interest in these compounds alive.

Schiff bases are obtained by reaction with primary amines in the presence of aldehydes or ketones. The first step of the Schiff base synthesis, which takes place in two steps, is the condensation of the carbonyl carbon and the primary amine. In the second step, Schiff base is formed over the intermediate product.

Whether the transition from the carbonyl compound to the Schiff base occurs or not can be examined with the help of thin layer chromatography during and at the end of the reaction. In IR spectroscopy, it can be seen that the carbonyl band disappears during the synthesis and is replaced by the imine group band [2]. In NMR spectroscopy, the configuration, conformation, and constitution changes can be observed clearly. In addition, theoretical characterization and optimization studies support experimental studies and contribute significantly to the elucidation of the synthesized molecule.

In this study, in order to carry out the reaction of acetone and isophorondiamine (IPDA) Schiff base, the mixture is stirred under reflux at 70 °C with a magnetic stirrer for 5 hours and then left to crystallize at room temperature. The crystals obtained are washed with cold ethanol, dried and examined.

The main aim of the study is to synthesize the compounds experimentally and to clarify these compounds correctly, to compare the experimental and theoretical spectroscopic properties of the molecules as well as to examine the physicochemical properties.

**Keywords:** Schiff Bases, spectroscopy, physicochemical properties

### References

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**Presentation Method: Oral**

## Electronic Structure and Nonlinear Optical Properties of 1-Butyl-3-Methylimidazolium Dicyanamide Ionic Liquid

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The electronic structure, spectroscopic features, polarizability, and first-order and second-order hyperpolarizabilities of 1-butyl-3-methylimidazolium dicyanamide (BmimDCN) ionic liquid have been explored via density functional theory modeling at M06-2X 6-31G(d), M06-2X 6-311++G(d,p), and M06-2X aug-cc-PVTZ levels. The frontier molecular orbitals, electrostatic potential surface, and electron density difference maps have been obtained to visualize the electrostatic characteristics. Interionic interactions have been characterized through reduced density gradient method to reveal and distinguish hydrogen bonding and other non-covalent interactions. The hyperpolarizability calculations indicate that BmimDCN has a significant potential to be used in electro-optics Pockels effect, second-harmonic generation, and electro-optical Kerr effect applications.

**Keywords:** BmimDCN; Ionic liquid; Hyperpolarizability; DFT

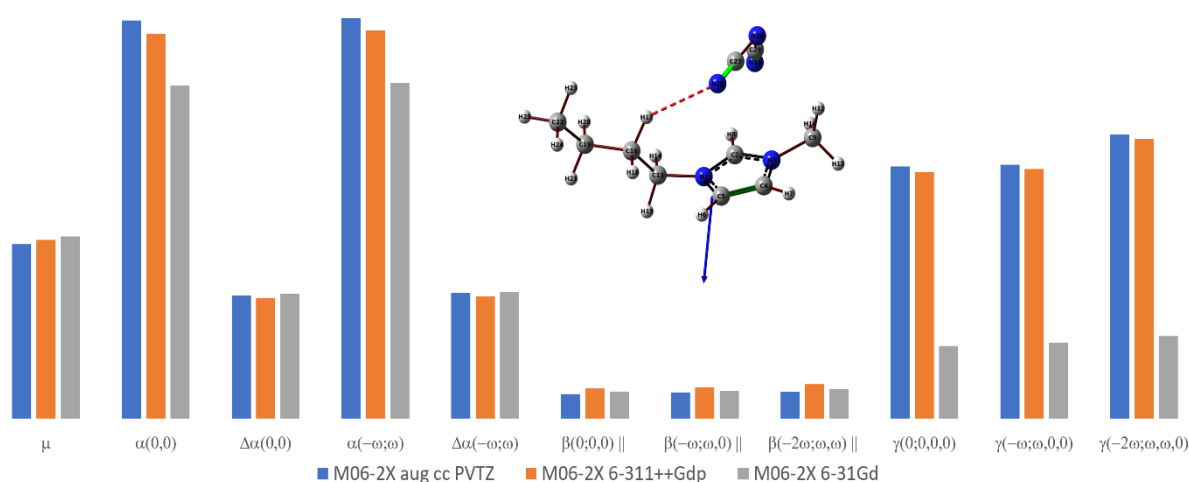


Fig. 1: The permanent electric dipole moment, linear electric polarizability and polarizability anisotropy, static and frequency-dependent first-order and second-order hyperpolarizabilities of 1-butyl-3-methylimidazolium dicyanamide obtained at M06-2X 6-31G(d), M06-2X 6-311++G(d,p), and M06-2X aug-cc-PVTZ levels.

### Acknowledgements

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**Presentation Method: Oral**

## Non-Invasive Spectroscopic Profiling of Spent Embryo Culture for Predicting the Cell Free DNA Content of Embryos in Women Undergoing *in vitro* Fertilization

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Embryonic DNA is frequently detectable in blastocoel fluid of blastocysts and in spent embryo culture media of embryos during *in vitro* fertilization (IVF) treatment. In this study it was aimed to determine if metabolomic profiling and cell free DNA content of embryo culture media (ECM) show differences between day 3 and day 5 embryos. The metabolomic analysis of the embryo is made by detecting the specific substances consumed around the culture medium or the metabolites secreted from the embryo into the culture medium. Since the midIR spectrum represent the whole “-omics” of a biological sample well, FTIR spectroscopy can be used to obtain a fingerprint pattern of metabolites that could differentiate and classify samples. A total of 21 patients scheduled for IVF with single embryo transfer were included in the study. Spent culture media samples collected from day 3 and day 5 embryos. After the embryos were removed from the culture and snap frozen in liquid nitrogen, the spent culture media were stored at -80 °C until analysis. Before analysis, the samples were thawed at room temperature (21°C). The ECM samples were analyzed in the 4000–450 cm<sup>-1</sup> spectral region by Attenuated Total Reflectance Fourier Transform Infrared (ATR-FTIR) spectroscopy. The spectra were preprocessed by calculating the second derivative (using Savitzky-Golay method with 9-point smoothing) in the regions 2800–3000, 1480–1800, 1200–1480 and 800–1200 cm<sup>-1</sup>. These preprocessed FTIR data from ECM samples were subjected to multivariate analyses by the unsupervised pattern recognition techniques such as hierarchical cluster analysis (HCA) and principal component analysis (PCA). The present study indicated the successful discrimination of ECM samples using ATR-FTIR spectroscopy in combination with chemometric approaches. PCA loading plots are the spectral origin of the variations which differentiate the data groupings according to the wavenumbers. The bands at 1170, 1122, 1046, 1033 and 835 cm<sup>-1</sup> contribute to the separation of day 3 and day 5 embryos culture media. The peak at 835 cm<sup>-1</sup> which is assigned to A- and B-form helix conformation of DNA contribute strongly for this clear separation of the groups. PC1 represents 67% of the explained variance and allows the discrimination between the groups in 800–1200 cm<sup>-1</sup> region, while it represents 74% of the explained variance in 800-960 cm<sup>-1</sup> spectral region with only strong contribution of the so-called DNA peak. The discovery of DNA within the blastocoel fluid of blastocysts and in embryo culture media has led to development of non-invasive methods of preimplantation genetic testing. The differences in DNA content of culture media may foresee the amount of the DNA on the day 3 and day 5 embryos and also predict the aneuploid cells. The results of this preliminary study will shed light on further studies to assist embryo selection.

**Keywords:** ATR-FTIR spectroscopy, embryo culture medium, multivariate analysis, PCA, HCA.

**Presentation Method: Oral**

## What We Can Learn from Infrared Spectra About the Structurally Flexible Molecules in Liquids and Solutions with Quantum Chemical Computations

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Tautomeric and conformational transformations and hydrogen bonding are the important phenomena in organic chemistry and biology. As any variations of the tautomeric/conformational state and H-bonding of compounds are reflected in their vibrational spectra, IR spectroscopy is one of the most sensitive spectroscopic techniques used for the structural analysis of H-bonded systems. To derive information about structural forms present in a sample and estimate their relative abundance, input is required from quantum chemical calculations at computational levels that match the experimental resolution and accuracy. The latter condition is achievable in most cases of gas-phase studies, but it is very problematic for the condensed state, especially for compounds forming hydrogen bonds with their environment. Recently [1] we have proposed an efficient protocol for accurate quantum mechanical simulation of IR spectra of such systems, in which (i) structural ensembles for the system under consideration are computed with the use of the recently developed efficient CENSO protocol to implicit quantum mechanical modeling of non-rigid molecules in solution [2]; (ii) Boltzmann populations calculated with CENSO for each implicitly solvated single tautomer/conformer are used to weight the IR spectra of such species explicitly solvated by the first shell of solvent molecules. An automated cluster generation algorithm was applied to construct these clusters that were re-optimized at a reasonable but efficient level of DFT [3]. Herein we will demonstrate by both published and yet unpublished examples of molecular [4] and ionic [5] liquids, and various solutions of structurally flexible compounds, an accuracy of such IR spectra simulations and efficiency of their use for interpretation of the corresponding experimental spectra.

**Keywords:** IR spectra; quantum chemistry; condensed state; conformers; hydrogen bonding

### Acknowledgements

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**Presentation Method: Oral**

## A Contribution to AH-B Sweetness Theory: Theoretical Infrared and Raman Spectroscopic Investigation on Artificial Sweetener Alitame

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Molecular nature of sweetness is of particular importance due to it is strongly connected to diseases such as diabetes, hyperlipemia, hypoglycemia etc. There is still no consensus explaining the sweetness of compounds and how this is related to the molecular structures. According to a study by Guley and Uhing [1], a sweetener should have a proper molecular shape and electronic configuration to bind itself to a receptor and it also should be miscible in the chemical surrounding related receptor. Earlier studies focused on finding specific glucophores, i.e., specific atoms or group of atoms that could impart sweetness of molecules. In 1914, Cohn proposed that a molecule should contain specific structural groups called ‘sapophores’. According to Cohn, molecules containing several hydroxyl groups and those containing chlorine atoms are often sweet [2,3]. Importance of the presence of a hydrogen bond donor (AH) and a hydrogen bond acceptor (B) spaced 2-4 Å was previously defined [4] and our findings of these distances are between 2.2 and 3.6 Å which are in line with this data [4]. Up to our knowledge, our work is the first report of vibrational spectra (Infrared and Raman) and optimized geometric structure of alitame by quantum chemical computations (Fig. 1). We found a strong hydrogen bond (1.702 Å) between aspartic moiety backbone-side chain and C=O-OH portion. We recently reported that the dihedral angle ( $-19.4^\circ$ ) between  $H_{36}-N_6-N_7-H_{41}$  and two adjacent C=O groups might be responsible for the sweetness of alitame [5]. Here, we report that related dihedral angles of alitame could be linked to the sweetness.

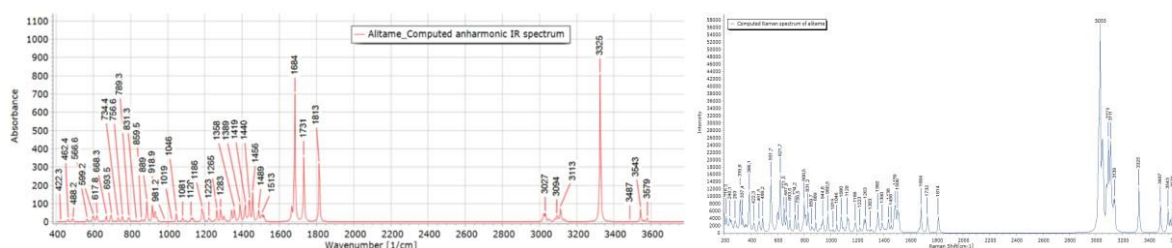


Fig. 1. Computational vibrational spectra of alitame (left: IR spectrum, right: Raman spectrum).

**Keywords:** Alitame, AH-B sweetness theory, DFT, artificial sweetener, IR spectroscopy, Raman spectroscopy

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**Presentation Method: Oral**



## Computed Vibrational Spectra of Hexamethylenetetramine and Its Derivatives

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This work is relevant to the hexamethylenetetramine (HMT) that may form organic compounds in interstellar medium. Organic compounds can be synthesized in laboratories and modeling the energetic and thermal processing of interstellar ice analogs. HMT (C<sub>6</sub>H<sub>12</sub>N<sub>4</sub>) is one of these organic compounds [1-4]. The exogenous distribution theory, which states that organic molecules were carried to the early earth surface by joining comets and asteroids. HMT is a key source of C-N moieties for the synthesis of organic compounds in this environment [5-6]. Theoretical IR and Raman spectroscopy investigations on HMT and some derivatives (HMTCONH<sub>2</sub>, and HMTCOOH) were performed in this study. Infrared (IR) and Raman spectra for HMT and its variants were computed using Gaussian 09 software by DFT/B3LYP theory level with the 6311++G(d,p) basis set. This work was carried out on Mars, Mercury, and Venus conditions in various pressure and temperature settings. Figure 1 shows comparative IR spectra of HMT and its variations under such conditions. This study contributes vibrational spectra of organic compounds which might be detected at such planetary environments.

**Keywords:** Hexamethylenetetramine, IR spectroscopy, Raman spectroscopy, planetary geology.

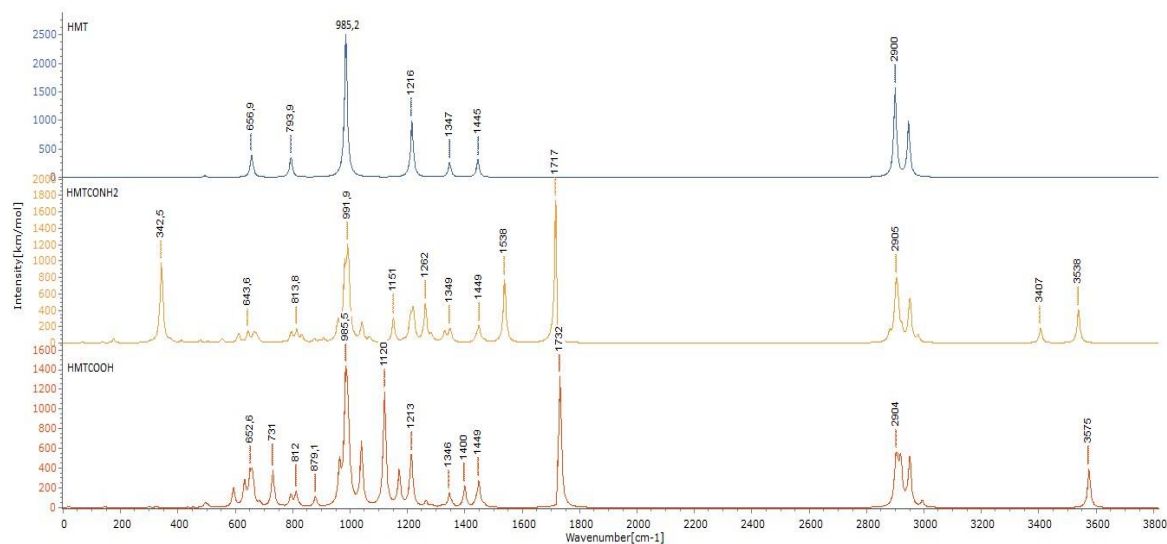


Fig. 1. Comparative IR spectra of HMT and its selected derivatives.

### Acknowledgements

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**Presentation Method: Oral**

## Bonding and Molecular Surface Analysis of Actinide Carbides

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Actinide carbides are supposed to be the form of nuclear fuel for IV. generation nuclear reactors. In addition to this potential use, the compounds of actinides have special attraction due to their unique property related to highly relativistic effect. Therefore, they are subject to experimental and theoretical studies extensively [1]. In this study, actinide carbides ( $AnC$  and  $AnC_2$ ) were studied by using TPSS functional of Density Functional Theory [2]. Orca 5 [3] and Gaussian 09 [4] quantum chemical program packages were used to optimize the structures. The optimized structure of  $CmC_2$  is given in Fig.1. As seen from the figure,  $CmC_2$  has the structure with  $C_{2v}$  symmetry. Although other  $AnC_2$  compounds have similar structures, there is no systematic change as a function of actinide Z. However, the Mulliken charge of actinide decreases with Z as expected. The optimized structures have been analyzed for bonding and molecular surface analysis by using Multiwfn 3.8 [5]. Bond orders and some QTAIM parameters [5] obtained from this package were also analyzed to get an insight for their variation across the f block. Several bond order models give contradictory results which can be explained in their own definitions. Electron density at the bond critical points shows that some An-C bonds have partially ionic character in contrast to others fully covalent character. Molecular surface analyses were also done by using Multiwfn 3.8 [5]. The variation of molecular volume, surface, and molecular surface electrostatic potentials as a function of atomic number were interpreted for the estimation of some physical properties. Molecular polarity index and internal charge separation values decrease with Z of actinide in correlation with Mulliken charge.

**Keywords:** Actinide; QTAIM; Molecular Surface Analysis; Bond Order, DFT.

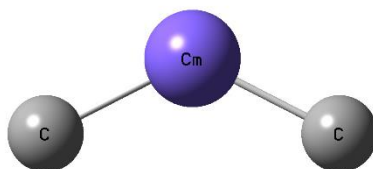


Fig. 1. The optimized structure of  $CmC_2$ .

### Acknowledgements

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