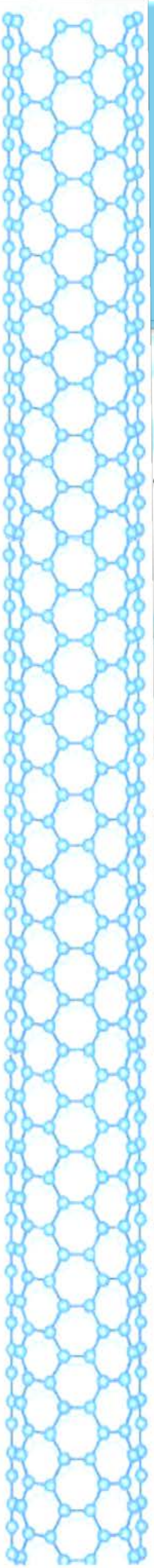

TUCr2014
4th NATIONAL CRYSTALLOGRAPHIC MEETING
With International Participation

ABSTRACT BOOK

17-19 May 2014
Dicle University, Diyarbakır / Turkey

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PREFACE

With international participation 4th National Congress of Crystallography (TUcr2014) hosted by Dicle University in Diyarbakir will be held between 17 and 19 May 2014 under auspices of Dicle University and National Crystallography Association. 2014 has been declared as the International Year of Crystallography by UNESCO, United Nations that gives more to gain importance to this meeting.

The aims of this meeting are bring scientists who are working in this area together and to supply various discussions by playing important role about crystallography. To realize these aims, novelties will be shared with presentations made by invited national and international scientists who are expert in their research area.

The meeting intends to multi discipliner works in the areas of; Physics, Chemistry, Biology, Material science, Pharmacy, Molecular Structure, Molecular Interaction and Chemical Properties in different fields of science, Crystallographic and Chemical Calculations, Macromolecular Crystallography, X-Ray Powder Diffraction Applications, Crystal Engineering and Supramolecular Structures, Mineral and Inorganic Crystallography Material Science, SAXS, Nano Crystallography.

For this purpose expert scientists were invited from Turkey and abroad; Mohamed Bououdina, The Bahrayn University, Bahrain, Lars Eriksson, University Of The Stockholm, Stockholm Sweden, Ferdi Karadaş, Bilkent University, Ankara, Engine Kendi, Hacettepe University, Ankara, İhsan Kılıç, Taek, Ankara, Mustafa Köksal, Izmir Institute Of Technology, Izmir, Maryam Ranjbar , İrost, Tehran, Iran, Emrah Özensoy, Bilkent University, Ankara, C.L. Azanza Ricardo University Of Trento, Trento, Italy, Abdelmalek Thalal, Marrakech University, Marrakech, Morocco, Paolo Scardi, Trento University, Trento, Italy, Dinçer Ülkü, Hacettepe University, Ankara, Omar Yavaş, Ankara University, Ankara, Fikret Yildiz, Gebze Institute Of Technology, Kocaeli, Hilmi Yurdakul, Dumlupınar University, Kütahya. I thank to the esteemed scientists who were accepted our invitations participates our meeting.

Our meeting includes 12 oral presentations and 114 poster presentations determined by the Board of Science among the participants. For this purpose, our presentation will begin at May 17, 2014 morning with opening program and will continue until noon session at May 19, 2014, sessions will end with our closing program.

We especially thank to the Dicle University Rector Prof. Dr. Ayşegül Jale Saraç for with material and moral support to the meeting, DUBTAM Manager and Coordinator of DUBAP Prof. Dr. Hamdi TEMEL, the Diyarbakir Governor's Office with financial support, Diyarbakir Chamber of Commerce and Industry, TUBITAK, TAEAK, Bruker, Nanospek, Anton Paar, Turgut Laboratory would like to thank the companies.

I hope that TUCR2014 Crystallographic Meeting is useful for all paticipant.

Ömer ÇELİK

Chair of Organizing Committee

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Mohamed Bououdına	Bahrain University	Bahreın
Lars Erıksson	Stocholm University	Sweden
Ferdi Karadaş	Bilkent University	Ankara, Turkey
Engin Kendi	Hacettepe University	Ankara, Turkey
İrfan Koca	TAEK	Ankara, Turkey
Mustafa Köksal	Izmir Institute Of Technology	İzmir, Turkey
Maryam Ranjbar	IROST	Teheran, Iran
Emrah Özensoy	Bilkent University	Ankara, Turkey
C. L. Azanza Rıcardo	Trento University	Trento, Italy
Abdelmalek Thalal	University Cadi Ayyad	Marrakech, Morocco
Paolo Scardi	Trento University	Trento, Italy
Dinçer Ülkü	Hacettepe University	Ankara, Turkey
Ömer Yavaş	Ankara University	Ankara, Turkey
Fikret Yıldız	Gebze Institute of Technology	Kocaeli, Turkey
Hilmi Yurdakul	Dumlupınar University	Kütahya, Türkiye

SCHEDULE

17 MAY 2014 SATURDAY	
08:30 -9:00 09:00-09:40	**Registration** **Opening Ceramony**
I. Session	**Chair** Süheyla Özbey
09:40-10:30	Invited Speaker **Engin Kendi**, Hacettepe University 100 Years of Crystallography and Paris Meeting
10:30-10:50	**Coffe Break**
II. Session	**Chair / Co Chair** Orhan Büyükgüngör /Hümeyra Paşaoğlu
10:50-11:40	Invited Speaker **Abdelmalek Thalal**, Marrakech – Morocco *Symmetry in Art and Architecture of the Western Islamic World*
11:40-12:30	Invited Speaker **Dinçer Ülkü**, Hacettepe University *Crystallography: From Past to Present*
12:30-13:30	**Meeting Photo and Lunch**
III. Session	**Chair / Co Chair** Dinçer Ülkü / Sevgi Bayarı
13:30-14:20	Invited Speaker **Paolo Scardi**, Trento University, Italy *Powder diffraction study on nanocrystalline metal catalysts*
14:20-14:40	Oral Presentation **Haluk Koralay**, Gazi University *The Investigation of Microstructural Properties of Cu0,2Bi1,8Sr2Ca2Cu3-xZnxO10+δ Ceramic Structure*
14:40-15:00	Oral Presentation **Mehmet Fatih Danışman,** METU *Helium Diffraction Studies of Organic Thin Films on Metal Surfaces*
15:00-16:00	**POSTER SESSION**
IV. Session	**Chair / Co Chair** İrfan Açıkgöz /Yusuf Selim Ocak
16:00-16:50	Invited Speaker **Emrah Özensoy,** Bilken University Analysis of Single Crystal and Ultrathin Film Surfaces via Surface Sensitive Spectroscopic and Diffraction Techniques
16:50-17:10	Oral Presentation **Mehmet Büyükyıldız**, Yalova University *Analysis of coloration in stainless steels, combined with the method of MIG brazing, via XRD and SEM*
20:00-22:00	**Dinner**

18 MAY 2014	**SUNDAY**
I. Session	**Chair / Co Chair** Leyla Yıldırım / Mehmet Aslantaş
08:30 -09:20	Invited Speaker **Ferdi Karataş,** Bilkent University Crystallization Techniques in Metal-Cyanide Chemistry
09:20-10:10	Invited Speaker **Mustafa Köksal,** İzmir Institute of Technology Expanding the Structural Biology of Terpenoid Biosynthesis: From Taxol® to Methylisoborneol & More
10:10-10:30	Oral Presentation **Didem Sutay Kocabaş,** Karamanoğlu Mehmetbey University Crystallization of Scytalidium thermophilum Xylanase by Vapor Diffusion
10:30-10:50	**Coffe Break**
II. Session	**Chairman / Co Chairman** Rıdvan Durak / Cengiz Arıcı
10:50-11:40	Invited Speaker **Fikret Yıldız,** Gebze Institute of Technology *Investigation of Non-collinear Magnetic Configuration in Exchanged Coupled Multilayered Structure*
11:40-12:00	Oral Presentation **Mustafa Öztürk,** Gebze Institute of Technology Structural and magnetic properties of exchange biased Pt/Co/(Pt,Cr)/CoO multilayers
12:00-12:30	Oral Presentation **Yusuf Selim Ocak**, Dicle University Investigation of Nanostructured Coated Oxides Films by X-Rays, UV-Vis-IR and AFM
12:30-13:30	**Lunch**
III. Session	**Chairman / Co Chairman** Ahmet Erdönmez / Betül Kaynak
13:30-14:20	Invited Speaker **Lars Eriksson,** Stockholm University Electron density determinations using in-house instrumentation
14:20-14:40	Oral Presentation **Barış Alkan**, METU Synthesis and characterization of selenium-doped hydroxyapatite as therapeutic bone substitute
14:40-15:00	Oral Presentation **Irmak Karaduman**, Gazi University Selective Carbon Monoxide Schottky Diode Gas Sensor
15:00-16:00	**POSTER SESSION**
IV. Session	**Chairman / Co Chairman** Mehmet Akkurt /Oral Oltulu
16:00-16:50	Invited Speaker **Ömer Yavaş**, Ankara Universityy *Türk Hızlandırıcı Merkezi Işınım Kaynağı Tesisleri ve Araştırma Potansiyelleri*
16:50-17:40	Invited Speaker **İhsan Kılıç,** TAEK SESAME and the TAEA's Support Policy
17:40-18:30	**Visit to Dicle University of Science and Technology Application and Research Center**
20:00-22:00	**Dinner**

19 MAY 2014	**MONDAY**
I. Session	**Chairman / Co Chairman** Engin Kendi /Mühittin Aygün
08:30 -09:20	Invited Speaker **Hilmi Yurdakul,** Dumlupınar University *Some Applications of Electron Diffraction in Scanning and Transmission Electron Microscopy*
09:20-10:10	Oral Presentation **Semra İde**, Hacettepe University *Nanoscale Structural Analysis of a self assembled liquid crystal system and Sulfonated Composite Proton Exchange Films*
10:30-10:50	**Coffe Break**
II. Session	**Chair / Co Chair** Muharrem Dinçer /Numan Akdoğan
10:50-11:40	Invited Speaker **Maryam Ranjbar,** IROST, Tahran Synthesis and characterization of Cu(II) and Pb(II) supra molecules: new precursors for CuO and PbO nanoparticles
11:40-12:00	Oral Presentation Molecular Structure, Electrochemical Properties and Theoretical Spectroscopic Studies on 2'-Hydroxyl-4''-Dimethylaminochalcone **Çağlar Karaca,** Celal Bayar University
12:00-12:30	**Closed Ceramony**
13:00-18:00	**Trip:Diyarbakır City**

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TABLE OF POSTER PRESENTATIONS

PRESENTATIONS OF INVITED SPEAKERS

100 Years of Crystallography and Paris Meeting

Engin Kendi*

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The year 2014 has been declared by the United Nations as the International Year of Crystallography (IYCr2014) . The year is being organized by jointly by the IUCr and UNESCO. The idea of an IYCr originated in the centennials af the famous experiments carried out by Max von Laue and father and son Braggs in the second half of 1912 and early 1913. IYCr2014 has been declared to celebrate 100 years of success following the first Nobel prize related to crystallography, awarded in 1914 to Max von Laue. IYCr2014 started with the Opening Ceremony on January 20-21, 2014 at the UNESCO Building in Paris. As mentioned many speakers; even though crystallography underpins all the sciences today, it remains relatively unknown to the general public. One aim of the Year will be to promote education and public awareness through a variety of activities.

Symmetry in Art and Architecture of the Western Islamic World

Abdelmalek. Thalal, Y. Aboufadil*

Faculty of Sciences – University Cadi Ayyad – Marrakech – Morocco

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Since the conquest of Andalusia by the Arab-Berber Muslim and the establishment of the Umayyad Caliphate in Cordoba the 8th century until the fall of Granada in the 15th century, the history of the Maghreb was closely linked to that of Andalusia.

The mixing of populations of different ethnic groups gave birth to a civilization, which spread throughout the world by its science and culture. This brilliant civilization has particularly favoured the development of an original, rich and varied art that integrated geometry in the construction of complex patterns that appear on the architectural ornament. This highly stylized form of Moorish art has evolved over centuries from simple to complex geometric drawings, involving a high degree of symmetry.

The Great Mosque of Cordoba, the madrassas (schools) of Fez and the Alhambra Palace the wonder Moorish architectural, are so many historic buildings that reflect the development of art and architecture during the golden age of the western Islamic world.

After the fall of Granada, Moorish decorative art continued to flourish in Maghreb especially in Morocco. In the late of 80s, the King Hassan II gave new impetus to this ancestral art by building the Great Mosque in Casablanca. Academic research on Moroccan geometric art from the viewpoint of crystallography is also conducted in the Moroccan universities.

Analysis of the Moroccan geometric patterns reveals that, despite of their great diversities, all the 17 crystallographic groups are not presents in the ornamental art. Our recent works (Aboufadil et al, 2013) show, that it is possible to generate the missing groups (Figure 1), by using craftsmen rules (Thalal et al, 2011), and symmetry laws.

Furthermore, the similarity between the zellige panel (fine mosaics) found in the Madrasa (school) Attarine in Fez constructed in the 14th century, and the quasicrystal structure discovered by D. Shechtman (1984) aroused our interest for this type of symmetry (Figure 2). We first describe this panel in term of Penrose tiling (Penrose, 1974), to prove the quasiperiodicity of this pattern. For this, we use the multigrid method developed by De Bruijn (1981) and reformulated by D. Gratias (2002) to obtain a quasiperiodic tiling. We then propose a method of construction of heptagonal, enneagonal, tetradecagonal and octadecagonal quasiperiodic patterns, not encountered in the Moroccan ornamental art Figure 3). These patterns are built from tiling (skeleton) generated by the multigrid method and decorated by motifs obtained by the craftsmen method (Aboufadil et al, 2014).

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Figures

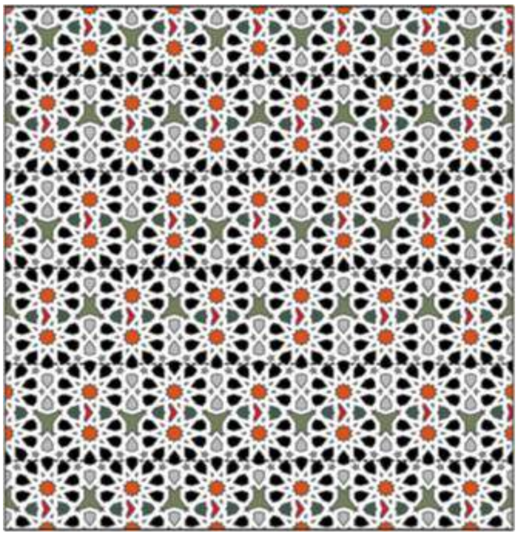
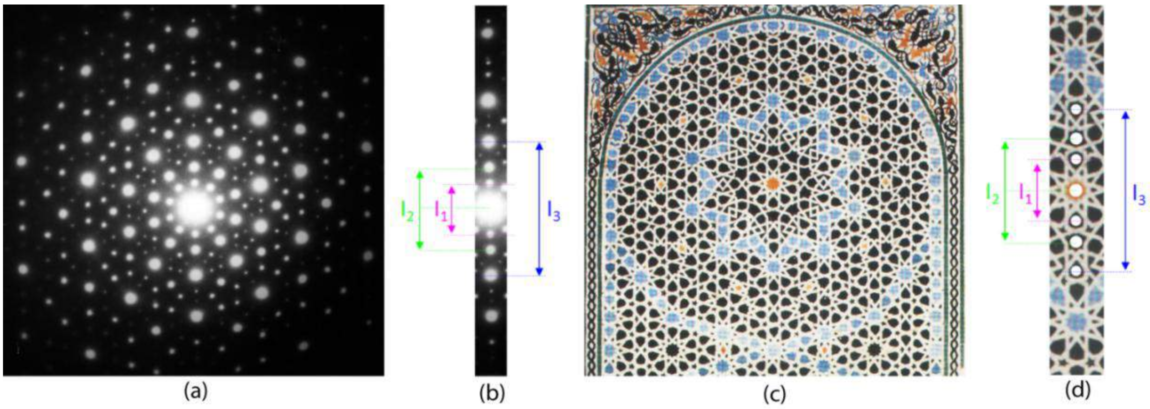


Figure 1: Symmetry group pg



(a) (b) (c) (d)

Figure 2 :

(a) Diffraction pattern of the quasicrystal AlMn (R. Portier)

(c) Quasiperiodic zellige pattern from Madrasa Attarine (Fez)

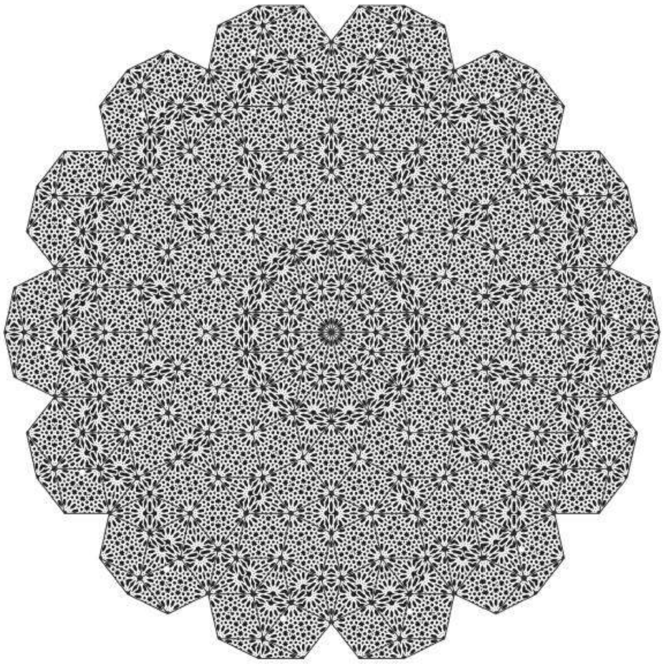


Figure 3 : Tetradecagonal quasiperiodic patterns

Crystallography: From Past to Present

Dinçer Ülkü*

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This presentation will focus on the historical developments in crystallography. Fascinated with the beauty of crystals, mankind always tried to understand their formation, inner structure and properties. In the 16th century, analogy to fruit-bearing plants was used to explain crystal formation. Corpuscular explanations of crystal structure was generally accepted in the 17th century. Physical properties such as double refraction, plane polarization through double refracting crystal, optical activity, law of constant interfacial angles were discovered and used for identification of crystals in the 18th century. Mathematical considerations of crystalline symmetry, together with the discovery of x-rays in the 19th century, has led to the development of a new science. Starting with Max von Laue's x-ray diffraction experiment on crystals in 1912, crystallography evolved into a mature science during the last hundred years. Crystallography studies condensed matter of any origin from the structural point of view at atomic resolution. This is important where structure–property or structure–function relationships play a role. Developments in x-ray sources, data collection techniques and computers paved the road for an extremely important interdisciplinary science which has been crowned so far with 28 Nobel Prizes. Structure determinations of biological molecules constitute the foundation of Molecular Biology. Unfortunately this well established scientific discipline came to Turkey with half a century delay. This presentation includes also a brief history of crystallography in Turkey.

Powder diffraction study on nanocrystalline metal catalysts

Paolo Scardi[1*] and Cristy L. Azanza Ricardo[1]

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Most properties of nanocrystalline materials depend on details of the nanostructure, primarily including size and shape, but also the atomic arrangement of surfaces, which results from the generally different coordination and chemical environment of surface atoms. Nanocrystals are special object for crystallography too: most frequently symmetry rules of corresponding bulk materials are not fulfilled, for the presence of defects (like multiple twinning) or just the very surface of the crystalline domain, which clearly breaks translational symmetry. As a consequence, the study of nanocrystalline materials requires special, dedicated methods, which can only partly be adapted from traditional crystallography.

Understanding the true shape and atomic arrangement in nanoparticles is especially important for metal catalysts, where the reactivity, for example in oxidation processes is directly related to the fine features discussed above. In the present contribution some recent results of an ongoing study on Pd nanocrystals by Synchrotron Radiation X-ray Diffraction are briefly reviewed. A realistic description of the nanoparticles is also necessary to correctly analyze results, and to that purpose atomistic models are used within a Molecular Dynamics approach. The key to success is in the atomic-level modelling of nanocrystals, and proper consideration of multiple techniques in the joint effort to describe the studied systems with the required detail.

Analysis of Single Crystal and Ultrathin Film Surfaces via Surface Sensitive Spectroscopic and Diffraction Techniques

Emrah Özensoy[1*]

[1] *Bilkent University, Department of Chemistry, 06800, Ankara, Turkey*

* ozensoy@fen.bilkent.edu.tr

In this talk, we will focus on understanding the structures of model catalyst surfaces which are comprised of single crystals and ultrathin films using surface sensitive diffraction (e.g. Low Energy Electron Diffraction, LEED) and spectroscopic (e.g. X-ray Photoemission Spectroscopy, XPS) techniques. Two different genres of TiO_2-promoted $DeNO_x$ catalysts with NO_x storage capabilities will be discussed [1-10]. The first genre of catalysts to be discussed is TiO_2-promoted NO_x-Storage Reduction (NSR, or Lean NO_x Traps, LNT) catalysts for automotive applications. [1-6]. Experimental results from ultra high vacuum (UHV) applications on atomically well-defined planar model catalysts [3,4,7] as well as realistic high-surface area (mesoporous) materials [1,2,5] will be combined with theoretical Density Functional Theory (DFT) modeling results [6]. Through these results, surface functionalization of conventional NSR materials (i.e. BaO/Al_2O_3) with TiO_2 is presented as an effective strategy to *"fine-tune"* the surface dispersion of the catalytically active nano-domains, to obtain superior NO_x storage capacity and to enhance tolerance against catalytic sulfur poisoning.

Inspired by the thermally-activated automotive catalysts given above, a second genre of photochemically-activated TiO_2-promoted $DeNO_x$ catalysts will also be presented [8-10]. These novel photochemically activated systems operate under ambient conditions offering a hybrid platform combining thermal catalysis and photocatalysis.

***Keywords*:**Single Crystals, Ultrathin Films, Catalysis, Low Energy Electron Diffraction.

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Crystallization Techniques in Metal-Cyanide Chemistry

Ferdi Karadaş

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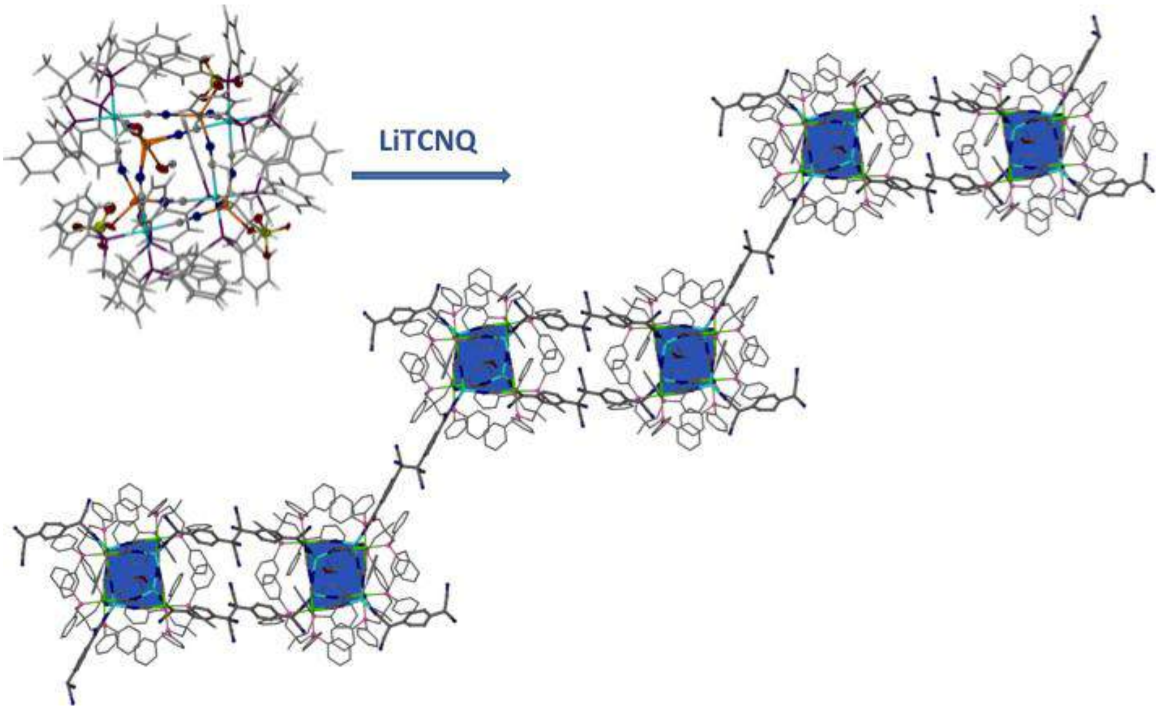
The cyanide ligand is an excellent linker for clusters with interesting magnetic and electronic properties due to its ability to provide an efficient pathway for superexchange between metal centers that are bound in an end-to-end fashion.In addition to their potential applications in magnetism and catalysis, extended cyanometalate clusters have also been investigated for their gas capture capacities due to their microporous behavior.

One of the common synthetic approaches in cyanide chemistry is the incorporation of capping ligands via a building-block approach to prepare cyanide-bridged molecular clusters. Since direct reaction of metal ions with cyanide precursors lead to the formation of a powder product, convenient crystallization techniques should be applied in order to obtain uniform crystals for characterization via X-ray single Crystal technique. Several crystallization techniques used in this field will be introduced. The design, preparation, characterization and magnetic properties of square- and cube-shaped molecular clusters will also be the focus of this presentation.



Expanding the Structural Biology of Terpenoid Biosynthesis: From Taxol® to Methylisoborneol & More

Mustafa Köksal[1*]and David W. Christianson[2]

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Enzymes are the frontrunners of sustainability in nature due to their catalytic efficiency, ease of production, reusability, and biodegradability. Most of the time, however, catalytic capacities of enzymes are restricted to a small range of substrates or products. Their structural features are keys to understanding their advantages, limitations, and potentials. Utilization of the structural and chemical knowledge about enzymes' catalytic mechanisms allows us to inhibit their activity for treatment of a disease, to enhance their activity for more efficient production of a product, or to divert their mechanism to obtain a novel product. Terpenoid biosynthesis exemplifies how enzymes are used in nature to catalyze mechanistically simple or complex reactions in biosynthesis of complex natural products with an astonishing diversity and a wide spectrum of biological activity. RecentX-ray crystallographic structural studies on taxadiene synthase and *ent*-copalyl diphosphate synthase suggested a "modular architecture" for enzymes involved in terpenoid biosynthesis. Later, structural studies on geranyl diphosphate *C*-methyltransferase expanded the frontier to modified precursors and using these precursors for the development of novel terpenoids. In this seminar, results from the studies on structural biology of enzymes involved in biosynthesis of important terpenoids will be presented along with current directions in related fields.

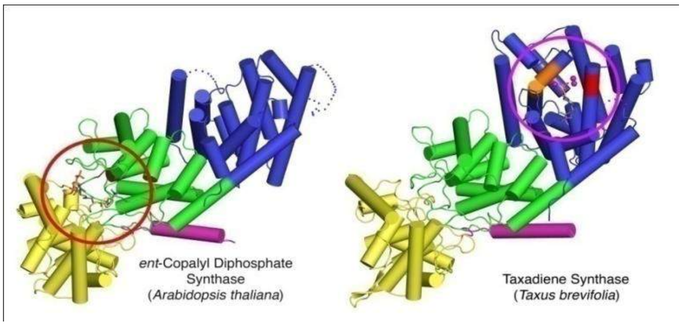

Figure 1. Structures of *ent*-copalyl diphosphate synthase and taxadiene synthase.

***Keywords*:** Macromolecular X-ray crystallography, Protein Structure, Terpenoid Biosynthesis, TerpeneSynthase

Investigation of Non-collinear Magnetic Configuration in Exchanged Coupled Multilayered Structure

Fikret Yıldız

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Magnetic layers separated by non-magnetic spacers have been extensively investigated in last decade due to applications in magnetic data storage and magnetic sensors. In most cases magnetic easy axis is in the direction of the film plane and some cases in the film normal. In this study these structures were combined. The easy axis of the following layers is oriented orthogonally or non-orthogonally. The procedure how to get such magnetic configurations can be found elsewhere [1-3]. This was managed by choosing suitable materials and arranging magnetic anisotropies of the layers. It is expected sensing lower magnetic fields with this kind of magnetic structure [4]. Magnetic properties and orientation of magnetization direction of each magnetic layer have been studied by ferromagnetic resonance (FMR), magneto-optical Kerr effect (MOKE) and soft X-ray resonant magnetic reflectivity (SXRMR). Particularly FMR and SXRMR techniques are layer sensitive and allows figuring out each magnetic layer separately.

Acknowledgements: This work was supported by TUBITAK through the Project no 112T940.

Keywords**:** Magnetic multilayer, Magnetic anisotropy, Non-collinear magnetic configuration, FMR, MOKE, SXRMR

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Electron density determinations using in-house instrumentation

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The electron density distribution of various chemical substances can be obtained with reasonable accuracy using an in-house diffractometer within approximately one day. Ideally one should measure at lowest possible temperature, shortest possible wavelength and to high resolution, at least 0.5 Å. Presently we are aiming at finding partial charges of surface atoms for different solid materials, to be used as input for classical simulations of adsorbance of various small molecules onto surfaces. Several methods have been used for obtaining the deformation density. X(all)-X(high), X-N and multipole refinements. The multipole functions are included in the refinement, thus all reflections can be used in the determination of the deformation density [1]. However even “normal” difference density calculations with traditional least square software as SHELXL [2] can still reveal considerable details of the deformation density. Synchrotron radiation and neutron diffraction may also be of great help in future studies. A short review should be given about the coming MAX4 [3] and ESS [4], both being built in south of Sweden.

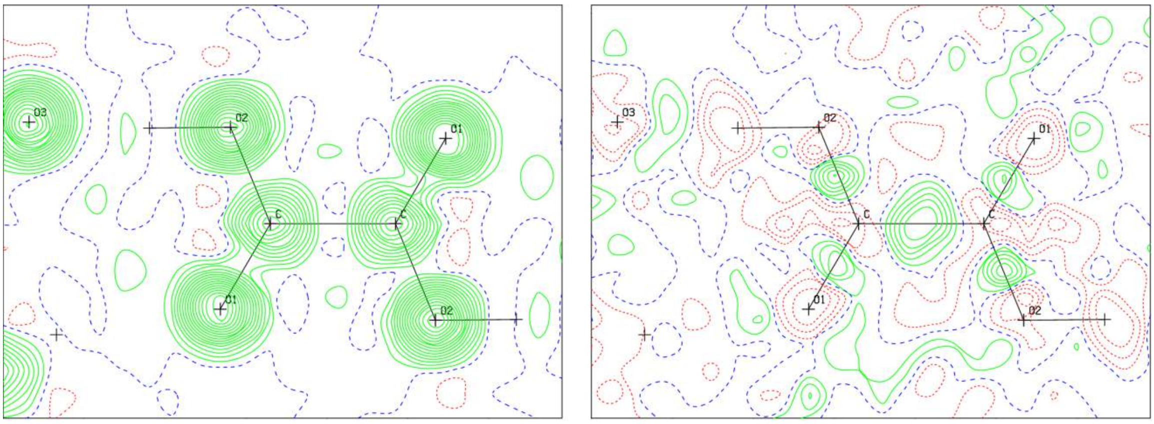

Figure 1. Total density and difference density of oxalic acid dihydrate.

Keywords**:** Electron density, Multipoles, Syncrothron radiation, Neutron diffraction

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Türk Hızlandırıcı Merkezi Işınım Kaynağı Tesisleri ve Araştırma Potansiyelleri

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Türk Hızlandırıcı Merkezi (THM) Projesi çalışmaları konusunda gelinen aşama ve geleceğe yönelik planlamaların yanı sıra proje kapsamında kurulum ve tasarım çalışmaları sürdürülen ışınım kaynağı tesisleri hakkında bilgiler sunulacaktır. Ankara Üniversitesi Gölbaşı Kampüsünde kurulumu devam eden Elektron Hızlandırıcısına dayalı Serbest Elektron Lazeri ve Frenleme Işınımı tesisinin (TARLA) yapısı, Ar-Ge ve uygulama potansiyeli ele alınacaktır. Ayrıca, THM'de yer alması öngörülerek tasarım ve projelendirme çalışmaları sürdürülen 3. nesil ışınım kaynağı olarak Sinkrotron Işınımı (TürkAY) ve 4. nesil ışınım kaynağı olarak SASE Serbest Elektron Lazeri (TürkSEL) tesislerinin yapıları, ana parametreleri, ışınım karakteristikleri ve araştırma potansiyelleri ele alınacak ve bu tesislere yönelik olarak son yıllarda gerçekleştirilen Uluslararası Kullanıcı Konferanslarının sonuçları üzerinde durulacaktır.

SESAME and the TAEA's Support Policy

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Turkey, being one of the founding states of the SESAME (Synchrotron-light for Experimental Science and Applications in the Middle East) International Research Center, fosters the development of scientific cooperation amongst nations through the Middle East and Mediterranean region. Since the approval of Membership, the Turkish Atomic Energy Authority (TAEA) represents our country at the SESAME Council and contributes to the construction and operation of the facility. However, in May 2012 a letter of commitment has been signed by Turkey and three other member states, namely Iran, Israel and Jordan, each to provide 5M USD as a voluntary contribution to the investment budget of the facility, scheduled to be operational by the end of 2015. Meanwhile, the TAEA is providing training and education of young researchers and students as well as the scientific community through schools, user meetings and workshops, etc. And lately, a new support mechanism is being sought for research and training of potential national user community.

Keywords**:** SESAME, TAEA

Some Applications of Electron Diffraction in Scanning and Transmission Electron Microscopy

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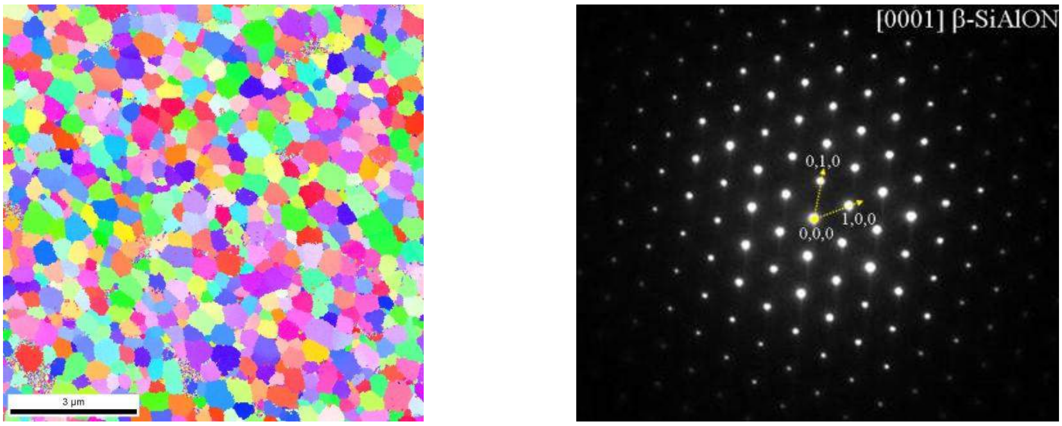
Electron microscopy is a powerful tool to examine crystallographic features down to the nano-scale, and is a crucial technique to research the internal structure of materials. Electron Back Scattering Diffraction (EBSD) is the most popular technique based on the analysis of the Kikuchi pattern through excitation of electron beam on the surface of sample at nano-scale in a scanning electron microscope (SEM). The crystal structure, orientation, texture, grain boundary types and misorientations can be easily acquired by this technique. Currently, nano-scaled precession 3D diffraction tomography and orientation phase mapping similar to EBSD in SEM significantly extend the crystallographic applications of transmission electron microscopy (TEM). Besides, selected area electron (SAE) and nano beam electron (NBD) diffraction routes can be generally used to identify crystal structures and defects as small as several hundred nanometers size. Here, the potential crystallographic applications of electron diffraction techniques at nanometer scale in electron microscopy will be presented.



(a) (b)

Figure 1 (a) EBSD pattern of sintered ZrO_2 ceramic and (b) SAED pattern acquired from the [0 0 0 1] low index zone axis of hexagonal β-SiAlON crystal [1,2].

***Keywords*:** Electron Diffraction, Electron Microscopy, EBSD, SAED, NBED

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Synthesis and characterization of Cu(II) and Pb(II) supra molecules: new precursors for CuO and PbO nanoparticles

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In this study we report crystal structure determination of Cu(II), $[Cu(dmph)\text{-}\mu\text{-}I]_2$ (**I**), {dmph= 2,9-dimethyl-1,10-phenanthroline (neocuproine)} and Pb(II), $\{[Pb(pydc)(pydc.H_2)(H_2O)_2]_2\}_n$ (**I**), where $[pyda.H_2]^{2+}[pydc]^{2-}$ (pyda= 2,6-pyridinediamine, and pydc.H_2= 2,6-pyridinedicarboxylic acid) (**II**), supra molecules. Also **I** and **II** nanostructures have been synthesized by sonochemical methods. Characterization of the compounds were performed by scanning electron microscopy (SEM), X-ray powder diffraction (XRD), FT-IR spectroscopy and elemental analyses, thermal gravimetric (TG/DTA) and the structures were determined by single-crystal X-ray diffraction. The crystal structure of compound **I** has been found to be a binuclear coordination compound while the compound **II** is a polymer. Pure phase CuO and PbO nanoparticles were simply obtained by calcination of nano-sized compounds **I** and **II** at 700 and 600 °C under air atmosphere respectively. This study demonstrates that the supramolecular compounds may be suitable precursors for the simple one-pot preparation of nanoscale metal oxide materials with different and interesting morphologies.

Keywords: Supramolecular; Crystal structure; Nano-structures; Sonochemical method

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ORAL PRESENTATIONS

Helium Diffraction Studies of Organic Thin Films on Metal Surfaces

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Helium diffraction is a very convenient technique for study of soft organic films on metal surfaces due to very low energies of the helium atoms employed. These low energies not only prevent film damage but also cause the helium atoms to scatter only from the topmost layer without any penetration to bulk which result in very high sensitivity to adsorbate coverage and surface corrugation. Here we will present our helium diffraction studies about the low coverage phases of long chain alkanethiolself assembled monolayers (SAMs)and asymmetric disulfide SAMs on Au(111) surface and pentacene thin films on Ag(111) and Au(111) surfaces, grown in vacuum by supersonic molecular beam deposition[1-4]. Crystals structures, phase behaviors and desorption energies of these films determined by helium atom diffraction technique will be discussed.

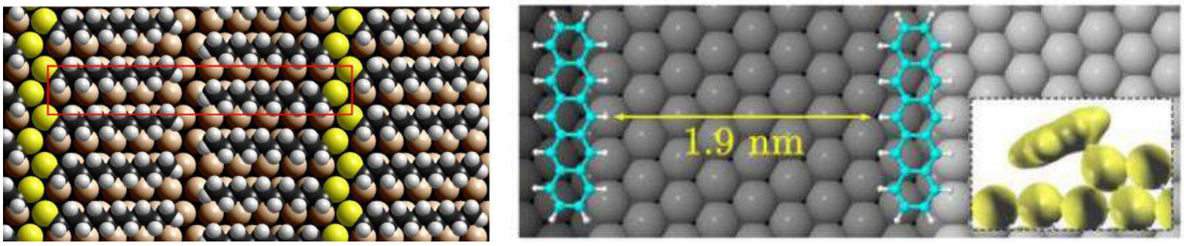

Figure 1. Schematic models of (left) decanethiol SAM on Au(111) and (right) isolated pentacene molecules on Ag(233)

***Keywords*:**Helium diffraction, low energy atom scattering, Ag(111), Au(111), pentacene, self assembled monolayers, self assembled monolayers, organic thin films.

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Analysis of coloration in stainless steels, combined with the method of MIG brazing, via XRD and SEM

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Resistance of stainless steels against corrosion is provided by thin and sensitive chrome oxide layer on the surface. This layer occurs of atmosphere effect and called passivity layer. When chromium rate in the metal reaches %12 - %13, passivity layer resists to the corrosion adequately. Because of the fact that weld zone of metals welded with melting method remains under the influence of high temperature during the process and however due to the presence of possible air, adverse reactions may occur, especially on the surface of stainless steels. In stainless steels temperature range of 200°C – 1200°C, especially in the root zone of the material occurs coloration form chrome yellow to brown-gray. This case affects negatively properties of the material such as technological and mechanical and thus may lose their suitability for use. In welding technology, in order to avoid undesirable these changes is an accurate method the use of gases we call the root shielding gases. The purpose of this study, is investigate this coloration, which affects phase structure and mechanical properties of material via XRD and SEM methods of analysis.

***Keywords*:** SEM, XRD, COLORATION

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Crystallization of *Scytalidium thermophilum* Xylanase by Vapor Diffusion

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The main heteropolymers of the hemicellulosic fraction of plant biomass are xylan, mannan, galactans and arabinans [1]. Xylan is a complex molecule mainly consisting of a five-carbon sugar D-xylose. Due to the complex structure of xylan, synergistic action of different hemicellulase enzymes is required for complete hydrolysis. Endoxylanases are one of the most important enzymes in this enzyme group. Microbial xylanase producers are mainly bacteria and fungi [2]. Filamentous fungi produce extracellular xylanase which makes fungal xylanases favorable at industrial scale such as animal feed production, manufacture of bread, food and drinks, pharmaceutical and chemical applications, textiles, pulp and paper. For crystallographic purposes, xylanase from *Scytalidium thermophilum* was purified to homogeneity by a two-step column chromatography technique including gel filtration and anion exchange, 21.8 fold with 9.6% yield. Xylanase crystallization was screened using ready-to-use screening kits by sitting drop vapor diffusion technique in 96-well plates. After dye test of observed crystals, xylanase-crystal forming conditions were optimized in 24-well plates by hanging drop vapor diffusion technique. So far, best crystals, having potential for X-ray structure studies, were obtained using ammonium citrate dibasic and sodium acetate trihydrate at 18°C at 3 mg/ml protein concentration as shown in Figure 1.

Figure 1. Crystals of *Scytalidium thermophilum* xylanase

Keywords: *Scytalidium thermophilum*, xylanase, crystallization, vapor diffusion

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Structural and magnetic properties of exchange biased Pt/Co/(Pt,Cr)/CoO multilayers

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Exchange bias is related to interfacial exchange coupling between ferromagnetic (FM) and antiferromagnetic (AFM) materials when the system is field cooled through the Néel temperature of AFM material and it manifest itself as a shift of hysteresis loop [1-7]. In this study, exchange bias in perpendicularly magnetized thin films has been manipulated by changing ferromagnetic film thickness or spacer layer at the interface. Structural and magnetic properties of Pt/Co(4Å)/Pt(5Å)/CoO/Pt {S1}, Pt/Co(Å)/Pt(5Å)/CoO/Pt {S2} and Pt/Co(4Å)/Cr(5Å)/CoO/Pt {S3} thin films grown on top of Si substrates were investigated by using x-ray reflectivity, x-ray diffraction, magneto-optic Kerr effect and vibrating sample magnetometry. The detailed analysis of exchange bias data indicates that the spacer layer properties strongly affect the interactions at the common interface. The data obtained from the simulation of x-ray reflectivity measurement give that the density of CoO is less than the bulk value that means the sample has mixed CoO phases which lower the blocking temperature of the system. This work was supported by TÜBİTAK (The Scientific and Technological Research Council of Turkey) through the project number 112T857.

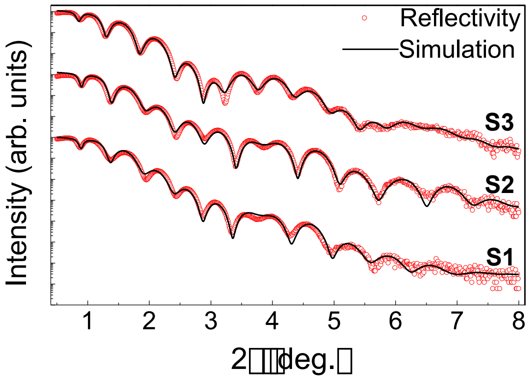

Figure 1. *X-ray reflectivity data and fit for the samples*

Keywords: Exchange bias, interface interactions, sputtering, multi layered thin films, magnetic anisotropy

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Investigation of Nanostructured Coated Oxides Films by X-Rays, UV-Vis-IR and AFM

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Structural, optical and surface properties of layers based on Zinc oxide have been investigated. Nanostructures of ZnO grown at several temperatures 250-400 °C by ultrasonic spray pyrolysis process have been successfully achieved. The effect of substrate temperature (T_S) on films' properties is studied. X-ray pattern confirms that the as-synthesized ZnO phase is grown along a (002) preferential orientation. It is revealed that the crystalline structure is improved with a substrate temperature of 350°C. The UV-Vis-IR measurement reveals that the sprayed films are high transparent in visible and IR bands. Moreover, the morphology of as-grown films, analyzed by AFM, shows nanostructures which grown along c-axis. The (3µm x 3µm) area scanned AFM surface studies give the smooth film surface Rms<40 nm.

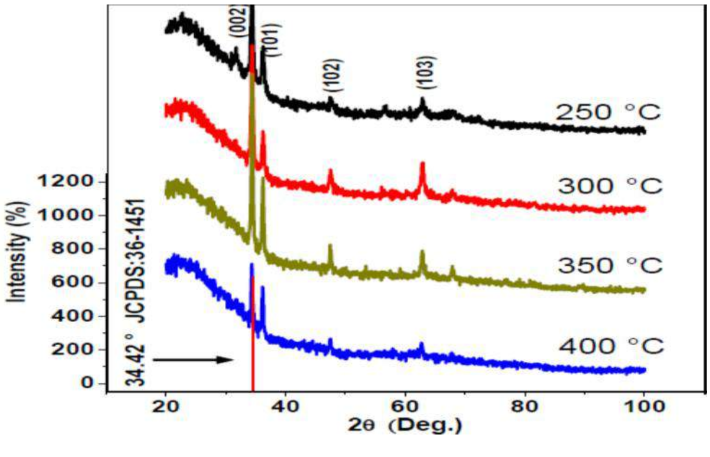

Figure 1. X-ray pattern of ZnO grown at T_S ranged within 250-400°C.

Keywords: ZnO; Spray pyrolysis; X-ray pattern; AFM observation; Nanostructures

Synthesis and characterization of selenium-doped hydroxyapatite as therapeutic bone substitute

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In case of severe bone damage or fracture, synthetic bone grafts such as hydroxyapatite (HAp) and related materials have long been applied for replacing natural bone tissue. Recent advances in this area have led to development of dual-functional synthetic hard tissue analogs exhibiting high biocompability/osteoconductivity together with therapeutic effect. Metallic ions are promising therapeutic agents in treatment of bone tumors due to their high physiological stability and availability compared to other alternative therapeutic agents such as recombinant proteins, therapeutic nucleic acids and anti-cancer drugs. Selenium, in that respect, is effective therapeutic agent with promising anti-oxidant and anti-carcinogenic effect when used in proper doses. In this study, selenium-doped HAp (HAp:Se) particles have been synthesized by modified aqueous precipitation method using calcium) and phosphate salts with sodium selenite. The effect of Se dopant in different amounts and calcination temperatures on the physical, chemical and crystal structure of resultant HAp powders have been investigated. Complete chemical analyses were performed with spectroscopical analyses including fourier transform infrared and X-ray photoelectron spectroscopy to elucidate the mechanism and chemical nature of Se doping in HAp. Meanwhile, x-ray diffraction studies by rietveld refinement have conducted to explain changes in the HAp crystal structure upon Se doping.

Keyword: Bone Grafts, Selenium, Rietveld Refinement

Selective Carbon Monoxide Schottky Diode Gas Sensor

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In recent years, since several years, urban air quality has become a problem of public health. Among all pollutants, carbon monoxide (CO) is a major problem. CO come from cars exhausts and combustion processes. Along the years, different methods have been proposed to increase the performance of these sensors. Most of the sensor characteristics depend on the physical properties of the material. Metal oxides have been widely exploited as sensing elements in semiconductor gas sensors, because they provide featured active sites to adsorb gas molecules and catalyze reactions [1-2]. In this study, Al/Al_2O_3/p-Si and Al/HfO_2/Al_2O_3/p-Si Schottky diodes were fabricated and investigated as a gas sensor. Measurements are taken at different temperature (25-150 ^{0}C) for different CO gas concentrations (10-60 ppm). The response increases with increasing temperature. The main sensing mechanism is attributed to the chemisorptions of oxygen on the oxide surface and the chemical reactions between adsorbed oxygen and tested gas. And also the influence of sensing mechanism of the heterointerface gas sensor has been discussed.

Keywords: Gas sensors, electrical characterization, CO

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Nanoscale Structural Analysis of a self assembled liquid crystal system and *Sulfonated Composite Proton Exchange Films*

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The obtained nanoscale structural knowledge determined by SAXS analysis was widely used to develop novel materials (which have industrial and technological importance) to explain the relation of structure-properties.

In the content of this presentation, pioneer SAXS analysis focused on two different groups of nanostructured samples will be mentioned before two detailed researches and investigations.

In the first part of the study, the ionic effect of salt addition to a lyotropic liquid crystal (LLC) system was investigated. NH_4Br salt was added to TTAB+water+decanol ternary system and the structural changes in lyotropic phases were characterized. The obtained polydisperse oblate ellipsoids indicate that these samples may play an important role in biological systems developed for technical applications [1].

In the second part, microstructure of sulfonated proton exchange membranes were investigated by SAXS and WAXS so as to identify the shape and size of the transport tunnels formed at dry and humidified states. With the help of this information, controlling of the proton transfer will be also possible and these type novel materials will be useful in fuel cells for energy applications. Shape and size of the mentioned tunnels determine the level of proton conduction and amount of undesirable fuel permeation which decreases fuel cell performance [2]. Elastomeric forms of the studied samples will be also important for new technological applications.

Keywords**:** liquid crystal, Sulfonated Composite, Proton Exchange Films.

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Molecular Structure, Electronic Properties, NBO Analysis And Spectroscopic Characterization Of 4-fluorophenyl)(4-hydroxy-3-methylphenyl)methanone Using Quantum Chemical Calculations

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The present communication deals with the quantum chemical calculations of energies, geometrical structure and vibrational wavenumbers of 4-fluorophenyl)(4-hydroxy-3-methyl-phenyl)methanone using density functional (DFT/B3LYP) method with 6-311++G(d,p) basis set. [1]. The computational vibrational wavenumbers and also ground state equilibrium conformations were carried out by using density functional method with 6-311++G(d,p) basis set. The vibrational frequencies were also computed using B3LYP method of DFT with 6-311++G(d,p) basis set. The fundamental assignments were done on the basis of the total energy distribution (TED) of the vibrational modes, calculated with scaled quantum mechanical (SQM) method. The hybrid DFT method is very useful in forecasting accurate vibrational structure as seen the vibrational results of the study. Also the ^{13}C and ^{1}H nuclear magnetic resonance (NMR) spectra were operated by using the gauge-invariant atomic orbital (GIAO) method, showing a consistency with literature data. Apart from these, the excitation energies, wavelengths, HOMO and LUMO energies, density of state (DOS) diagrams, thermo dynamical properties and molecular electro-static potential (MEP) were appreciated.

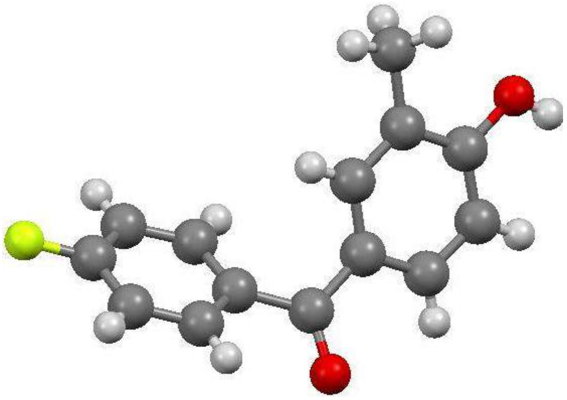

Figure 1. The crystal structure and optimized geometry of the title molecule.

Keywords: 4-fluorophenyl)(4-hydroxy-3-methylphenyl)methanone, DFT; NMR, UV, Infrared and Raman spectra; HOMO–LUMO, DOS.

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POSTER PRESENTATIONS

Molecular Geometryand Supramolecular Architecture of One-Dimensional CoordinationPolymer Containing Pyromelliticacid and Isonicotinamide.

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Mixed-ligand coordination polymer$[Cu_2(H_2O)_2(pm)(ina)_2]_n.3nH_2O$(pm=tetraanion of pyromellic acid, ina=isonicotinamide) was investigated mainly from the point of supramolecular architecture in their respective crystal packings. The structural properties of complexwere characterized by X-ray diffraction (XRD) technique, Thermalanalysis and Fourier transform infrared (FT-IR) spectroscopy. It has been observed that complex has crystallized in the monoclinicspacegroup $P2_1/c$. The Cu(II) ionis five-coordinated in a trigonalbipyramidalgeometrybytwo O atomsfromdiffrenttwopyromellitateligandsandby a N atom from a isonicatinamideandbytwowaterligands.The metal center is bridged by pyromellitate ligands to form 1D polymer chains of *2,4 ribbon*type. The polymer chains are connected by O–H···O hydrogen bonds to form sheet structures. Thiscomplexconsists of a 3Dstructurewithcontainingplanarhexacyclicanddimericwaterrings.The FT-IR investigation of the complex was performed within the mid-IR region, mainly focusing on the characteristic vibrations of pyromellitic acid and isonicotinamidemoieties by considering their free states and ligand behaviour in the case of complex formation.

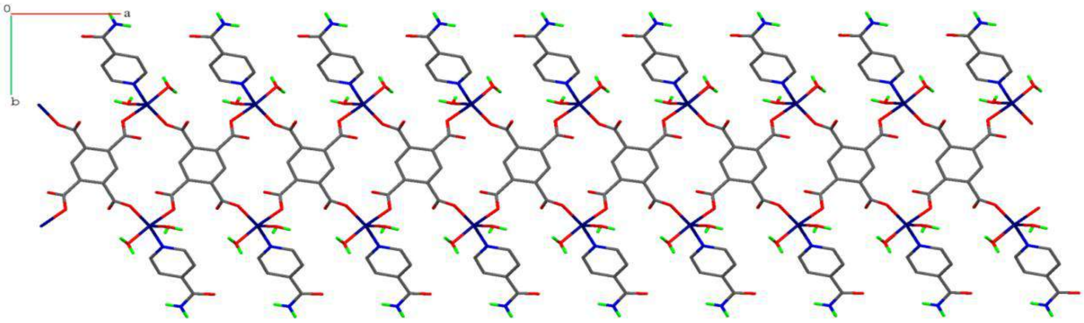

Figure1. CrystalStructures of $[Cu_2(H_2O)_2(pm)(ina)_2]_n.3nH_2O$

Keywords: Pyromellitic acid, Isonicotinamide, X-ray, IR and Copper complex

Average Particle Size and Microstrain Calculation of $Ca_{(3-x)}M_{(x)}Co_4O_9$ (M=Sb and B) Thermoelectric Materials

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In this study, we have prepared and characterized $Ca_{3-x}M_xCo4O9$ (M= B and Sb, x=0, 0.5, 0.75 and 1) thermoelectic materials [1]. These compounds have been synthesized by conventional solid state reaction process. Which material can be called “misfit layered” because this systems occurring between the two subsystems. One is rocksalt-type Ca_2CoO_3, named sublattice-1, and the other is CdI2-type CoO_2, named sublattice-2. The crystal structure analysis, lattice parameters, crystallite size and micro-strain effects of the samples were calculated from XRD pattern of the samples.

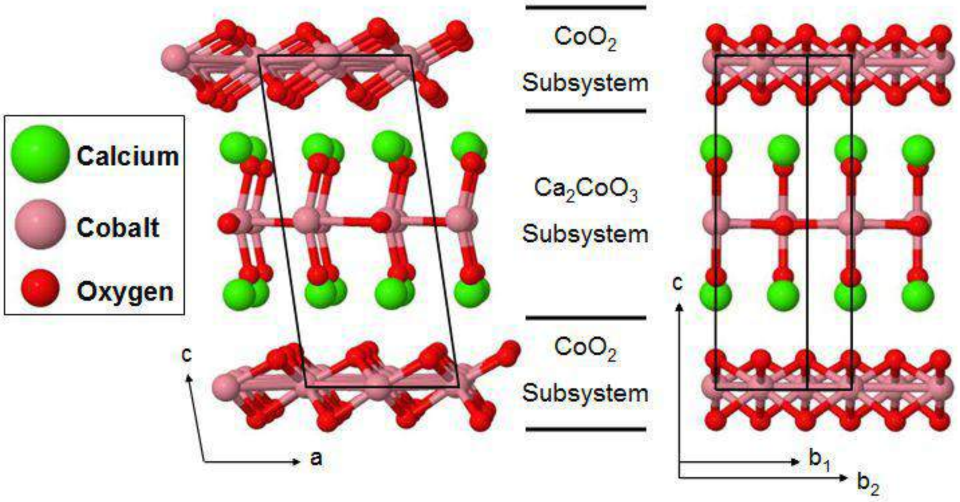

Figure 1. $Ca_3Co_4O_9$ crystal structure [2].

Keywords: $Ca_3Co_4O_9$, thermoelectric, misfit layered

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Evaluation of Average Grain Size and Microstrain in $LiCo_{1-x}B_xO_2$ Cathode Materials by the Williamson–Hall Method

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We report the average grain size and the microstrain in $LiCo_{1-x}B_xO_2$ cathode materials by applying the Williamson-Hall (WH) technique to XRD line broadening. According to the XRD patterns, the samples are well crystallized. Our data agree well with the standard PDF card (PDF#50-0653) and previous repots on $LiCoO_2$. All the diffraction peaks in the XRD pattern of the x=0 sample are indexed with the $LiCoO_2$ phase which has a rhombohedral symmetry with R3m space group. The $x \leq 0.25$ samples have no detectable impurity phases indicating that B^{3+} substitutes for Co^{3+} ions in the $LiCoO_2$ as reported in the studies. As the boron content increases, the $LiBO_2$ and $Li_6B_4O_9$ impurity phases become visible for $x>0.25$ samples. Based on our calculations, the strain increases with increasing boron content up to x=0.375 and then starts to decrease. There are three possible scenarios for these conditions depending on where the B ions settle in the lattice. If B ions substitute for Co in the lattice, the unit cell should shrink while if they are located in crystallographic sites different than Co sites, no reduction of the lattice volume is expected. The other possibility is the B ions settle the interstitial region in the lattice which can cause an increase in the lattice volume. Based on our experimental results regarding the change in the lattice volume with increasing boron content, we propose that some of the B ions settle interstitial region while the rest of them occupy the Co sites for $x \leq 0.375$.

Keywords: Williamson–Hall method, microstrain, grain size, $LiCo_{1-x}B_xO_2$ cathode.

Acknowledgement: This study was supported by TÜBİTAK (The Scientific and Technical Research Council of Turkey) under grant no TUBITAK 112M487.

Investigation of microstructure, electrical and mechanical properties of Ti-6Al-4V alloys

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In this study, the microstructure of the Ti-6Al-4V alloys with 5x40x130 mm (grade 5) dimensions heat treated with different conditions was investigated. The residual strains formed by the heat treatments were determined by micro-structure, hardness analysis. The average grain size and the microstrain in Ti-6Al-4V alloys were analyzed by applying the Williamson-Hall (WH) technique to XRD line broadening. The elemental distribution of the commercially obtained Ti-6Al-4V alloys (Ti-) were given as %Ti=91-88.75, %Al=5.5-6.75 and %V=3.5-4.5. The lattice parameters and microstructure of the samples were changed by heat treatment temperatures and cooling process such as quenching or constant cooling rates. According to XRD analysis, we observed□, □□ and β phase of Ti-6Al-4V alloy depending on the fabrication conditions. The lattice parameters of the samples were calculated by Rietvelt refinement technique. The electrical properties of the sample were measured with four probe technique down to 5 K and it was found that the resistivity of the quenched samples was increased.

Keywords: Ti-6Al-4V alloys, crystallite size, lattice strain

Synthesis and Characterization of Magnesium Cobalt Orthoborate

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Metal borates display a wealth of structural diversity, because of their potential applications as reinforcements in electronic ceramics, wide band gap semiconductors, antiwear additive, nonlinear optical devices [1]. Borates are stable at high temperature and have high luminescence which has applications in laser, optical glasses and phosphors. Structurally, borates can be coordinate to oxygen both in triangular (BO_3) or tetrahedral (BO_4) geometry.[2].Among the known borates, nickel orthoborate (isomorphous with magnesium orthoborate) have been studied by Gotz et al and Pardo et al [3,4]. Later on, Effenberger et al. have been reported the three kotoite type of compounds $M_3(BO_3)_2$ (M=Mg, Co and Ni) through the solid state reactions [5]. Lately, two new binary metal orthoborate compounds, $Co_2Ni(BO_3)_2$ and $CoNi_2(BO_3)_2$ have been successfully synthesized in kotoite structure with the space group of Pnmn, the crystal system is orthorhombic, by high temperature solid state reaction method using three reagents ($Co(NO_3)_2.6H_2O$, $Ni(NO_3)_2.6H_2O$ and H_3BO_3) and mol ratio 2:1:2, 1:2:2 respectively [6,7]. In this work, magnesium cobalt orthoborate**,** $MgCo_2(BO_3)_2$, has been prepared through the solid state reaction of $Co(NO_3)_2.6H_2O$, MgO and H_3BO_3.The obtained compound was characterized using XRD, FTIR, SEM and DTA methods [8].

Keywords: Solid state synthesis, X-ray powder diffraction, kotoite structure.

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X-Ray Diffraction results of polyurethane nanocomposites

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Polyurethanes (PUs) are an important class of polymers that have wide application in a number of different industrial sectors. Polyurethane (PU) composites were obtained with different organoclay contents (1, 3, 5 and 10 wt.% in for all cases). Firstly, quaternary ammonium salt, which is 1 methyl- dinonyl-1-phenyl ammonium iodide (QAS-1) was synthesized for modified of Na^+-montmorillonit. For polymer-organoclay composites substantial we preferred polyurethane polymer because it can be used large usage area and ıt is resistant material. Using method is mixing method from solution. The characterization of PU/organoclay composites was carried out by means of fourier transform infrared and X-ray diffraction.

Keyword: Polyurethane, quaternary ammonium salts, Na^+-montmorillonite, organoclay, nanocomposites

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Structural and Magnetic Properties of Exchange Biased $[Ni/CoO]_n$ Multilayers

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Exchange bias (EB) is a result of interfacial exchange coupling between ferromagnetic (FM) and antiferromagnetic (AF) materials after magnetic field cooling (FC) the system below to the Néel temperature of AF. The need of strong, controllable, predictable, and also low-energy consuming devices for the technology motivates the researchers studying more to understand the scientific basis of this phenomenon. With this motivation, we have investigated bilayered and multilayered exchange bias systems with different materials [3-7]. In this study, the exchange bias properties of four polycrystalline multilayer stack samples of AF CoO and FM Ni in the form of $[Ni/CoO]_n$ with n = 1, 2, 3, and 4 are reported. The samples were grown on top of Si (111) substrates by using magnetron sputtering method. X-ray photoelectron spectroscopy (XPS) and X-ray diffraction (XRD) were used to determine the structural properties of the samples. XPS measurements of cobalt oxide layer revealed the coexistence of different phases in cobalt oxide as CoO and Co_3O_4, the latter of which lowers the blocking temperature. The detailed analysis of magnetization measurements related to the structural properties was also provided.

This work was supported by TÜBİTAK through the project number 112T857.

Keywords: Exchange bias, antiferromagnetic, ferromagnetic, interfacial exchange coupling, spintronic.

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Low Concentration of CO gas sensor by Atomic Layer Deposition

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Increasing of the hazardous gases or other chemicals into the environment have led to the increased attention on development of gas sensors. Make measurements at low concentrations is becoming more and more important for human health. Gas sensors has developed by different production methods (RF sputtering, chemical vapor deposition (CVD), thermal evoparation, atomic layer deposition (ALD) and so on…) that shows different response to hazardous gases. Due to the saturative nature of the reaction steps, a uniform thickness, thin film growth at atomic scale, ALD is a unique process that can allows intended layer production of the desired and offers many advantages for low temperature gas sensors [1]. In this work, we fabricated Al/TiO_2/Al_2O_3/p-Si by ALD method and investigated as a gas sensor between 27-177 ◦C. The sensitivity is increasing with increased gas concentration and temperature which have a direct effect on sensing surface. The maximum sensitivity of sensor was obtained for 80 ppm at 177 ◦C. The obtained response to CO could be explained with the surface adsorption theory and conduction band theory associated with temperature [2].

Keywords**:** Gas Sensors, CO, Conduction Band Theory

[1] M.R. Saleem, R. Ali, S. Honkanen, J. Turunen, Thin Solid Films 542 (2013) 257–262
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The polyhedron cluster analyses of alloy system under rapid quenching conditions by using simulation

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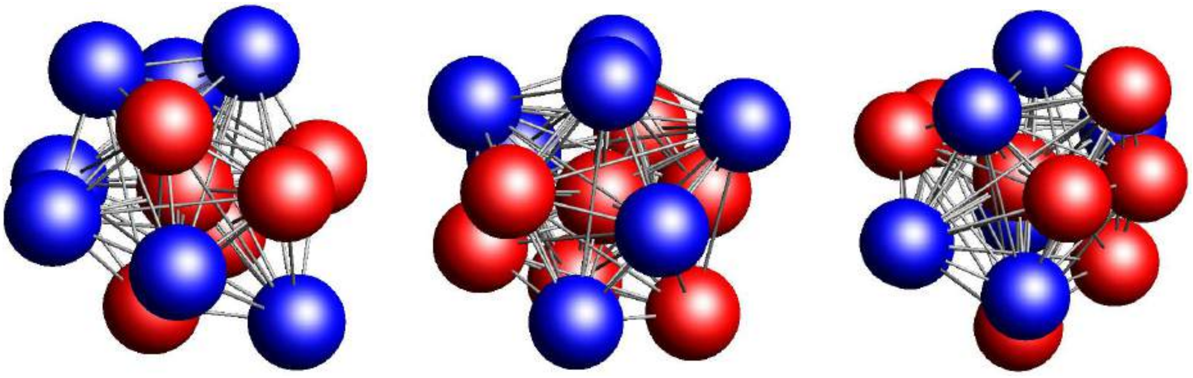
In this study, the formation mechanism of polyhedron clusters in $Cu_{50}Ag_{50}$ binary alloy system have been have been investigated by using molecular dynamics simulations based on embedded atom method (EAM) during the rapid cooling processes. The cluster-type index method (CTIM) has been used to describe the evaluation properties of clusters. The simulation results show that the amorphous phase is formed main bonded pairs of 1551, 1541 and 1431 in the system, and ideal icosahedral (icos) cluster (12 0 12 0) and other basic polyhedron clusters, such as defective icos, Frank-Kasper, Bernal polyhedral play a critical role under the rapid cooling conditions. The results of our simulations have been disclosed that high cooling rate favours the icos and defective icos clusters for model alloy system.



(a) **(b)** **(c)**

Figure 1. Schematic diagrams of typical polyhedron clusters in the system expressed by CTIM **a)** ideal icos, **b)** deficos **c)** FK polyhedron.

***Keywords*:** CuAg alloy; molecular dynamic simulation; bond-type index method; cluster-type index method.

Two dimensional coordination polymers with 3,30-thiodipropionate: An unprecedented coordination mode and strong hydrogen-bond network

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The design and synthesis of metal organic coordination polymers constructed with transition metals and organic linkers have received much attention due to their fascinating structures and potential applications [1]. In this study, four novel coordination polymers with 3,3´-thiodipropionic acid (tdpH_2), nicotinamide, isonicotinamide and Co(II), Cu(II) and Zn(II) ions have been synthesized and structurally characterized.

The asymmetric units of **1**-**3** contain one M(II) ion (M(II)=Co(II) in **1**, Cu(II) in **2** and Zn(II) in **3**), two ina ligands and one 3,3´-thiodipropionate (tdp) ligand (Figure 1), while the asymmetric unit of **4** contain one Zn(II) ion, two na ligands and one 3,3´-thiodipropionate (tdp) ligand (Figure 2).

Topological analysis results showed that the complexes display five-connected 2D layers with a point symbol of $3^3 \cdot 4^3 \cdot 5^4$ (Figure 3).

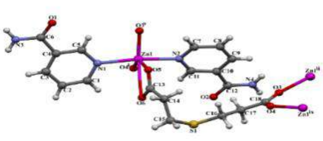


Figure 1. The molecular structure of complexes 1-3

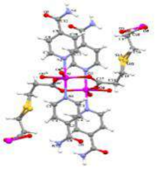


Figure 2. The molecular structure of 4

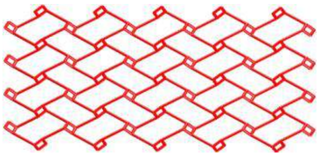


Figure 3. Schematic view of the 2D layers of complexes 1-4

The M(II) ions and tdp ligands generate 2D polymeric chains with 40-membered rings (Figures 4 and 5).

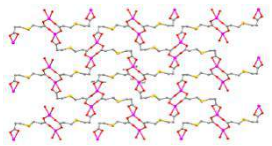
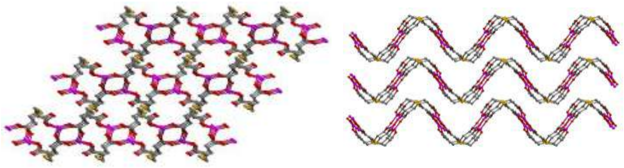


Figure 4. An infinite 2D layer of complexes **1-3** (ina ligands are omitted)



(a) (b)

Figure 5. An infinite 2D layer of complex **4** [(a) *ac* plane and (b) *ab* plane] (nicotinamide ligands are omitted)

***Keywords*:**3,30-Thiodipropionate complex, Two-dimensional complex

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Low Concentration of CO_2 gas sensor by Atomic Layer Deposition

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Increasing of the hazardous gases or other chemicals into the environment have led to the increased attention on development of gas sensors. Make measurements at low concentrations is becoming more and more important for human health. Gas sensors has developed by different production methods (RF sputtering, chemical vapor deposition (CVD), thermal evoparation, atomic layer deposition (ALD) and so on…) that shows different response to hazardous gases. Due to the saturative nature of the reaction steps, a uniform thickness, thin film growth at atomic scale, ALD is a unique process that can allows intended layer production of the desired and offers many advantages for low temperature gas sensors [1]. In this work, we fabricated Al/TiO_2/Al_2O_3/p-Si by ALD method and investigated as a gas sensor between 27-177 ◦C. The sensitivity is increasing with increased gas concentration and temperature which have a direct effect on sensing surface. The maximum sensitivity of sensor was obtained for 80 ppm at 177 ◦C. The obtained response to CO could be explained with the surface adsorption theory and conduction band theory associated with temperature [2].

Fig 1. Schematic Diagram Of Sample

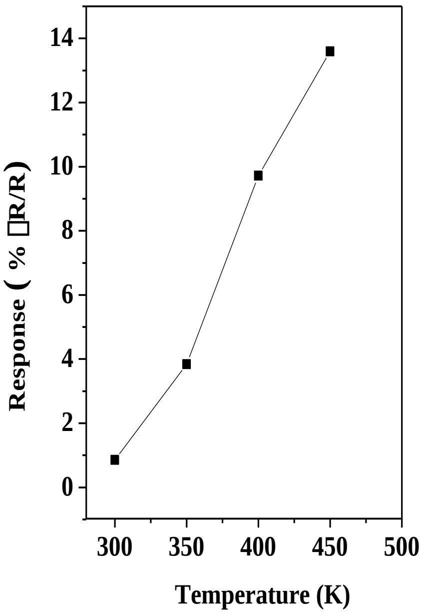

Fig 2. The variation of response vs. temperature

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Crystal structure of 1-[3-(Morpholin-4-yl)propyl]-4-(3-nitrophenyl)spiro[azetidine-3,90-xanthen]-2-one

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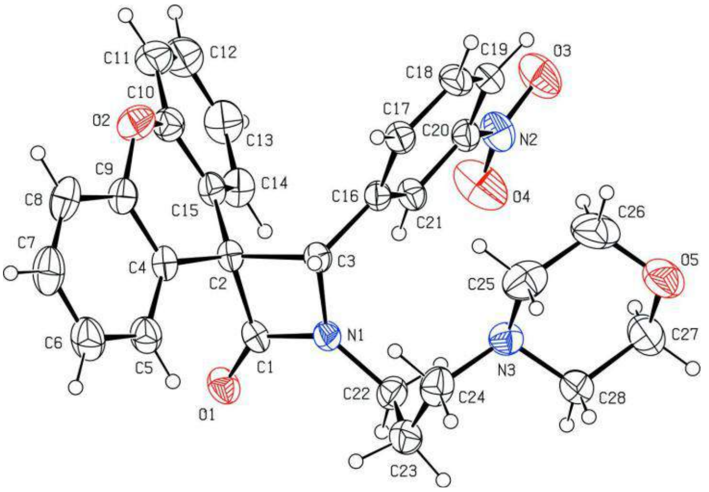
β-lactams occupy a central place among medicinally important compounds due to their unique structure and their antibacterial activities [1-3]. The title compound, $C_{28}H_{27}N_3O_5$, crystalizes in the monoclinic space group $P2_1/n$ with a = 9.2637 (6) Å, b = 11.4091 (5) Å, c = 23.3310 (15) Å, β= 96.930 (5)°, V = 2447.9 (2) Å^3, Z = 4 at room temperature. The β-lactam ring of the compound makes dihedral angles of 75.77 (5)°, 52.78 (9)° and 88.72 (5)°, respectively, with the benzene ring, the least-squares plane formed by the four C atoms of the morpholine ring, which adopts a chair conformation, and the xanthene ring system. In the crystal, C—H…O hydrogen bond contacts connect neighbouring molecules into infinite zigzag chains running parallel to [010].



Keywords**:** β-lactams, single-crystal X-ray study, crystal structure.

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Synthesis and Structures of Hg(II) and Zn(II) metal complexes containing multimodal cyclotriphosphazene ligand

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Coordination polymers are interesting not only their intriguing molecular structures but also their potential applications such as gas storage, luminescent material, catalyser, non-linear optic and magnetic material [1-3]. The cyclophosphazene compounds are capable to bind metal ions through endocyclic and exocyclic ring nitrogen atoms (Figure 1). Cyclotriphospahazatrien containing pyridyloxy groups have used as ligand in a lot of studies [4]. In this study, Hg (II) and Zn (II) metal complexes were synthesized using fully substituted cyclotriphosphazatriene ligands containing 3-hydroxypyridyloxy groups. Hg (II) (**1**) and Zn (II) (**2**) complexes have monoclinic P2_1/c and monoclinic P*n* space groups, respectively according to crystallographic analysis. Whereas compound **2** has two-dimensional (2D) crystal structure, interestingly, compound **3** arranged a three-dimensional (3D) framework, which comprised of two interpenetrating 3D nets.

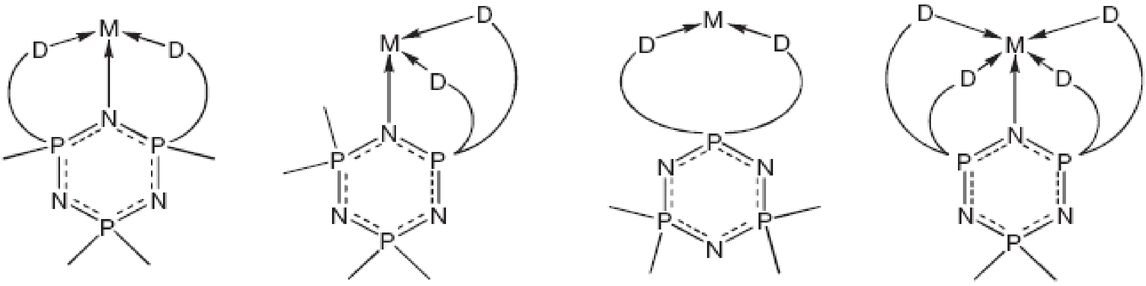

Figure 1. Various coordination modes of multimodal cyclophosphazene ligands

Keywords: Cyclotriphosphazene ligand, metal complex, crystal structure

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Phenol substituted ansa fluorodioxy cyclotriphosphazenes

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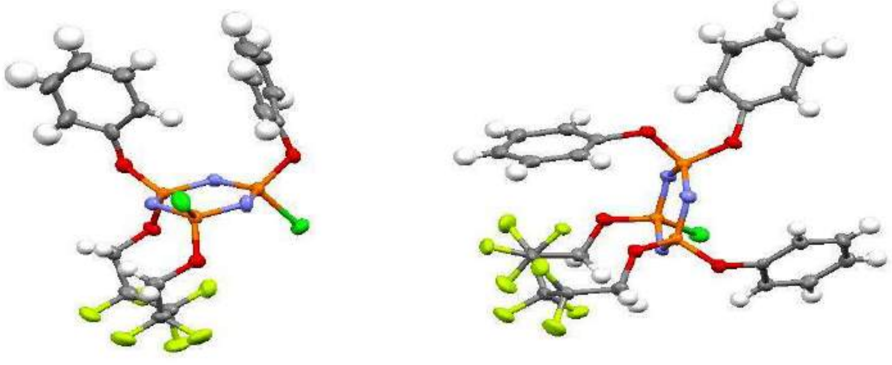
The nucleophilic substitutions reactions are interest centre of investigations in the cyclophosphazene chemistry due to the complexity and variability of the reaction mechanisms and the broad range of regio- and stereo- chemical outcomes of these reactions [1, 2]. We have investigated the reactions of sodium salt of phenol with fluorodioxy cis-ansa derivatives of cyclotriphosphazene; the hexafluoropentanedioxy derivative, $N_3P_3Cl_4[OCH_2(CF_2)_3CH_2O]$ (**1a**) and the octafluorohexanedioxy derivative, $N_3P_3Cl_4[OCH_2(CF_2)_4CH_2O]$ (**1b**) in THF at different molar ratios (1:1, 1:2 and 1:3). The important details were obtained about the mechanism and pathways of the reaction of the mono-ansa fluorodioxy cyclophosphazene derivatives (**1a**, **1b**). X-ray crystallographic studies of two compounds (**7a** and **8b**) demonstrated unambiguously that nucleophilic substitution reactions at the ansa-ring PCl(OR) phosphorus atoms of the cyclotriphosphazene compounds $N_3P_3Cl_4[OCH_2(CF_2)_nCH_2O]$ $n = 3$ (**1a**) and 4 (**1b**) occurred with retention of configuration for both the 10- and 11-membered fluorodioxy ansa rings, respectively (Figure 1).



7a **8b**

Figure 1. Molecule Structures of Compounds **7a** and **8b**

***Keywords*:** Cyclophosphazene, Phenol, Mechanism, X-Ray Diffraction

The authors thank to the Scientific and Technical Research Council of Turkey (TÜBİTAK) for financial support (Project No: 112T066).

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Structural Properties of 2-Naphthylamine Substituted Cyclotriphosphazenes

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Cyclophosphazenes, composed of alternating nitrogen and phosphorus atoms, have many applications including organic light emitting diodes, biomedical materials, anticancer-antimicrobial agents and liquid crystals [1-3]. In most cases, cyclotriphosphazene (hexachlorocyclotriphosphazene, $N_3P_3Cl_6$,) can be readily modified with a variety of substituents via nucleophilic substitution reactions. In the current study, six novel cyclotriphosphazene compounds were synthesized and fully characterized by MALDI-TOF mass spectrometry, ^{1}H, ^{13}C, ^{31}P NMR spectroscopies and elemental analysis. The molecular structure of compounds; mono-, geminal bis and tetrakis 2-naphthylamino cyclotriphosphazenes were also determined by x-ray crystallography.

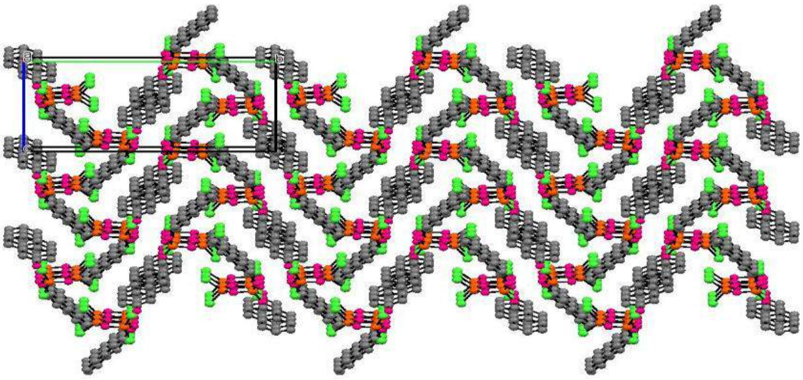

Figure 1. 3-D channel formation in the crystal packing of geminal bis-compound.

Keywords: Hexachlorocyclotriphosphazene, 2-naphthylamine, ^{31}P NMR spectroscopy, X-ray crystallography.

The authors thank to the Scientific and Technical Research Council of Turkey (TÜBİTAK) for financial support (Project No: 111T085).

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Paraben Substituted Cyclotetraphosphazenes

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Cyclophosphazanes, (NPXY)n, are important class of inorganic compounds. Different kinds of cyclophosphazenes could be synthesized by the reaction of chlorines substituted cyclophosphazenes containing different nucleophils groups. Chemical and physical properties of phosphazene derivatives depend on change of inorganic side group [1, 2]. Amongst the widest used antimicrobial preservatives in body care, pharmaceutical and food products are esters of phydroxybenzoic acid, referred to generally as parabens [3]. In the present work, paraben substituted cyclotetraphosphazenes were designed, synthesized and characterized for the first time. All paraben-substituted cyclotetraphosphazene compounds were fully characterized by elemental analysis, IR, MALDI-TOF mass spectrometry, ^{1}H and ^{31}P NMR spectroscopies. The molecular structures of compounds were also determined by x-ray crystallography.

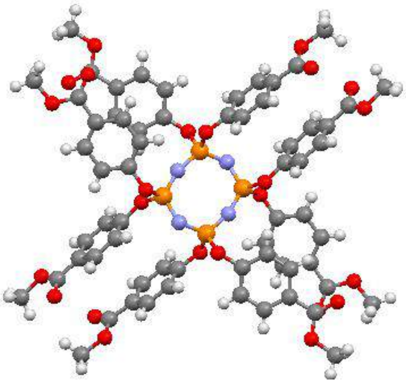

Figure 1. Molecule structure of methyl paraben substituted cyclotetraphosphazene

Keywords: Oktachlorocyclotetraphosphazene, paraben, ^{31}P NMR spectroscopy, X-ray crystallography.

The authors thank the Gebze Institute of Technology (GIT) for the provided financial support (Grant no: BAP 2013-A-013).

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Cyclooctaphosphazenes

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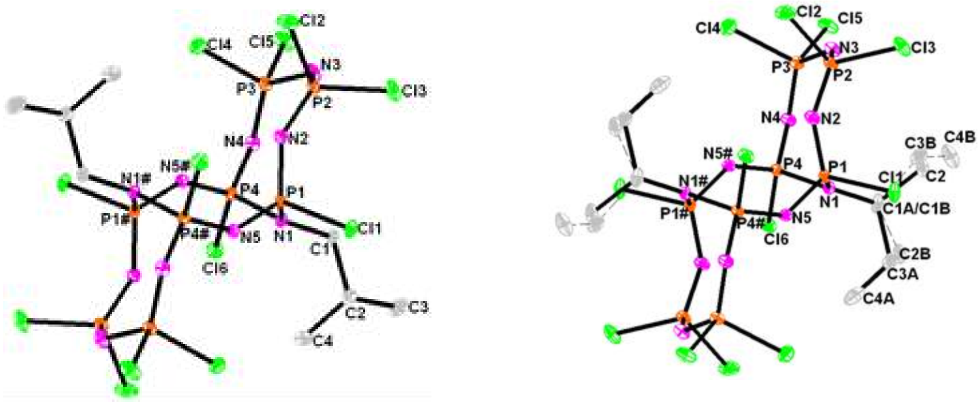
In the present work, the de-protonation reactions of mono amino cyclotetraphosphazene derivatives were studied to see whether or not de-protonation reaction occurred for cyclotetraphosphazene derivatives and, if so, to compare the results (variety of products, yield, stability etc.) with analogous reactions using mono amino cyclotriphosphazene derivatives [1-3]. Therefore, cyclotetraphosphazene derivatives having butyl-amino groups in the side chain, [$N_4P_4Cl_7$(NHR); R = *n*–butyl, *i*–butyl and *sec*–butyl], were reacted directly with sodium hydride in a 1:1 molar ratio in THF at room temperature for 2h under an argon atmosphere resulting in novel types of tris–cyclic compounds having 16–membered cyclooctaphosphazene (P_8N_8) rings bridged by the two amino alkyl groups. The molecular structures of compounds **2b** and **2c** were established by X-ray structure analysis. Compound **2b** has a triclinic system, space group *P-1* and compound **2c** has a monoclinic system, space group *P21/n* and the molecules in both structures sit on inversion centers (Figure 1).



2b **2c**

Figure 1. Molecule Structures of compounds **2b** and **2c**.

***Keywords*:** De-protonation, Cyclotetraphosphazene, Cyclooctaphosphazene, X-Ray analysis,

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A theoretical study on 4-Hydroxy-N'–[(1E)-1-(4-methylphenyl) ethylidene] benzohydrazide

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The chemistry of hydrazones has been extensively investigated in the recent years due to their strong tendency to form chelate complexes with transition metals and their pharmacological properties [1-3].The optimized geometries of 4-Hydroxy-N'–[(1E)-1-(4-methylphenyl) ethylidene] benzohydrazide have been calculated using density functional theory (DFT) method. The calculations were performed with Becke's nonlocal three-parameter hybrid functional in combination with the Lee, Yang, and Parr correlation functional (B3LYP) using the 6-311++G(d, p) basis set. We calculated the infrared frequencies and intensities of the most stable conformers in order to assist in the assignment of the vibrational bands in the experimental spectrum. The fundamental vibrational modes were characterized depending on their total energy distribution (TED%) using scaled quantum mechanical (SQM) force field method. ^{1}H and ^{13}C nuclear magnetic resonance chemical shifts of the compound were calculated using the gauge independent atomic orbital (GIAO) method. All the calculated results were compared with the available experimental data of the title compound [4].

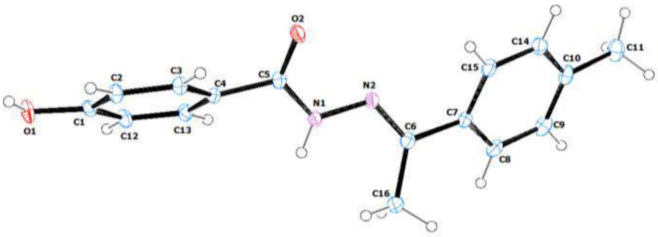

Figure 1. Molecule Structure.

***Keywords*:** Hydrazone, DFT, B3LYP, Vibrational Properties, NMR

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Measurement of mass attenuation coefficients around the K absorption edge of some Ce compounds

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Accurate data of total mass attenuation coefficients for gamma rays required in many fields such as dosimetry, radiation biophysics, tomography, spectrometry and crystallography. The total mass attenuation coefficient parameter is theoretically determined using WinXCOMprogram, a Windows version of XCOM. This program is used the mixture rule. The mixture rule is a practice to assume that the contribution of each element to the attenuation is additive. The mixture rule is valid when the effects on the atomic wavefunction of molecular bonding and chemical or crystalline environment are negligible. This study was realized to observe the chemical effect.

The total mass attenuation coefficients for element Ce and compounds $CeCl_3.7H_2O$, $Ce(SO_4)_2$, $Ce(OH)_4$ and Ce_2O_3 were measured at the different energies between 31.817-51.698 keV range by using secondary excitation method. Ba, La, Ce, Pr, Nd, Sm, Eu, Gd and Tb were chosen as secondary exciter. 59.54 keV gamma rays emitted from an Am-241 annular source were used to excite secondary exciter and $K\alpha_2$, $K\alpha_1$, $K\beta_1$ and $K\beta_2$ lines emitted of secondary exciter were counted by a Si(Li) detector with a resolution of 160 eV at 5.9 keV. The validity of mixture rule was discussed around the absorption edge for compounds. Obtained values were compared with theoretical values.

Keywords:Total mass attenuation coefficient, EDXRF, Mixture rule.

X-ray attenuation coefficients of Gd compounds in the K edge region at different energies

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The total mass attenuation coefficients for element Gdand compounds Gd_2O_3, $Gd_2(CO_3)_2.H_2O$, $Gd_2(C_2O_4).H_2O$ and $Gd_2(SO_4)_3$were measured at the different energies between 39.522-57.142keV range by using secondary excitation method. Sm, Eu, Gd, Tb, Dy, Ho and Er were chosen as secondary exciter. 59.54 keV gamma rays emitted from an Am-241 annular source were used to excite secondary exciter and $K\alpha_2$, $K\alpha_1$, $K\beta_1$ and $K\beta_2$ lines emitted of secondary exciter were counted by a Si(Li) detector with a resolution of 160 eV at 5.9 keV. The validity of mixture rule was discussed around the absorption edge for compounds. Obtained values were compared with theoretical values.

***Keywords*:** Total mass attenuation coefficient, EDXRF, Mixture rule.

The effects of Gd doping on ZnO and SnO_2 transparent conductive thin films

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Undoped and Gadolinium (Gd) doped zinc oxide (Gd:ZnO) and tin oxide (Gd:SnO_2) transparent conducting oxide thin films were deposited on soda lime glass and p-Si substrates by spin coating technique. Zinc acetate dihydrate and tin(IV) chloride pentahydrate were used as starting materials and Gd (III) chloride hexahydrate was used as dopand source. They were dissolved in methanol and several drops of diethylamide were added very slowly to solutions as a stabilizer at room temperature with a Gd/Zn ratio of 0, 1, 3 and 5%. The films were annealed at 450 °C for 1 h in a quartz tube furnace. Morphological and optical properties of the films were investigated as a function of Gd doping by using x-ray diffraction (XRD), scanning electron microscopy (SEM) and UV-Vis spectroscopy. Furthermore, Gd:ZnO/p-Si and Gd:SnO_2/p-Si heterojunctions were fabricated to see the effect of Gd doping on the performance of devices. It was seen that Gd doping has strong effects on optical properties of thin films and electrical properties of heterojunctions.

***Keywords*:** Gd doping, ZnO, SnO_2, SEM, XRD, optical properties

Tuning exchange bias in PtCo/CoO multilayers

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Exchange bias (EB) is a result of interfacial Exchange coupling between ferromagnetic (FM) and antiferromagnetic (AF) materials after magnetic field cooling (FC) the system below to the Néel Temperature of AF. It manifests itself as a shift of the FM hysteresis loop along magnetic field axis generally to the opposite direction of the cooling field. It has great application relevance for the fabrication of spintronic based technological devices like magnetic data storage units and nonvolatile memory devices. There are many studies related to exchange bias in the literature with different systems [1-7].In this study, PtCo thickness dependence of exchange bias in PtCo/CoO multilayers is investigated. After field cooling below the Néel temperature of CoO layer, the multilayer with AF/FM interfaces exhibits EB effect. A detailed structural analysis of antiferromagnetic CoO has been done by x-ray photoelectron spectroscopy (XPS). . The role of PtCo thickness on the interfacial interactions between ferromagnetic and antiferromagnetic layers, and the effect of superstoicbhiometric CoO on blocking temperature are also discussed.

This work was supported by TÜBİTAK (The Scientific and Technological Research Council of Turkey) through project numbers 112T857, 106T576 and 212T217.

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Crystal structure andtheoretical calculations of (Z)-4-(((Z)-(2-oxonaphthalen-1(2H)-ylidene)methyl)amino)-N-(thiazol-2(3H)-ylidene)benzenesulfonamide

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The experimental geometry of the title compound, (Z)-4-(((Z)-(2-oxonaphthalen-1(2H)-ylidene)methyl)amino)-N-(thiazol-2(3H)-ylidene)benzenesulfonamide, $C_{20}H_{15}N_3O_3S_2$, was characterized by X-ray diffraction analysis (XRD) and compared with those obtained from DFT method in gas phase. For theoretical calculations, B3LYP with 6-31+G(d) basis set was performed. SEM study of the sample which belongs to molecular structure reveals the external morphology. An Ortep-3 [1] view of the molecule of (I) is shown in Fig.1

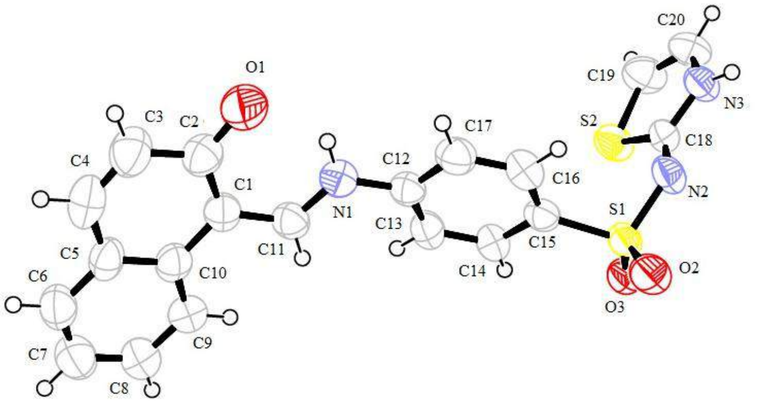

Figure.1 Ortep 3 diagram of the molecular structure

Keywords: XRD, DFT, SEM

[1] L. J. Farrugia, J. Appl. Cryst.**1997** 30, 565.

X-ray crystallographic and computational studies of N-(1,3-dioxoisoindolin-2yl)benzamide

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Single crystal of the molecular structure, $C_{15}H_{10}N_2O_3$, synthesized and crystallizes in monoclinic form, space group P 2_1/c with a = 13.5324(11) Å, b =9.8982(8) Å, c = 9.7080(8) Å, β= 95.425(6)°, V = 1294.53(18) Å^3. In addition to XRD analysis, SEM analysis and theoretical calculation methods were used for the further investigation of the crystal structure. An Ortep-3 [1] view of the molecule of (I) is shown in Fig.1

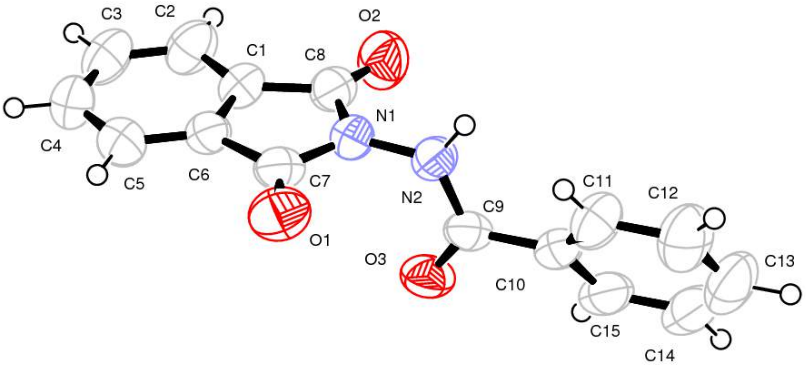

Figure.1 ORTEP plot of molecule with displacement ellipsoids drawn at 50% probability

Keywords: Single crystal, X-Ray Diffraction, SEM.

[1] L. J. Farrugia, J. Appl. Cryst. **1997** 30, 565.

Effect of total thickness on structural and magnetic properties of electrodeposited Co/Cu multilayers

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Co/Cu multilayers were produced by electrodeposition on polycrystalline Cu substrate having a strong (100) texture. The Co and Cu layer thicknesses were fixed at 3 and 0.5 nm respectively. The bilayer number of the multilayers was varied between 86 and 571, namely the total thickness was changed from 0.3µm to 2 µm. The structural characterization was carried out usingthe X-ray diffraction (XRD) technique. The XRD patterns indicated that all films have characteristic peaks of face centered cubic (fcc) structure. Furthermore, the appeared peaks increase as the total thickness increases (Fig 1). Also the lattices parameter calculated by the method of least squares increase and shifted tothat of Cu with increasing total thickness, due to increasing Cu amount of the films. The preferential orientation was found in the [100] direction and it is compatible with the Cu substrate [1]. The magnetic properties were investigated by vibrating sample magnetometer (VSM).Saturating magnetization, remnant magnetization and coercivity were determined from hysteresis curves.The magnetic moment per volume decreases as the total thickness decreases. Magnetoresistance(MR) measurements were made in the magnetic fields of ±12 kOe using the Van der Pauw method. Giant magneto resistance (GMR) values decreases with increasing total thickness.

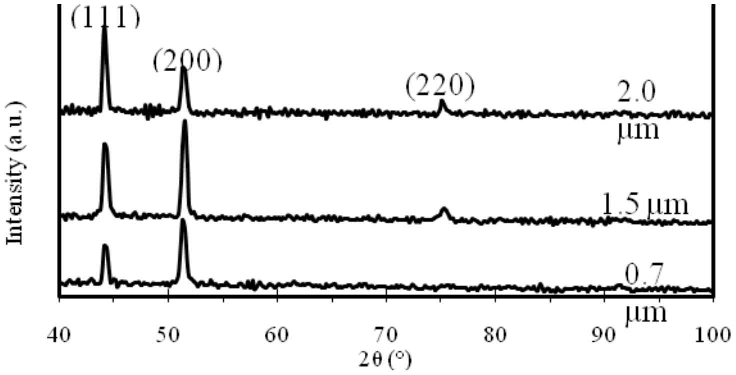

Figure 1.XRD spectra of Co/Cu multilayerswiththethicknesses of 0.7, 1.5 and 2.0 µm

***Keywords*:**Co/Cu multilayers, electrodeposition, GMR

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CrystalStructure, SpectroscopicStudiesand Quantum Mechanical Calculations of 2-[(3-Iodo-4-methyl)phenylimino)methyl]-5-nitrothiophene

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Schiff bases (azomethines, imines) belongto a widelyusedgroup of organic intermediates important for a production of chemical specialties, e.g. pharmaceuticals, oradditivestorubber. A basicreactionsynthesisinvolves an aromaticamineandaldehyde[1–3].

The title compound, 2-[(3-Iodo-4-methyl)phenylimino)methyl]-5-nitrothiophene, $C_{12}H_9O_2N_2I_1S_1$, was synthesized and characterized by IR, UV-V is and single-crystal x-ray diffraction technique. The molecular structure was optimized at the B3LYP levels of density functional method (DFT) with 6-311G+(d,p) basis set. By using TD-DFT method, electronicabsorptionspectra of the title compound recorded in the both gas phase and ethanol solvent. The harmonic vibrational frequencies of the title compound were calculated by using sam emethods with the 6-311G+(d,p) basis set. The calculated results were compared the experimental determination results of the compound. The energetic behavior of the compound in solvent media was examined using the B3LYP method with the 6−311G+(d,p) basis set by applying the On sagerand the polarizable continuum model (PCM). The molecular orbitals (FMO) analysis, the molecular electrostatic potential map (MEP), the nonlinear optical properties (NLO) and thermodynamic properties 6-311g(d,p) for the title compound were obtained with the same level of theory.

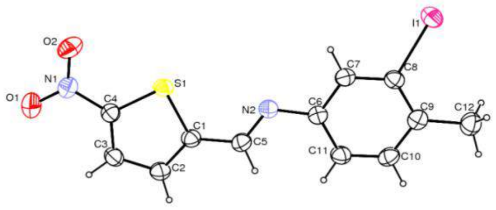

Figure1. Themolecularstructure of thetitlecompoundshowingthe atom-numberingschemeand 30% probabilitydisplacementellipsoids.

Keywords:Schiff Base, X-Ray Analysis, Density Functional Theory (DFT), Non-linear optical properties (NLO).

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Crystal structure of Zn(II) and Cd(II) complexes of 2,9-dimethyle 1,10-phenantroline

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In this study we report crystal structure determination of Zn(II) and Cd(II) complexes, [M(dmph)I_2], {dmph= 2,9-dimethyl-1,10-phenanthroline (neocuproine)}. the Zn(II) and Cd ions are four-coordinated in a distorted tetrahedral configuration by two N atoms from a neocuproine ligand and two terminal I atoms. Also **I** and **II** nanostructures have been synthesized by solvothermal methos Characterization of the compounds were performed by scanning electron microscopy (SEM), X-ray powder diffraction (XRD), FT-IR spectroscopy and elemental analyses, thermal gravimetric (TG/DTA) and the structures were determined by single-crystal X-ray diffraction.

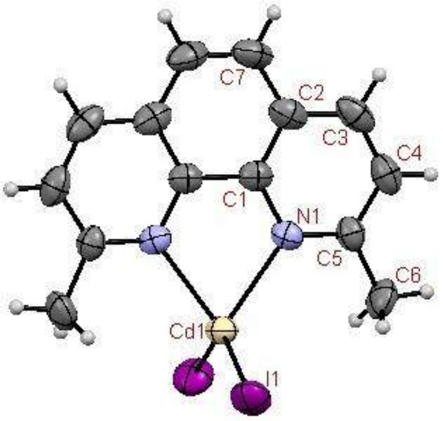

Figure 1. Molecule Structure.

***Keywords*:** Crystal structure; Cd(II) complex; solvothermal method.

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Determination of structural and optical properties of reactive sputtered MoO_3 thin films

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MoO_3 thin films were grown on soda lime glass and Si substrates by reactive magnetron sputtering technique. The depositions were executed by DC and RF magnetron reactive sputtering of Mo target in various O_2 atmospheres and temperatures. The samples were also annealed at 500 °C for 30 min in a quartz tube furnace. Morphological and optical properties of annealed and annealed films were investigated by using x-ray diffraction (XRD), scanning electron microscopy (SEM), electron dispersive spectroscopy (EDS) and UV-Vis spectroscopy. Furthermore, MoO_3/Si heterojunctions were fabricated to see the effect of grown condition on the performance of devices. It was seen that growing condition has strong effects on morphological and optical properties of thin films and electrical properties of heterojunctions.

***Keywords*:** MoO_3, Reactive sputtering, SEM, XRD, optical properties

Synthesis, Crystal Structures and ab initio Study of Sandwich-Layered 2D Ag(I) Coordination Polymers

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Metal-Organic Frameworks (MOFs) or Coordination Polymers (CPs) are one of the most attractive materials, appearing promising in the last years in the fields of catalysis, gas absorption, magnetic materials, second-order nonlinear optics (NLO), luminescence [1]. Among CPs, the d^{10} Ag(I) CPs have received great attention in the last two decades as being one of the most interesting research fields in supramolecular coordination chemistry due to the flexible coordination geometries varying from linear to trigonal, tetragonal, square pyramidal, and octahedral, corresponding to coordination numbers ranging from 2 to 6 [2]. These versatile coordination geometries of Ag(I) ions contribute significantly to the structural topologies of Ag(I) CPs with different dimensionalities (1D, 2D and 3D) [3].

In this study, we synthesized Ag(I) CPs containing variable Ag···Ag argentophilic contacts, and investigated the significant delocalization effects around the silver ions. Presently, density functional theory methods are frequently utilized to understand the electronic structure of transition metal systems, and as well as their chemical properties, reactions and bonding characteristics [4]. Natural Bond Orbital (NBO) analysis is a helpful tool to understand intra and intermolecular interactions among the filled orbitals and virtual orbitals.

Keywords**:** Coordination polymers, silver(I) complex, argentophilicity, crystal engineering, dicarboxylate ligands, NBO

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Structural Characterisation of Three Novel Isonicotinic Acid Hydrazide Base Schiff Bases: Hydrogen Bonding and Π-Π Interactions

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The condensation reaction of aromatic aldehydes with primary amines form compounds called Schiff bases. Schiff base compounds exhibit a wide range of biological activities and applications. Hydrazones possessing the azomethine –NHN=CH– groups, have been shown to possess antibacterial, anticonvulsant, antitubercular, and antitumor activities [1–3]. Intermolecular interactions such as hydrogen bonding and π-π stacking have a crucial role in supramolecular chemistry, materials science as well as biological systems. Hydrogen bonds are extremely important in biological systems and they stabilize and determine the structure of large macromolecules such as proteins and nucleic acids [4]. In this study, three novel hydrazone compounds were synthesised and structurally characterised by single crystal X-ray diffraction study. Molecular packing of all three compound are directed by hydrogen bonding and π-π interactions. Molecular structure of two compounds are shown in Figure 1.

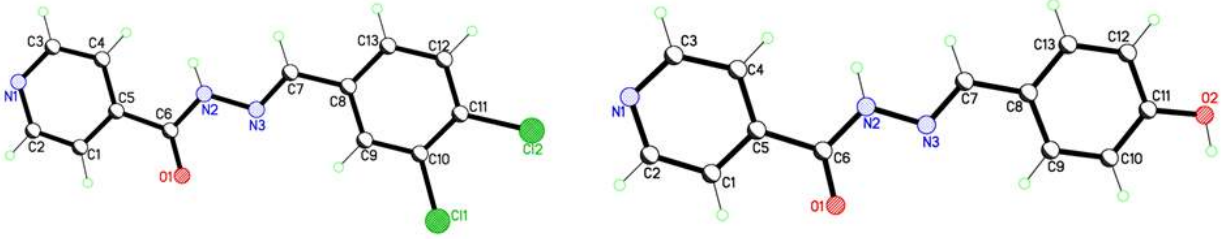

Figure 1 Molecular structure of two hydrozone compounds.

Keywords: Schiff Bases, Hydrazone, Hydrogen Bonding, π-π Interactions.

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Molecular Structure of A Novel La(III) Complex and Its Photo-luminesence Properties

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Lanthanide(III) complexes are of special interest due to their wide range of applications in different scientific areas ranging from chemistry to material science to the life science [1–3]. Because of their unique properties and potential applications, lanthanide complexes are used to design Ln-doped semiconductors, magnetic, catalytic, fluorescent, and nonlinear optical materials [4, 5]. Lanthanide complexes usually exhibit high coordination numbers and structural diversity. It is very difficult to predict the coordination number and geometry of lanthanide complexes in the solid state unlike their transition metal counterparts. In this study, a novel La(III) complex of a Schiff base (H_2L) was synthesised and characterised by single crystal X-ray diffraction study (Fig. 1). In the structure, La(III) ion is 10-coordinated by O atoms, five of which come from three nitrate ions, four come from the two Schiff base ligands and one from methanol oxygen atom. Photoluminesence properties of the complex was investigated.

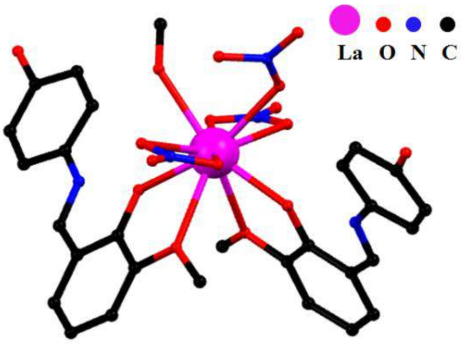

Figure 1 Molecular structure of La(III) complex.

Keywords: Lanthanide(III), X-ray Structure, Schiff base, Photoluminesence

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Hydrogen Bonding Interactions Between 2,6-Dichloro-*p*-Nitrophenol with 1,4-Dioxane: X-Ray Characterization

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Phenol derivatives are interesting molecules for theoretical studies due to their relatively small size and similarity to biological species [1]. Crystal structure of 2,6-Dichloro-p-Nitrophenol with dioxane is depicted in Fig. 1. A single crystal of dimensions 0.61 x 0.52 x 0.35 mm^3 was chosen for the diffraction experiment. X-ray diffraction data for the compound was collected at 150(2) K on a Bruker Apex II CCD diffractometer using Mo-Kα radiation ($\lambda = 0.71073$ Å). The structures were solved by direct methods and refined on F^2 using all the reflections [2]. The compound crystallizes in monoclinic, crystal system, $P_{21/n}$ space group with unit cell parameters a= 11.9935(7), b= 5.1491(3), c= 16.8775(10) Å, β= 105.9360(10)°, 1002.23(10) Å3 and Z=4. All the bond lengths and angles are within the normal ranges. All bond lengths and angles in the phenyl ring have normal Csp^2- Csp^2 values with small distortions. In the structure, two molecules of 2,6-dichloro-4-nitrophenol moiety are connected by an 1,4-dioxane molecule via strong hydrogen bonding (O3H……O4). The molecules lie about an inversion centre and asymmetric unit contains half of the structure. Six-membered 1,4-dioxane ring has an ideal chair conformation, and all the geometric parameters in the ring are quite normal.

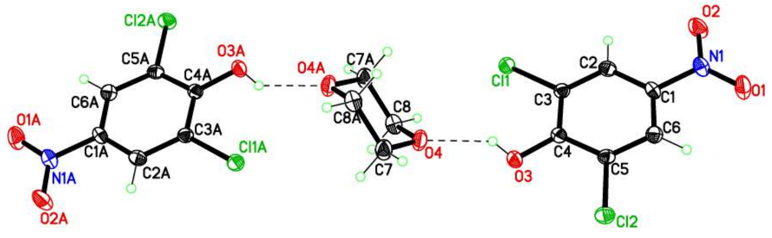

Figure 1. Molecular structure of DCNP with 1,4-dioxane with atom numbering, thermal ellipsoid 50% probability, symmetry operation -x+1,-y+2,-z.

Keywords: Phenol, Crystal Structure, Hydrogen Bonding, 1,4-dioxane.

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Synthesis, Structural Characterization of the 4- Heptyloxy -3-Methoxy Benzaldehyde Compound and Investigation of the Its Photoluminesence Properties

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Mehmet Tümer[1], and Vickie McKee[2]

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In a broad sense, liquid crystals (LCs) can be considered as prototypical self-organizing molecular materials of today [1]. Liquid crystals stand between the isotropic liquid and the strongly organized solid state. Similarly, life stands between complete disorder which is death, and complete rigidity, which is death again [2]. In materials science, non-covalent interactions have been used to obtain well-defined, self-assembled architectures in neat systems as well as in solvents. LCs belong to one of such systems. LCs are unique functional soft materials that combine both order and mobility on a molecular, supramolecular, and macroscopic level [3]. Molecular structure and photoluminesence properties of a novel alkyloxy compound (4-heptyloxy-3-metoxy benzaldehyde) were investigated.

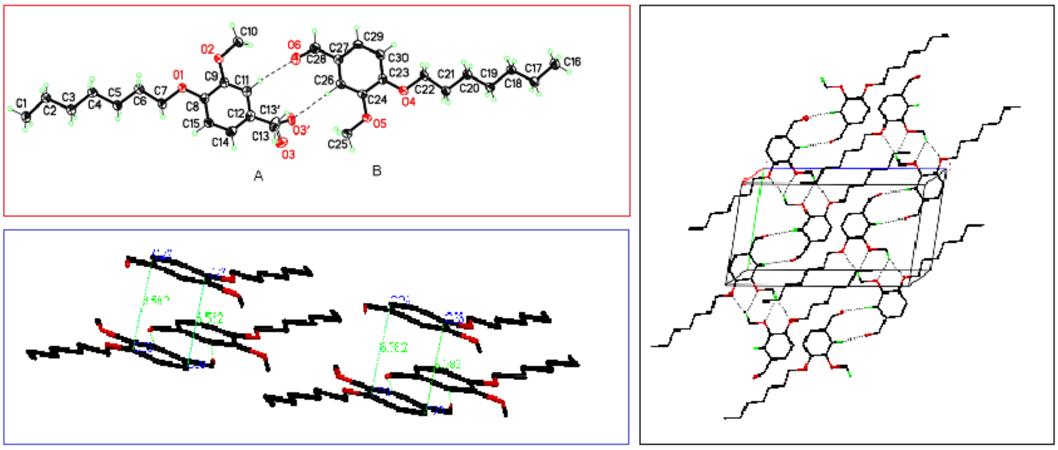

Figure 1. X-ray structure of 4-heptyloxy-3-metoxy benzaldehyde.

Keywords: Luquid crystal, Molecular Structure, Photoluminesence.

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Synthesis, Crystal Structure of A Novel Three-Dimensional Metal−Organic Framework Containing One-Dimensional Ag···Ag cluster

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The constitution of metal–organic frameworks (MOFs) with appropriate metal ions and ligands have attracted great interest because of their fascinating structures and potentially useful properties for ex. porosity, luminescence, catalysis, conductivity, magnetism and like these [1]. In this study, a novel three dimensional polynuclear Ag(I)-5-hydroxyisophthalate complex $\{[Ag_2(\mu_6\text{-hip})(H_2O)]\cdot H_2O\}_n$ (H_2hip = 5-hydroxyisophthalic acid) has been synthesized. The molecular structure of complex has been determined by the single crystal X-ray diffraction. The complex has been observed to crystallize in the triclinic space group *P*-1. There are two different Ag(I) ions, Ag1 ion exhibits a distorted square pyramidal geometry by two hip^{2-} which act bidentate, two Ag(I) ions and one aqua ligand. Whereas Ag2 ion has octahedral geometry by three hip^{2-} which act four dentate and two Ag(I) ions. The hip^{2-} ligand acts as a sixdentate bridging ligand with a new coordination mode. The most important feature is the hip^{2-} ligand coordinated to metal ion through –OH group, in the hip literature none of synthesized complexes have coordinated to metal ions through –OH group [2, 3]. In this complex, there is a one-dimensional chain consisting Ag···Ag interactions.

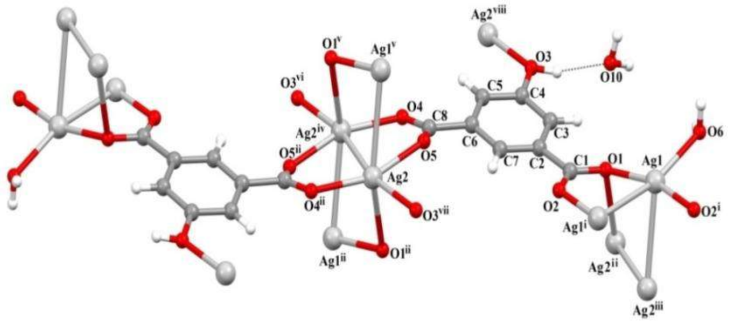

Figure 1. The molecular structure of **1** showing the atom numbering scheme.
(i: 3-x, 3-y, 2-z, ii: 2-x, 3-y, 1-z, iii: x, y, 1+z, iv: 2-x, 3-y, -z, v: x, y, -1+z, vi: 1-x, 2-y, -z,
vii: 1+x, 1+y, z, viii: -1+x, -1+y, z).

Keywords**:** 5-hydroxyisophthalic acid, three-dimensional complex, new coordination mode, Ag···Ag interaction.

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Synthesis, Crystal Structure of A Novel Two-Dimensional Coordination Polymer with 5-hydroxyisophthalate

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Polymers play a substantial role due to the vast variety of their physical and chemical properties as well as their wide commercial application [1]. In this study, a novel polynuclear Zn(II)-5-hydroxyisophthalate complex $[Zn(\mu\text{-hip})(bpp)]_n$ **(1)** (H_2hip = 5-hydroxyisophthalic acid, bpp: 1,3-bis(4-pyridyl)propane) has been synthesized. The molecular structure of complex has been determined by the single crystal X-ray diffraction. The compound was characterized by elemental analysis, spectroscopic measurements (UV-Vis. and FT-IR), photoluminescence and thermal analysis (TG, DTG and DTA). The complex has been observed to crystallize in the triclinic space group *P*-1. Zn(II) ion has tetrahedral geometry by two oxygen atoms (O1 and $O5^i$) from carboxylate groups and nitrogen atoms (N1 and $N2^i$) from bpp ligand. The hip^{2-} ligand acts as bidentate bridging ligand which links two Zn(II) ions (in different unit cell) to each other. In the literature $\{[Zn(hip)(bpp)]\cdot H_2O\}_n$ formulated complex has been synthesized [2]. But this complex is different from our complex with one hydrate molecule and unit cell parametres. This complex **(1)** is a 2-dimensional polymeric complex. The photoluminescence of the complex in the solid state at room temperature will be examined.

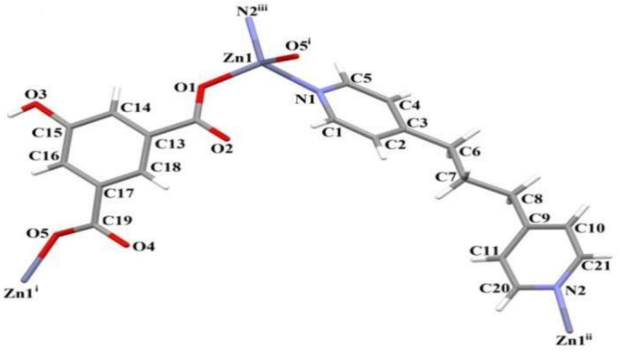

Figure 1**.** The molecular structure of **1** showing the atom numbering scheme.
(i: ½-x, ½+y, ½-z, ii: 1+x, y, 1+z, iii: -1+x, y, -1+z)

Keywords**:** 5-hydroxyisophthalic acid, zinc(II) complex, luminescence.

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Synthesis, Crystal Structure, Spectroscopic and Thermal Studies of $(Hda)(Him)_2(V_5O_{14})$ Complex

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The design and assembly of supramolecular architectures are quite an active research area due to crystal engineering of functional materials involving potential applications in optical, electronic, magnetic, liquid crystal, porous materials, etc. [1–2]. A new supramolecular compound formulated $(Hda)(Him)_2(V_5O_{14})$ **(1)** (im= imidazole, da = diethylamine) was synthesized with hydrothermal method at 150 °C for 96 hours and characterized by elemental analysis, magnetic, spectroscopic measurements (UV-Vis. and FT-IR), thermal analysis (TG, DTG and DTA) and single crystal X-ray diffraction technique. In the experimental process V_2O_5(1:1), H_3BO_3(1:1), im, 1 mL da and 10 mL water was used. The complex **1** is crystallized in the monoclinic crystal system space group $P2_1/c$. The asymmetric unit of the complex **1** consists of $V_5O_{14}^{3-}$ cluster and protonated diethylamine and two protonated imidazole groups. Imidazolium cations are held on to each others with $\pi\cdots\pi$ interaction. There is C-H$\cdots\pi$ interaction between Hda^+ and imidazolium cation. The $V_5O_{14}^{3-}$ cluster hangs on to structure through strong inter-molecular hydrogen bonding. Due to these interactions three-dimensional supramolecular framework occurred.

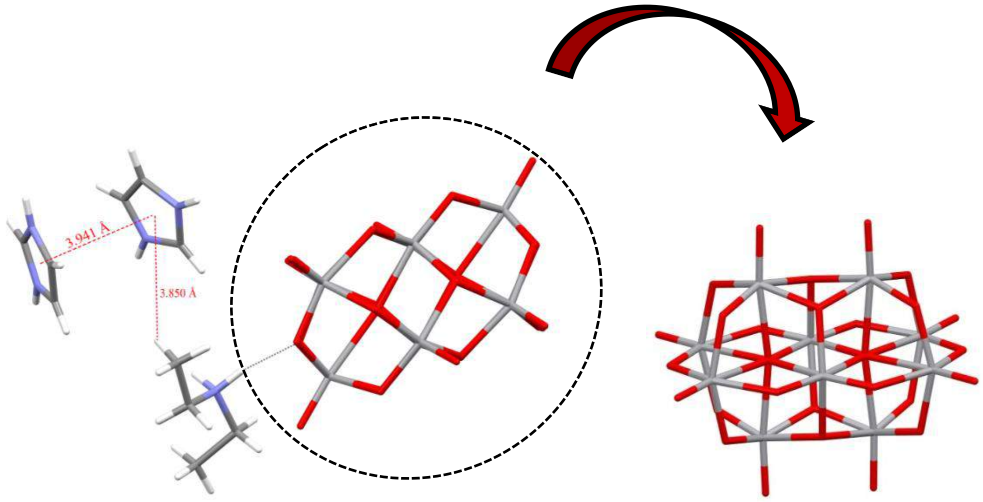

Figure 1. The molecular structure of $(V_5O_{14})(HDa)(Him)_2$ **(1).**

Keywords: Vanadium, imidazole, vanadiumoxide cluster.

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Structure Of 2,3-Dihydro-4-Phenyl-1,4-Benzoxazine -6,7-Dicarbonitrile

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Phthalocyanine compounds are used in electrochromism, batteries, photodynamic therapy(PDT), semiconductive materials, liquid crystal and non-linear optics [1,2]. The title molecule, $C_{16}H_{11}N_3O$, contains a benzene ring fused to an oxazine ring and one phenyl ring bound to the N atom. The two aromatic rings are not coplanar because of steric hindrance, the shortest H…H contact being 2.45 (4) Å. The dihedral angles between these two rings is 52.28 (1)°. Crystal data, $C_{16}H_{11}N_3O$, Monoklinik, $P2_1/c$, Z=4, a=14.3999(14)Å, b=7.5806(4)Å , c=13.1208(14)Å, β=114.879(7)^0, V=1296.6(2)Å^3, R=0.050, $\Delta\rho_{max.}$=0.18eÅ^{-3}, $\Delta\rho_{min.}$= -0.16eÅ^{-3}, λ(MoKα)= 0.71073 Å.

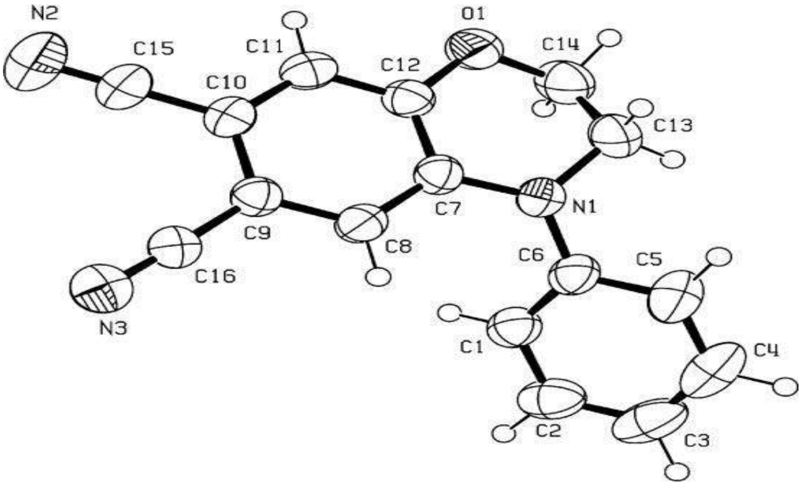

Figure 1. The molecular structure of $C_{16}H_{11}N_3O$ and the crystallographic numbering scheme adopted. Displacement ellipsoids are drawn at the 50% probability level.

Keywords: Phthalocyanine, Photodynamic therapy (PDT), Semiconductive.

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Structure Of (*E*)-2-Hydroxy-3-Methoxy-5-[(3- Methoxyphenyl) Diazenyl]Benzaldehyde

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[2]Ondokuz Mayıs University,Faculty of Arts and Sciences, Department of Chemistry, Samsun, Turkey
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Azobenzenes have a wide variety of potential applications for organic non-linear optics, optical storage media, chemosensors, and photochemical switches because of their characteristic colour and photoresponsive properties [1]. In addition, azo compouds represent the dominant class of synthetic colourants employed in the textile, printing, agrochemical and pharmaceutical industries [2]. The molecule of the title compound, $C_{15}H_{14}N_2O_4$, is approximately planar and displays a trans configuration with respect to the N=N double bond. The molecules are linked by intermolecular C-H…O and C-H…π interactions, forming a three-dimensional network. Crystal data, $C_{15}H_{14}N_2O_4$, Monoklinik, $P2_1/c$, Z=4, a=11.8486(14)Å, b=9.9295(9)Å, c=12.6574(15)Å, β=112.441(9)^0, V=1376.4(3)Å^3, R=0.083, $\Delta\rho_{max}$.=0.12eÅ^{-3}, $\Delta\rho_{min}$.=-0.13eÅ^{-3}, λ(MoKα)= 0.71073 Å.

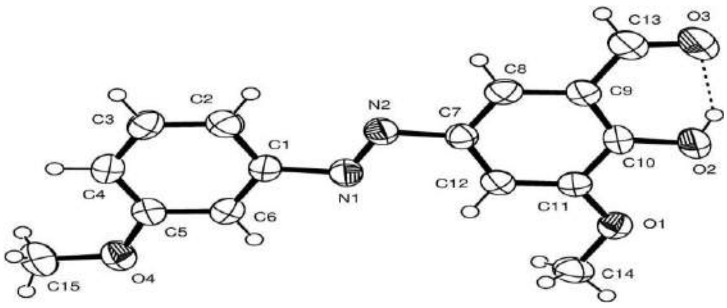

Figure 1. The molecular structure of $C_{15}H_{14}N_2O_4$ and the crystallographic numbering scheme adopted. Displacement ellipsoids are drawn at the 50% probability level.

Keywords: Agrochemical, chemosensors, photochemical switches.

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Synthesis, Crystal Structure And Vibrational Spectroscopy Of A Mixed Ligand Cu(II)-Pentaborate

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In recent decades, borate materials have been extensively studied because of their rich structural chemistry and potential applications, especially in mineralogy, nonlinear optics and photoluminescence [1]. Compared to the expansion of inorganic metal borates found in high-temperature/pressure solid-state synthetic and mineral forms, the metallo-organically templated borate is less explored [2]. A metallo-organically templated pentaborate $[Cu(im)_4Cu(\mu\text{-}ac)_2(H_2O)_2(im)_2][B_5O_6(OH)_4]_2$ has been synthesized by hydrothermal reaction and characterized by single-crystal X-ray diffraction and FT-IR spectroscopy. The crystal structure of this compound consists of two copper center and two discrete $[B_5O_6(OH)_4]^-$ anions. These are linked together through intensive hydrogen bonding interactions. The two different copper are connected by acetate molecule. A anion of $[B_5O_6(OH)_4]^-$ is composed of two B_3O_3 rings which is constituted of two BO_3 planar triangles an done BO_4 tetrahedron connected of common oxygen atom. This complex was synthesized by You et al. in 2010 [3]. But we synthesized the same complex by using different method.

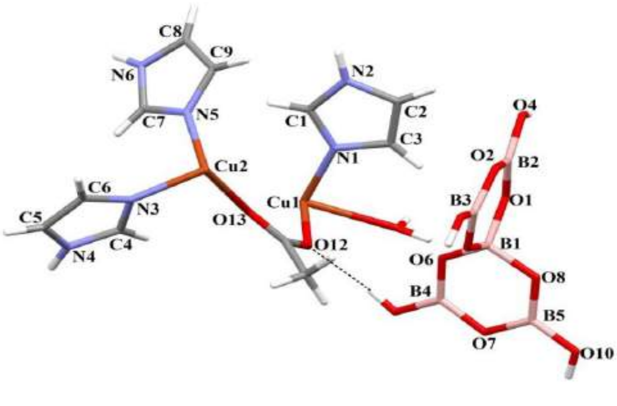

Figure 1. Asymetric unit of **1.**

Keywords**:** borate, crystal structure, transition metal complexes

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Unprecedented 4/5-methylimidazole linkage isomerism within $[Cu(dpa)(4\text{-}meim)_3]\cdot H_2O$

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Lately, many the mixed ligand complexes of transition metal(II) ions have been designed and constructed due to their significance in chemical, biological, environmental, catalytic and ion exchange [1, 2]. A novel Cu(II) diphenate complex with the 4-methylimidazole ligand was synthesized and characterized through elemental analysis, thermal analysis, magnetic susceptibilities, spectral methods and X-ray diffraction techniques. X-ray crystallographic study of $[Cu(dpa)(4\text{-}meim)_3]\cdot H_2O$ (**1**) revealed that the Cu(II) ion has distorted trigonal bipyramidal geometry with three 4-methylimidazole and one diphenate ligands (Fig. 1.). The most striking feature of complex **1** is that the structure contains two coordination modes of the 4(5)-meim ligand in same coordination sphere. Moreover, another interesting feature of this complex is the presence of C–H···Cu weak hydrogen bonding interactions.

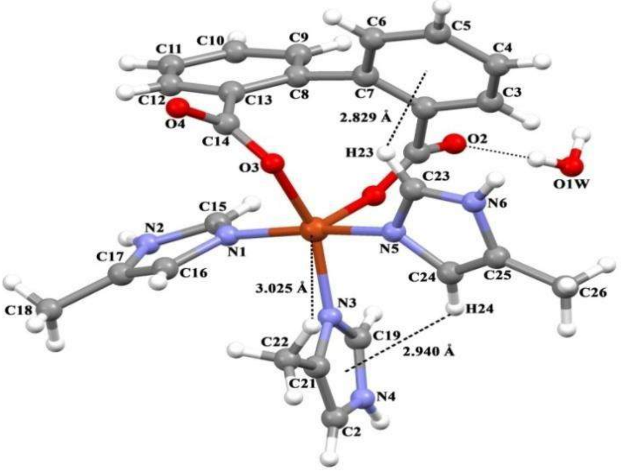

Figure 1. The molecular structure of **2.**

Keywords**:** Linkage isomerism, Mixed ligand complex, Diphenate Complexes

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The Synthesis and Characterization of Copper(II)–3,3'–Thiodipropionate Complexes With Imidazole Derivatives

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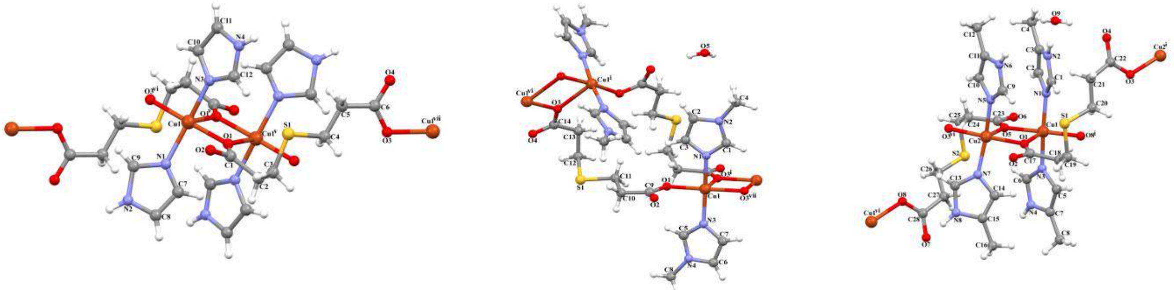
Synthesis and characterization of coordination polymers have attracted interest because of their tunable structure and potential applications in the fields such as gas adsorption/separation, catalysis, conductivity, magnetism and non linear optic [1]. In this study, three new coordination polymers, 3[Cu(μ_3–tdp)(im)$_2$]$_n$ (**1**), {[Cu(μ_3–tdp)(1–mim)$_2$]·0.5H_2O}$_n$ (**2**), {[Cu_2(μ_3–tdp)$_2$(4–mim)$_4$]·H_2O}$_n$ (**3**), [tdpH_2=3,3'–thiodipropionic acid, im=imidazole, 1–mim=1–methylimidazole and 4–mim= 4–methylimidazole], were synthesized using 3,3'–thiodipropionic acid (tdpH_2) and imidazole derivatives. These complexes were characterized by IR spectroscopy, elemental analysis, magnetic measurements, thermal analyses and single crystal X–ray diffraction. Complexes **1–3** crystallize in the monoclinic system with the space groups of C2/c and P2$_1$/c, respectively (Fig. 1). In complexes **1–3**, the tdp ligand acts as a bridging ligand to form 1D chain, which are extended into a 2D layer by hydrogen bonding and π···π interactions. The 3,3'–thiodipropionate ligand exhibits an unexpected coordination mode in **1-3**.



1 **2** **3**

Figure 1. The molecular structures of **1-3.**

Keywords: 3,3'–thiodipropionic acid; 3,3'–thiodipropionate complexes; imidazole complexes

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Dinuclear And Polynuclear Copper(II) Complexes With 3,3'-Thiodipropionate And Unprecedented Coordination Mode

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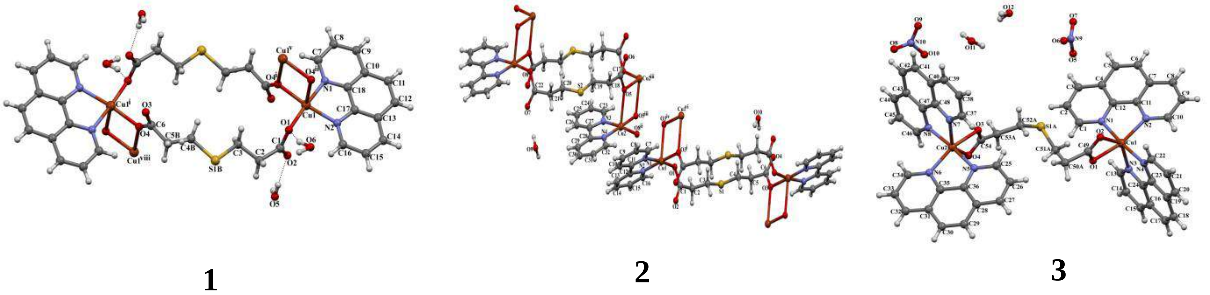
The syntheses of coordination polymers have received great interest owing to their magnetic, luminescence, gas storage/separation, catalytic properties [1]. In the syntheses of coordination polymers, aromatic and aliphatic polycarboxylates have been widely utilized due to the fact that they can adopt various coordination modes in the self-assembly process. In this study, we described the synthesis, crystal structure, thermal properties of three new coordination compounds, namely, ({[Cu(μ_3–tdp)(phen)]·$2H_2O$}$_n$ (**1**), {[Cu(μ_3-tdp)(bipy)]·H_2O}$_n$ (**2**), [Cu_2(μ_2-tdp)(phen)$_4$](NO_3)$_2$·$2H_2O$ (**3**)) using flexible 3,3′-thiodipropionic acid (H_2tdp) with phen and bipy. The complexes were characterized by the IR spectroscopy, elemental analysis, magnetic measurements and single crystal X-ray diffraction. Thermal behaviors and thermochromic properties of the complexes were investigated in detail. Complexes **1** and **2** are 1D coordination polymers while complex **3** is dinuclear structure. In complexes **1** and **2**, the tdp acts as a tridentate bridging ligand to coordinate the two different Cu(II) centers to form 1D chain, which are extended into a 3D networks by hydrogen bonding and $\pi\cdots\pi$ interactions. The 3,3'–thiodipropionate ligand adopts a new coordination mode in **3**. Furthermore, complex **3** changed the color from blue to green at 140 °C at solid state.



1 **2** **3**

Figure 1. The molecular structures of **1-3.**

Keywords: 3,3'–Thiodipropionate Complexes, Copper(II) Complexes, Dinuclear Complex, *Thermochromism*

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Synthesis and Crystal Structure of 4-Methylbenzene-1-{(*E*)-[(6-hydroxycyclohexa-1,4-dien-1-yl) methylidene] amino}-5-(4-methylbenzoyl)pyrimidin-2(1*H*)- one

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Zülbiye Önal[1]

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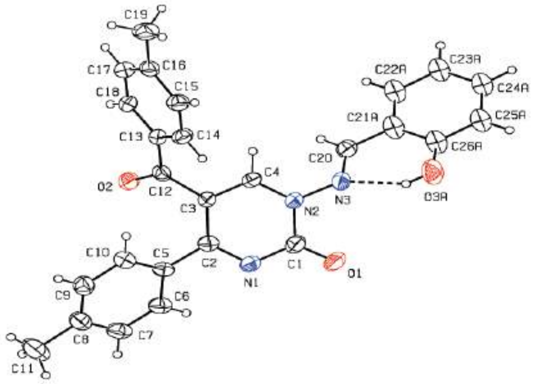
The compound, $C_{26}H_{21}N_3O_3$ (I), has been synthesized and characterized by elemental analysis, IR, ^{1}H NMR and ^{13}C NMR. The crystal structure of (I) has been determined by single crystal X-ray diffraction method. It crystallizes in monoclinic space group C2/c, with unit cell dimensions a = 26.787 (3), b = 11.0216 (9), c = 23.221 (3) Å, β = 140.546 (7)°, V = 4356.5 (10) Å^3, Z = 8. The atoms of the phenol group are disordered over two sites [occupancies = 0.697 (19) and 0.303 (19)] and the major and minor components of the disordered ring are oriented at a dihedral angle of 12.6 (6)°. The molecular structure is stabilized by an S(6) ring motif, owing to an intramolecular O—H...N hydrogen bond. In the crystal, the components are linked into a three-dimensional framework by intermolecular C—H...O hydrogen bonds. The crystal packing also features two C—H...π interactions. Moreover, π-π stacking interactions with a centroid-centroid distance of 3.756 (3) Å are observed between the pyrimidine rings of the neighbouring molecules.



(I)

***Keywords**: Pyrimidine, single crystal X–ray, disorder, crsytal structure*

The *thrinuclear* Mn(II) complex containing thiophene-2-carboxylate and aqua ligands

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The complexes of thiophene-2-carboxylic acid were known antifungal and anti-tumor properties, with some transition metals such as Cu(II), Ni(II), Zn(II) and Co(II) [1]. The compound was synthesized by mixture of Mn^{+2}, thiophene-2-carbocylic acid and *1-vinylimidazole* in ethanol. The suitable crystals for X-ray single crystal analyses were deposited by slow evaporation of the filtered solution of the reactants. There were two different types of aqua and thiophene-2-carbocylate ligands in the thrinuclear complex which crystallized in the space group P-1 (Fig. 1). The one type of thiophene-2-carboxylate and aqua ligands acted in bridging manners and the other type of them acted as monodentate ligands (Fig. 1). Interestingly the *1-Vinylimidazole was not coordinated to the metals* (Fig. 1) *and* has found its place among molecular layer by formation of π···π stacking interactions with the five membered thiophen rings and C-H···O interactions in protonated cationic form. The compound has shown three dimensional molecular architectures. For this, the both type of aqua ligands acted as hydrogen bond donors and the π···π stacking interactions were also detected between the thiophen rings in the solid state.

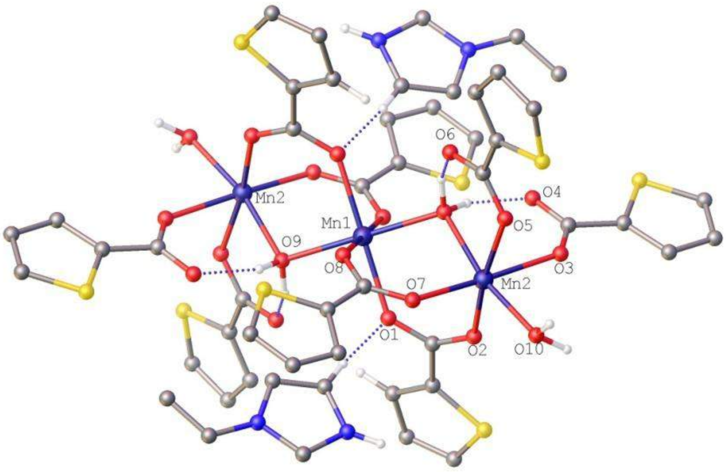

Figure 1. The structure of the compound (some hydrogen atoms were omitted for clarity).

Keywords: thiophene-2-carbocylic, three nuclear complex, π···π stacking

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Influence of doping on the X-ray Diffraction patterns of nanostructured CdO films

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Cadmium oxide (CdO) is a n-type semiconductor that has a variety of optoelectronic applications like, solar cells, optical communications, flat panel display [1-3]. For transparent conducting oxide (TCO) films doping is a powerful tool to organize the physical properties. The structural, morphological and optical properties of CdO can also be controlled by doping. Among various materials, tin can easily replace cadmium (Cd^{2+} = 0.087 nm and Sn^{4+} = 0.062 nm) and doping with tin can reduce grain size [4]. Pure and tin-doped CdO films were prepared by SILAR method. The film's structural, morphological and optical properties have been investigated by X-ray diffraction (XRD), field emission scanning electron microscope (FESEM) and UV-Vis spectrophotometer. XRD results showed that all of the films are polycrystalline cubic CdO. Doping of tin enhances the film's (111) preferred orientation and causes slight shift in the (111) Bragg angle towards higher value. Increasing tin concentrations causes decrease in the intensities of (111) and (200) peaks. From the FESEM images, it was seen that tin-doping concentration affects the shapes of the nanostructures [5]. The optical properties and thus the band gap of CdO films can be controlled by tin doping rate.

Keywords: *CdO, XRD, FESEM*

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$Be_{1-X-Y}Ca_xLi_y$te Alaşimlarinin Yapisal, Elektronik, Elastik Ve Optiksel Özelliklerinin Ab-Initio Metodla İncelenmesi

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Bu çalışmada, $Be_{1-x-y}Ca_xLi_yTe$ alaşımının bazı yapısal, elektronik ve optik özellikleri yoğunluk fonksiyon teorisi (YFT)' yi temel alan CASTEP paket programı kullanılarak, Local Density Approximation (LDA) ile incelenmiştir. Yapılan hesaplamada $Be_{1-x-y}Ca_xLi_yTe$ Alaşımlarının; örgü parametreleri, bant yapıları, durum yoğunluğu, Kramer-Kronig bağıntıları kullanılarak, dielektrik fonksiyon, kırılma indisi, soğurma katsayısı ve enerji kayıp fonksiyonu hesaplandı. Dielektrik fonksiyonun soğurma başlangıç noktasının, bant aralığı enerjisi ile uyumlu olduğu görülmüştür. Elastik sabitleri yardımı ile bulk modülü, Young ve izotropik shear modülleri, poisson oranları ve diğer özellikleri hesaplandı.

***Anahtar kelimeler**:* Yoğunluk fonksiyon teori, dielektrik fonksiyon, LDA, optik özellikler, örgü parametreleri, kırılma indisi, vs.

2-[(2E)-2-(2-chloro-6-fluorobenzylidene)hydrazinyl]pyridine

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Hydrazones are formed by the condensation of hydrazines with aldehydes or ketones. These are typically crystalline compounds with sharp melting points. Therefore, these compounds can be used to identify the aldehydes and ketones from which the hydrazones have been formed. Hydrazones are more efficient than oximes in this reaction, because their greater molecular weight causes lower solubility in most solvents. Therefore, they can be easily isolated and recrystallized [1]. Hydrazones are also useful for the synthesis of metal complexes as they easily form stable complexes with most transition metal ions. Therefore, hydrazones and their metal complexes have gained a special attraction and growing interest in chemistry and biology, analytical chemistry. Also, hydrazones possessing an azomethine —NHN□CH— proton constitute important class of compounds for new drug development [2]. Also, hydrazones have been intensively investigated mostly for pharmacological applications due to their potential application as anticancer, antiviral, antibacterial, and antifungal agents [3-7]. In this work, 2-[(2E)-2-(2-chloro-6-fluorobenzylidene)hydrazinyl]pyridine, $C_{12}H_9N_3FCl$, schiff base molecule has been synthesized and characterized by single crystal X-ray determination. This compound crystallizes in the monoclinic system, $P2_1/n$ space group with unit cell parameter a = 3.9415(3) Å, b = 22.8712 (19) Å, c = 12.3809 (10) Å, β=95.149 (4)°.

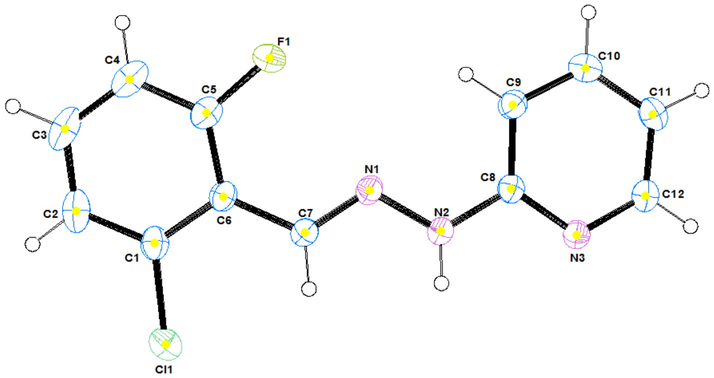

Figure 1. ORTEP drawing of the title compound.

Keywords: Hydrazone, crystal structure, X-Ray.

Crystal Structure, Spectroscopic Properties and Density Functional Theory Study of (Z)_1_[(2,4_Dimethoxyphenylamino) Methylene] Naphthalen_2(1H)_One

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The Schiff base (Z)_1_[(2,4_dimethoxyphenylamino)methylene] naphthalen_ 2(1H)_one was synthesized from the reaction of 2_hydroxy_1_naphthaldehyde with 2,4_dimethoxyaniline. The title compound has been characterized by FT_IR, UV–Vis and, X_ray single_crystal techniques. The present X_ray investigation shows that the compound exists in the keto_amine tautomeric form. Molecular geometry and vibrational frequencies of the compound in the ground state have been calculated using the density functional theory (DFT) with 6_311G(d,p) basis set and compared with the experimental data. The calculated results show that the optimized geometry is compatible with the crystal structure and the theoretical vibrational frequencies are in good agreement with the experimental values. Besides, molecular electrostatic potential (MEP), frontier molecular orbital analysis (HOMO_LUMO) and nonlinear optical (NLO) properties of the compound were investigated using the same theoretical calculations

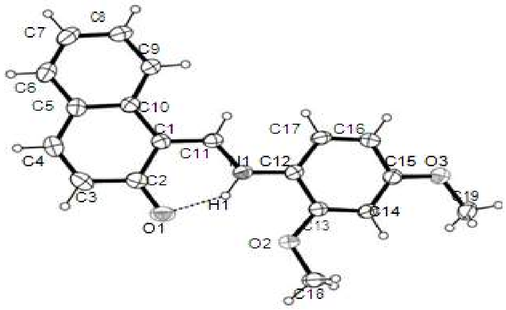

Figure 1. Ortep3 diagram of the title compound. Displacement ellipsoids are drawn at the 30% probability level. The intramolecular hydrogen bond is shown as a dashed line.

Keywords: Schiff base, crystal calculations, tautomeric form

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The Synthesis, Characterization and study of luminescent properties of Ba_2CaWO_6:Dy^{3+} Phosphor Compound

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The earth alkali orthotungstate compounds are very stable and have different crystallographic structures. Therefore they have been investigated intensively for their structural properties [1]. Although the Ba_2CaWO_6 phase is well known as home phase [2], but as doped phosphor hasn't been investigated yet. The Ba_2CaWO_6:Dy^{3+} phosphor was synthesized first time in this study, characterized structurally by powder diffraction method. Its structural parameters found as: cubic, space group Fm3m, cell parameters are a=b=c=8.384 Å (JCPDS File Number: 22-0509). Luminescence properties of this phase, Ba_2CaWO_6:Dy^{3+}, were investigated by photoluminescent spectrophotometer, and its exciting and emission spectrum is shown in fig. 1. Strong and broad bands belong to charge transfer transitions of the home phase. The Dy^{3+}-O^{2-} charge transfer band and $^6H_{15/2}\rightarrow{}^4M_{17/2}$ transition band of Dy^{3+} are overlapped entirely by home-phase charge transfer bands. $^6H_{15/2}\rightarrow{}^4M_{15/2}$ and $^6H_{15/2}\rightarrow{}^6P_{7/2}$ transition bands of Dy^{3+} observed near 360 nm, and $^4F_{9/2}\rightarrow{}^6H_{15/2}$ ve $^4F_{9/2}\rightarrow{}^6H_{13/2}$ transition bands observed at 493 and 585 nm respectively. The weak transition bands of Dy^{3+} ($^4F_{9/2}\rightarrow{}^6H_j$ (j=11/2, 9/2)) were observed between 650-800 nm [3].

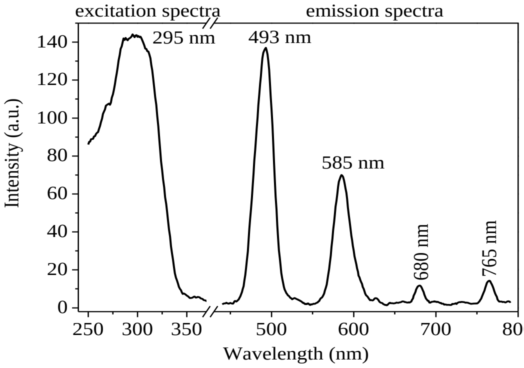

Figure 1. The exciting and emission spectrum of Ba_2CaWO_6:Dy^{3+} phase.

Keywords: Ba_2CaWO_6:Dy^{3+} phosphor, structure, luminescence spectra

Acknowledgment: This work financially supported by Turkish Scientific and Technical Research Council, TUBİTAK, (Project Nr: 107T392) and Mersin University Research Fond (Project Nr: BAP-FBE KB (RA) 2013-2 YL)

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Comparison of Crystallite Size and Lattice Strain of YBCO (123) and YBCO (358) High Temperature Superconductors

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The new Y-based (Y358) high-temperature superconductor (HTSC) is synthesized by using the standard solid-state reaction method. This superconductor shows the Meissner effect at liquid nitrogen temperature (77 K). The XRD spectra were performed and it was seen that they have a similar crystalline structure with Y123 with some impurity peaks. We studied to determine the lattice strain and the average crystallite size calculated in a direction perpendicular to the surface of the superconductor specimens by X-ray peak broadening analysis. As a result, the crystal size of Y358 superconductor was seen to be about 3 times larger than Y123 superconductor crystal size.

Keywords: High Temperature Superconductors, YBCO-358, Crystallite Size, Lattice Strain

Crystal Structure of N-(5-((m-tolylimino)methyl)pyridin-2-yl)pivalamide

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The structure of title compound N-(5-((m-tolylimino)methyl)pyridin-2-yl)pivalamide $C_{18}H_{21}N_3O$, has been synthesized. The Schiff base compound has been characterized by single–crystal X-ray diffraction. The compound crystallizes in the monoclinic space group P 1 21/c 1 with the following unit-cell dimensions a=5.5719(25)Å, b=24.9671(11)Å, c=12.2380(5)Å, α=90.000(0)^0, β=106.529(3)^0 , γ=90.000(0)^0, V=1632.13(17)Å^3 Z=4 . The crystal structure contains intramolecular N-H…N hydrogen bond. X-ray measurements $C_{18}H_{21}N_3O$ was carried out on a STOE IPDS II diffraction diffractometer with MoK$_\alpha$ radition. The molecular structure was solved by direct metod using SHELXS97 [1] and refiment by full-matrix least-squares on F^2 using SHELXL97 [1] program. An Ortep-3 [2] view of the molecule of title compound is shown in Fig. 1.

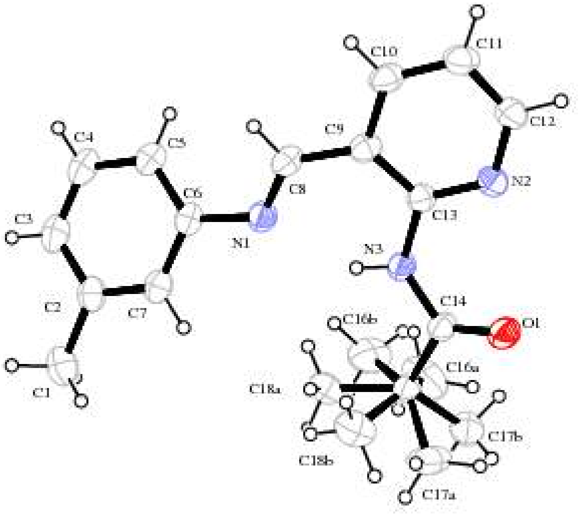

Figure 1. Ortep-3 diagram of the title compound.

Keywords: Schiff base, single crystal, X-ray diffraction

[1] Sheldrick, G. M. (2008). Acta Cryst. A64, 112-122

[2] Farrugia, L.J.,J. Appl. Cryst., 30(1997)

Crystal Structure of N-(3-((3-hydroxy-4methylphenylimino)methyl)pyridin-2-yl)pivalamidine

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The schiff base compound N-(3-((3-hydroxy-4methylphenylimino)methyl)pyridin-2-yl)pivalamidine $C_{18}H_{21}N_3O_2$, was characterized by single–crystal X-ray diffraction. The parameters that belong to this structure are a=5.8594(3)Å, b=18.8756(8)Å, c=16.0649(9)Å, α=90.000(0)^0, β=108.130(4)^0 , γ=90.000(0)^0, V=1688.56(23)Å^{3}Z=4. The compound crystallizes in the monoclinic, space group P 1 21/c 1.The crystal structure contains intramolecular N-H…N hydrogen bond. X-ray measurements $C_{18}H_{21}N_3O_2$ was carried out on a STOE IPDS II diffraction diffractometer with MoK$_\alpha$ radition. The molecular structure was solved by direct metod using SHELXS97 [1] and refiment by full-matrix least-squares on F^2 using SHELXL97 [1] program. An Ortep-3 [2] view of the molecule of title compound is shown in Fig. 1.

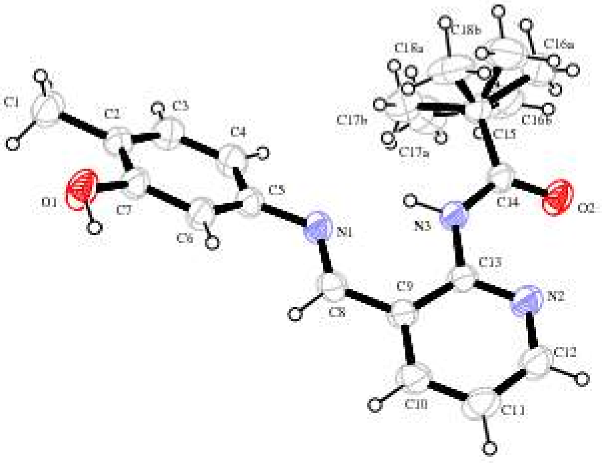

Figure 1. Ortep-3 diagram of the title compound

Keywords: X-ray diffraction, schiff base, crystal structure

[1] Sheldrick, G. M. (2008). Acta Cryst. A64, 112-122

[2] Farrugia, L.J.,J. Appl. Cryst., 30(1997)

An experimental and theoretical study of one redox-active ligand

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The crystal and molecular structure of *bis*(2-isobutyrylamidophenyl)amine has been determined from single crystal X-ray diffraction data [1]. It crystallizes in the triclinic space group *P-1*, Z = 2 with a = 9.5377(9) Å, b = 10.9710(10) Å, c = 18.6693(15) Å, α = 76.644(6)°, β = 80.010(6)°, γ = 81.379(7)°, and D_{calc} = 1.212 mg/m^3. The molecular structure, vibrational frequencies and infrared intensities of *bis*(2-isobutyrylamidophenyl) amine were calculated by ab initio Hartree-Fock and Density Functional Theory methods (BLYP, B3PW91 and B3LYP) using the 6-31G(d,p) basis set [2]. The calculated geometric parameters were compared to the corresponding X-ray structure of the title compound. The harmonic vibrations computed for this compound by the B3LYP/6-31G(d,p) method are in good agreement with the observed IR spectral data. Theoretical vibrational spectra of the title compound were interpreted by means of PEDs using the SQM 2.0 program. A general better performance of the investigated methods was calculated by PAVF 1.0 program.

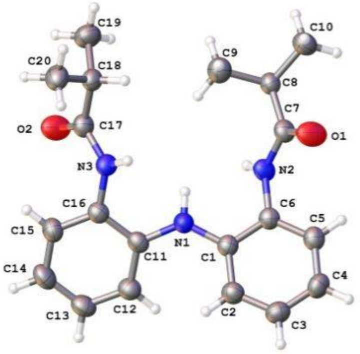

Figure 1. Molecular structure of *bis*(2-isobutyrylamidophenyl)amine.

***Keywords*:** Redox-active ligand, Ab-initio calculations, Infrared spectrum, DFT, B3LYP, BLYP, B3PW91.

***Acknowledgement*:** This work was financially supported by the Technological and Scientific Research Council of Turkey, TUBITAK, [TBAG (112T322)].

[1] S. K. Sharma, P. S. May, M. B. Jones, S. Lense, K. I. Hardcastle, C. E. MacBeth, *Chem. Commun*. **2011**, *47*, 1827-1829.
[2] M. J. Frisch, *et. al*. Gaussian 03, Revision C.02, Gaussian Inc., Pittsburgh, PA, **2003**.

Experimental and molecular modeling investigation of (*E*)-*N*-{2-[(2-hydroxybenzylidene)amino]phenyl} benzenesulfonamide

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and Nilgün Ö. Kalaycıoğlu[2]

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[2]Department of Chemistry, Faculty of Science, Erciyes University, 38039, Kayseri
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The compound has been synthesized and characterized by spectroscopic and single-crystal X-ray diffraction techniques. The crystal structure was solved by direct methods using SHELXS-97 [1] and refined by full-matrix least-squares method using SHELXL-97 [1]. In addition, quantum chemical calculations employing density functional theory (DFT) method with the 6−311++G(d,p) basis set by Gaussian 03W [2] were performed to study the molecular, spectroscopic and some electronic structure properties of the title compound, and the results were compared with the experimental findings. There exists a good correlation between experimental and theoretical data. Enol-imine/keto-amine tautomerization mechanism was investigated in the gas phase and in solution phase using the polarizable continuum model (PCM) approximation. The energetic and thermodynamic parameters of the enol-imine → keto-amine transfer process show that the single proton exchange is thermodynamically unfavored both in the gas phase and in solution phase. However, the reverse reaction seems to be feasible with a low barrier height and is supported by negative values in enthalpy and free energy changes both in the gas phase and in solution phase. The solvent effect is found to be sizable with increasing polarity of the solvents for the reverse reaction.

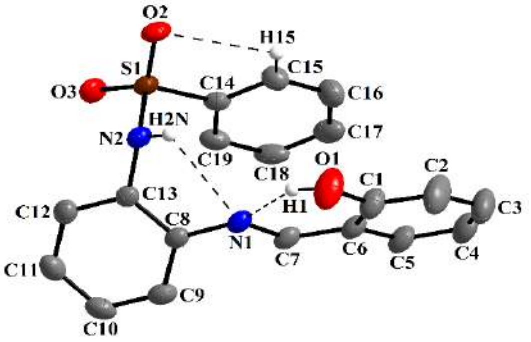

Figure 1. Molecule Structure.

***Keywords*:** Crystal structure, DFT, Enol-imine/keto-amine tautomerism

[1] G. M. Sheldrick, *SHELXS-97 and SHELXL-97*. University of Göttingen, Göttingen, **1997**.
[2] M.J. Frisch et al., *Gaussian 03W, Revision E.01*, Gaussian, Inc., Wallingford, CT, **200**

Synthesis, characterization and crystal structure of *N*-((3-methoxyphenyl)carbamothioyl)cyclohexanecarboxamide

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N-((3-Methoxyphenyl)carbamothioyl)cyclohexanecarboxamide was synthesized in excellent yield following the method described by Douglass and Dains [1]. The obtained compound was characterized by elemental analyses, IR spectroscopy and ^{1}H NMR spectroscopy. Title compound was also characterized by a single crystal X-ray diffraction study. Molecule formula of this compound, $C_{15}H_{20}N_2O_2S$: monoclinic, space group C2/c (no. 15), a = 16.454(3) Å, b = 6.6034(13) Å, c = 28.559(6) Å, β = 106.51(3)°, V = 2975.0(10) Å^3, Z = 8, μ(MoKα) = 0.221 mm^{-1}, $Dcalc$ = 1.306 g/mm^3, 8979 reflections measured ($5.96 \leq 2\Theta \leq 50.3$), 2643 unique ($R_{\text{int}}$ = 0.0318) which were used in all calculations. The final R_1 was 0.0328 (>2sigma(I)) and wR_2 was 0.0683 (all data). The bond lengths and angles in the thiourea moiety are typical for thiourea derivatives; the C8-S1 and C9-O1 bonds both show a typical double-bond character with 1.672(2) and 1.228(2) Å, respectively. The intramolecular hydrogen bond N1-H1···O1 (1.882(1) Å) forms a 6-membered ring with C8, N2 and C9 [2].

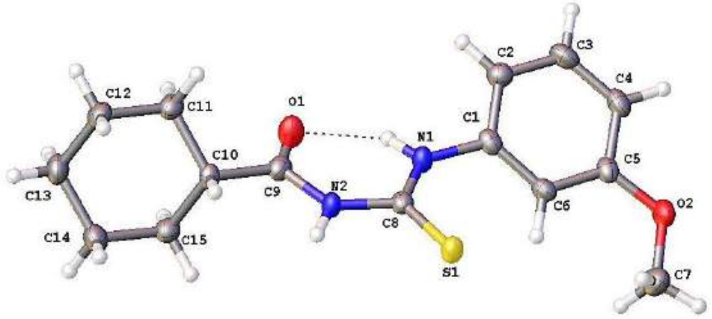

Figure 1. Molecular structure of title compound.

Keywords**:** Thiourea, Cyclohexanecarboxamide, X-ray single crystal diffraction, Synthesis, Thiourea derivatives.

Acknowledgement**:** This work was financially supported by Mersin University Research Fund (BAP.SBE.TB(CKO) 2007-1YL).

[1] I.B. Douglass, F.B. Dains, *J. Am. Chem. Soc*. **1934**, *56*, 719-721.
[2] C.K. Özer, *Synthesis and characterization of the transition group metal complexes of the various thiourea derivatives*, MSc. Thesis, Mersin University, Mersin, Turkey, **2008**.

Single-Crystal X-ray Crystallography Study of Cu(II) complex with *N*-polyfluorophenyl-3,5-di-*tert*-butylsalicylaldimine ligand

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[1]Dept. of Physics, Dicle University, Diyarbakır, Turkey.
[2]Dept. of Chemistry, Harran University, Şanlıurfa, Turkey
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Synthesis and crystallographic characterization of the title compound, [$C_{84}H_{88}N_4O_4F_{16}Cu_2$] has been reported in this study. Single-crystal X-ray diffraction method was also used to obtain the single crystal structure of the compound and its crystal and molecular structure was solved and refined by WinGX package programme [1, 2]. It crystallizes in a monoclinic system P121/c1 space group, with a= 23.7519(7) Å, b= 4.2504(9) Å, c= 10.7424(3) Å, b = 93.392(1)°, V= 8723.8(4) Å^3, Z=19, μ (MoK$_\alpha$)= 3.931 mm^{-1}. The refined molecule is shown in Figure 1. Its bond lenghts, bond angles, torsion angles and dihedral angles were determined.

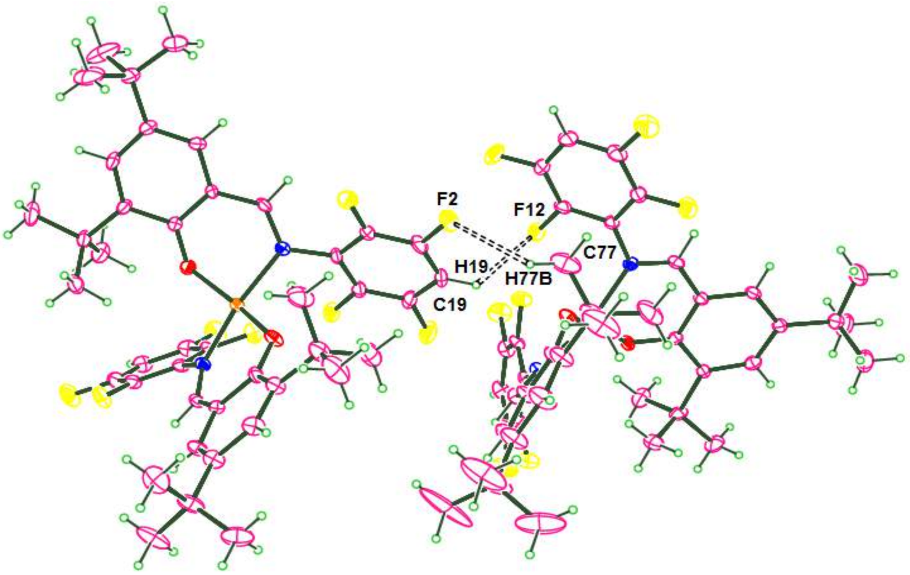

Figure 1. Mercury 1.4.2 diagram of the compound, showing the molecular numbering scheme. Displacement ellipsoids are drawn at 50% probability for all atoms except H.

Keywords: Single crystal X-ray structure refinement, WinGX, Cu(II) complex

[1] Farrugia, L. J. **(1997)** J. Appl. Cryst. 30, 565.
[2] Sheldrick, G. M. **(2008)** Acta Cryst. A64, 112-122.

Synthesis, Single-Crystal X-ray Diffraction and Density Functional Modelling Studies of a Schiff Base Combining Salicylaldehyde and Tyramine

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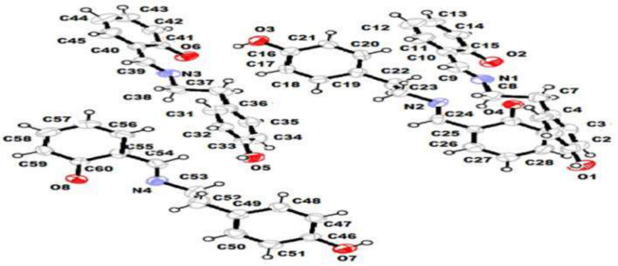
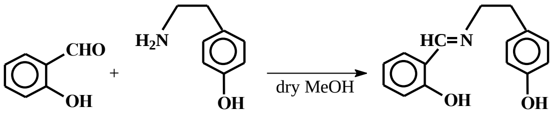
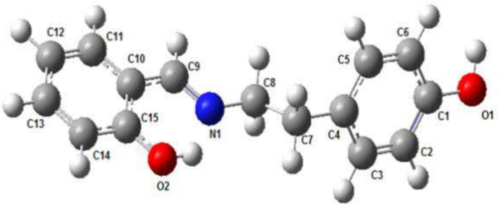
Schiff bases are the compounds carrying imine or azomethine (–C=N–) functional group and condensation products of primary amines with carbonyl compounds [1]. These compounds have a common integral feature of a variety of medicinal agents. In this study, the synthesis, crystallographic characterization and density functional modelling studies of the Schiff base ligand, 2-((*E*)-{[2-(4-hydroxyphenyl)ethyl]imino}methyl)phenol were reported. The molecular structure obtained from X-ray single crystal diffraction of the compound was compared using Hartree-Fock (HF) and density functional theory (DFT) calculations with 6-31G(d) basis set [2,3]. In addition to the optimized geometrical structures, atomic charges and molecular electrostatic potential (MEP) of the compound were investigated by using DFT. To investigate the tautomeric stability, some properties such as total energy, HOMO and LUMO energies of the tautomeric forms of the compound were obtained at B3LYP/6-31G(d) level in the gas phase. The calculated results showed that the phenol-imine form of the compound was more favorite than keto-amine form. Moreover, a good correlation between experimental and theoretical data for phenol-imine form of the compound was found.



The crystal structure of the compound





The theoretical geometric structure of the compound

This study was financially supported by The Scientific and Technological Research Council of Turkey (Grant No. 113Z861).

***Keywords*: Schiff Base, Molecular Orbitals, DFT, Tautomerism, Cystal Structure**

[1] H. Schiff, *Justus Liebigs Annalen der Chemie* **1864**, 118–119.
[2] H. B. Schlegel, *Journal of Computational Chemistry* **1982**, 214–218.
[3] C. Peng, P. Y. Ayala, H. B. Schlegel, M. J. Frisch, *Journal of Computational Chemistry* **1996**, 49–56.

Synthesis, characterization and crystal structure of *N*-((4-chlorophenyl)carbamothioyl)pivalamide

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Ümmühan Solmaz [1,2], Cora E. MacBeth [4], and Hakan Arslan [1,2,4,*]

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We report the synthesis of *N*-((4-chlorophenyl)carbamothioyl)pivalamide of an benzoylthiourea derivative formulated as $C_{12}H_{15}ClN_2OS$. The structure of compound has been characterized by single-crystal X-ray diffraction analysis. It crystallizes in the triclinic, space group P-1 (no. 2), with unit cell dimensions of a = 5.8690(19) Å, b = 11.110(4) Å, c =20.564(7) Å, α =89.551(5)°, β =88.197(5)°, γ =80.962(5)°, V = 1323.6(7) Å^3, Z = 4, μ(MoKα) = 0.432 mm^{-1}, $Dcalc$ = 1.359 g/mm^3, 26983 reflections measured ($3.72 \leq 2\Theta \leq 61.24$), 8047 unique ($R_{\text{int}}$ = 0.0472) which were used in all calculations. The final R_1 was 0.0420 (>2sigma(I)) and wR_2 was 0.1088 (all data). The bond lengths and angles in the thiourea moiety are typical for thiourea derivatives; the C2-S1 and C1-O1 bonds both show a typical double-bond character with 1.6675(16) and 1.220(2) Å, respectively. Similar shortening for the C-N bonds C1-N2 1.384(2) Å, C2-N2 1.3904(19) Å, C2-N1 1.333(2) Å, and C7-N1 1.4311(19) Å also indicates a partial double-bond character. The intramolecular hydrogen bond N1-H1···O1 (1.972(3) Å) forms a 6-membered ring with C1, N2 and C2.

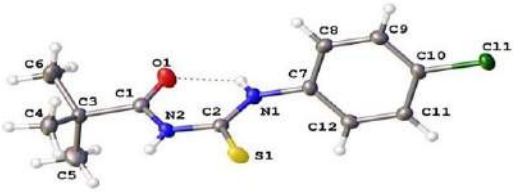

Figure 1. Molecular structure of *N*-((4-chlorophenyl)carbamothioyl)pivalamide.

Keywords**:** Thiourea, Pivaloyl thiourea, X-ray single crystal diffraction, Synthesis, Pivalamide derivatives.

Acknowledgement**:** This work was financially supported by Mersin University Research Fund (BAP-SBE AK (HÖ) 2010-2 YL).

[1] H. Gedik, *Synthesis and characterization of the various urea compounds*, MSc. Thesis, Mersin University, Mersin, Turkey, **2012**.

Structural, spectroscopic and magnetic studies of sulfathiazole-zinc(II) complex with diethylenetriamine

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New sulfathiazole (4-amino-N-(1,3-thiazol-2-yl)benzene sulfonamide, Hstz)-zinc(II) complex with dien (diethylenetriamine) has been synthesized and characterized by single crystal X-ray diffraction, EPR and IR methods. The single crystal XRD analysis indicated that the compound crystallizes in the monoclinic space group *Pc* with Z=4. The sulfathiazole anion acts as a monodentate ligand through the thiadiazole N atom contiguous to the deprotonated sulfonamido group. The metal centre adopts a near regular trigonal-bipyramidal geometry. Some comparisons with related structures are made and the most important features of its IR spectrum were also discussed. The powder EPR spectrum of Cu^{2+}doped Zn(II) complexes at room temperature was recorded. The EPR spectral analysis has led to that the ground state wave function of the unpaired electron of copperion is $d_{x^2-y^2}$.

Keywords: Zn(II) complex; sulfathiazole; X-ray crystalstructure; EPR; IR

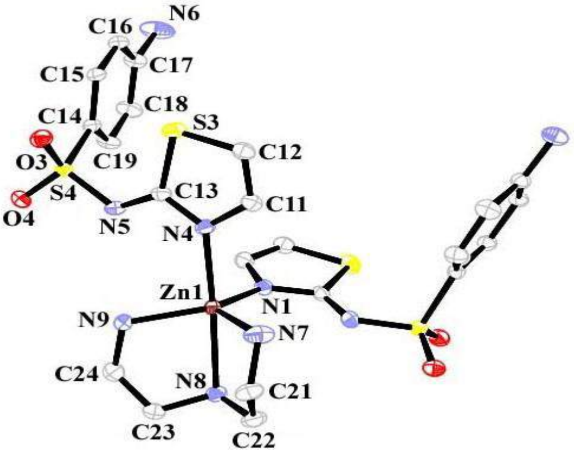

Figure 1. Themolecularstructure of **:**[Zn(stz)$_2$dien] with atom-labelingscheme.

Synthesis, characterization and crystal structure of *cis-Bis*[*N*-(dipropylcarbamothioyl)cyclohexane carboxamido-κ^2O,S]copper(II)

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Don VanDerveer [3], and Hakan Arslan [1,2]

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cis-Bis[*N*-(dipropylcarbamothioyl)cyclohexanecarboxamido-κ^2O,S] copper(II) has been synthesized and characterized by elemental analyses, FT-IR and NMR methods [1]. The obtained metal complex was also characterized by a single crystal X-ray diffraction study. Molecule formula of the title compound, $C_{28}H_{50}CuN_4O_2S_2$: monoclinic, space group $P2_1/n$ (no. 14), $a = 10.025(2)$ Å, $b = 21.724(4)$ Å, $c = 14.848(3)$ Å, $\beta = 100.60(3)°$, $V = 3178.5(11)$ Å^3, $Z = 4$, μ(Mo Kα) = 0.848 mm^{-1}, $Dcalc = 1.259$ g/mm^3, 22069 reflections measured ($5.88 \leq 2\Theta \leq 50.2$), 5639 unique ($R_{\text{int}} = 0.0630$) which were used in all calculations. The final R_1 was 0.0488 (>2sigma(I)) and wR_2 was 0.1277 (all data). Title compound shows the Cu ion is four-coordinated by two O and two S atoms (S(1)-Cu-O(2) 155.91(8)°, O(1)-Cu-S(2) 157.47(8)°). The dihedral angle between the S(1)Cu(1)O(1) and S(2)Cu(1)O(2) planes of 31.7(1)° indicates strong distortion from square planar towards tetrahedral geometry.

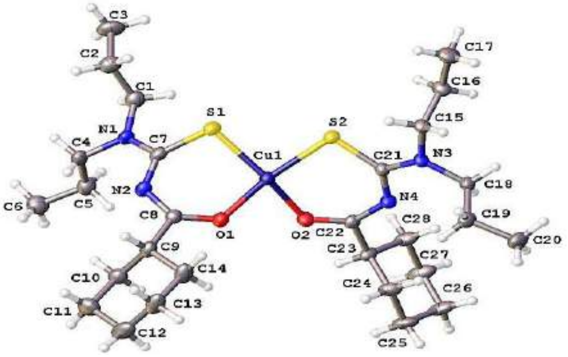

Figure 1. Molecular structure of title compound.

Keywords**:** Copper complex, Thiourea, Cyclohexanecarboxamide, X-ray single crystal diffraction, Synthesis.

Acknowledgement**:** This work was financially supported by Mersin University Research Fund (BAP.SBE.TB(CKO) 2007-1YL).

[1] C.K. Özer, *Synthesis and characterization of the transition group metal complexes of the various thiourea derivatives*, MSc. Thesis, Mersin University, Mersin, Turkey, **2008**.

Single crystal structure of *bis*(2-methyl-*N*-(diethylcarbamothioyl) benzamido)copper(II) complex

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Bis(2-methyl-*N*-(diethylcarbamothioyl)benzamido)copper(II) complex has been synthesized and characterized by elemental analyses, FT-IR and NMR methods [1,2]. The obtained metal complex was also characterized by a single crystal X-ray diffraction study. Molecule formula of the title compound, $C_{26}H_{34}CuN_4O_2S_2$: monoclinic, space group $P2_1/c$ (no. 14), $a = 11.7617(14)$ Å, $b = 9.1338(11)$ Å, $c = 26.558(3)$ Å, $\beta = 109.822(5)°$, $V = 2684.1(5)$ Å^3, $Z = 4$, $\mu(\mathrm{MoK}\alpha) = 1.000\ \mathrm{mm}^{-1}$, $Dcalc = 1.391\ \mathrm{g/mm}^3$, 22933 reflections measured ($3.68 \leq 2\Theta \leq 55.76$), 6392 unique ($R_{\mathrm{int}} = 0.0400$, $R_{\mathrm{sigma}} = 0.0415$) which were used in all calculations. The final R_1 was 0.0447 (>2sigma(I)) and wR_2 was 0.1168 (all data). In this compound, the copper atom is coordinated by two sulphur and two oxygen atoms from two 2-methyl-*N*-(diethylcarbamothioyl)benzamide molecules forming an distorted square-planar geometry (S(1)-Cu-O(1) 94.59(6)°, O(2)-Cu-S(2) 93.84(6)°). The dihedral angle between the S(1)-Cu-O(1) and S(2)-Cu-O(2) planes of 19.91° confirms distortion from square planar towards tetrahedral geometry.

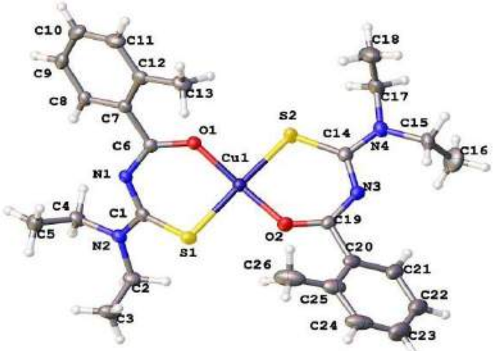

Figure 1. Molecular structure of title compound.

***Keywords*:** Copper complex, Thiourea, Benzoyl thiourea X-ray single crystal diffraction, Synthesis.

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Synthesis, characterization and crystal structure of *cis*-*Bis*[4-chloro-*N*-(diphenylcarbamothioyl) benzamido-κ^2O,S]platinum(II)

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cis-*Bis*[4-chloro-*N*-(diphenylcarbamothioyl)benzamido-κ^2O,S]platinum(II) has been synthesized and characterized by elemental analyses, FT-IR and NMR methods. The obtained metal complex was also characterized by a single crystal X-ray diffraction study. Structure of *cis*-*bis*[4-chloro-*N*-(diphenylcarbamothioyl)benzamide-κ^2O,S]platinum(II) was confirmed using infrared, ^{1}H nuclear magnetic resonance, and mass spectral data. Molecule formula of the title compound, $C_{80}H_{56}Cl_4N_8O_4Pt_2S_4$: triclinic, space group P-1 (no. 2), $a = 9.0138(2)$ Å, $b = 14.9355(3)$ Å, $c = 15.9076(3)$ Å, $\alpha = 109.9660(10)°$, $\beta = 99.5280(10)°$, $\gamma = 104.3810(10)°$, $V = 1874.62(7)$ Å^3, $Z = 1$, $\mu(\mathrm{MoK}\alpha) = 4.037$ mm^{-1}, $Dcalc = 1.642$ g/mm^3, 39243 reflections measured ($3.08 \leq 2\Theta \leq 52.74$), 7649 unique ($R_{\mathrm{int}} = 0.0510$) which were used in all calculations. The final R_1 was 0.0370 (>2sigma(I)) and wR_2 was 0.0646 (all data).0 A square-planar coordination geometry is formed around the Pt atom by two S atoms and two O atoms of the 4-chloro-*N*-(diphenylcarbamothioyl)benzamide ligands, which are in a *cis* configuration. Synthesized compound was tested *in-vitro* against two Gram-positive (*S. aureus* and *S. pneumoniae*) and three Gram-negative bacterial strains (*E. coli*, *P. aeruginosa*, and *A. baumannii*), two fungal strains (*C. albicans* and *C. glabrata)*.

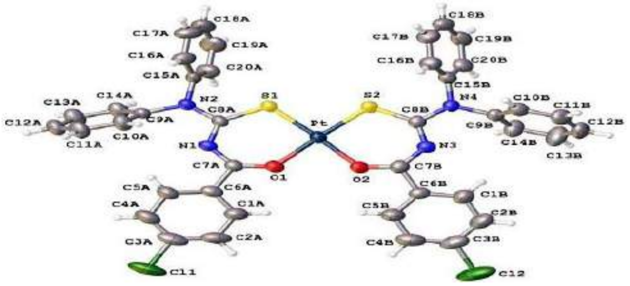

Figure 1. Molecular structure of title compound.

Keywords**:** Platinum complex, Thiourea, Benzoyl thiourea X-ray single crystal diffraction, Synthesis, Antimicrobial activity.

Acknowledgement**:** This work was financially supported by Mersin University Research Fund (BAP-ECZ F TEB (HA) 2010-5 A).

Synthesis, characterization and crystal structure of *cis-bis*[4-chloro-*N*-(dibutylcarbamothioyl) benzamido-κ^2O,S]palladium(II)

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cis-*Bis*[4-chloro-*N*-(dibutylcarbamothioyl)benzamido-κ^2O,S]palladium(II) has been synthesized and characterized by elemental analyses, FT-IR and NMR methods [1]. The obtained metal complex was also characterized by a single crystal X-ray diffraction study. Molecule formula of the title compound, $C_{64}H_{88}O_4S_4Cl_4Pd_2N_8$: orthorhombic, space group $P2_12_12_1$ (no. 19), $a = 8.5141(9)$ Å, $b = 16.5890(17)$ Å, $c = 51.924(6)$ Å, $V = 7333.8(13)$ Å^3, $Z = 4$, $\mu(\mathrm{MoK}\alpha) = 0.798$ mm^{-1}, $Dcalc = 1.373$ g/mm^3, 26461 reflections measured ($2.578 \leq 2\Theta \leq 66.352$), 13708 unique ($R_{\mathrm{int}} = 0.0755$) which were used in all calculations. The final R_1 was 0.0604 ($I > 2\sigma(I)$) and wR_2 was 0.1350 (all data). Title compound shows the palladium ion is four-coordinated by two O and two S atoms (S(1)-Pd-O(2) 179.1(3)°, O(1)-Pd-S(2) 178.7(2)°). In the title complex, the Pd atom has a *cis*-square-planar geometry defined by two 4-chloro-*N*-(dibutylcarbamothioyl)benzamide ligands (The dihedral angle between the S(1)PdO(1) and S(2)PdO(2) planes: 0.08(1)°).

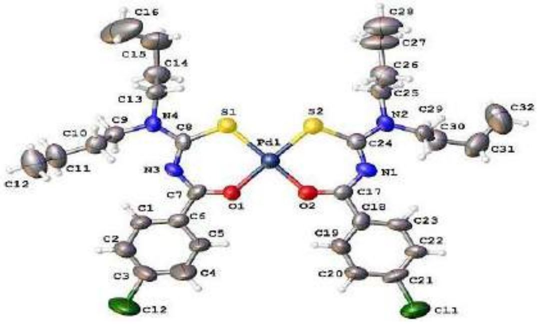

Figure 1. Molecular structure of title compound.

***Keywords*:** Palladium complex, Thiourea, Benzoyl thiourea X-ray single crystal diffraction, Synthesis.

***Acknowledgement*:** This work was financially supported by Mersin University Research Fund (BAP-FBE KB (ÜK) 2013-1 YL).

[1] U. Solmaz, *Synthesis and characterization of palladium complexes of thiourea derivatives*, MSc. Thesis, Mersin University, Mersin, Turkey, **2014**.

Synthesis, characterization and crystal structure of *trans*-dichloro *bis*[4-chloro-*N*-(dibutylcarbamothioyl) benzamido-*κ*S]palladium(II)

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Trans-[$PdCl_2(HL\text{-}S)_2$] (HL=*N*,*N*-di-*n*-butyl-*N*'-4-chloro benzoylthiourea) complex was formed from the reaction between $PdCl_2$ and *N*,*N*-di-*n*-butyl-*N*'-4-chloro benzoylthiourea in acetonitrile. Pd(II) complex has been characterized by spectral (FT-IR, ^{1}H NMR and ^{13}C NMR, LC-MS/MS) techniques. The molecular structure of the title complex has been confirmed by X-ray crystallography. Molecule formula of the title compound, $C_{32}H_{46}Cl_4N_4O_2PdS_2$: monoclinic, space group C2/c (no. 15), a = 12.282(5) Å, b = 18.682(5) Å, c = 16.893(5) Å, β = 97.604(5)°, V = 3842(2) Å^3, Z = 4, μ(MoKα) = 0.903 mm^{-1}, *Dcalc* = 1.437 g/mm^3, 29360 reflections measured ($4 \leq 2\Theta \leq 66.62$), 7356 unique ($R_{\text{int}}$ = 0.0233) which were used in all calculations. The final R_1 was 0.0443 (>2sigma(I)) and wR_2 was 0.0993 (all data). Title compound shows the palladium ion is four-coordinated by two S and two Cl atoms. The palladium atom in *trans*-[$PdCl_2(HL\text{-}S)_2$] is located on a center of inversion so that the *trans*-Cl_2S_2 donor set is planar. The observed molecular conformation is stabilized by an intramolecular N-H···Cl interaction [1].

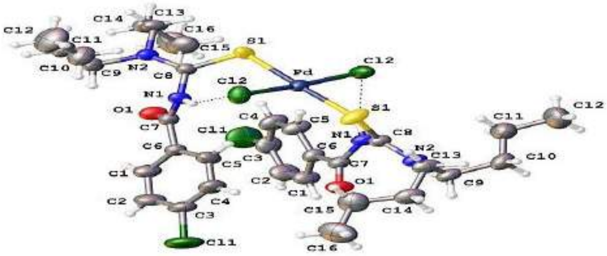

Figure 1. Molecular structure of title compound.

***Keywords*: Palladium complex, Thiourea, Benzoyl thiourea X-ray single crystal diffraction, Synthesis.**

***Acknowledgement*:** This work was financially supported by Mersin University Research Fund (BAP-FBE KB (ÜK) 2013-1 YL).

[1] U. Solmaz, *Synthesis and characterization of palladium complexes of thiourea derivatives*, MSc. Thesis, Mersin University, Mersin, Turkey, **2014**.

Polymeric Copper(II) Succinate Complex with N,N-Diethyl-ethylenediamine: Spectral and Structural Characterization (68)

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The crystal and molecular structure of $[Cu(succ)(deed)]_n{\cdot}4nH_2O$ complex (deed=diethyl-ethylenediamine) was synthesized and determined by IR, UV and single-crystal x-ray diffraction. In complex, the metal centers are bridged by succinate ligands to form 1D polymer chains. Each of the Cu atoms is octahedrally coordinated by four O atoms of two carboxylate moiety of the bridging succinate group and two N atoms of deed ligand in chelating form [1]. The crystal structure is monoclinic, space group $P2_1/c$ with parameters a=15.7523(8) Å, b=7.1201(3) Å, c=15.9540(8) Å, α=γ=90°, β=112,709(4)°, V=1650.65(30) Å^3, Z=1. The polymer chains are connected by O–H···O and N–H···O hydrogen bonds to form sheet structures. This complex consists of a 3D structure with containing planar hexameric and tetrameric water rings [2]. The IR spectra of polymeric copper(II) complex were discussed in relation to other compounds containing N,N-diethyl-ethylenediamine and succinate complexes.

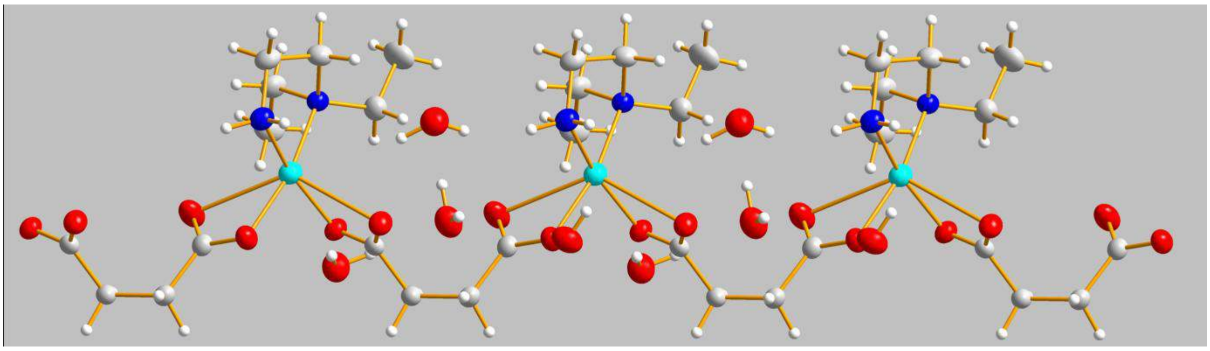

Figure 1. Molecular structure of $[Cu(succ)(deed)]_n{\cdot}4nH_2O$.

Keywords: Succinic acid, N,N-diethylethylenediamine, X-ray, IR, UV.

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Metisiline Dirençli *Staphylococcus aureus* (MRSA) EPS Yapısının SAXS Yöntemiyle İncelenmesi

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Metisiline dirençli *Staphylococcus aureus* bakterileri, dünyada en tehlikeli enfeksiyon hastalıklarına neden olmaktadır. Bu bakteriler, tıbbi cihazlarda, kateterlerde, kalp kapakçıklarında biyofilm oluşturarak ölümlere yol açmaktadır. Biyofilm, ekzopolimerik materyallerle yüzeylere tutunan mikroorganizmalar topluluğudur ve biyofilmin %90'nı ekstrasellüler polimerik materyal (EPS) olarak isimlendirilen kompleks bir polimerdir. EPS; hücre agregasyonu, hücre adezyonu, biyofilm oluşumu ve patojen bakterinin konağın immün sisteminden kaçmasında önemli rol oynar. Biyofilm EPS'si, genel olarak "çözünebilir EPS" ve "membrana bağlı EPS" olmak üzere iki kısımdan oluşur. MRSA kaynaklı infeksiyonların önlenmesi önemli sağlık politikalarının başında gelmektedir [1]. EPS'lerin sulu çözeltilerde oluşturdukları nano yapılar ile farklı çözücü koşulları altında ortaya çıkan yapısal değişimler, Küçük Açı X-Işını Saçılması (SAXS) yöntemi kullanılarak incelenmiştir. SAXS incelemesinden elde edilen sonuçlara göre, EPS'nin sulu ortamda oluşturdukları nano boyutlu yapılarının şeklinin yayvan (prolate) olduğu görülmüştür [2-5]. Bu yüzden, biyofilm matriksinin temel yapısı olan EPS'nin yapısının aydınlatılması biyofilm oluşumunun önlenmesi için önemlidir.

Teşekkür: PAÜ BAP Koordinasyon Birimine desteklerinden dolayı (2013FBE026) teşekkür ederiz.

Keywords**:** *Staphylococcus aureus*, EPS, Biofilm, SAXS.

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Synthesis, Spectroscopic Thermal and Structural Properties of $Zn(3\text{-}Aminopyridine)_2Ni(CN)_4$ Hofmann Type Complex

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$Zn(3\text{-}Aminopyridine)_2Ni(CN)_4$ Hofmann type complex has been synthesized in the powdered form and characterized by FT-IR spectroscopy, thermal analysis, powder XRD analysis method and elemental analysis. Its FT-IR spectrum has been reported in the range of (4000-400) cm^{-1}. General information was acquired about structural properties of this complex from IR spectra by considering changes at characteristic peaks of the cyano group and 3AP. The thermal behavior of this complex has been also investigated in the range of (25-750) ^{o}C. Thermal behavior of this complex was studied using TG and DTG methods. Structural and crystal properties of this complex was studied using powder XRD analysis in the range of (4-70)^{o}. The powder XRD analyses showed that this complex was in crystalline form.

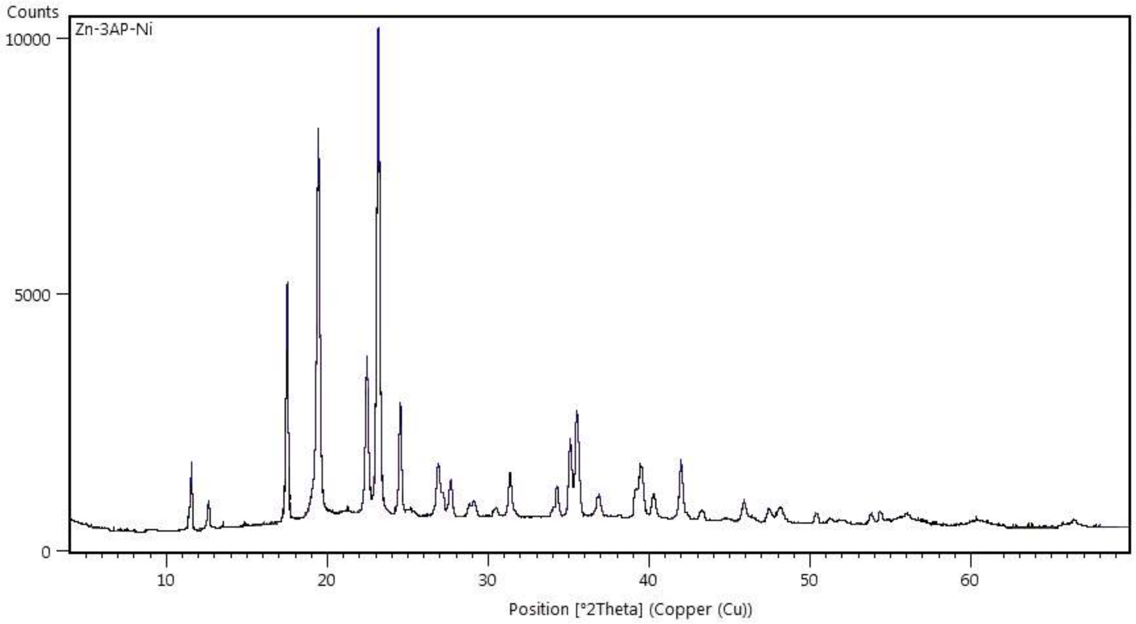

Figure 1: Diffraction pattern of $Zn(3\text{-}Aminopyridine)_2Ni(CN)_4$ Hofmann type complex.

Keywords: 3-Aminopyridine complexes, Hofmann type complexes, Zn complexes, FT-IR spectroscopy, powder XRD analysis, thermal analysis

Optical Properties of Reactive Sputtered Cuo Thin Films

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There are two stable copper oxide phases according to oxygen composition. One is cupric oxide (CuO), monoclinic phase, the other one is cuprous oxide (Cu_2O), cubic phase. These oxides are natural p-type semiconductors having a band gap of 1.2-1.9 eV for CuO and 1.8-2.5 eV for Cu_2O [1]. However, Gupta et al. [2] reported band gap value of CuO as 2.05 eV. In this study, we prepared CuO films by reactive magnetron sputtering and those films were annealed at from 250 °C to 550 °C with 100 °C step in ambient. The structural properties of the films were investigated by X-ray diffraction. The optical properties such as transmittance, reflectance and optical band gap from absorption data were determined using a spectrophotometer in the range between 300 nm and 900 nm. Optical band gap values varied from 2.52 to 2.18 eV for the films that of 250 °C to 550 °C annealing temperatures, respectively.

Keywords: Optical properties, CuO, p-type, Crystal structure

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Synthesis, Crystal Structure Analysis of 1-(3,4-Methoxyphenyl)-3-phenoxy-4-(4-{[1-(prop-2-en-1-yl)-1*H*-1,2,3-triazol-4-yl] methoxy}phenyl)azetidin-2-one

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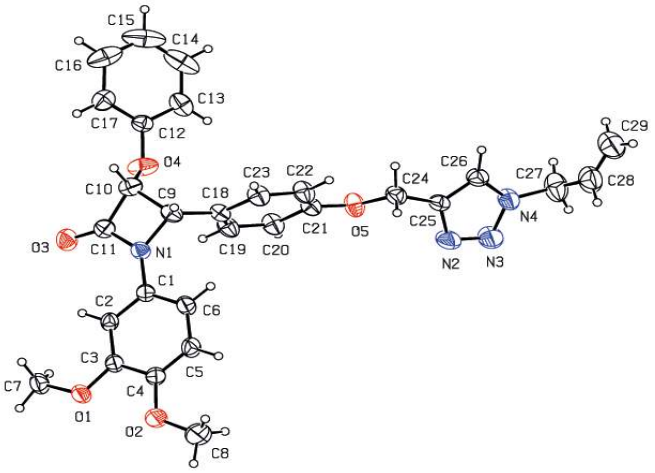
In the compound $C_{29}H_{28}N_4O_5$, (**1**), the four-membered □-lactam ring is essentially planar, with a maximum deviation of -0.011(2) Å for the N atom, and has long C—C distances of 1.525(3) and 1.568(4) Å. The mean plane of this group makes dihedral angles of dihedral angles of 60.03(16), 5.54(14), 51.52(16) and 83.72(14)° with the 1H-1,2,3-triazole ring system, the benzene ring of the 3,4-methoxyphenyl group, the phenyl and benzene rings of the two phenoxy groups, respectively.

In the crystal structure, molecules are linked by C—H...O and C—H...N hydrogen bonds, forming infinite chains running along the [010]-axis. Molecular packing exhibits sheets parallel to (011). In addition, C—H...π interactions and π-π stacking interactions [centroid-centroid distances = 3.6762(15) and 3.8099(16) Å] stabilize the molecular packing of **1**.



(**1**)

Keywords**:** β-lactam, crystal structure, hydrogen bond

Cobalt(II)-2,2'-Thiodiacetate Complex with Imidazole Ligand: $[Co(tda)(im)_3]\cdot H_2O$

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The thiodiacetate (tda) is versatile ligand that has been widely explored as multidentate and chelating units for one or more metals of a different nature. It contains five atoms that are potential donors, four of which come from two carboxylate groups and one from the thioether [1]. This ligand can bind a single metal in a tridentate manner, with the two "exo" oxygen donor atoms of the carboxylate groups being capable of additional coordination of another metal or external electrophiles. In this study, thiodiacetate-cobalt(II) complex, $[Co(tda)(im)_3]\cdot H_2O$ synthesized and characterized by elemental analysis IR spectroscopy, single crystal X-ray diffraction techniques and thermal analysis (TG, DTG and DTA). Complex **1** was synthesized by the reaction of $Co(CH_3COO)_2\cdot 2H_2O$ (1 mmol), 2,2'-thiodiacetic acid (1 mmol) and imidazole (3 mmol) at 70 °C in water. After two weeks, red crystals of **1** were isolated. Single-crystal X-ray analysis demonstrates that tda ligand binds to Co(II) ion as tridentate. The asymmetric unit of complex **1** contains one Co(II) ion, one tda, three imidazole ligands and aqua molecule (Fig. 1).

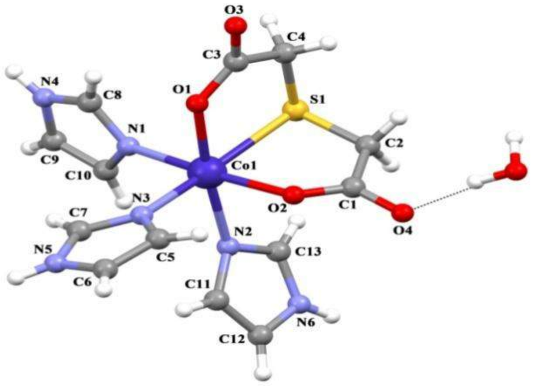

Figure 1. The molecular structure of **1**

Keywords**:** 2,2'-Thiodiacetate Complex, Imidazole Complex, Cobalt(II) complex

[1] A. Grirrane, A. Pastor, E. Alvarez, C. Mealli, A. Ienco, A.Galindo, *Inorg. Chem. Commun.* **2006** , 160-163.

The Synthesis and Crystal Structure of Zinc(II)-2,2'-Thiodiacetate Complex with Isonicotinamide

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Although the study of the thiodiacetate (tda, $S(CH_2COO)_2$) transition metal chemistry was initiated several decades ago [1], the interest for the structural aspects of thiodiacetate compounds has remarkably increased in the recent years [2]. In this study, mixed-ligand zinc complex, $[Zn(tda)(ina)(H_2O)_2]\cdot 2H_2O$ (**1**) was synthesized and characterized by elemental analysis IR spectroscopy, single crystal X-ray diffraction techniques and thermal analysis (TG, DTG and DTA). Complex was synthesized by the reaction of $Zn(CH_3COO)_2\cdot H_2O$ (1 mmol), 2,2'-thiodiacetic acid ($tdaH_2$) (1 mmol) and isonicotinamide (1 mmol) at 80-100 ºC in the solvent mixture of ethanol-water. One week later, white crystals of the complexes were obtained. The molecular structure of **1** with the atom numbering scheme is shown in Figs. 1 The asymmetric unit of **1** contains one zinc (II) ion, one tda, one ina, two aqua ligands and two uncoordinated water molecules (Fig. 1). The coordination geometry around the Zn(II) ion can be described as a distorted octahedral geometry. Tda ligand binds to zinc(II) ion as tridendate from sulphur and oxygen atoms. Moreover, thermal and photoluminescent properties of the complex **1** were studied.

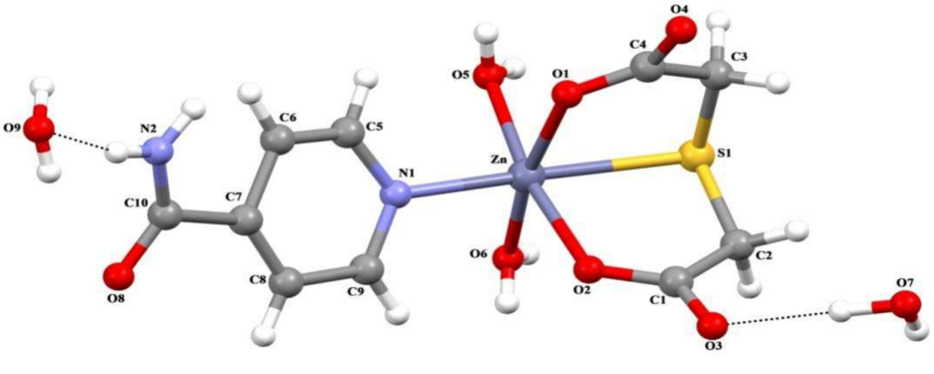

Figure 1. The molecular structure of **1.**

Keywords**:** 2,2'-Thiodiacetate Complex, Isonicotinamide Complex, Zinc(II) complex

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Structural and Spectroscopic Investigations of 1:2 Cocrystal Prepared by Pyromellitic Acid and Isonicotinamide (Pyridine-4-carboxamide)

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In this study, a cocrystal of pyromellitic acid with isonicotinamide (Fig. 1) has been characterized by X-ray diffraction (XRD) technique and Infrared (IR) spectroscopy. XRD studies were performed by mainly focusing on non-covalent interactions responsible for the packing network. XRD results show that moderate strength hydrogen bonds of N-H···O type between the amide and carboxylate groups play an important role in stabilizing the cocrystal by constructing the chain structures parallel to (010) and interconnecting them. It is also seen that lattice waters are effective in crystal packing by participating in O-H···O hydrogen bonds with the functional groups of pyromellitate and pyridinium-4-carboxamide. IR studies have been carried out by considering the characteristic frequencies. Investigation of fundamental modes shows shifts andsplittings in FT-IR spectrum, being in agreement with XRD results.

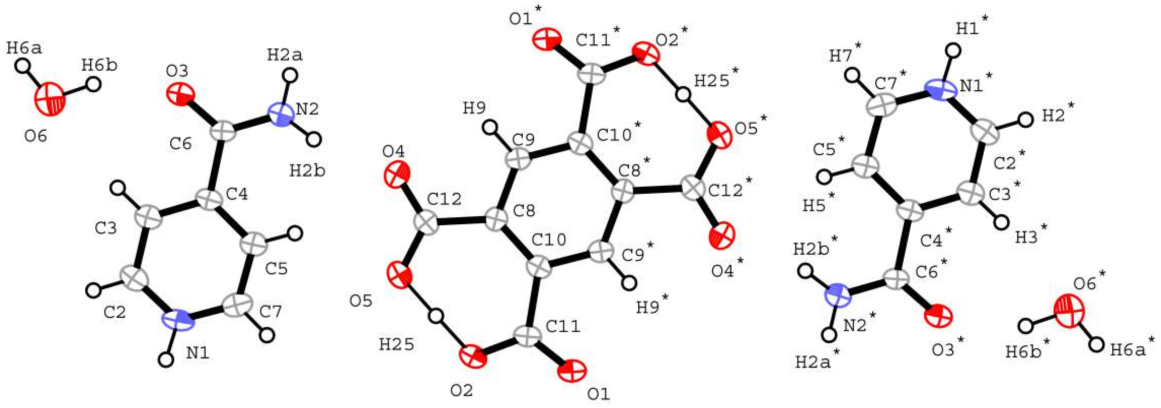

Figure 1. The structure of 1:2 cocrystal prepared by pyromellitate and pyridinium-4-carboxamide

Keyword: Pyromellitic Acid, Isonicotinamide, X-ray, IR.

Determination of crystallinity of biological apatites by X-ray diffraction and FTIR spectroscopy

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Bone and tooth dentin are an inorganic-organic nanocomposite, in which hydroxyapatite type [HA, unit cell can be represented as $Ca_{10}(PO_4)_6(OH)_2$, hexagonal] nanocrystallites and collagen fibres are well arranged in a hierarchical architecture [1]. Biological apatite also contains significant carbonate substitutions, OH- deficiencies, and imperfections in the crystal lattice. Crystallinity is a measure of crystallite size and mechanisms of growth of calcium phosphates in biological mineralized tissues. The crystallinity index (CI) is a measure of the percentage of crystalline material and also correlated to the degree of order within the crystals. CI can be determined with both X-ray diffraction and Fourier Transform Infrared Spectroscopy. Both methodologies are complementary. The infrared (FTIR-CI) index is a mathematical calculation based on spectral data, is simplest method but gives relative values. However, FTIR does allow for the examination of carbonate content and ionic substitution, that it is sensitive to CI changes and that carbonate content is more influence on FTIR results than XRD. To calculate the XRD crystallinity index (XRD-CI) from XRD diffraction pattern can be used two or three different methods. To investigate similarities and differences between the two techniques, the CI values of biological apatites obtained by these techniques will be compared in this work.

Keywords**:** Mineral, Crytallinity index, FTIR, X-ray diffraction

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Two different natural materials: Investigation of the porous structures with SAXS method

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In this study, SAXS analysis of two natural materials: a lava rock (*Scoria, basaltic pumice*) and an ocean sponge (*Cliona varians*)] which are investigated as part of our TUBİTAK project (No: 113F014) are presented.

Dynamic interactions with fluids of nano-sized pore structures of these two natural materials which are widely used in many sectors such as buildings, cosmetics, glass, chemicals, electronics, metal-plastic, furniture and agriculture are still not exactly understood today [1,2]. Sponges and lava stones are used to clean sea and environmental waste waters, respectively. This property and the other physical/chemical properties cause the usage of these materials as remarkable scientific samples and models in the design and development of new materials.

The data related with dry and wet samples were used to find the convenience of the various structural models. As a result of the study, nano-structural parameters, related to the porous structure such as size, shape, distribution, porosity and the electron density of the matrix are described. As conclusion, it may be said that, the nano-sized pores dynamically interact with fluids in a short time and the pore surfaces reach more clear and smooth forms. In the next phase of the study, the interaction waste fluid and harmful gases with pores will be examined using a flow cell attached to main SWAXS system in the content of the mentioned project.

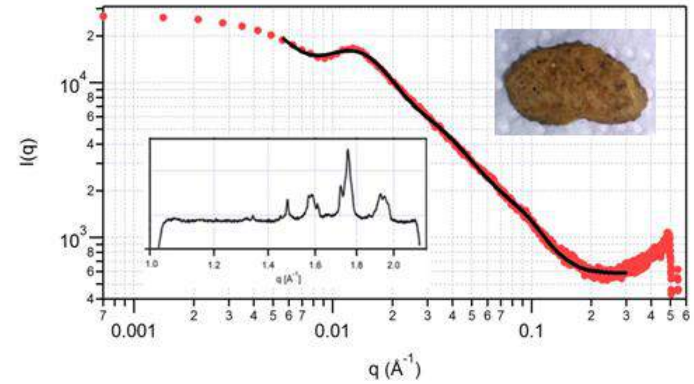

Figure1. Fit result and SWAXS illustrations for sponge sample

Keywords: SAXS, sponge, pumice, porous materials

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Structural and optical properties of Mn-doped CuO thin films deposited by the SILAR method

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Transition metal oxides in the nanoscale region are of great interest in the current research because of their interesting properties with a variety of applications. Among them, cupric oxide (CuO) is an important p-type transition metal oxide with a narrow band gap (E_g = 1.2 – 1.9 eV) [1,2]. CuO has received considerable attention in recent years due to its unique properties and wide application range in gas sensors, biosensors, solar cells, catalysts [3-5], etc. In this research influence of Mn-doping concentration on the structural and optical properties were studied X-ray diffraction (XRD) and UV-vis spectrophotometry. From the XRD patterns it was seen that the crystallite size of the films decreases at low doping concentrations but at higher concentrations it starts to increase again and reach even to higher values than the undoped samples. From the optical investigations the optical band gap of the films were increased (from 1.47 eV) and saturated at 6-7 at.% doping values first, but with higher doping concentrations it was started to increase again up to 2.08 eV. From these characterizations it was understood that Mn-doping affects the structural and optical properties of CuO films.

Keywords: CuO; Mn-doping; thin film

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Nanostructural Analysis Of Ti-6Al-4V and CoCrW Implants

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In this research, 12 implant samples have been investigated using small angle X-ray scattering and X-ray diffraction methods. Samples are produced with the SLM method and chosen according to their production angle, annealing temperature and production shape. Aim of this work is to determine external effects of the production media such as annealing temperature, production angle and dimensions. By examining resulting SAXS data, best production parameters will be determined.[1]–[3]

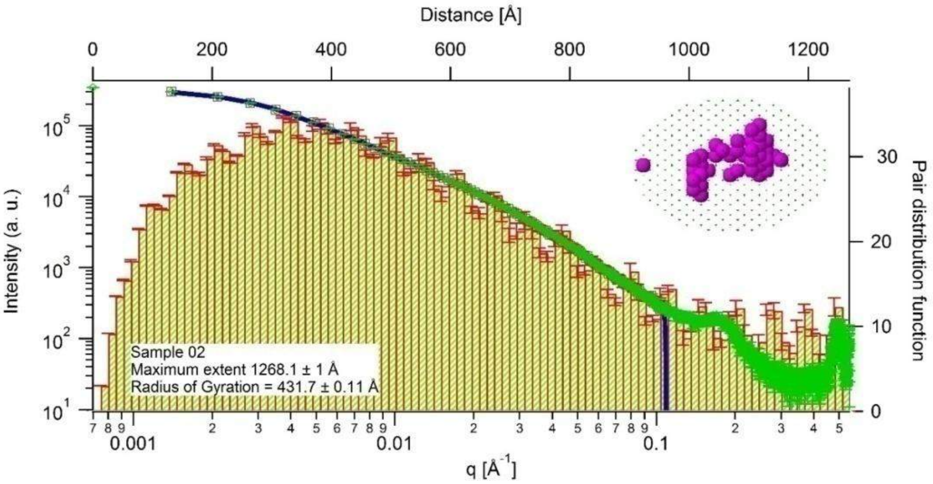

Figure 1. PDDF and DAMMIN output of sample with production angle of 45^0

***Keywords*:** SAXS, XRD, SLM, Titanium, Implant.

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Nanostructural Analysis of a Natural and a New Prepared Mesocrystals

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Some curve-shaped inner surfaces and substrates, crystal/crystalline/amorphous layers along several orientations, are appeared and included differently from 3D ordered single crystal structures, when natural bio-minerals are structurally investigated. Self-assembled and curve-shaped nano size layers in these bio-minerals can be examined with X-ray scattering analysis (SAXS-WAXS) which are different from classical crystal structure analysis[1].The information gained at the end of these analyses,may be guidefor the synthesis of mineral hetero structures and the creation of organic/inorganic nano-hybrid structures[2].In modern crystallography, these type bio-mineral structures like sea urchin are called "natural mesocrystals", as an abbreviation of “mesoscopically structured crystal”[3].The synthesis of the un-natural mesocyristals are depend on parallel crystallization operations and self-assembled colloidal formations. Applying the process called mesocristallation, it’s possible to synthesis of perfectly designed organic/inorganic hybrid materials which has complex morphology, hierarchical order and superior properties[4]. In this study, one of the natural mesocyristal structure, sea urchin structure which is a new model for engineering materials are investigated with X-ray scattering methods SAXS and WAXS[5]. Also on this natural structures, self-assembling nano-crystal-layer formation has tried to be built using various metallic Nano-Powders (Ti, Zr, and Ag) and bioactive organic compounds.Thesynthesized structures will be analyzed with the SAXS-WAXS, XRD and SEM methods in detail.Acknowledgement: In this study, a flow cell equipment (adopted to the SWAXS system and installed with a TUBITAK Project 114F013) was used.

Keywords :Mesocyristal, SAXS, WAXS.

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Calculation of molecular properties of safrole by density functional theory

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Safrole (shikimol) is a naturally-occurring genotoxic compound found in Sassafras root and Areca (betel) quid (Figure 1). It is a precursor in the synthesis of insecticides, fragrances, and the psychoactive drug ecstasy, (MDMA). The structural and vibrational properties of the safrole were investigated using density functional theory at B3LYP/6-31++G(d,p) level. The calculation of molecular properties (the geometric, electronic and spectroscopic) with density functional theory (DFT) allows a connection between theory and experiment of the systems. Experimental geometric data of the safrole have not been reported. Thus, our computed optimized geometric values (bond lengths and angles) were compared with the crystal data of MDMA which is determined by X-ray diffraction. The experimental vibrational frequencies were compared with those obtained theoretically from DFT calculation. The highest occupied molecular orbital energy (E_{HOMO}), the lowest unoccupied molecular orbital energy (E_{LUMO}), the energy gap between E_{HOMO} and E_{LUMO}, dipole moment and electronegativity of safrole were also calculated and discussed.

Keywords**:** Safrole, DFT, Molecular properties

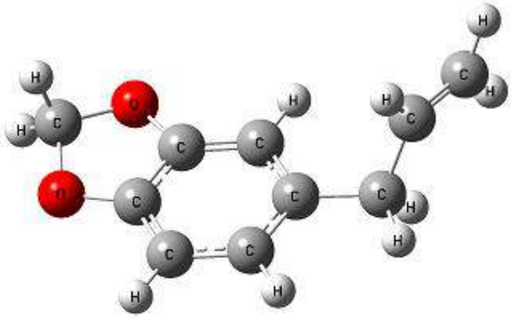

Figure. 1. Optimized structure of safrole (DFT/B3LYP/631++G(d,p)

Synthesis, Structural Characterization, Thermal and Biological Analyses of $[Co(H_2O)_6]_2(C_7H_7SO_3)$Complex

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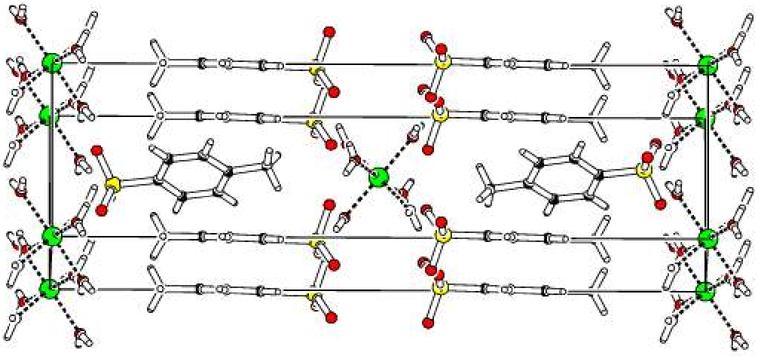
Metal complex,$[Co(H_2O)_6]_2(C_7H_7SO_3)$, was synthesized from the reaction between 4-methylbenzenesulfonic acid and 2-aminobenzamide in the presence of cobalt(II) sulfate, and characterized by means of thermal (TG/DTA) and X-ray single crystal diffraction methods. The crystallographic analysis reveals that the complex crystallizes in the monoclinic system, space group$P2_{1/n}$. In the complex, the geometry around the cobalt ion has a distorted octahedral geometry by sixH_2O molecule. The O-H…O strong intra- and 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 104°C. 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,The Biotechnology Laboratory in Biology Department, KSU and DÜPTAM, University of Dicle, staff for their assistance without which this work could not have been accomplished.

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

Crystal Structure Analysis of 4-(1-(2-phenylhydrazono)ethyl)benzene-1,3-diol and Its Electrochemical Properties

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The 4-(1-(2-phenylhydrazono)ethyl)benzene-1,3-diol, ($C_{14}H_{14}N_2O_2$), was prepared by the reaction of 2,4-dihydroxy acetophenon with phenylhydrazine and characterized by single crystal X-ray diffraction, and its electrochemical properties studied using Cyclic Voltammetry (CV) technology. The title compound crystallizes in the orthorhombic system, space group $P2_1$, a=5.3078(3), b=14.3756(8), c=16.1397(8)*Å* and *Z*=4. The crystal structure is stabilized by O-H···O strong intramolecular (Fig.1) and C-H···O, N-H···O and O-H···O intermolecular hydrogen-bond interactions. According to the CV measurement, the highest occupied molecular orbital-lowest unoccupied molecular orbital energy levels and the electrochemical band gap (E_g') of 4-(1-(2-phenylhydrazono)ethyl)benzene-1,3-diol were found to be -5.602, -3.577 and 2.025 eV, respectively.

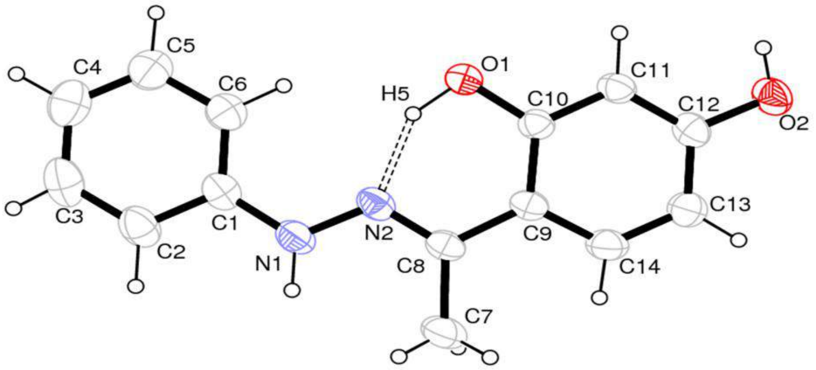

Figure 1. Molecular structure of the title compound.

We would like to thank DÜBTAM, University of Dicle, staff for their assistance without which this work could not have been accomplished.

Keywords: Crystallography, Hydrogen-Bond Interactions, Electrochemistry.

Earth – Mars: Recent Crystallographic Investigations and Geochemical Results

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In this review, information about the 4.4 billion years old antique zircon crystal, antique ice crystals from Earth and the first extraterrestrial crystalline peaks obtained from Mars via robotic rover Curiosity is mentioned. The zircon crystal which has the most antique history, has been found on Australia in 2001 and it gives us valuable information such as;

- During the formation of Earth, it cooled down so sudden then we think.
- Considering that oldest sign of a life form that we know is a bacteria which is 3,4 billion years old, it can be concluded that there might be older life forms.

In 2013, the first Debye rings of sand samples collected from (Rocknest Eolian Bedform) scoop5 region of Mars were recorded as evidence of crystalline compounds [1]. After Rietvelt refinement of the data, the crystallographic contents were showed the presence of andesine (43%), forsterite (21%), augite (17%), pigeonite (11%), magnetite (2%), quartz (2%) and with the possibility of occurrence sanidine, anhydrite, hematite and limonite signs are observed.

***Keywords*:** Mars, Crystallography, Geochemical.

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Projection of Crystallography Science on Postage Stamps

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Postage stamps , firstly printed and used in national postages in England with Sir Rowland Hill's efforts in 1840. Nowadays , all contries except the UK print the postages by typing the country's name with images that show country's historical and touristical places , important occasions and the message they want to give . So, the postage stamps are also represent their countries by describing an ocassion or a subject and immortalizing the people who served their community well. In today's world , even though mailing is not used widely , their postage stamps are always attract attention by it's images and graphs on it. Also shese stamps that printed in limited edition are an important source for collectors.

In this study, because of 2014-The International Year of Crystallography, postage stamps around the world are investigated to see how the scientific researches on crystallography reflected on postage stamps in years. Starting from the discovery of X-rays, which is origin of crystallography, up to the present, it has been tried to examine this historical process and the shown interest in this subject and the existence of scientific importance were also visualited by using views of the stamps of different countries.Two important scientific reflections on stamp visuals may be seen in fig.1

Figure 1. Two pioneer traces of crystallography science on stamps related with the diffraction of X-rays by crystals (Max von Laue) and first crystallographic analyses (W.H. Bragg and W.L Bragg)

Keywords: Stamps, History of Crystallography, IYCr stamps

Crystallographic Symmetries in Turkish Architecture and Artworks

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Rich symmetries and aesthetic high visual qualities of crystal structures have taken attention since 1913 (after the declaration of first crystal structure analysis) till these days. Especially, artists and architects are inspired from crystallographic symmetries and they create a lot of new designs by using this symmetry information.

Crystallographers, who are the eyewitnesses of these perfect crystallographic structures, started to cooperate with graphic designer M.C Escher in 1964, who is internationally specialist on drawings and lithography techniques[1,2]. So, presentations of the matching the patterns on designs of arts and architectures with the crystallographic symmetry become a tradition in crystallography activities.

This presentation was prepared to focus Turkish crystallographers' and artists' attention on this subject in 2014 which is celebrated as The International Year of Crystallography. In this study, artworks symmetries(Fig.1) are newly included beside of our previously presented and focused work on Turkish Architecture Patterns [3].

Figure 1. Symmetry usage on Turkish carpets, rocks, wooden and tile artworks

Keywords: Symmetry, Turkish art-architecture

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Organic Semiconductor based Gas Sensors

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In gas sensor applications, Inorganic semiconductors, such as SnO_2, Fe_2O_3, and ZnO, either undoped or doped have been studied extensively. The disadvantages of semiconductor oxide sensors are their high operating temperature (350–450^{0}C) which increases power consumption, reduces sensor life, and limits the portability [1]. During the past few decades, organic semiconductor materials have become attractive Because of they can operate at low temperatures or even at room temperature. Among them Poly(3-hexylthiophene) (P_3HT) is one of the important conducting polymers due to its electrical conductivity, electroluminescence, and optical properties [2]. They can be used for some applications such as solar cell, photovoltaic and gas sensor. In this study, Au/P_3HT/6H-SiC/Au Schottky diode was fabricated and investigated as a gas sensor. Measurements are taken at room temperature for different NO_2 gas concentrations. The response increases with increasing gas concentrations. According to the results, response which is obtained at room temperature could be explained with the presence of P_3HT. P_3HT are also used to fix the interface state density of sample [2].

Keywords**:** Organic semiconductors, gas sensors, electrical characterization

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Structural Investigation of New Prepared Salt Composites

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It has been known that salt and its new designed composites are useful in industrial applications and in protecting human health. Turkey has very rich salt reserves and the effective usage of these reserves can cause financial, scientific and technological benefits. Salt composites are already in our daily lives as various objects and building materials to benefit from their humectants and ionizer functions [1]. It is also used with the same functions in apiculture regions to control humidity and ion in hives. In this research, the novel composites were prepared and their structures were examined by using SAXS, WAXS and XRD methods. CEM I 52,5 R cement (M_1), 42.5% M_1 H_2O (M_2) and 80.0 % (M_1+M_2) NaCl (M_3) were used to reach the most uniform distribution of nanosize salt crystallites (with mean radius of 32.29 ±0.02 nm) in the composite structure (Fig.1). So after these preliminary studies, it was obtained that, the best percentages of the mixture can be used to prepare macroscopic size nanocomposites and environmental conditions on the sample structure may be tested for their usage in hives. A project including university-industry cooperation on these type composites will be able to realize after these pre-results.

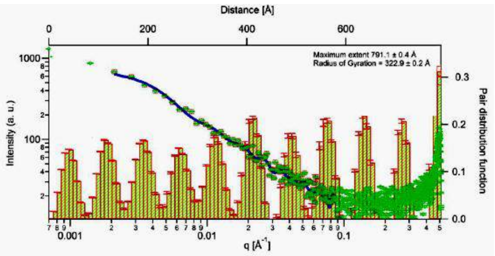

Figure 1. SAXS data analysis and PDDs of the nanocrystallites

Keywords: SAXS, WAXS, XRD, Salt Composites

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Crystal Structure and Theoretical Calculations of 2-oxo-1,2-diphenylethyl-2-bromopropanoate

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In this study, the structural properties of the 2-oxo-1,2-diphenylethyl-2-bromopropanoate has been investigated by X-ray diffraction and molecular modelling tecniques. The compond is crystallized in the monoclinic system, space group C 2/c, with lattice parameters; a=31.759(5)Å, b=5.965(5) Å, c=17.467(5) Å, β=111.564(5)°, Z=4, S=1.030, R=0.045 and wR=0.103 for 2201 observed reflections. The structures were solved by direct methods using the SHELX-97 program and refined on F^2. On the other hand, density functional theory (DFT) calculations are useful to model orbital energies of the polymers[1]. Molecular orbital calculations were carried out by using Gaussian 09 software package. HOMO and LUMO energies of the title compound by using B3LYP method with 6–311G(d) and 6-31G(d) basis set.

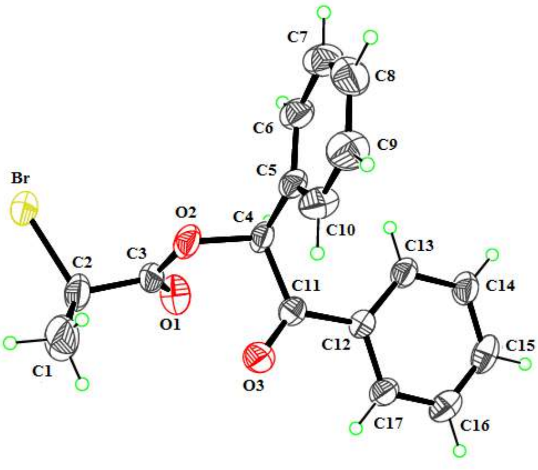

Figure 1.Ortep diagram of 2 -oxo-1,2-diphenylethyl-2-bromopropanoate

***Keywords*:** DFT, X-ray diffraction, HOMO-LUMO

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The excellent harmony between the X-ray structure and theoretical calculations : Bis-[2-hydroxy-2-(3-methyl-3-phenyl-cyclobutyl)-ethyl]-amine

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[2]*Ondokuz Mayıs University, Arts and Sciences Faculty, Department of Physics, 55139-Samsun, Turkey*
[3]*Fırat University, Sciences Faculty, Department of Chemistry, 23119-Elazığ, Turkey*
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In recent years, experimental and theoretical comparison of molecules has become popular. The geometries of the compounds can be determined X-ray diffraction method in the laboratory and also theoretically calculated in computer. The accuracy of the theoretical data can be controlled by the correlation calculation and superposition drawings.

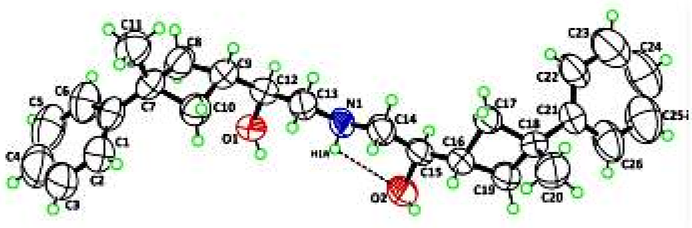

Figure 1. Molecule Structure.

In this study, bis-[2-hydroxy-2-(3-methyl-3-phenyl-cyclobutyl)-ethyl]-amine was theoretically investigated. The molecular geometry were those obtained from the X-ray structure determination [1] was optimized using density functional theory (DFT/B3LYP) method with the 6-31G(d) basis set in ground state. From the optimized structure, geometric parameters (bond lengths, bond angles, torsion angles) of molecule were obtained. This theoretical results were compared with experimental findings and an excellent harmony between the two data was ascertained. In addition to the molecular electrostatic potential (MEP) and Mulliken population analysis of the title compound were investigated by theoretical calculation results.

***Keywords*:** Cyclobutane, Density Functional Theory, Molecular Electrostatic Potential, Mulliken Population Analysis

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Structural Properties of $TlPb_{0,3}Sr_2Ca_{2-x}Se_xCu_3O_y$ Superconductors

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Highly-refined chemical powder were synthesized by having them ready in appropriate stoichiometric proportions with conventional solid state reaction method so that they would produce the superconductor as $TlPb_{0,3}Sr_2Ca_{2-x}Se_xCu_3O_y$ (x=0,0.2,0.4,0.6,1). The conventional solid state reaction method was used in this study. The solid state reaction method contains mixing the materials as homogenous and subjecting to some heat treatments in the high temperature ovens of these mixed materials. In this study annealing process carried out at 860°C for 4 hours. This project aims to understand selenium substitution effect on the structural properties. Structural properties were observed by using XRD and SEM. The XRD pattern resembles that there are peaks belonging to Tl-1223 (086-0458-ICDD) and as an impurity of CaSrCuO (048-0761-ICDD) and Tl_2O_3 (001-0849-ICDD) structures within the pure and substituted samples.

***Keywords*:** Superconductivity, TSCCO, Selenium

Magnetron sputtered MoS_2 thin films for MoS_2/p–Si heterojunction

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The optical, electrical and structural characteristics of the magnetron sputtered MoS_2 films were analyzed by uv-vis spectrophotometry, Hall effect measurements, scanning electron microscopy, and X-ray diffraction techniques. Furthermore, Au/MoS_2/p–Si heterojunction was obtained by forming a thin film of MoS_2 on p–Si and by evaporating Au metal on MoS_2/p–Si structure. It was observed that structure exhibit excellent rectifying behavior. Electrical properties of the device including ideality factor, barrier height and series resistance were determined using its current-voltage (*I-V*) measurements at room temperature. The capacitance–voltage (*C–V*) measurements of the heterojunction were executed for various fruquencies. The barrier height value obtained by *C-V* data was compared with the one obtained by *I-V* data.

Key Words: MoS_2, barrier height, series resistance, heterojunction, XRD, SEM, Band gap

Theoretical Study of $C_{17}H_{21}NO_2S_2$

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Semi empirical AM1 calculations of the title compound were carried out with WinMopac 7.2 software [1, 2]. The spatial view of the single molecule of (I) calculated as closed-shell in a vacuum is shown in Fig. 1 with atomic labels. The dihedral angle between the thiophene rings is 49.08 ° and is different from that in the x-ray result which the molecule is disordered. The dipole moment, the HOMO and LUMO energy levels are calculated as about 2.530 Debye, -9.1202 and -.0523 eV, respectively. We may state that the theoretical calculation of (I) supports the suggestion that the present intra and intermolecular interactions in (I) influence crystal packing.

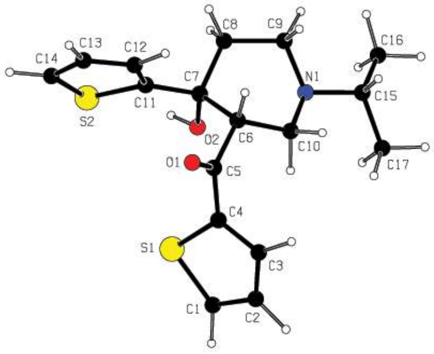

Figure 1. The spatial view of (I) calculated, using the *AM1* method.

***Keywords*: **Semi Emprical, AM1, Theoretical study

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Novel Bidentate Schiff base ligands containing functional groups: Structural Characterisation, Electrochemical and Photoluminescence Properties

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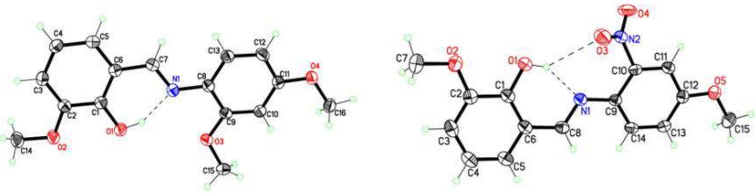
Schiff base compounds are versatile ligands in coordination chemistry due to their ease of preparation via condensation reaction of primary amines with aldehydes/ketones [1]. Schiff base ligands play a seminal role in the development of coordination chemistry because of their high affinity to transition metals [2]. Methoxy group containing Schiff base ligands have strong conjugation. Therefore, these compounds can be used in the preparation of floresance materials [3]. In this study, two novel Schiff base ligands containing methoxy (HL1) and nitro group (HL2) were prepared and characterised by FT-IR, ^{1}H-NMR, ^{13}C-NMR, MS, TG/DTA, elementel analysis and X-ray diffraction technique. Cu(II) complexes of the ligands were prepared and structurally characterised by single crystal X-ray diffraction study. Electrochemical and photoluminescence properties of the compounds were investigated. Molecular structures of Schiff base compounds are shown in Figure 1.



HL1 HL2

Figure 1. Molecular structures of Schiff base ligands

Keywords: Schiff Bases, Methoxy group, Electrochemical and Photoluminescence.

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Synthesize, X-ray *Structure* and DFT Studies of 1-amino-5-(4-methoxybenzoyl)-4-(4-methoxyphenyl) pyrimidine-2(1H)-one

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Pyrimidine derived Schiff base ligands and their complexes have been extensively investigated in recent years biological activities, including antimalarial, antibacterial, antitumor, antiviral activities etc [1,2]. Because of the importance of this compound, the structure of "1-amino-5-(4-methoxybenzoyl)-4-(4-methoxyphenyl) pyrimidine-2(1H)-one" (Figure1) was characterized by single crystal X-ray diffraction and DFT methods as theoretically and experimentally. According to X-ray diffraction results, **c***ompound* (Figure1) *crystallizes in the monoclinic space group* P 21/c with a = 13.9150 (6) Å, b = 10.4860(4) Å, c = 20.8720(9) Å and β = 131.605(2) °, Z = 4. The molecular geometry was also calculated by using Gaussian 03 software and structure was optimized by using HF/B3LYP method with the 6-31+g basis sets in ground state. It was seen that optimized structure is in excellent agreement with the X-ray crystal structure of (Figure1).

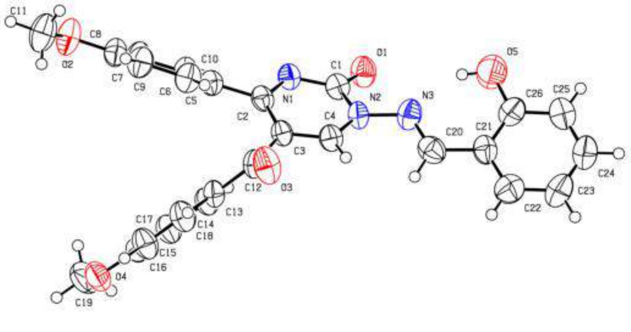

Figure 1. The molecular structure of 1-amino-5-(4-methoxybenzoyl)-4-(4-methoxyphenyl) pyrimidine-2(1H)-one.

Keywords: X-ray diffraction, Quantum chemical calculations, Density functional theory.

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The Structural, Electronic And Thermodynamical Properties Of 2,6-Bis(bromo-meth-yl)pyridine

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The structural, electronic and thermodynamical properties were analyzed of 2,6-Bis(bromo-meth-yl)pyridine (26BMP)acid in this work. The experimental geometrical results are combined the theoretical calculations using DFT calculations to reinforcement of the study[1]. The calculated spectroscopic studies were record and common spectroscopic techniques for adequate working. The theoretical explication were performed both FT-IR and FT-Raman spectra computed by using DFT (B3LYP) with 6-311++G(d,p) basis set calculations. The vibrational wavenumbers were remedied for scale number to take preferable result according to literature data. The scaled quantum mechanics (SQM) method were used total energy distribution (TED) of the vibrational modes for the assignments of the title molecule. The hybrid DFT method is very useful in forecasting accurate vibrational structure as seen the vibrational results of the study. Also the ^{13}C and ^{1}H nuclear magnetic resonance (NMR) spectra were operated by using the gauge-invariant atomic orbital (GIAO) method, showing a consistency with literature data. Apart from these, the excitation energies, wavelengths, HOMO and LUMO energies, density of state (DOS) diagrams, thermo dynamical properties and molecular electro-static potential (MEP) were appreciated. At the end of this work, the results were proved our paper had been needful for the literature contribution.

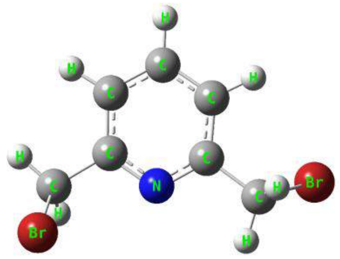

Figure 1. The crystal structure and optimized geometry of the 26BMP

***Keywords*:** 2,6-Bis(bromo-meth-yl)pyridine, DFT; NMR, UV, Infrared and Raman spectra; HOMO–LUMO.

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Microstructual defect properties of InGaN/GaN solar cell structures as depending on annealing tempratures

Çelik A[1]., Tamer M[4]*, Öztürk MK[1*], Özçelik S[1],Gültekin A[1] , and Özbay E[3]

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The structural and morphological properties of InGaN/GaN Solar cell structures grown by metal-organic chemical vapor deposition (MOCVD) with different In graded and ungraded content types, and with the aim of the higher performance values have been studied by high-resolution X-ray diffraction (HRXRD) and atomic force microscopy (AFM) at increasing temperatures (IT) up to 500 °C. Annealing has made in the atmospheric environment since nitride structures has stable more [1]. It is found that the tilt, lateral and vertical coherence lengths (CLs) of mosaic blocks, twist angles, grain size, screw and edge dislocation densities of GaN and InGaN layers, and surface roughness monotonically vary with In content type, and increasing annealing temperatures. [2,3].

Table I. HRXRD and AFM results for samples A, B, and C.

Samples GaN, InGaN/ InGaN	In content (%)	heterogenous strain ($\times 10^{-4}$)	Late. CL	Verti. CL	Tilt angle ($\times 10^{-3}$)	Screw TDD ($\times 10^{4}$, $10^{5}/10^{6}$)	Edge TDD ($\times 10^{6}$, $10^{7}/10^{7}$)
-	-	-	nm	nm	deg.	cm^{-2}	cm^{-2}
A(b2556)	10.5/18.4	-3.75, 2.25/4.75	9000, 900/250	321, 265/346	1.70, 4.2/1.03	7.51, 4.43/2.68	5.50, 0.806/290
B(b2557)	13.6/24.9	-4.00, 1.0/3.75	9000, 900/265	321, 450/281	1.70/ 5.0/1.03	7.51, 6.56/2.82	5.56, 1.06/361

Keywords*: *HRXRD ,AFM, twist angles, grain size, screw and edge dislocation.

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Structural And Optical Properties Of InGaN/GaN Solar Cell Nanostructure

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The structural and morphological properties of InGaN/GaN Solar cell structures grown by metal-organic chemical vapor deposition (MOCVD) with different In graded and ungraded content types, and with the aim of the higher performance values have been studied by high-resolution X-ray diffraction (HRXRD) and atomic force microscopy (AFM) at increasing temperatures (IT) up to 500 °C. Annealing has made in the atmospheric environment since nitride structures has stable more [1]. It is found that the tilt, lateral and vertical coherence lengths (CLs) of mosaic blocks, twist angles, grain size, screw and edge dislocation densities of GaN and InGaN layers, and surface roughness monotonically vary with In content type, and increasing annealing temperatures. [2,3]. As a result it is shown that In graded structure, the (004) peak broadening of InGaN layer shows a dramatic behavior with parallel trend when the broadening of the GaN (004) reflection peaks varies smoothly at IT, but In ungraded structure, these changes in the GaN layer is same but that of the InGaN exhibits a more dramatic behavior with parallel trend again at IT. Furthermore, AFM images for every two structure show a parallel behavior at IT. GaN, InGaN and their alloys have the hexagonal stucture and their qualities can be measured with the broadening of symmetric peaks. Even, the broadening of the symmetric or asymmetric rocking curves in such layers are the results of the tilt and twist angles and the lateral CL parallel to the substrate surface [4].

Table I.HRXRD and AFM results for samples A, B, and C.

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***Keywords**: HRXRD ,AFM, twist angles, , screw and edge dislocation.*

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Structural, morphological, and optical properties of AlGaN/GaN heterostructures with AlN buffer and interlayer

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AlxGa1−xN / GaN □x □ 0.3□ heterostructures with and without a high-temperature □HT□ AlN interlayer □IL□ have been grown on sapphire □Al2O3□ substrates and AlN buffer/Al2O3 templates by metal organic chemical vapor deposition. The effects of an AlN buffer layer □BL□ grown on an Al2O3 substrate and an AlN IL grown under the AlGaN ternary layer □TL□ on structural, morphological, and optical properties of the heterostructures have been investigated by high-resolution x-ray diffraction, spectroscopic ellipsometry, atomic force microscopy, and photoluminescence measurements [1]. The AlN BL improves the crystal quality of the AlGaN TL. Further improvement is achieved by inserting an AlN IL between GaN BL and AlGaN TL. However, experimental results also show that a HT AlN IL leads to relatively rough surfaces on AlGaN TLs, and an AlN IL changes the strain in the AlGaN TL from tensile to compressive type. In addition, an AlN BL improves the top surface quality of heterostructures[2-3].

Samples GaN, InGaN/ InGaN	In content (%)	heterogenous strain ($\times10^{-4}$)	Late. CL	Verti. CL	Tilt angle ($\times10^{-3}$)	Screw TDD ($\times10^{4}$, $10^{5}/10^{6}$)	Edge TDD ($\times10^{6}$, $10^{7}/10^{7}$)
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Table I. HRXRD and AFM results for samples A, B, and C.

Keywords*: *HRXRD ,AFM, twist angles, grain size, screw and edge dislocation.

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Structural and Magnetic Characterization of FeRh Thin Films

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The iron-rhodium alloys have very interesting magnetic ordering and phase transition depending on chemical composition and crystallographic structure. When iron and rhodium ratio is around equal, the composition has antiferromagnetic order at room temperature. However the system makes a transition to a ferromagnetic state above a critical temperature. This transition was named first phase transition and lattice parameter changes about %0,3. Ferromagnetic – antiferromagnetic transitions were explained by a strong dependence of the exchange interaction on the crystalline lattice parameter [1]. This material has a potential for using heat assisted magnetic data storage system. In our study we examine effects of growing parameters, using buffer and cap layers on magnetic ordering and phase transition. We deposited FeRh thin films on MgO (100) substrate at different growing conditions by sputter technique. Effect of buffer layer and top layer were investigated by depositing Rh and Pt. Structural properties of the film were investigated by X-ray diffraction. Magnetic phase transition was clarified by magnetization measurement as a function of temperature. And magnetic anisotropy was determined by ferromagnetic resonance analysis.

Keywords: Iron-rhodium thin film, magnetic phase transition, magnetic anisotropy

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A Mononuclear Cu(II) Complex Derived from a Salen Type Ligand Containing Azo-benzene Moiety

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Both Schiff bases and azo compounds are also important structures in medicinal and pharmaceutical fields and it has been suggested that the azomethine linkage might be responsible for the biological activities displayed by Schiff bases. These compounds have also received special attention because of their mixed soft–hard donor characters, versatile coordination behavior, optical and pharmacological properties and thermal properties [1-3]. In the last few decades many copper complexes have been reported. The growing interest on the coordination compounds of copper with various *N*-donor ligands, comes mainly from their capability of combining characteristic structural flexibility [4]. Single crystal X-ray diffraction study is very useful tool for structural-reactivity comparison in biological and catalytic systems.

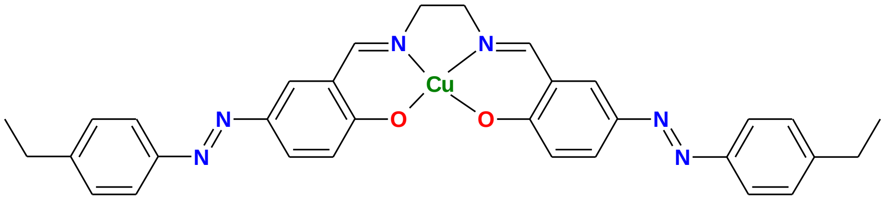

Figure 1. The structure of Cu(II) complex.

In this study, Cu(II) complex of a salen type ligand containing azo-benzene moiety was prepared and characterized. Molecular structure of the copper(II) complex of the tetradentate ligand was determined by single crystal X-ray diffraction study. In the structure, Cu(II) is coordinated to two imine nitrogen and two phenolate oxygen atoms in an approximate square planar geometry. The structure of the complex was shown in Figure.

Keywords: X-ray structure, Schiff base, Azo-benzene, Cu(II) complex

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Purification, structural characterization and homology modeling of a novel neurotoxic peptide (Acra3) from the scorpion *Androctonus crassicauda*

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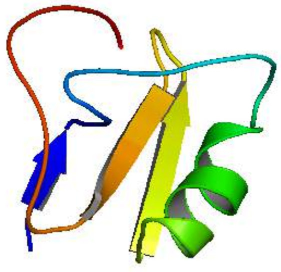
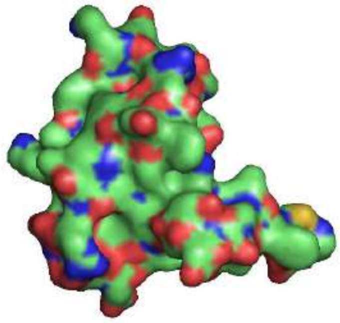
Androctonus crassicauda is one of the Southeastern Anatolia scorpions of Turkey with ethnomedical and toxicological importance. Information on the biochemistry, pharmacology, active principles and mechanism of action of the venom is crucial for the development of specific antivenoms. The venom group in the Biology Department of Eskisehir Osmangazi University is focused at the characterization of the main components of this scorpion venom, due to the fact that very little is known thus far on this species.The isolation of neurotoxic peptide Acra3 by chromatographic separations (HPLC and TSK-gel sulfopropyl) and its chemical and functional characterization were also performed and recently reported (Caliskan et al. 2012, *Peptides* 37: 106–112). Acra3 is a 7620 Da molecular weight peptide, with 66 amino acid residues and has eight cysteine residues, crosslinked by four disulfide bridges.We have currently carried out the structural characterization of Acra3 peptide by using the small angle x-ray solution scattering. From the small angle scattering data overall structural parameters of the protein e.g. molecular radius of gyration (R_g), particle volume (V), molecular mass (MM), maximum particle diameter (D_{max}) were derived. Furthermore, three-dimensional structure modeling of Acra3 was also predicted by amino acid sequence alignment and then homology modeling by using FASTA and CLUSTALW EBI and Swiss Model servers. These models will be used as the starting point for nanosecond-duration molecular dynamics simulations.





Investigation of Dose-Response Curves of Azelaic Acid Powders

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Azelaic acid or chemically 1,7-Heptanedicarboxylic acid, is a natural substance that is produced by Malassezia furfur (also known as Pityrosporum ovale), a yeast that lives on normal skin. In this study, powder formed of azelaic acid is irradiated at 1, 5, 7, 10, 25 irradiation doses and paramagnetic centers in the sample upon irradiation are characterized by Electron Paramagnetic Resonance (EPR)tecnique. In some cases, dose- response curves were investigated. It is observed that non irradiated AA display no EPR signal, irradiated AA were observed to present an EPR spectrum. First Derivative EPR spectra were obtained on Bruker X-band spectrometer.

Keywords: Irradiation, EPR, dose-response

Synthesis, Characterization and XRD Investigation of Boron Bearing N, O Type Ligands

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Boron compounds have versatile aspects in most fields such industry, agriculture, textile, automotive, electronics, medicine, pharmaceutical researches, cosmetic, energy, construction, communication tools etc.[1-3]. Furthermore, the synthesis of boron compounds has become widespread manner for science and technology in recent years due to their enormous applications [3-4]. N, O donor atom bearing ligands was applied to synthesize novel compounds including boron and its derivatives. The structures was illuminated by various spectroscopic techniques such XRD, ^{1}H & ^{13}C NMR, LC- MS/MS, TGA/DTA, UV-Vis., Elementel Analysis, SEM, FT-IR. The molecular structures and the powder XRD patterns are depicted in **Figure 1**.

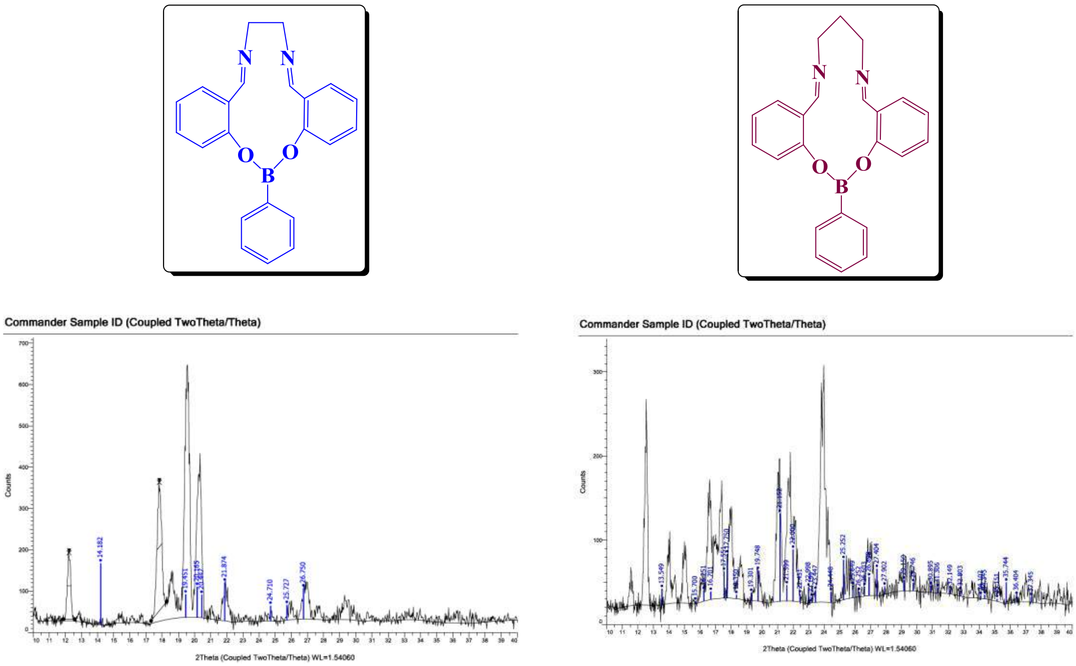

Figure 1 The illustration of molecular structures and the XRD patterns of compounds

Keywords: Boron compounds, spectroscopic techniques, powder XRD

[1] X. Zhang, and S. Zhang, *Spectrochimica Acta Part A* **2005** 61(6), 1045–1049.
[2] G. E. Morse, and T. P. Bender, *ACS Appl. Mater. Interfaces*, **2012** 4, pp. 5055−5068.
[3] A. Kilic, M. Aydemir, H. Temel and et al. *Journal of Fluorine Chemistry* **2014** 162, pp.9-16.

The Synthesis, Characterization and IntermolecularInteractions of [Ag_4(1,2dimim)$_4$ (μ-ssal)$_4$] Complex

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In this study we synthesized new [Ag_4(1,2dimim)$_4$ (μ-ssal)$_4$] complex with 5-sulfosalicylic acid and 1,2-dimethylimidazole [ssal= 5-sulfosalicylate, 1,2dimim= 1,2-dimethylimidazole]. The complex was characterized by IR spectroscopy, elemental analysis, thermal analyses and single crystal X-ray diffraction. Complex crystallized in the triclinic system with the space group of P-1 (**Fig. 1**). In the complex ssal ligand coordinated to metal atoms with tetradentad and formed 1D polymeric chain. The oxygen atoms which are belonging to ssal ligand and the hydrogen atoms which are belonging to 1,2dimim formed the C···H···O hydrogen bonds between the chains which extend the structure into a 2D layer by hydrogen bonding (**Fig. 2**). In the complex although the distance of trans Ag1···Ag1 atoms is 2,839 Å, the distance of Ag1···Ag2 atoms is 3,042 Å. All these values are shorter than the van der Waals radius (3.44 Å) and form strong argentophic interactions between argentad ions.

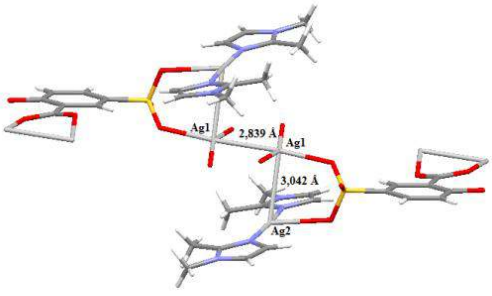

Figure 1. The molecular structures of complex**.**

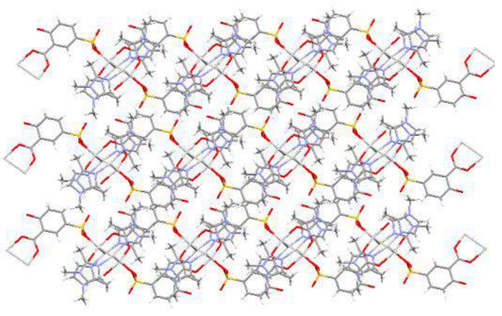

Figure 2. 2D structure of complex

Keywords**:** 5-sulfosalicylic acid, 1,2-dimethylimidazole, X-ray analysis

[1] S. R Fan., *Journal of Molecular Structure*, **2007 827**, 188-194,.

Influence of γ-irradiation on the Signal Intensity of Green Olive Seeds: An EPR study

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Dosimetric properties of unirradiated and irradiated green olive seeds cultivated in Turkey were investigated through Electron Paramagnetic Resonance (EPR) technique. In unirradiated samples singlet EPR signals which are results of polyphenol oxidation in plants were obtained. Two satellite peaks on the sides of the central singlet signal attributed to cellulose radicals were observed after the samples were irradiated up to 7 kGy. In order to describe the variation of EPR signal intensity with absorbed radiation dose, several mathematical equations were tried. Correlation coefficients between the absorbed doses and their corresponding EPR signals were identified from EPR signals. Moreover time dependency of the intensity of the central EPR signal of the irradiated sample was analyzed to study the stability of the free radicals. Based on the results of the study, it can be concluded that EPR technique can be used to identify unirradiated and irradiated green olive seeds even after two months.

Keywords: Electron Paramagnetic Resonance (EPR), food irradiation, absorbed dose.

Theoretical Calculations of Capacitance-Conductance-Frequency (*C*-*G*-*f*) on Semiconductors

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In the present study, Theoretical capacitance-conductance-frequency *(C-G-f)* values of some semiconductor in used electronic and optoelectronic technology were performed and graphs were drawn. This graphs depended on interface density (N_{ss}) and series resistance (Rs). Series resistance changes depending on the graphs were drawn and compared with literature.

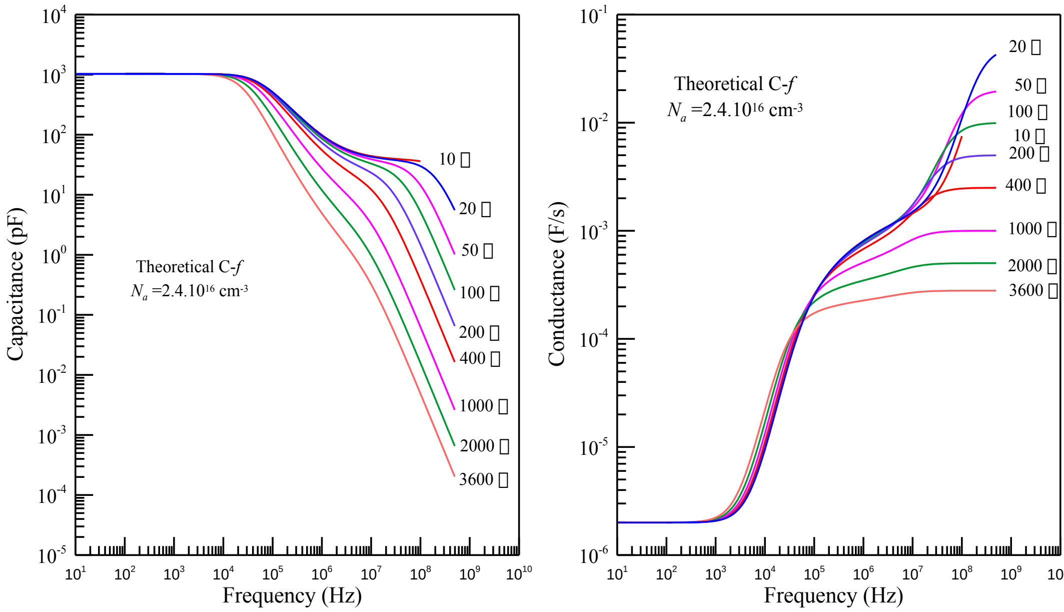

Figure 1. Theoretical graphs of *C*-*G*-*f* values depend on series resistance.

Keywords: Theoretical calculation, Interface density, Series resitance

Indentation Size Effect Study of Biomedical CoCrMo Alloy

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CoCrMo alloys are nowadays commonly used for dental restorations such as customized abutments, crown and bridges in the anterior and posterior region, telescope and conical crowns, and screw-retained restorations. In this study Cobalt-based alloy is produced by the investment casting process. An allotropic g-to-e (face-centred cubic (fcc)-to-hexagonal close-packed (hcp)) phase transformation can be seen to occur during cooling. Scanning Electron Microscopy, X-Ray Diffraction and hardness tests are used to examine the mechanical properties of the material. Examinations reveal that hardness decreases with increasing indentation test load. Also, the materials examined exhibit significant peak load dependence (i.e., indentation size effect (ISE)). All ISE models have a term which accounts for the load dependence of the hardness. The traditional Meyer's law, proportional specimen resistance (PSR) model, modified PSR (MPSR) model, and Hays Kendall model were used to analyze the indentation size effect of the materials.

Keywords: CoCrMo, XRD, Indentation

DFT Study and Conformational Analysis of 2-(2-fluoro-4-nitro-phenoxy)-3-nitropyridine

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In the present study, the molecular structure, vibrational and electronic transition, isotropic chemical shifts analysis of 2-(2-Fluoro-4-nitrophenoxy)-3-nitropyridine [1] were presented using quantum chemical calculations. To determine lowest-energy molecular conformation of the title molecule, the selected torsion angle is varied every 10° and molecular energy profile is calculated from 0° to 360°. The molecular structure and spectroscopic data of the molecule in the ground state were computed by density functional theory (DFT) using 6-31++G(d,p) basis set. The complete assignments of all vibrational modes were performed on the basis of the total energy distributions (TED) of the vibrational modes, computed with scaled quantum mechanics (SQM) method. Also the ^{13}C and ^{1}H nuclear magnetic resonance (NMR) spectra were operated by using the gauge-invariant atomic orbital (GIAO) method, showing a consistency with literature data. Apart from these, the excitation energies, wavelengths, HOMO and LUMO energies, density of state (DOS) diagrams, thermo dynamical properties and molecular electro-static potential (MEP) were appreciated.

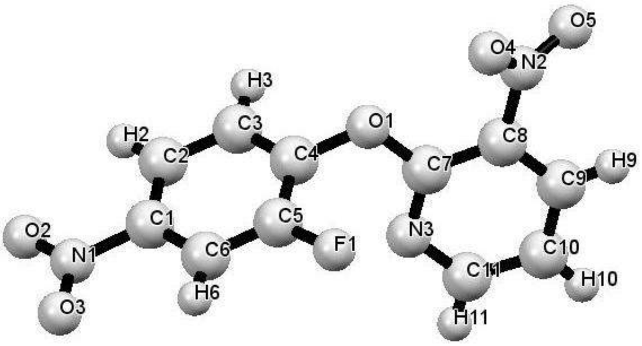

Figure 1. The crystal structure and optimized geometry of the 2-(2-Fluoro-4-nitrophenoxy)-3-nitro-pyridine

Keywords**:** 2-(2-Fluoro-4-nitrophenoxy)-3-nitropyridine, DFT; NMR, UV, Infrared and Raman spectra; HOMO–LUMO

[1] L. Cui and X. He, Acta Crystallographica, Section E 58 2014, o100

X-Ray Structural And Thermal Analysis Of A Novel Copper Compound Containing Dissymmetric Independent 5- And 6-Coordinate Cul(H_2O)$_N$ (N=2,3) Units And Hydrogen Bond Bridges

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The synthesis, thermogravimetric and X-ray structure analysis of an unprecedented copper compound prepared from a chiral tridentate Schiff base ligand is reported. The compound is essentially composed of two independent CuL(H_2O)$_x$ complexes, one of which has bound one more water molecule than the other, resulting in distorted square pyramidal and octahedral geometries. It is suggested that this may be a particularly clear model for the substrate association step of copper-based enzymes. Data were absorption-corrected within the CrysAlis program [1]. Using Olex2 [2], the structure was solved with the SHELXS [3] structure solution program using the Patterson Method and refined with the SHELXL refinement package using Least Squares minimization.

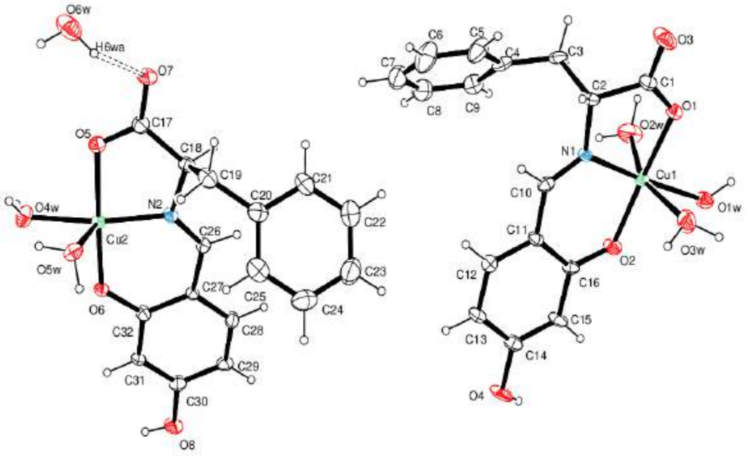

Figure 1. The molecular structure of the title compound in the asymmetric unit, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 20% probability level. Dashed line indicates the inter-molecular hydrogen bond.

Keywords**:** Schiff base Cu(II) complex, Crystal structure, 2D supramolecular structure.

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[3] G.M. Sheldrick, *Acta Cryst. A*, **2008,** *64*, 112-122.

[(S)-2,4,6-trimethyl-N-(pyrrolidin-2-ylmethyl)aniline](chloro)(p-cymene)ruthenium(II)

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The title compound, [(S)-2,4,6-trimethyl-N-(pyrrolidin-2-ylmethyl)aniline](chloro)(p-cymene)ruthenium(II), was synthesized and characterized by elemental analysis, infrared absorption spectra (IR) and its molecular structure was also determined by X-ray structure analysis. The complex crystallizes in monoclinic space group $P2_1$, a = 9.2088(6), b = 12.1642(6), c = 12.6561(11) Å, β= 100.322(6)°, V = 1394.76(17) Å^3 and Z = 2.The structure exhibits a typical three legged piano-stool structure with Ru^{II} coordinated by two nitrogen atoms of the N-heterocyclic carbene ligand and Cl atom The coordination geometry around Ru^{II} is that of a distorted octahedron in which three sites are occupied by the p-cymene ligand (with an η^6 coordination mode), two by N-heterocyclic carbene and one by the Cl ligand. The distance between the Ru^{II} ion and the leastsquares plane of the p-cymene aromatic ring is, 1.6849 Å, in good agreement with those found in other (*p*-cymene) ruthenium (II) complexes. [1,2].

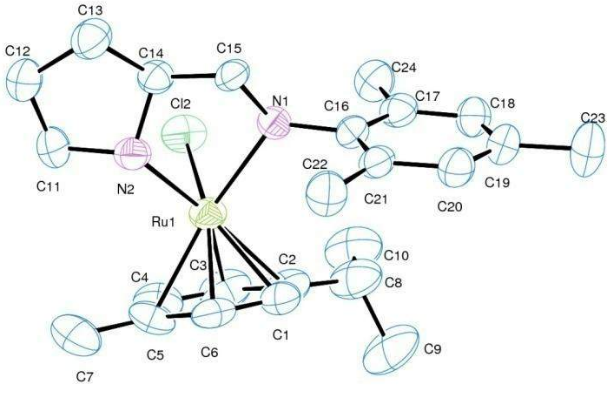

Figure 1. The molecular structure of the title compound, showing displacement ellipsoids at the 50% probability level. H atoms have been omitted for clarity.

Keywords: Ruthenium(II), p-cymene, Crystal structure.

[1] M. Aitali, L.E. Firdoussi, A. Karim, A.F. Barrero, M. Quiros, *Acta Crystallographica* **2000** C56, 1088-1089.

[2] T. Brietzke, D. Kässler, A. Kelling, U. Schilde, H.J. Holdt, *Acta Crystallographica* **2014** E70, m39-m40.

Structural Analysis of AA 5000 Series Aluminum Alloys by XRD and DTA Methods

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In this study, structural analysis of AA 5000 aluminum alloys was investigated by XRD and DTA methods. Cryogenic process for AA 5000 series aluminum alloys were carried out at -146 °C for 12 and 24 h. For comparison, samples without cryogenic process were also prepared. Phases in these samples were investigated by using XRD powder method between 2□=10-70° angles using Cuk□□source. Crystal sizes of the samples were calculated by using Scherrer equation. Phase transitions were examined by Differential Thermal Analyzer (DTA).

Keywords: *XRD, DTA, AA 5000, Cryogenic*

Structural Analysis for a Plastic Work Tool Steel and a Hot Work Tool Steel by XRD Method

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In this study, structural analysis for work tool steels was investigated by XRD method. Heat treatments were carried out for a plastic work tool steel and a hot work tool steel samples in order to obtain working conditions. After that, 55 HRC and 52 HRC hardness values were measured from these samples respectively. Phases in these samples were investigated by using XRD powder method. Crystal sizes of the samples were found between 20 nm and100nm by using Scherrer equation. Crystal parameters were determined and microstructural investigation was carried out by optical microscopy.

Keywords: *XRD, Work Tool Steel,*

Partly Substituted *spiro-ansa-spiro* (*sas*) Phosphazene

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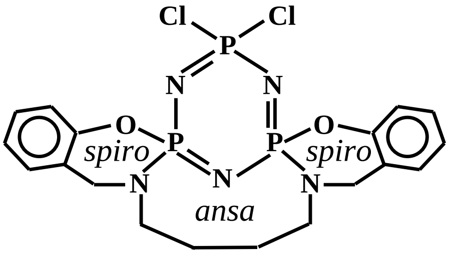
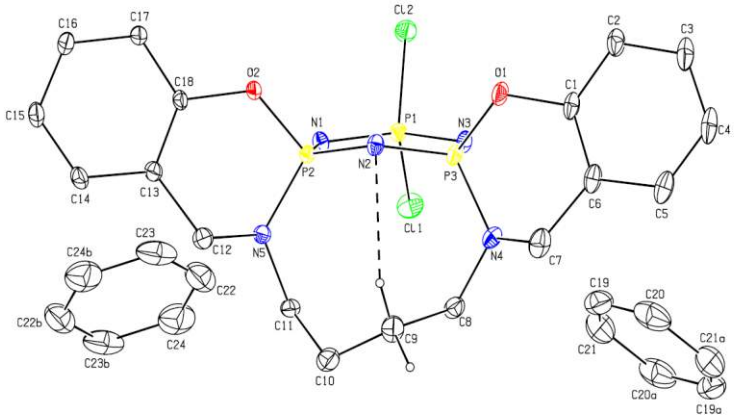
The word phosphazene refers to a broad range of molecules containing phosphorus and nitrogen atoms joined by formally unsaturated bonds [1]. In this study, the crystal structure of partly substituted *spiro-ansa-spiro* (*sas*) phosphazene was determined by the single X-ray crystallography. The phosphazene ring [P1/N1/P2/N2/P3/N3], *ansa*-ring [P2/N2/P3/N4/C8/C9/C10/C11/N5] and the *spiro*-rings [P2/N5/C12/C13/C18/O2 and P3/O1/C1/C6/C7/N4] are in twisted conformations. The bicyclic system made up of phosphazene and *ansa*-rings of the compound is in a sofa conformation. This bicyclic system contains V-shaped rings with the nonplanar two halves (P2/N1/P1/N3/P3) and (P3/N4/C8/C9/C10/C11/N5/P2) with one of the two halves (P2/N1/P1/N3/P3) being essentially planar, while the other half (P2/N5/C9/C8/N4/P3) is a crown conformation. The sums of the bond angles around the atoms N4 and N5 [354.2(3)° and 357.9(3)°] show the hybridizations of the N-atoms are trigonal planar. P2–O2 and P3–O1 are bonded to *cis*-fashion. The stereogenic P2 and P3 atoms have (*R*)- and (*S*)-configurations (*meso* form). The average endocyclic PN bond lengths of the compound [1.581(3) Å] is considerably shorter than the average exocyclic PN bonds [1.636(3) Å]. In the phosphazene ring, the endocyclic angles N2–P3–N3 and N1–P2–N2 [113.6(2)° and 114.6(2)°] are decreased with respect to the corresponding value in the "standard" compound $N_3P_3Cl_6$ [118.3(2)°] [2].



sas-Phosphazene



This study was financially supported by Ankara University Scientific Research Projects (BAP) (Grant No. 10B4240008) and Hacettepe University Scientific Research Unit (Grant No. 02 02 602 002).

***Keywords*:** Phosphazene, *spiro-ansa-spiro*-Phosphazene, Cystal Structure

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Theoretical and Experimental Studies on 5-Methoxy-2-({[4-(3-methyl-3-phenyl-cyclobutyl)-thiazol-2-yl]-hydrazono}-phenyl-methyl)-phenol

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A new compound ($C_{30}H_{34}N_2O_2S_1$), was synthesized and characterized by IR spectroscopy and single-cyrstal X-ray diffraction. The compound cyrstallizes in the triclinic space group *P*-1. There are two independent molecules A and B in the asymmetric unit. The crystal structure is stabilized by two O-H···O intermolecular hydrogen bonds. The conformational behavior and structural stability of the optimized geometry of the title compound were also investigated by utilizing ab- initio calculations with 6-31G(d) basis set at HF and B3LYP levels. The calculated parameters are in good agreement with the corresponding X-ray diffraction values.

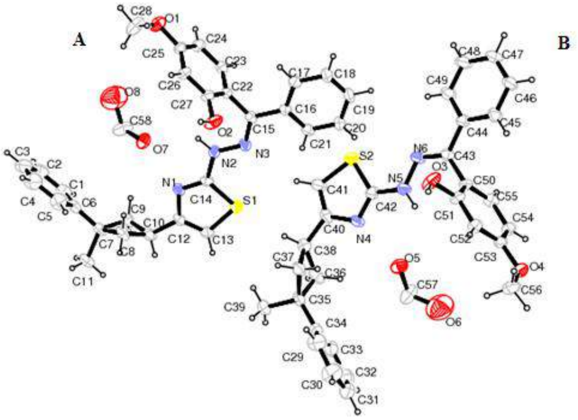

Figure1. Molecule Structure.

Keywords: X-ray, DFT and HF calculation, B3LYP, IR spectrum.

Investigation of Mechanical, Electronic, Vibrational and Thermodynamic Properties of α –V_3AsC_2 Composite with Ab-initio

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In this study, hexagonal (P63/mmc (# 194)) is α –V_3AsC_2 ground state properties of the compound Density Functional Theory (DFT) within the Generalized Gradient Approximation (GGA) were analyzed using the program based VASP package and were used in calculations potentially ultrasoft psedopotansiyel. First lattice constant (a), Bulk modulus (B), and pressure derivative of bulk modulus (B') with the total energy equation of state was fit to the data was found and compared with available data. From Band structure and density of states (DOS) density of states calculations, the compound is metallic. The elastic constants are calculated using stress-strain relationship and their corresponding elastic moduli of polycrystalline aggregate, including shear moduli (G), Young's moduli (E), Poisson's ratios (ν), and elastic anisotropy values (A) are obtained and also discussed. Calculated phonon spectra and the related DOS curves were calculated. Phonon frequency is found to be positive for the study of the structure was confirmed to be stable as dynamical. Called MAX phase structure is hexagonal crystals in space group 194 P63/mmc structure is stable. $M_{n+1}AX_n$ n = 1, 2, 3 may take the values. M = transition metal of the first part, A = A group elements, X is C or N [1]. MAX phases makes this so impressive physical, chemical, electrical and mechanical properties as well as metal and ceramic characteristics are showing [2]. MAX phases are solid, lightweight and rigid structure with high flexibility. Although a rigid structure MAX phases can be processed easily. GGA approach was used in this study. Calculation of the cut-off energy 800ev and 16x16x5 Monkhorst-Pack k- point network was used. α - V_3AsC_2'n total energy by minimizing and Murnaghan[3] the state equation By fitting lattice constant(a), Bulk module(B) and the bulk modulus based on the pressure derivative (B') and the formation enthalpy (□H°) theoretically found and the results in Table 1 with other experimental and theoretical studies are given. α-V_3AsC_2 crystalline lattice constants calculated using the high symmetry points of the Brillouin zone of the electronic band structure and DOS were obtained

Table 1: The structure parameters of α-V_3AsC_2

system	a(A°)	c(A°)	B (GPa)	B'	ΔH° (eV/atom)
Our work	3.07	10.88	238	4.32	-0.71

The elastic constants (C_{ij}) provide information about the stability and stiffness of materials, and their first principles calculation requires accurate methods. The compound satisfy all these stability conditions, and thus α –V_3AsC_2 compound is mechanically stable. Phonon spectra of linear response calculations help PHONOPY code method was utilized. Phonon frequencies using the 2x1x2 super-cell, was to obtain the phonon DOS and thermodynamic properties

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The Investigation of Microstructural Properties of $Cu_{0,2}Bi_{1,8}Sr_2Ca_2Cu_{3-x}Zn_xO_{10+\delta}$ Ceramic Structure

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In this work, effects of substitution ratio on the microstructural properties in $Cu_{0,2}Bi_{1,8}Sr_2Ca_2Cu_{3-x}Zn_xO_{10+\delta}$ system by taking the substitution ratio x= 0, 0,1, 0,5 and 1,0 were investigated. The samples prepared with glass ceramic method at 830 ^{o}C. In order to determine the crystalline phases, the heat treated samples were subjected to X-ray diffraction (XRD) analysis. The XRD analysis of the samples fabricated was performed using a Bruker D8 Advanced X-ray diffractometer with wavelength of Cu Kα radiation (□=1.5418). The scan rate was chosen as 3 min^{-1} in the range of 2θ=4-70^{o}. Two main phases (BSCCO 2212 and 2223) were observed in the x-ray data and the values of the lattice parameters quite agree with the known values for 2212 and 2223 phases. The crystallite size of $Cu_{0,2}Bi_{1,8}Sr_2Ca_2Cu_{3-x}Zn_xO_{10+\delta}$ bulk material increases as the substitution degree increases, from 51 nm (x = 0) to 54 nm (x = 1.0).

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Macromolecular Crystallography: Quantitative approach and choices in X-ray data acquisition strategies

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There are remarkable numbers of Synchrotron Radiation (SR) facilities which are being used for X-ray diffraction experiments for macromolecular crystallography. Main indicators on collecting optimum data for a macromolecular crystal involve a number of preferences including beam line structure, scavenger type, crystal sensitivity, wavelength, beam intensity, time and temperature dependences. If the choice of the synchrotron data acquisition strategies is not correct in crystallography, the result of the experiment and 3D structural analysis of macromolecules can be fail. Therefore many parameters involved in X-ray data collection for each experiment at high-brilliance synchrotron beam lines for macromolecular crystallography have to be considered individually and required careful attention. This study presents many important strategically points and notes on an optimum data collection derived from macromolecular crystallographic experimental results performed at 2nd and 3rd generating beam lines of X6A, X17B and X18B, respectively, of NSLS and ESRF.

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***Keywords*:** Macromolecular Crystallography, Optimum Data Collection, Beam Line.

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X-Ray *Structure* And *Dft Studıes* of 3-Chloro-N-(4-Sulfamoylphenyl)-Propanamıde

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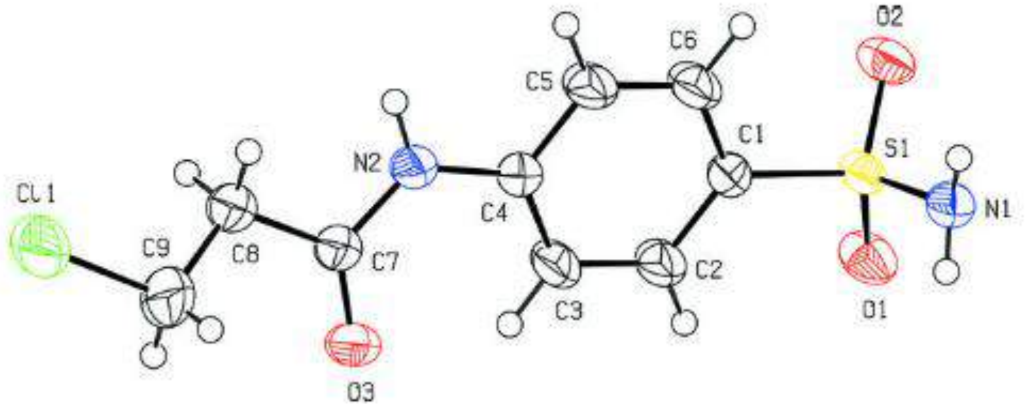
In this study, compound "3-chloro-N-(4-sulfamoylphenyl)-proponamide" (1) was synthesized and characterized by single crystal X-ray diffraction and DFT methods as theoretically and experimentally. According to X-ray diffraction results**,** c*ompound*(1) *crystallizes in themonoclinicspacegroup*$P2_1$/c with a = 7.7554 (4) Å, b = 14.8191 (8) Å, c = 9.7482 (5) Å and β = 94.181 (4) °, Z = 8.The crystal structure of (1) is stabilized by N—H···O type hydrogen bonds generate the two-dimensional network (double layer structure), and generates a ring of graph-set motif S(6). Crystal packing is influenced by weak π–π stacking interactions between nearby aromatic rings of the adjacent molecules, symmetry code: (iv) [1 - x, 1 - y, 1 - z].The molecular geometry was also calculated by using Gaussian 03 software and structure was optimized by using DFT/B3LYP method with the 6-31+g basis sets in ground state. DFT optimized structure is in excellent agreement with the X-ray crystal structure of (1).



(1)

Keywords: *3-Chloro-N-(4-sulfamoylphenyl)-proponamide X-ray diffraction, Quantum* *chemicalcalculations, Densityfunctionaltheory,*

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Zinc(II) and Cadmium(II)-Saccharinate Complexes with 1,2-Bis(imidazole-1ylmethyl)benzene

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Saccharinate (sac) is a well-known versatile ligand that has been widely used in the synthesis of complexes [1, 2]. Sac ligand coordinates to metal ions by means of its one imino nitrogen, one carbonyl oxygen and two sulfonyl oxygen atoms forming monodentate, bidentate and bis(monodentate) bridge ligand. In addition to these donor atoms, a sac may be regarded as a hydrogen bonding acceptor with a significant potential to generate supramolecular assemblies in the solid state. In this study, zinc(II) and cadmium(II) saccharinate coordination polymers with 1,2-bis(imidazole-1ylmethyl)benzene (1,2-bix),$[Zn(sac)_2(1,2\text{-bix})]_n$ (**1**) and $\{[Cd(sac)_2(1,2\text{-bix})_2]\cdot 2H_2O\}_n$ (**2**) were synthesized and characterized by IR spectroscopy, single crystal X-ray diffraction and thermal analysis techniques.X-ray diffraction analyses show that sac ligand coordinate to Zn(II) ion from nitrogen atom in complex **1** while sac ligand to Cd(II) ion from oxygen donor atom in complex **2**. 1,2-bix ligand acts as bridging ligand and generates one dimensional polymeric structure in both complexes. Moreover, the emission spectra of complexes in the solid state at roomtemperature are investigated.

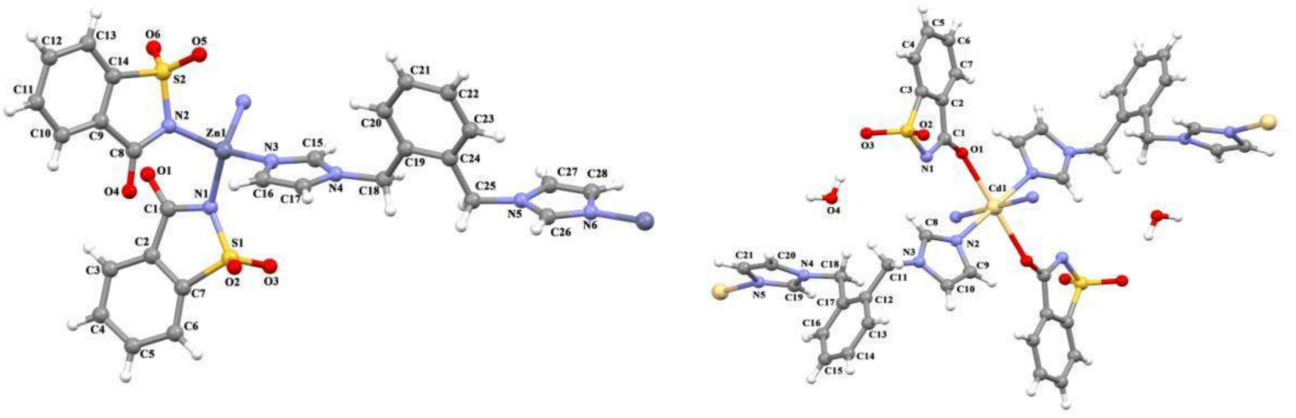

Figure 1. The molecular structures of **1**and **2**

Keywords: Saccharinate complexes, 1,2-bis(imidazole-1ylmethyl)benzenecomplexes

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