6th TURKISH NATIONAL CRYSTALLOGRAPHY MEETING

17-19 May 2026
Giresun University
Giresun
TÜRKİYE

ABSTRACTS BOOK

Editors

Prof. Dr. Sema Öztürk Yıldırım
Prof. Dr. Gökhan Alpaslan
Prof. Dr. Resul Sevinçek

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6th NATIONAL CRYSTALLOGRAPHY MEETING

17-19 May 2026

Giresun, TÜRKİYE

TOPICS

Macromolecular Crystallography
Material Science and Powder Diffraction Applications
Molecular Structures and Properties
Fundamental Concepts

INVITED SPEAKERS

Cengiz Arıcı (TÜBİTAK ARDEB, Türkiye)
Michael Richard Probert (Newcastle University, UK)
Mustafa Fatih Genişel (SESAME, Salt, Jordan)
S. Garcia-Granda (University of Oviedo, Spain)
Santanu Pathak (SESAME, Salt, Jordan)
Veysel Turan Yılmaz (Karadeniz Technical University, Türkiye)
William Clegg (Newcastle University, UK)
Zehra Sayers (Sabancı University, Türkiye)

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6th National Crystallography Meeting

17-19 May 2026 | Giresun University

Sunday, 17 May 2026 (Şehit Ömer Halisdemir Conference Hall)

10:00 - 12:00	**Registration, Opening Ceremony & Congress Opening Speeches**
12:00 - 13:30	**Visit to the Stands & Lunch**
13:30 - 14:00	**Session I (Invited Speaker)** *Prof. Dr. Santiago GARCIA-GRANDA (University of Oviedo, Spain)* New sustainable ceramic pigments based on solid solutions of Olivine and Diopside *Chairs: Prof. Dr. Zehra SAYERS & Prof. Dr. Sema ÖZTÜRK YILDIRIM*
14:00 - 14:30	**Session II (Invited Speaker)** *Prof. Dr. Zehra SAYERS (Sabancı University, Türkiye)* Bringing the invisible into focus with synchrotron radiation *Chairs: Prof. Dr. Metin KUL & Prof. Dr. Mehmet KABAK*
14:30 - 15:00	**Coffee Break**
15:00 - 15:30	**Session III (Invited Speaker)** *Assoc. Prof. Dr. Cengiz ARICI (TÜBİTAK, Türkiye)* ARDEB Programları ve Yenilikler *Chairs: Prof. Dr. Yelda BİNGÖLALPASLAN & Prof. Dr. Gökhan ALPASLAN*

Scientific Program – Oral Presentations (15:30 – 16:15)

Chairs: Prof. Dr. Orhan BÜYÜKGÜNGÖR & Prof. Dr. Can ALAŞALVAR

15:30 - 15:45	*Sultan Başak, Başak Koşar Kırca, Çiğdem Albayrak Kaştaş* Quantum Chemical Characterization and Molecular Docking Analysis of (E)-2-[(4-Chloro-3-nitrophenylimino)methyl]-3-methoxyphenol: A Novel Schiff Base Ligand with Potential Anticancer Activity
15:45 - 16:00	*Sema Öztürk Yıldırım, Metin Kul, Ray J. Butcher* Crystal Structure of S-2-Aminophenyl phenylcarbamothioate
16:00 - 16:15	*Onur Rauf Yılmaz, Çiğdem Albayrak Kaştaş, Canan Kazak* A Comparison of Isomeric Schiff Bases Featuring Halogens at Different Contact Points

Sunday, 17 May 2026 (Şehit Ömer Halisdemir Conference Hall)

Scientific Program – Poster Presentations (16:15 – 17:00)

Chairs: Prof. Dr. Birol ERTUĞRAL & Prof. Dr. Halil GÖKÇE

Poster 1	*Sema Öztürk Yıldırım, Zeki Büyükmumcu, Rahime Şimşek, Gökalp Çetin, Ray J. Butcher* Synthesis and Spectroscopic Characterization and DFT Study of benzyl 4-([1,1'-biphenyl]-4-yl)-2,6,6- trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate
Poster 2	*Rahime Şimşek, Zeki Büyükmumcu, Sema Öztürk Yıldırım, Gökalp Çetin, Cihat Şafak, Ray J. Butcher* DFT Studies, Synthesis, Biological Activity and Crystal Structure of Tert-Butyl 4-([1,1'-Biphenyl]-4-Yl)-2- Methyl-5-Oxo-1,4,5,6,7,8-Hexahydroquinoline-3-Carboxylate
Poster 3	*Sema Öztürk Yıldırım, Zeki Büyükmumcu, Rahime Şimşek, Gökalp Çetin, Cihat Şafak, Ray J. Butcher* Synthesis, Structural Characterization and Density Functional Studies of ethyl 4-(biphenyl-4-yl)-2,6,6- trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate – A non-merohedral Twinned Structure
Poster 4	*Gökhan Kaştaş, Çiğdem Albayrak Kaştaş, Cumhur Avşar* Structural, Catalytic, and Biological Evaluation of a Copper(II) Schiff Base Complex: bis{2-ethoxy-6-(E)-[(4- fluorophenyl)imino)methyl]phenolato-κN,κO}copper(II)·1.5H_2O
Poster 5	*Başak Koşar Kırca, Çiğdem Albayrak Kaştaş, Gökhan Kaştaş* Bis{2-ethoxy-6-(E)-[(4-bromophenyl)imino)methyl]phenolato-κN,κO}copper(II)
Poster 6	*Çiğdem Albayrak Kaştaş, Gökhan Kaştaş* Synthesis, Structural, and Spectroscopic Characterization of a Seesaw-Geometry Schiff Base Complex: bis{2- ethoxy-6-(E)-[(4-methylphenyl)imino)methyl]phenolato-κN,κO}copper(II)·monohydrate
Poster 7	*Tuğba Bayın, Onur Rauf Yılmaz, Erbil Ağar, Seda Nur Aygün, Canan Kazak* Substituent-Dependent Crystal Packing in Ortho-Hydroxy Schiff Bases
Poster 8	*Esengül Ejder* DFT and Molecular Docking Evaluation of a Novel Schiff Base (E)-2-(4-((2,4-dimethoxybenzylidene)amino)phenyl)ethan-1-ol: From Electronic Structure to Biological Interaction
17:00 - 20:00	**Social Events - Dinner**

Monday, 18 May 2026 (Mevlana Celaleddin-i Rumi Conference Hall)

09:30 - 10:00	**Session IV (Invited Speaker)** *Prof. Dr. Bill CLEGG (Newcastle University, United Kingdom)* Refining difficult structures and workshops *Chairs: Prof. Dr. Onur ŞAHİN & Prof. Dr. Resul SEVİNÇEK*
10:00 - 10:30	**Session V (Invited Speaker)** *Prof. Dr. Michael PROBERT (Newcastle University, United Kingdom)* Exploring the Crystallization Field Using High-Efficiency ENaCt Methods *Chairs: Prof. Dr. Ufuk ÇORUH ve Prof. Dr. Ümit CEYLAN*
10:30 - 11:00	**Coffee Break**
11:00 - 11:30	**Session VI (Invited Speaker)** *Ph.D. Mustafa Fatih GENİŞEL (SESAME, Jordan)* The Light of Science in the Middle East: SESAME and Research Opportunities *Chairs: Prof. Dr. Ahmet ERDÖNMEZ & Assoc. Prof. Dr. M. Hakkı YILDIRIM*
11:30 - 13:30	**Visit to the Stands & Lunch**
13:30 - 14:00	**Session VII (Invited Speaker)** *Prof. Dr. Veysel Turan YILMAZ (Karadeniz Technical University, Turkey)* Crystal structure–NMR spectra correlations: Two examples of metal complexes *Chairs: Prof. Dr. Ersin TEMEL & Prof. Dr. Fulya Aydın TEMEL*

Scientific Program – Oral Presentation (14:00 – 14:15)

Chairs: Prof. Dr. Ersin TEMEL & Prof. Dr. Fulya Aydın TEMEL

14:00 - 14:15	*Öznur Ölmez Nalcıoğlu, Mine Sulak, Ayşe Gül Caniklioğlu, Bahadır Koz* Transforming PET Bottle Waste into Multifunctional ZnO@MIL-101(Cr) Material via Moss-Mediated Synthesis: Characterization and Antimicrobial Evaluation
14:15 - 14:45	**Session VIII (Invited Speaker)** *Assoc. Prof. Dr. Santanu PATHAK (SESAME MS/XPD Beamline, Jordan)* The MS/XPD Beamline at SESAME: Capabilities, Applications and User Opportunities *Chairs: Prof. Dr. Veysel Turan YILMAZ & Prof. Dr. Aytaç GÜDER*
14:45 - 15:45	**Coffee Break & Poster Session** *Chairs: Prof. Dr. Serkan DEMİR & Assoc. Prof. Dr. Selbi KESKİN*
Poster 1	*Nuri Yıldırım* Crystal and molecular structure of N-(3,5-diphenyl-4H-1,2,4-triazole-4-yl)thiophene-2-carboxamide

Monday, 18 May 2026 (Mevlana Celaleddin-i Rumi Conference Hall)

Poster 2	*Nuri Yıldırım* Crystal and molecular structure of N-(3,5-di-p-tolyl-4H-1,2,4-triazol-4-yl)thiophene-2-carboxamide
Poster 3	*Ceyda İÇSEL* Crystal and molecular structure of a new binuclear silver(I) complex with bridging chlorido and 1,4- bis(diphenylphosphino)butane ligands
Poster 4	*Murat Tekingündüz, Resul Sevinçek* Electronic Structure Engineering of Pentagraphene via Site-Selective B and N Substitution: A First-Principles Study
Poster 5	*Selim Adıgüzel, Resul Sevinçek* Ti_2BN Monolayer as a Novel MBene: A First-Principles Study of Stability and Electronic Structure
Poster 6	*Hanifi Özşanlı, Gülnur Odabaş, Ufuk Çoruh* Detailed examination of 4-[(4-Ethyl-5-phenyl-4H-1,2,4-triazol-3-yl)sulfanyl]phthalonitrile crystal packing, Hirshfeld surface analysis, and 2D fingerprint map
Poster 7	*Berru Özkaya, Emine Berrin Poyraz, Mustafa Şanlı, Metin Yavuz, Ufuk Çoruh* Investigation of the Crystal Structure of a 4,5-Dicyanobenzene Derivative via Hirshfeld Surface Analysis and Energy Frameworks Method
Poster 8	*Gül Yakalı, Zeynep Türkmen Bulca, Merve İzmirli, Resul Sevinçek* Charge Mobility Analysis of Phenanthroline Derivatives via Density Functional Theory: Role of Reorganization Energy and Charge Transfer Integrals
Poster 9	*Merve İzmirli, Hasan Karabıyık, Gül Özkan, Resul Sevinçek, Hande Karabıyık, Muhittin Aygün* Crystal Structure and Hirshfeld Surface Analyses of some PEPPSI Type Pd(II)NHC Complexes
15:45 - 17:00	**Closing Ceremony**
19:00 - 23:00	**Gala Dinner**

Tuesday, 19 May 2026

10:00 - 18:00	**Giresun Tour** Social program and city tour in Giresun.

INVITED SPEAKERS (I)

I-01: New sustainable ceramic pigments based on solid solutions of Olivine and Diopside

[1]M. A. Tena, [2]M. S. M. Abdelbaky, [3*]S. Garcia-Granda

[1]*University Jaume I, School of Technology and Experimental Sciences, Inorganic and Organic Chemistry Department, Castellón, Spain*
[2]*Salamanca University, Faculty of Chemical Sciences, Physical Chemistry Department, Salamanca, Spain*
[3]*Oviedo University-CINN, Chemistry Faculty, Physical and Analytical Chemistry Department, Oviedo, Spain*

* E-mail: sgg@uniovi.es

Abstract
The incorporation of elements or ions in the crystalline structures by the formation of solid solutions in materials changes the composition of the materials and therefore its properties allowing the design of materials of industrial interest. The formation of solid solutions allows to increase the melting point of a material, to change gradually its color, to increase its hardness, to increase its conductivity, and to increase its magnetism, or other properties.

Formation of solid solutions with Mg(II) in materials can be used to decrease the nickel and/or cobalt amount in compositions of ceramic pigments reducing the toxicity of the materials while making them less expensive. This work presents the results obtained in the crystallization of olivine solid solutions as a single phase or together with others crystalline phases in compositions: $MgCo_xNi_{1-x}SiO_4$ $(0.0 \leq x \leq 1.0)$, $Na_2Co_xNi_{1-x}Si_4O_{10}$ $(0.0 \leq x \leq 1.0)$, $Na_2Mg_{1-x}Co_xSiO_4$ $(0.0 \leq x \leq 1.0)$ and the crystallization of diopside solid solutions in $CaMg_{0.5}Co_xNi_{0.5-x}Si_2O_6$ $(0.0 \leq x \leq 0.5)$ compositions.

The colour of samples containing Co(II) ions is pink-violet or blue-violet in compositions which include olivine structure and pink in compositions with diopside structure at 1000 and/or 1200 °C and green and blue colourations were obtained from $CaMg_{0.5}Co_xNi_{0.5-x}Si_2O_6$ enamelled samples. These colourations are similar to those obtained in the $MgNiSiO_4$ - $MgCoSiO_4$ system or in $Na_2Co_xNi_{1-x}Si_4O_{10}$ compositions and blue in the $Na_2Mg_{1-x}Co_xSiO_4$ compositions. These solid solutions were dissolved in the commercial glaze tested. A reduction of cobalt amount is achieved with respect to the 56.1 %-weight in Co_2SiO_4 until 33.7 %-weight of Co(II) in $MgCoSiO_4$ composition, 15.62 %-weight in $Na_2CoSi_4O_{10}$, 12.6 %-weight of Co(II) in $CaMg_{0.5}Co_{0.5}Si_2O_6$ composition, or between 7.0 and 24.8 % in $Na_2Mg_{0.8}Co_{0.2}SiO_4$ $(x = 0.2)$ and $Na_2Mg_{0.2}Co_{0.8}SiO_4$ $(x = 0.8)$ compositions respectively.

Key Words: Olivine, Diopside, Solid solution, Ceramic, Pigments

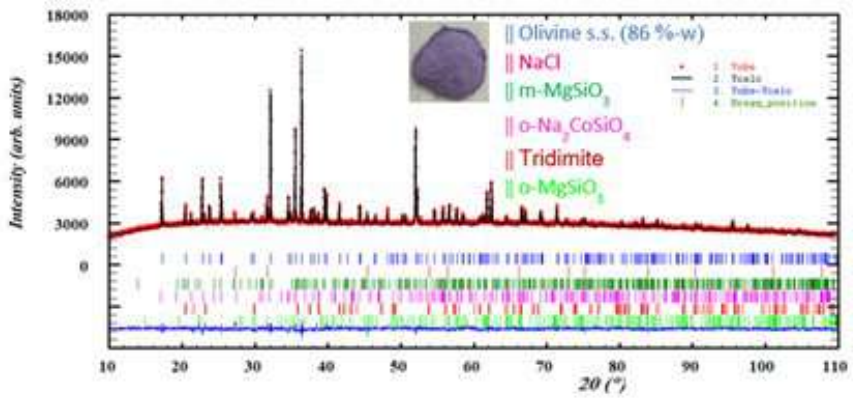

Fig. 1: The diffraction profile by Rietveld's method from $Na_2Mg_{0.4}Co_{0.6}SiO_4$ composition fired at 1200 °C.

References

[1] Tena, M.A., Mendoza, R., Trobajo, C., García J. R., García-Granda, S., (2023). Green and blue materials for the ceramic industry from pink $MgCo_xNi_{1-x}SiO_4$ $(0 \leq x \leq 1)$ solid solutions. *Ceramic International*, 49, 12021-12033.

[2] Tena, M. A., Abdelbaky, M. S. M., Trobajo, C., García J. R., García-Granda, S., (2024). Synthesis and structural characterization of $CaMg_{0.5}Co_xNi_{0.5-x}Si_2O_6$ $(0 \leq x \leq 0.5)$ solid solutions as a colouring substance. *Ceramic International*, 50, 20391-20401.

[3] Tena, M. A., Abdelbaky, M. S. M., Trobajo, C., García-Granda, S., (2025). Crystallization of M_2SiO_4 (M = Ni, Co) olivine solid solutions from $Na_2Co_xNi_{1-x}Si_4O_{10}$ $(0.0 \leq x \leq 1.0)$ compositions. *Ceramics International*, 51(27). Part B 53154-53168.

Acknowledgements: We gratefully acknowledge the financial support provided by Principality of Asturias (IDE/2024/000742).

I-02: Bringing the invisible into focus with synchrotron radiation

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Abstract Synchrotron radiation (SR) facilities provide powerful "microscopes" in modern science, enabling studies on biological structures that are out of reach for conventional methods. In this talk, I will outline the unique properties of synchrotron light and its essential role in advancing structural biology. Using examples from our work on the cornea, chromatin, and fibrous proteins like actin and keratin, along with metal-binding systems, I will try to illustrate how my pursuit of structure-function relationships using SR has shaped my career.

I will also provide an inside look at a landmark achievement: the establishment of the SESAME SR laboratory in Jordan. As the Middle East's first international center of excellence, and the world's first synchrotron powered entirely by renewable energy, SESAME is fostering a new era of collaborative research. I will discuss how this unique facility is bringing new scientific frontiers into focus for both the regional and global scientific communities.

Key Words: Synchrotron Radiation (SR), Structural Biology, Structure-Function Relationships

I-03: Refining difficult structures

William Clegg*

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Abstract The refinement of small-molecule crystal structures is usually performed with least-squares techniques. Numerical parameters consist mostly of atomic coordinates and anisotropic displacement parameters, but atomic occupancy factors may also be included in cases of structural disorder. For well-behaved ordered and untwinned structures the procedure is straightforward and routine. Free refinement of all parameters may be unsatisfactory when there is disorder, and in such cases a range of available constraints and restraints can help. In this tutorial presentation I will explain the difference between constraints and restraints (as usually understood, particularly in the widely used program SHELXL1), outline some of the most common and useful constraints and restraints, and illustrate their use with specific examples.

Key Words: refinement, constraints, restraints

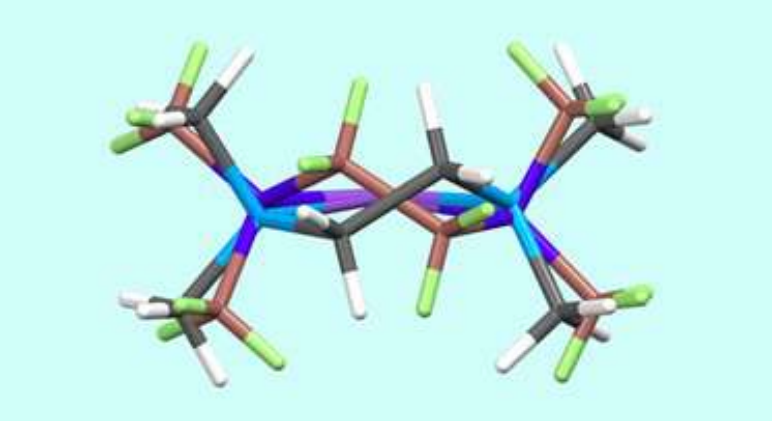

Fig. 1: Two-component disorder of a tetramethylethylenediamine (TMEDA) ligand refined with the help of restraints.

References

[1] Sheldrick, G. M. (2015). *Acta Crystallographica Section C*, 71, 3–8. Crystal structure refinement with SHELXL.

I-04: Encapsulated Nanodroplet Crystallisation – a modern method to obtain crystals and enhance structural characterisation

Michael Probert*

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Abstract Crystallisation is a key requirement to enable the analysis of chemical species by diffraction methods. Classically non-systematic, large scale, approaches have been used to generate the required crystals. However, these methods are becoming less applicable to modern compounds and the pace of pharmaceutical development. A new approach, developed at Newcastle University, has caused a significant shift in this field, making access to crystalline material easier and more cost effective. This technique is known as Encapsulated Nanodroplet Crystallisation (ENaCt). It has successfully been employed on a diverse range of structurally challenging compounds from small molecules through inorganic complexes to natural products and their synthetic analogues. The method has the major advantages of the limited amount of material required (<10 mg material gives >1000 crystallisations) and ease of polymorph screening across a wide range of chemical environments.

The methodologies employed in the technique will be discussed with case studies highlighting the scientific and structural diversity of the method's applicability, along with the mechanisms for easy access to the technique.

Key Words: Encapsulated Nanodroplet Crystallisation, ENaCt, Crystallisation, Structural characterisation

I-05: The Light of Science in the Middle East: SESAME and Research Opportunities

Mustafa Fatih GENİŞEL*

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Abstract This talk aims to provide a comprehensive introduction to the scientific and institutional aspects of SESAME (Synchrotron-light for Experimental Science and Applications in the Middle East), a pioneering international research infrastructure located in the Middle East. Situated in the Allan district of Salt, Jordan, SESAME is not only a major center for advanced scientific research in the region, but also a powerful symbol of science diplomacy and international collaboration. Established under the auspices of UNESCO, the facility is a multinational organization with members including Cyprus, Egypt, Iran, Israel, Jordan, Pakistan, Palestine, and Türkiye.

In the first part of the talk, the fundamental principles of synchrotron radiation will be discussed, and the importance of this high-brightness electromagnetic radiation for fields such as materials science, biology, chemistry, and environmental science will be explained. The second part will introduce the historical background and governance structure of SESAME.

In the third part, the six active beamlines at SESAME will be examined from both technical and scientific perspectives: BM02 – IR (Infrared spectromicroscopy), BM08 – XAFS/XRF (X-ray Absorption Fine Structure and Fluorescence Spectroscopy), ID09 – MS/XPD (Materials Science and X-ray Powder Diffraction), ID10 – BEATS (BEAmline for Tomography at SESAME), ID11L – HESEB (HElmholtz–SESAME soft X-ray Beamline), and ID11R – TXPES (Turkish Soft X-ray Photoelectron Spectroscopy End Station). In the final part, the procedures for researchers to access and benefit from SESAME will be outlined. This presentation aims not only to highlight the scientific opportunities offered by SESAME, but also to emphasize the importance of a collaborative research culture at both regional and global scales.

Key Words: Synchrotron Radiation, SESAME, X ray, Spectroscopy, Tomography, Diffraction, Science Diplomacy

Fig. 1: SESAME Experimental Hall and Guest House

I-06: Crystal structure-NMR spectra correlations: Two examples of metal complexes

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Abstract Both single crystal X-ray crystallography and NMR spectroscopy are powerful techniques to determine the molecular structure of compounds. If one method alone is insufficient, another method may be helpful in elucidating the molecular structure. Here, we presented two examples of metal complexes in terms of crystal structure-NMR spectrum correlations. The crystallographic refinement studies of trans-[Pt(H)(sac)(PPhCy2)2] and trans-[Pt(H)(sac)(PCy3)2] initially resulted in corresponding tri-coordinate Pt(II) complexes, excluding the coordination of the hydride ion (H–), probably due to relatively low electron density. Although no hydride salt was used in the synthesis of these Pt(II) complexes, the formation and coordination of the hydride ion in both complexes were confirmed by 1H NMR spectra with a triplet at ca. –18 ppm, so that the hydrate ion was crystalographically located with the help of the NMR data as a Pt–H bond to complete the coordination number of 4. The other example is the Zn(II) complexes of 5-fluorouracil (5-FU), namely [Zn(5-FU)2(bpyma)]×2H2O and [Zn(5-FU)2(terpy)]×H2O. 5-FU shows tautomerism in solution, and usually coordinates to metal ions through the N3 donor site. However, the two 5-FU ligands in these Zn(II) complexes exhibit the linkage isomerism: one is coordinated via the N3 site, while the other one through the N1 site. The linkage isomerism for 5-FU was first observed in these complexes and well-established by X-ray crystallography. Additionally, the two well-separated signals in the 19F NMR spectra of both complexes further confirmed the coordination of the tautomeric forms of 5-FU.

Key Words: Crystal structure, NMR spectrum, Structure-spectra correlation.

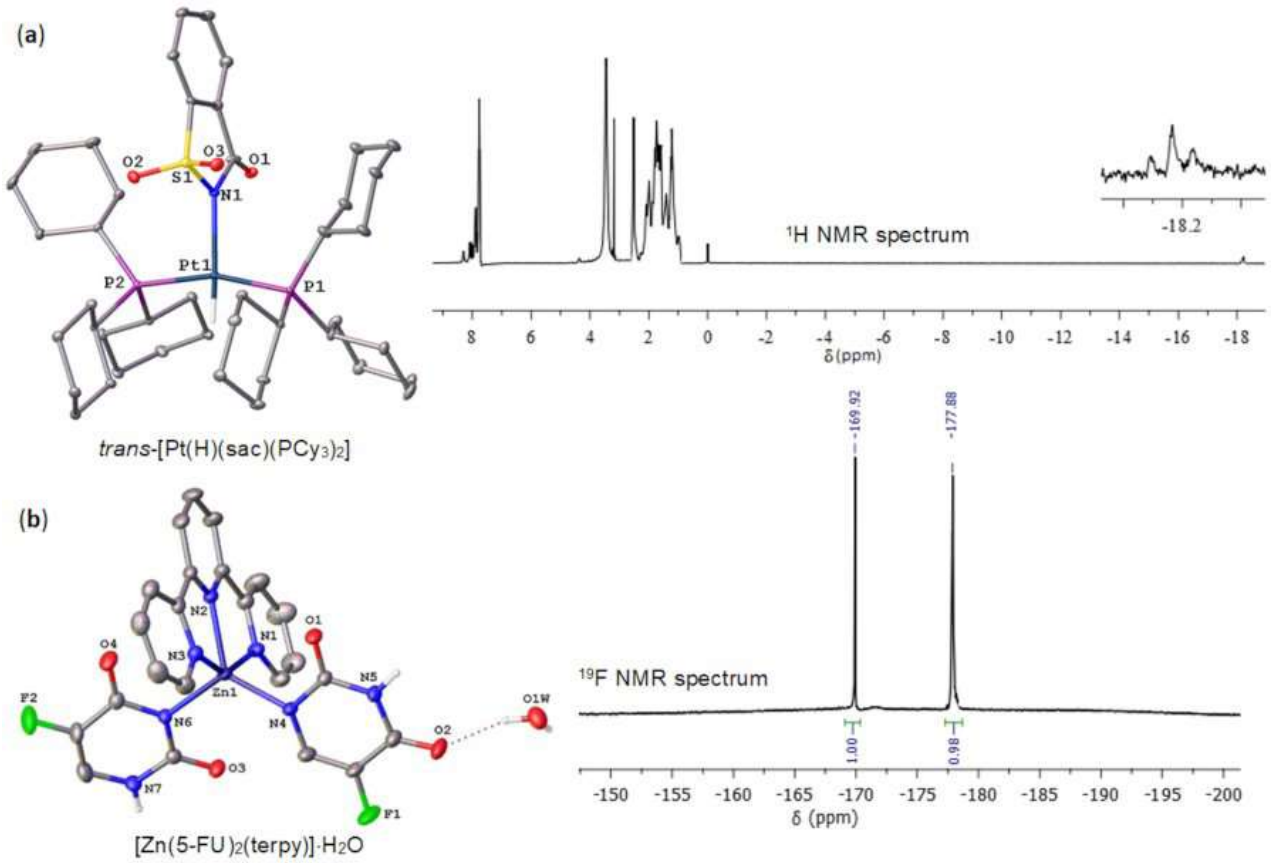

Fig. 1: (a) the molecular structure and 1H NMR spectrum of trans-[Pt(H)(sac)(PCy3)2], and (b) the molecular structure and 19F NMR spectrum of [Zn(5-FU)2(terpy)]×H2O.

References

[1] Yilmaz, V.T. et al. (2018). Synthesis, structures and anticancer potentials of platinum(II) saccharinate complexes of tertiary phosphines with phenyl and cyclohexyl groups targeting mitochondria and DNA, *Eur. J. Med. Chem.*, 155, 609.

[2] Icsel, C. et al. (2022). Novel 5-fluorouracil complexes of Zn(II) with pyridine-based ligands as potential anticancer agents, *Dalton Transact.*, 51, 5208.

I-07: The MS/XPD Beamline at SESAME: Capabilities, Applications and User Opportunities

Santanu Pathak*

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Abstract ID9- MS/XPD- Materials Science/X-ray Powder Diffraction is the dedicated beamline for hard X-ray diffraction in SESAME synchrotron facility. The primary purpose of the wiggler based beamline is to provide detailed information about the atomic-scale crystal structure and phase composition of materials. The high brilliance of the synchrotron beam, combined with instrumental resolution comparable to leading XRPD beamlines, enables precise and efficient analysis.

The beamline primarily operates in capillary (transmission) geometry in the 5-25 keV energy range (2 eV resolution), with a Dectris Pilatus 300K detector mounted on the diffractometer arm. The beamline is equipped with a hot air blower for high-temperature measurements and a liquid nitrogen system for low-temperature conditions. Available analysis tools include the PDF-4 database, Match! program for phase identification, and GSAS-II, FullProf for structural refinement. A robotic sample changer is currently being integrated to enable automated and rapid sample exchange, improving experimental efficiency.

The MS/XPD beamline supports a broad range of scientific disciplines, with a strong emphasis on physical sciences and materials research, particularly condensed matter physics. It also contributes significantly to chemical sciences, including metal–organic frameworks, nanomaterials, and catalysis, as well as applications in environmental science, cultural heritage, geochemistry, and emerging biological, medical research. Future research is expected to further broaden the scientific scope of the beamline.

Key Words: Powder X ray Diffraction, Synchrotron Radiation, SESAME

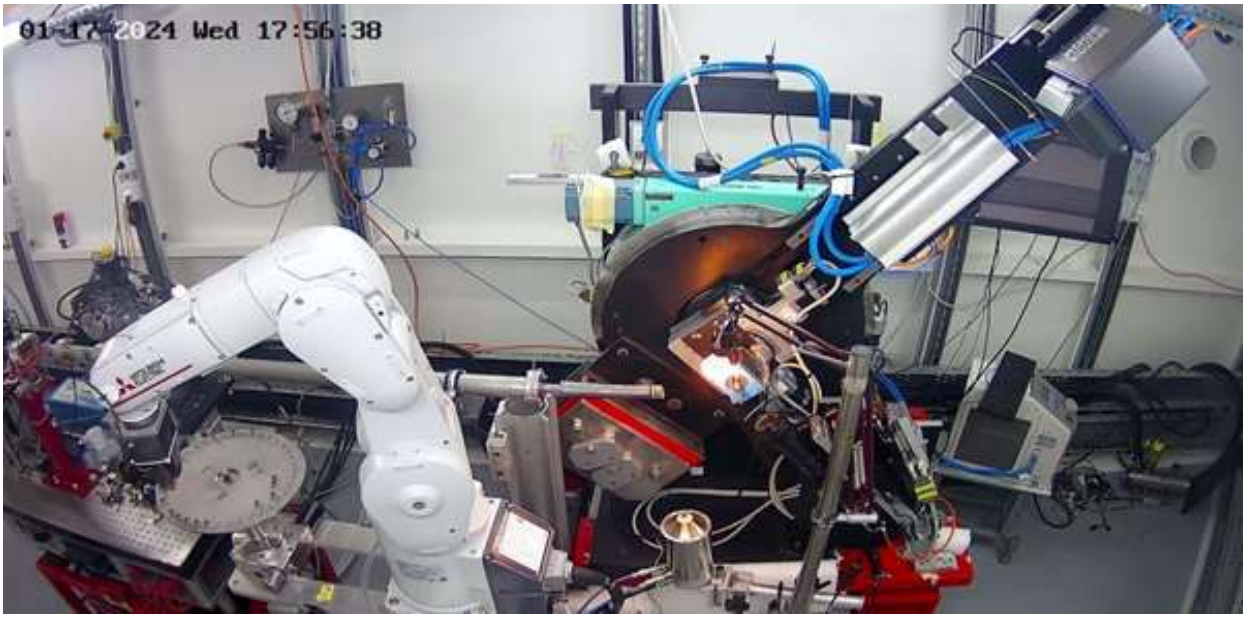

Fig. 1: ID9-MS/XPD Goniometer

ORAL PRESENTATIONS (O)

O-01: Quantum Chemical Characterization and Molecular Docking Analysis of (E)-2-[(4-Chloro-3-nitrophenylimino)methyl]-3-methoxyphenol: A Novel Schiff Base Ligand with Potential Anticancer Activity

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Abstract Schiff bases were first synthesized by the German chemist Hugo Schiff via condensation reactions between primary amines and aldehydes or ketones under azeotropic conditions. The presence of the characteristic imine (–C=N–) linkage plays a crucial role in the structural stability of these compounds. Due to their notable physical, chemical, and biological properties, Schiff bases have attracted considerable scientific attention and have found broad applications in chemistry, biochemistry, materials science, and medicinal research. In this study, the quantum chemical properties of the newly synthesized Schiff base (E)-2-[(4-chloro-3-nitrophenylimino)methyl]-3-methoxyphenol were investigated using Gaussian 03W. The calculated average linear polarizability (α), polarizability anisotropy ($\Delta\alpha$), and first-order hyperpolarizability (β) values indicate that the compound exhibits high polarizability, hyperpolarizability, and structural stability. Frontier molecular orbital analysis, along with donor–acceptor interactions and electrophilic–nucleophilic reactivity assessments, demonstrated strong internal consistency. Additionally, molecular docking simulations were carried out using AutoDock Vina 1.5.6 to explore the binding behavior of the compound with the tyrosine kinase receptor (PDB ID: 1T46). The in silico results revealed stable binding conformations supported by multiple intermolecular interactions. Furthermore, ADME–Tox parameters were evaluated to assess the pharmacokinetic and toxicity profiles, and these findings were found to be consistent with the calculated molecular properties. Overall, the results suggest that the compound is a promising candidate for further optimization and investigation.

Key Words: Schiff base, in silico, quantum chemical calculations

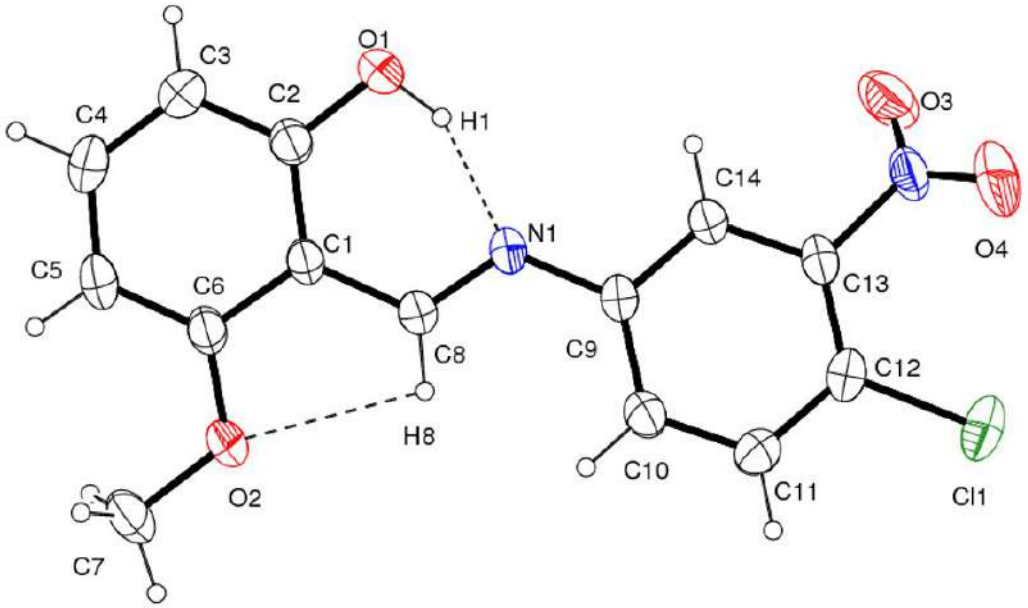

Fig.1: ORTEP3 diagram of the title compound showing thermal ellipsoids at the 30% probability level.

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O-02: Crystal Structure of S-2-Aminophenyl phenylcarbamothioate

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Abstract Organic carbamothioates are a class of compounds that play an important role in the synthesis of pharmaceuticals and agricultural chemicals. As part of our studies in this area, the title compound (Fig. 1) was obtained from the condensation reaction of 2-aminobenzenethiol with isocyanatobenzene. The dihedral angle between the aromatic rings is 83.5 (1)° and the major twist occurs about the C6—S1 bond [C1—C6—S1—C7 = 87.6 (2)°]. The C—S bond distances are comparable with those in related structures [average C—S = 1.778 (6) Å in S-phenyl 4-methoxybenzothioate and 1.7733 (2) Å in ethane-1,2-diyl bis(benzenedithioate)]. The least-squares plane through the S-methyl methylcarbamothioate unit (S1/C7/O1/N2) makes dihedral angles of 88.3 (1) and 6.9 (1)° with the C1–C6 and C8–C13 benzene rings, respectively. In the crystal, N—H—O and N—H—N hydrogen bonds connect the molecules into (001) sheets.

Key Words: Crystal structure, thiol, phenly-carbamothioate

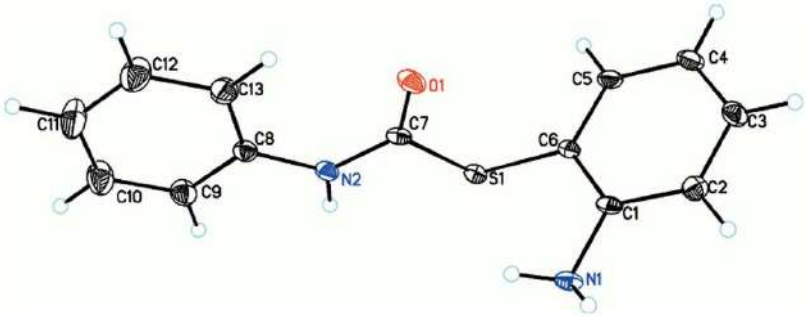

Fig. 1: Molecular Structure of the Compound

Acknowledgements: The title compound was synthesized by Şengül Dilem Doğan, Department of Pharmaceutical Basic Sciences, Faculty of Pharmacy, Erciyes University, Kayseri, 38039, Turkey.

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O-03: A Comparison of Isomeric Schiff Bases Featuring Halogens at Different Contact Points

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Abstract
We examined the structures (E)-2-Bromo-6-[(4-fluorophenylimino)methyl]-4-methylphenol and (E)-2-Bromo-6-[(2-fluorophenylimino)methyl]-4-methylphenol. A comparison of the crystal structures reveals that while both are monoclinic, the first compound crystallizes in the $P2_1/c$ space group, and the second in the $P2_1/n$ space group. Despite their apparent similarity, the fluorine atom's location near the phenol-imine hydrogen bonding motif in the second compound induces a pronounced coplanarity between the benzene rings, with a dihedral angle of only 2.57°. In contrast, the corresponding rings in the first structure adopt a twisted conformation, as evidenced by a much larger dihedral angle of 33.45°. This leads to a displaced stacked π-π interaction in the second structure, with a centroid–centroid distance of 3.622 Å—a feature absent in the first. This packing difference is directly evidenced by Hirshfeld surface analysis, which shows a marked increase in C···C contacts: 9.7% in the π-stacked structure versus 4.6% in the non-stacked analogue. This work examines the impact of a significant shift in the interplanar benzene angle, within a pair of highly similar molecular frameworks, on key electronic and structural properties: intermolecular contact geometries, electron polarization, and electron delocalization.

Key Words: Hirshfeld Surface Analysis, NBO, Schiff Base

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O-04: Transforming PET Bottle Waste into Multifunctional ZnO@MIL-101(Cr) Material via Moss-Mediated Synthesis: Characterization and Antimicrobial Evaluation

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Abstract Polyethylene terephthalate (PET) is widely used in the packaging industry due to its superior physical properties. However, its slow degradation in nature, inadequate waste management, and high consumption levels lead to the accumulation of large quantities of waste, posing a threat to living organisms. A sustainable and cost-effective approach to this problem is to recycle PET waste and convert it into valuable material. Metal-organic frameworks (MOFs) are next-generation adsorbents with a wide range of applications, from environmental remediation to medicine, owing to their crystalline structures, tunable porosity, and high surface areas.

n this study, PET bottle waste was converted into the advanced material MIL-101(Cr) using an environmentally friendly method. ZnO NPs and ZnO@MIL-101(Cr) materials were synthesized using the moss species *Isothecium myosuroides*, identified and collected from unpolluted areas in Giresun. Comprehensive characterization was conducted using FTIR, PXRD, TGA, BET analysis, FESEM, TEM, EDX, and DLS techniques. The antimicrobial activities of the materials were evaluated against Gram-positive bacteria, Gram-negative bacteria, and yeasts. It is anticipated that the environmentally friendly ZnO@MIL-101(Cr) composite will offer new application potentials in materials science, biomedicine, and biotechnology in the future.

Key Words: Upcycling, *Isothecium myosuroides*, green synthesis, MOF, ZnO@MIL-101(Cr), antimicrobial activity

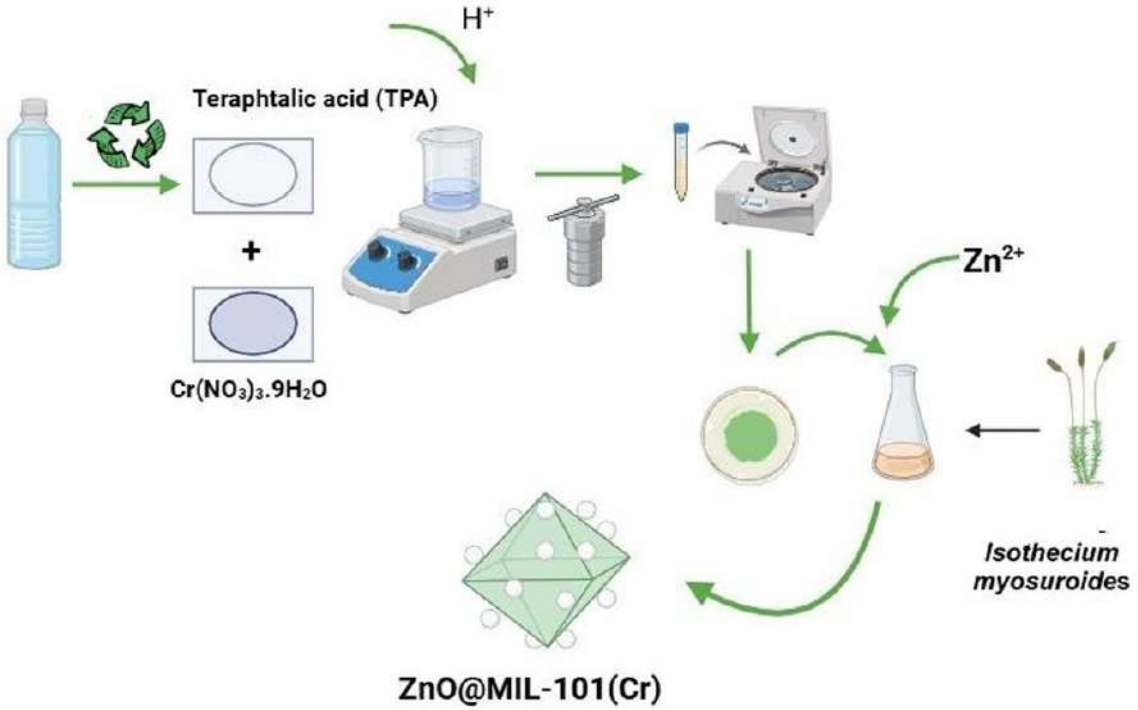

Fig. 1: Representative synthesis of ZnO@MIL-101(Cr) (Created in BioRender.com)

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POSTER PRESENTATIONS (P)

P-01: Synthesis and Spectroscopic Characterization and DFT Study of benzyl 4-([1,1'-biphenyl]-4-yl)-2,6,6-trimethyl-5-oxo-1,4,5,6,7,8hexahydroquinoline-3-carboxylate

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Abstract
Calcium channel blocker compounds act on L-type calcium channels and reducing the influx of extra-cellular calcium ions into the cell. These are divided into three main groups, one of which is 1,4dihydropyridine derivatives. In this study, a new compound bearing the hexahydroquinoline ring analogous to 1,4-dihydropyridine structure was synthesized and its structure proved by instrumental techniques such as mass spectroscopy, 1H NMR, 13C NMR, IR and elemental analysis. In addition to the spectral methods used, X-ray study has been carried out to realize advanced studies on the structure of the mentioned compound. The analyses of single crystal X-ray diffraction show that the title compound crystallized in the monoclinic system with space group $P2_1/n$. Lattice constants are $a = 7.1231(3)$ Å, $b = 30.0033(19)$ Å, $c = 11.8361(7)$ Å, $\beta = 95.698(4)^\circ$, $Z = 4$. Crystallographic studies also show that the molecular structure was stabilized by intramolecular and intermolecular hydrogen bonds. The 1,4-dihydropyridine (1,4-DHP) ring in the structure has a shallow boat conformation. The shallowness of the boat is indicated by the puckering parameters $Q = 0.2759(1)$ Å, $q = 75.73(1)^\circ$ and $\phi_2 = 182.3(1)^\circ$ for the atom sequence N1-C1-C2-C3-C4-C9.

Key Words: Hexahydroquinoline Synthesis, XRD, NMR, DFT

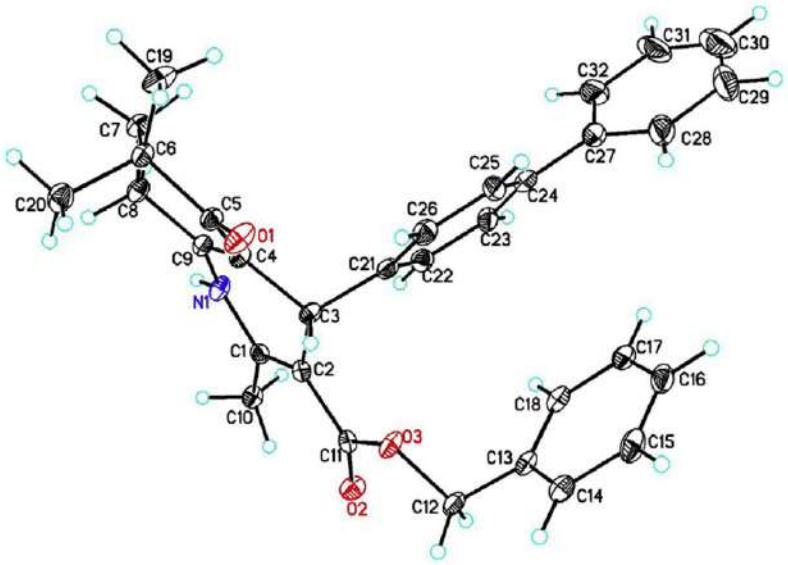

Fig. 1: Molecular Structure of the Compound

Acknowledgements: RJB is grateful for NSF award 1205608 for partial funding of this research, to Howard University Nanoscience Facility to access to liquid nitrogen, and the NSFeMRI program (grant No. CHE0619278) for funds to purchase the X-ray diffractometer.

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P-02: DFT Studies, Synthesis, Biological Activity And Crystal Structure of Tert-Butyl 4-([1,1′-Biphenyl]-4-Yl)-2-Methyl-5-Oxo-1,4,5,6,7,8-Hexahydroquinoline-3-Carboxylate

[1]Rahime Şimşek, [2]Zeki Büyükmumcu, [3]Sema Öztürk Yıldırım*, [4]Gökalp Çetin, [5]Cihat Şafak, [6]Ray J. Butcher

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Abstract

Calcium channel blocker compounds represent a chemically and pharmacologically diverse group of drugs widely used for treating cardiovascular system complications such as hypertension and angina. In this study, a novel compound bearing the hexahydroquinoline ring, obtained by the cyclic condensation of the 1,4-dihydropyridine ring, was synthesized using microwave irradiation, and its structure was proven by IR, 1H-NMR, 13C-NMR, HRMS, and elemental analysis. The antimicrobial activity of the compound has also been tested. The asymmetric unit of the title compound, $C_{29}H_{33}NO_3$, comprises three independent molecules (A, B, and C). Molecule C exhibits disorder in the 6-isopropylcyclohex-2-enone group, with site occupancies of 0.717(4) and 0.283(4) for the major and minor components, respectively. In the crystal, molecules are linked by C—H···O hydrogen bonds, generating [0 0 1] chains incorporating all three asymmetric molecules. The weak N—H···O and C—H···O interactions connect three independent molecules to each other along the c-axis direction. **Key Words:** Hexahydroquinoline, synthesis, crystal structure, DFT, antimicrobial activity

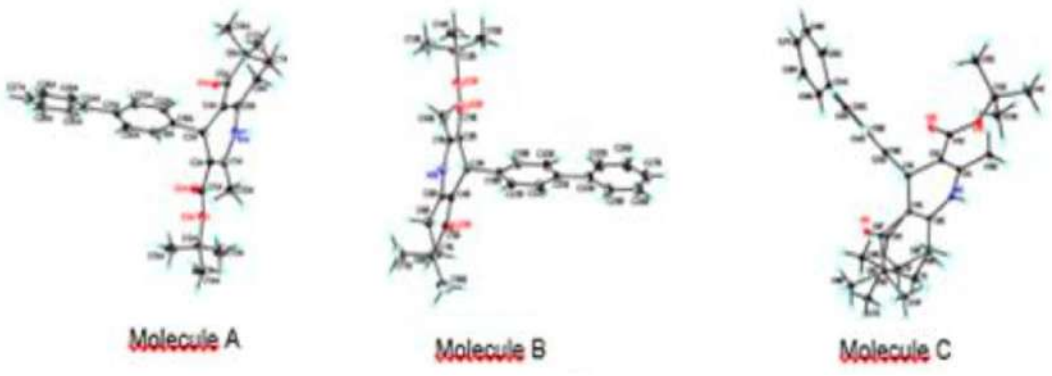

Fig. 1: Molecular Structure of the Title Compound

Acknowledgements: RJB is grateful for funding from NSF (award 1205608) and the Partnership for Reduced Dimensional Materials for partial funding, Howard University Nanoscience Facility for liquid nitrogen access, and the NSF–MRI program (grant No. CHE0619278). This study was supported by the Scientific Research Unit of Hacettepe University (Project no: THD 2017-13452). Antimicrobial screening was funded by the Wellcome Trust (UK) and The University of Queensland (Australia).

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P-03: Synthesis, Structural Characterization and Density Functional Studies of ethyl 4-(biphenyl-4-yl)-2,6,6-trimethyl-5-oxo-1,4,5,6,7,8hexahydroquinoline-3-carboxylate: A non-merohedral Twinned Structure

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Abstract
1,4-Dihydropyridine (1,4-DHP) derivatives are potent calcium channel blockers and antihypertensive agents due to their effect on reducing extracellular Ca^{2+} ion influx on L-type calcium channels. In this study, the biphenyl group was introduced into the 1,4-DHP structure to achieve an active calcium channel blocker compound. The structure was confirmed by IR, ^{1}H NMR, mass spectroscopy, X-ray crystallography, and elemental analysis. Crystallographic analysis revealed that the phenyl rings make dihedral angles of 84.4 (1)° and 87.5 (1)° with the 1,4-dihydropyridine ring. In the crystal, adjacent molecules are linked by N—H···O and C—H···O hydrogen bonds into chains parallel to [010]. The (C4–C9) cyclohexene ring adopts a sofa conformation, while the 1,4-dihydropyridine ring is in a slight boat conformation. The dihedral angle between the two phenyl rings is 40.65°.

Key Words: Structural analysis, Hexahydroquinoline, Non-merohedral twin

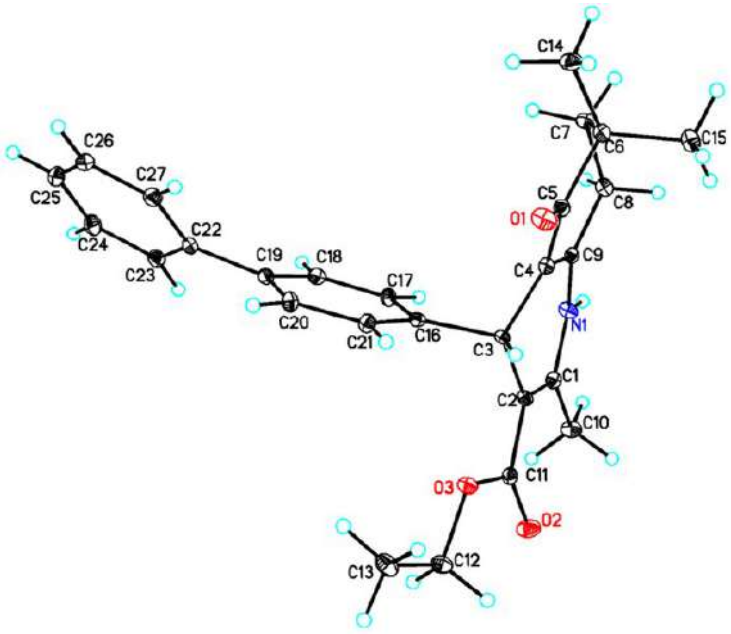

Fig. 1: Molecular Structure of the Title Compound

Acknowledgements: RJB is grateful for funding from NSF (award 1205608) and the Partnership for Reduced Dimensional Materials for partial funding, Howard University Nanoscience Facility for access to liquid nitrogen, and the NSF–MRI program (grant No. CHE0619278).

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P-04: Structural, Catalytic, and Biological Evaluation of a Copper(II) Schiff Base Complex: bis2-ethoxy-6-(E)-[(4-fluorophenyl)imino)methyl]phenolato-κN,κOcopper(II)·1.5H_2O

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Abstract
In this study, the copper complex of a Schiff base, bis2-ethoxy-6-(E)-[(4-fluorophenyl)imino)methyl]phenolato-κN, κOcopper(II)·1.5H2O has been synthesized. Its molecular and crystal structures were investigated using XRD technique, FT-IR, and UV-Vis spectroscopy. The complex crystallizes with two independent asymmetric units, and the Cu(II) ion adopts a seesaw coordination geometry. In the crystal packing, C-H···F, C-F···C and C-H···O interactions construct a 2D network. To investigate the effect of solvent polarity on the electronic transitions, UV–Vis spectra were recorded in dichloromethane (DCM) and ethyl alcohol (EtOH). Absorption bands at 214 nm and 273 nm (DCM) are related to π–π* transitions, while the band at 381 nm corresponds to the ligand-to-metal charge transfer (LMCT) transition. The weak broad band at approximately 650 nm is assigned to the d–d transition. The complex afforded a product yield of 5.06% in the Suzuki-Miyaura cross-coupling reaction. The complex showed notable activity against S. aureus and C. parapsilosis, while antioxidant assays indicated relatively weak antioxidant activity compared to ascorbic acid.

Key Words: Schiff base, copper complex, XRD

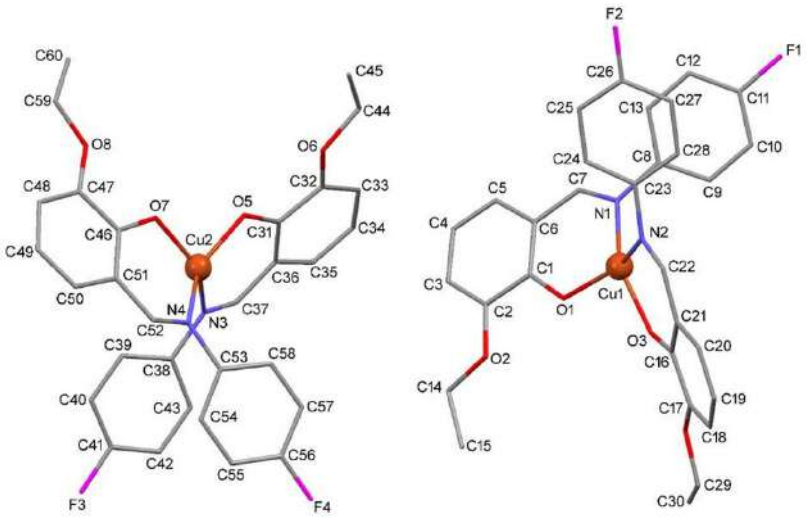

Fig. 1: The molecular structure of bis2-ethoxy-6-(E)-[(4-fluorophenyl)imino)methyl]phenolato-κN,κOcopper(II)

Acknowledgements: This study was supported by Sinop University Scientific Research Coordination Unit. Project Number: FEF-1901-21-006.

P-05: Bis2-ethoxy-6-(E)-[(4-bromophenyl)imino)methyl]phenolato-κN,κOcopper(II)

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Abstract
In this study, a Schiff base ligand containing an ortho-hydroxy group and its copper(II) complex were synthesized and characterized. The ligand was obtained by the condensation reaction of an amine with a salicylaldehyde derivative. The structure of the prepared copper complex was elucidated by single-crystal X-ray diffraction (XRD) analysis. The XRD data provide detailed information about the coordination geometry of the metal ion, the binding mode of the ligand, and important solid-state interactions in the molecular structure (e.g., hydrogen bonds, π-π stacking). The presentation will discuss the obtained crystal structure data together with the spectroscopic characterization results. The development of such metal complexes is important for their potential applications in catalysis, bioinorganic chemistry, and materials science. **Key Words:** X-Ray Diffraction, UV, IR

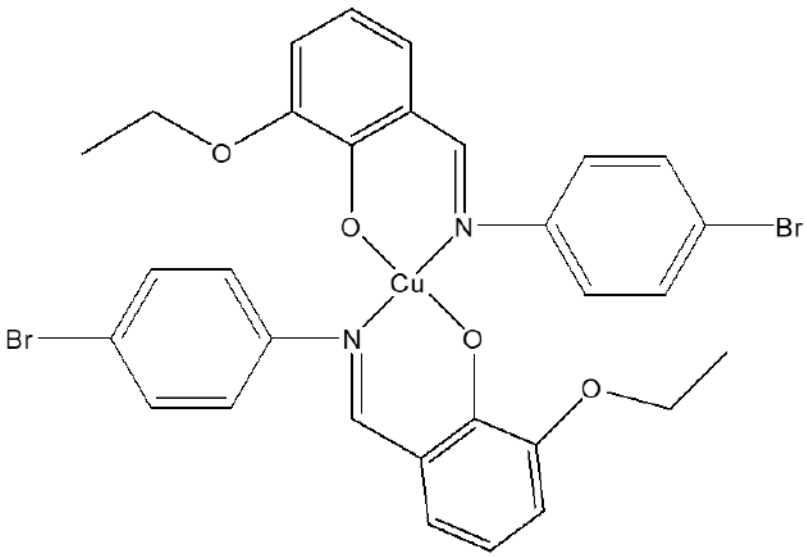

Fig. 1: Bis2-ethoxy-6-(E)-[(4-bromophenyl)imino)methyl]phenolato-κN,κOcopper(II) molekülü açık formülü

Acknowledgements: This study was supported by Sinop University Scientific Research Coordination Unit. Project Number: FEF-1901-21-006.

P-06: Synthesis, Structural, and Spectroscopic Characterization of a Seesaw-Geometry Schiff Base Complex: bis2-ethoxy-6-(E)-[(4-methylphenyl)imino)methyl]phenolato-κN,κO copper(II)monohydrate

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Abstract
In this study, the copper complex of a Schiff base, bis2-ethoxy-6-(E)-[(4-methylphenyl)imino)methyl]phenolato-κN,κOcopper(II)monohydrate has been synthesized. Its molecular and crystal structure have been investigated using X-ray diffraction technique (XRD), FT-IR, and UV-Vis spectroscopy. It was found that the Schiff base behaves as a bidentate ligand, chelating the Cu(II) ion through imine N atom and phenolic O atoms. The coordination polyhedron of the Cu(II) ion exhibits a slightly distorted seesaw geometry. In the crystal packing, aromatic C-H···C interactions form a one-dimensional (1D) structure, which is extended to two dimensions (2D) via C···C interactions. The UV-Vis spectrum in DCM shows bands at 215 nm and 273 nm related to π–π* transitions, a band at 378 nm corresponding to the ligand-to-metal charge transfer (LMCT), and a weak broad band at 650 nm resulting from the d–d transition. The complex exhibited 1.68% catalytic activity in Suzuki-Miyaura cross-coupling reactions with K_2CO_3, and 1.85% with hexamethylenetetramine.

Key Words: Schiff base, copper complex, XRD

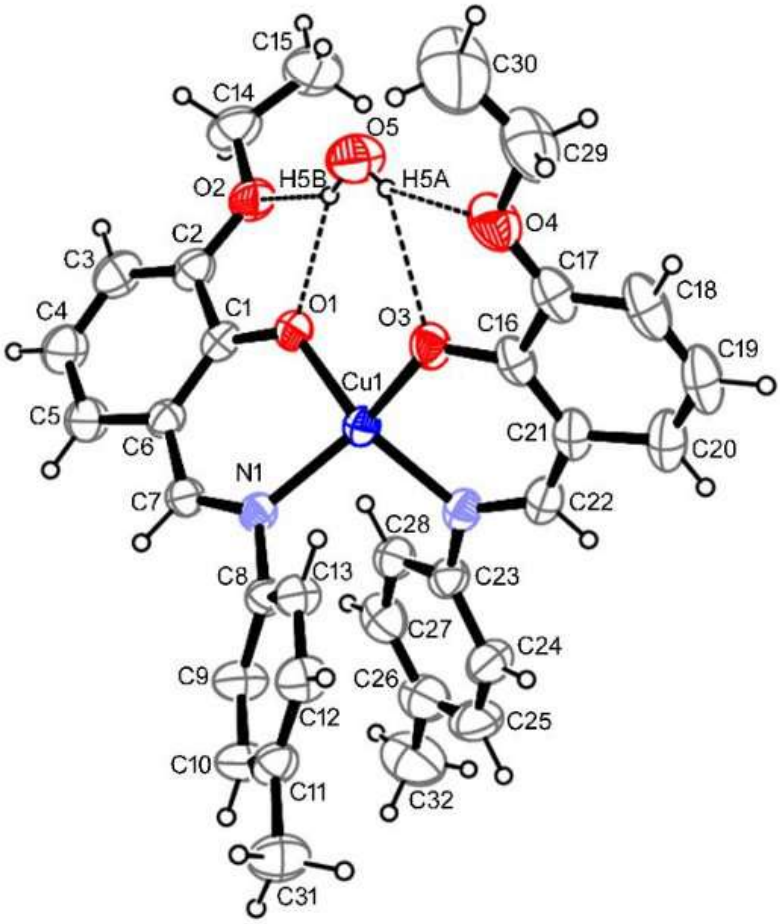

Fig. 1: The molecular structure of bis2-ethoxy-6-(E)-[(4-methylphenyl)imino)methyl]phenolato-κN,κOcopper(II)monohydrate

Acknowledgements: This study was supported by Sinop University Scientific Research Coordination Unit. Project Number: FEF-1901-21-006.

P-07: Substituent-Dependent Crystal Packing in Ortho-Hydroxy Schiff Bases

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Abstract
Two ortho-hydroxy Schiff bases, differing solely by the presence of 6-chloro and 6-methyl substituents on the aniline fragment, were comparatively investigated. Both compounds crystallize in the orthorhombic $P2_12_12_1$ space group, exhibiting a high degree of crystallographic symmetry. Graph-set analysis demonstrates that, in the first structure, one-dimensional chain motifs are generated via Br···Cl halogen–halogen interactions, giving rise to a $C(9)$ graph-set descriptor, whereas in the second structure the chain propagation occurs through Br···H–CH_2 contacts, resulting in a $C(10)$ chain motif. These results indicate that, despite the highly similar packing features of the two structures, the substituent sites that differentiate the molecules play an active role in governing the crystal packing.The atom-resolved fingerprint plots derived from the Hirshfeld surface analysis reveal notable differences between the two structures. The relative contributions of C···H/H···C and H···H contacts are 31.5% in the first molecule (23.8% in the second). In addition, atom-specific contributions involving chlorine, observed only in the second molecule, amount to Cl···H/H···Cl (6.9%) and Br···Cl/Cl···Br (5.9%). These quantitative variations are in good agreement with the graph-set analysis, further supporting the role of substituent-dependent intermolecular interactions in determining the crystal packing. In this study, comparative MEP, NBO, and molecular docking analyses were performed for these structurally similar molecules in order to investigate how this substitution, which does not alter the overall packing motif, influences the nature and strength of intermolecular interactions at the molecular level.

Key Words: Schiff bases, crystal packing, halogen bonding

P-08: DFT and Molecular Docking Evaluation of a Novel Schiff Base (E)-2-(4-((2,4-dimethoxybenzylidene)amino)phenyl)ethan-1-ol: From Electronic Structure to Biological Interaction

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Abstract Schiff bases, characterized by the presence of the azomethine group, have garnered significant attention due to their broad spectrum of applications ranging from biological activities to various industrial sectors. In this context, the structural and biological properties of a novel Schiff base (E)-2-(4-((2,4-dimethoxybenzylidene)amino)phenyl)ethan-1-ol were investigated in detail using both experimental and theoretical methods. To elucidate the molecular structure of the compound, experimental NMR spectra were recorded and compared with calculated theoretical values. The Molecular Electrostatic Potential (MEP) map was generated to identify the reactive sites of the molecule. Additionally, Frontier Molecular Orbitals (HOMO-LUMO) were analyzed to determine its chemical stability and reactivity. Theoretical calculations were performed using the DFT/B3LYP method with the 6-311++G(d,p) basis set. Finally, the biological activity of the compound was evaluated against the acetylcholinesterase (AChE) enzyme through molecular docking simulations.

Key Words: Schiff bases, DFT, Molecular Docking

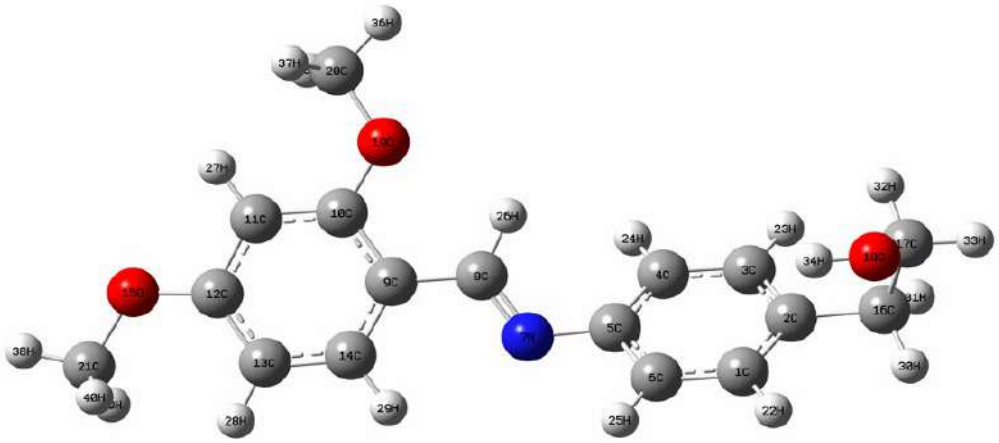

Fig. 1: Optimized geometry of the molecule obtained using the B3LYP/6-311++G(d,p) basis set.

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P-09: Crystal and molecular structure of N-(3,5-diphenyl-4H-1,2,4-triazole-4-yl)thiophene-2-carboxamide

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Abstract

The title compound was synthesized by the reaction of 3,5-diphenyl-4H-1,2,4-triazole-4-amine with 2-thiophenecarbonyl chloride according to the literature method, and crystallized from ethanol. Single crystal X-ray diffraction data showed that the compound crystallizes in the monoclinic crystal system with a space group of $P2_1/n$. The asymmetric unit of the molecule contains a hydrogen-bonded dimer of the molecules. Both phenyl groups, and the five-membered 1,2,4-triazole and thiophene rings are essentially planar. However, the orientation of these rings with each other are significantly different in the two molecules. The dihedral angles between two phenyl rings, and two phenyl rings with the triazole ring are 22.99°, 21.19° and 41.16°, respectively, in molecule A, while 68.48°, 34.49° and 36.90°, respectively in molecule B. The bond distances and bond angles of the triazole moiety are typical for the reported data of 3,5-diphenyl-4H-1,2,4-triazol-4-amine. The molecules in the crystalline state are connected by a number of strong N–H···N and N–H···O hydrogen bonds, forming a two-dimensional planar arrangement in the bc plane. Additionally, π–π stacking interactions are present between the phenyl rings (3.874 Å) and the thiophene rings (3.942 Å)

Key Words: 1,2,4-Triazole, Crystal structure, Molecular structure

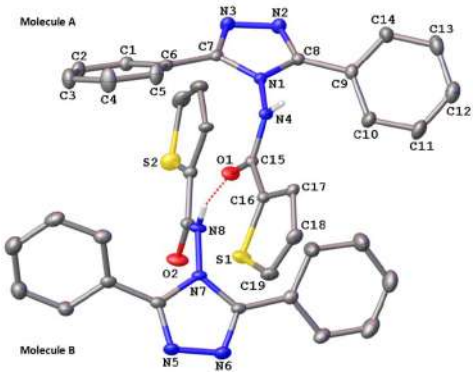

Fig. 1: Molecular structure of N-(3,5-diphenyl-4H-1,2,4-triazole-4-yl)thiophene-2-carboxamide.

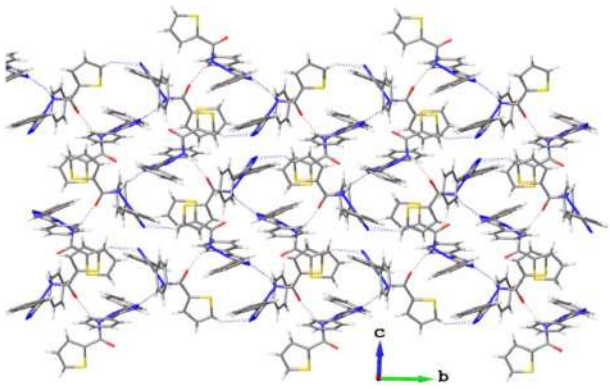

Fig. 2: Two-dimensional packing of molecules viewed down b.

References

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P-10: Crystal and molecular structure of N-(3,5-di-p-tolyl-4H-1,2,4-triazol-4-yl)thiophene-2-carboxamide

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Abstract

The compound was synthesized by the reaction of 3,5-di-p-tolyl-4H-1,2,4-triazol-4-amine with 2-thiophenecarbonyl chloride, and obtained as colourless crystals after crystallization from ethanol. Single crystal X-ray crystallography measurements indicated that the compound crystallizes in the orthorhombic crystal system with a space group of $Pna2_1$. The unit cell contains four molecules of the compound. The 1,2,4-triazole-4-amine group is bonded to two p-tolyl groups and a 2-thiophenecarbonyl group. The phenyl groups, the five-membered 1,2,4-triazole and thiophene rings are planar. The dihedral angles between these rings are similar to those of 3,5-diphenyl-4H-1,2,4-triazole-4-amine. In addition, the dihedral angle between the thiophene and 1,2,4-triazole rings is 69.77°.In the solid-state, the molecules of the compound are linked by strong N–H···N hydrogen bonds to create a one-dimensional linear chain running along the c axis. Interestingly, no π-π stacking interaction is present within the crystal structure, but a number of weak C–H···N, C–H···O and C–H···S hydrogen bonds further reinforce the crystal packing in a three-dimensional network.

Key Words: 1,2,4-Triazole derivative, Crystal structure, Molecular structure

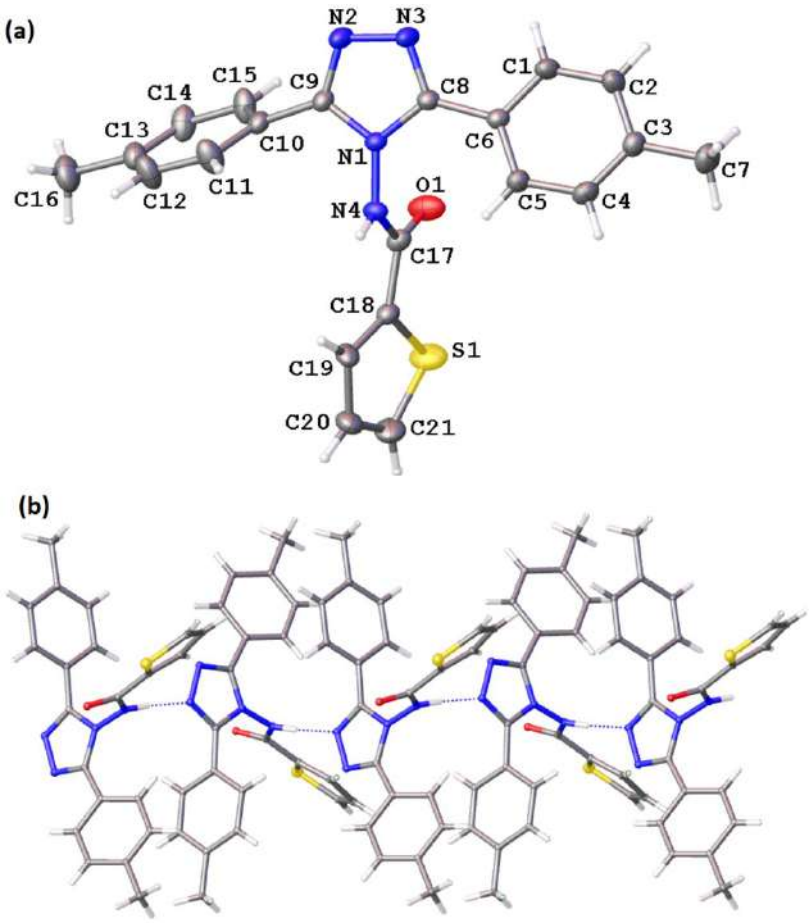

Fig. 1: (a) Molecular structure of N-(3,5-diphenyl-4H-1,2,4-triazole-4-yl)thiophene-2-carboxamide, and (b) one-dimensional hydrogen-bonded chains of the molecules running along the axis c.

References

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P-11: Crystal and molecular structure of a new binuclear silver(I) complex with bridging chlorido and 1,4-bis(diphenylphosphino)butane ligands

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Abstract

The crystal and molecular structure of $[Ag_2(\mu\text{-}Cl)_2(\mu\text{-dppb})_2]$ (dppb = 1,4-bis(diphenylphosphino)butane) was determined using single crystal X-ray crystallography. The silver(I) complex crystallizes in the monoclinic space group $P2_1/c$, and its asymmetric unit consists of a half of the molecule. The complex has a binuclear structure, in which the two silver(I) ions are doubly bridged by two dppb and two chloride ligands. Each silver ion is coordinated by two P and two Cl atoms in a distorted $AgCl_2P_2$ tetrahedral environment. The bridging of two silver(I) ions by two dppb ligands forms a 14-membered nonplanar metalloring of $Ag_2P_4C_8$. The Ag and P atoms are approximately coplanar, but the chloride ligands are located on either side of the plane. The chlorido-bridged Ag_2Cl_2 moiety forms a slightly distorted square with a Cl1–Ag1–Cl1^i bond angle of 91.30(11)°. In the solid state, the molecules are connected by relatively weak C–H···Cl intermolecular interactions to create a two-dimensional arrangement running through the bc plane.

Key Words: Binuclear silver(I) complex, Bridging chloride ligand, 1,4-bis(diphenylphosphino)butane

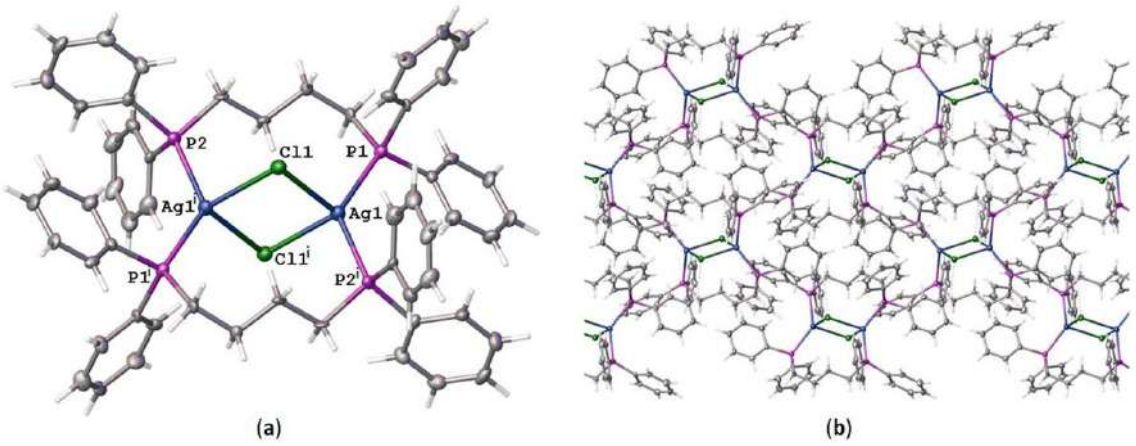

Fig. 1: (a) Molecular structure of $[Ag_2(\mu\text{-}Cl)_2(\mu\text{-dppb})_2]$, and (b) crystal packing of the molecules connected through C–H···Cl interactions viewed down the axis a.

Acknowledgement: I am thankful to Prof. Dr. M. Aygün for data collection and refinement.

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P-12: Electronic Structure Engineering of Pentagraphene via Site-Selective B and N Substitution: A First-Principles Study

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Abstract
Pentagraphene is a theoretically proposed two-dimensional carbon allotrope with a tetragonal lattice, composed of both sp^2- and sp^3-hybridized carbon atoms. The primitive unit cell contains six carbon atoms and is characterized by a lattice parameter of approximately 3.64 Å. This unique structural configuration gives rise to distinct electronic properties compared to graphene.In this work, we investigate the effect of site-selective boron (B) and nitrogen (N) substitution on the electronic structure of pentagraphene using density functional theory (DFT). A 3×3 supercell is constructed to model dilute doping conditions, allowing substitution at both sp^2- and sp^3-like carbon sites. This approach enables a direct comparison of how local hybridization environments influence the electronic response to doping. Band structure and projected density of states (PDOS) analyses reveal that the band gap can be tuned depending on the dopant species and its position within the lattice. In some configurations, impurity states emerge within the band gap, indicating potential applications in nanoelectronic and optoelectronic devices. These findings highlight the importance of hybridization-dependent doping strategies for tailoring the electronic properties of pentagraphene and provide valuable insight into the design of functional two-dimensional materials.

Key Words: Pentagraphene, Site-Selective Doping, sp^2–sp^3 Hybridization, B/N Substitution

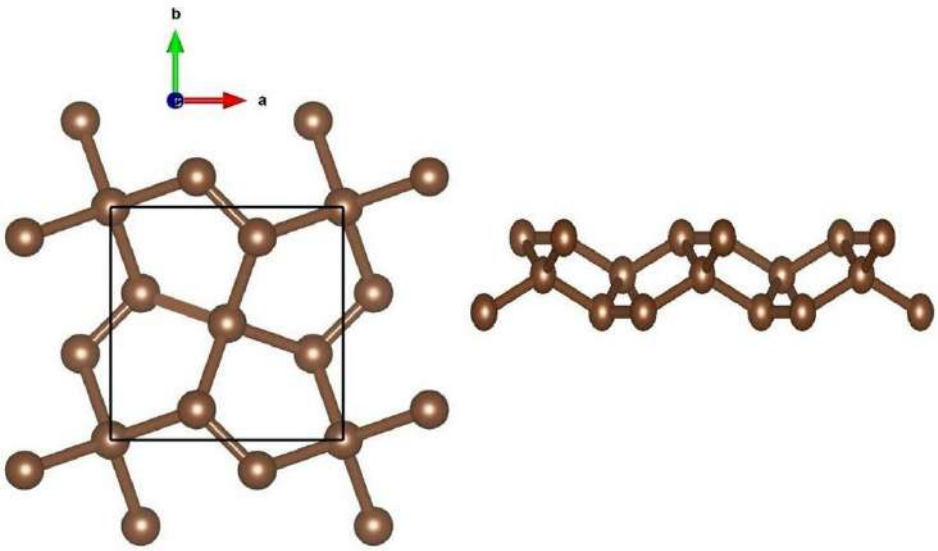

Fig. 1: Top (left) and side (right) views of the pentagraphene 1×1 unit cell. The top view illustrates the tetragonal lattice and the defined primitive cell, whereas the side view reveals the buckled geometry associated with the mixed sp^2–sp^3 hybridization of carbon atoms.

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Acknowledgements: Bu araştırmada yer alan tüm nümerik hesaplamalar TÜBİTAK ULAKBİM, Yüksek Başarım ve Grid Hesaplama Merkezi'nde (TRUBA kaynaklarında) gerçekleştirilmiştir.

P-13: Ti_2BN Monolayer as a Novel MBene: A First-Principles Study of Stability and Electronic Structure

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Abstract
Two-dimensional transition metal–based materials, including MXenes and their boron-containing analogues (MBenes)[1,2], have attracted increasing attention due to their versatile properties. In this study, the structural and electronic properties of the Ti_2BN monolayer are investigated using first-principles calculations within Density Functional Theory. Two different pseudopotential schemes (rrkj ultrasoft and kjpaw) are employed for validation, and on-site Coulomb interactions are included via a self-consistently determined Hubbard U parameter for Ti-d states. Phonon dispersion calculations confirm the dynamical stability of the structure through the absence of imaginary frequencies. Electronic structure calculations reveal that Ti_2BN is an indirect band gap semiconductor with a narrow band gap. The valence band maximum and conduction band minimum occur at different k-points, indicating indirect electronic transitions. Projected density of states analysis shows that Ti-d orbitals dominate near the band edges, with noticeable hybridization with B and N p states, suggesting mixed bonding characteristics. These results demonstrate that Ti_2BN is a dynamically stable MBene with semiconducting behavior, highlighting its potential for applications in nanoelectronics and optoelectronic devices.

Key Words: MBene, Density Functional Theory, 2D materials, phonon stability, electronic structure

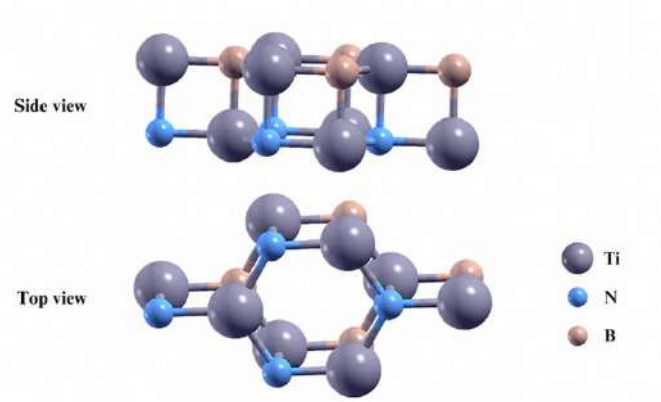

Fig. 1: Side and top views of the optimized Ti_2BN monolayer structure. Ti, N, and B atoms are shown in gray, blue, and light brown, respectively, illustrating the layered atomic arrangement.

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Acknowledgements: Bu araştırmada yer alan tüm nümerik hesaplamalar TÜBİTAK ULAKBİM, Yüksek Başarım ve Grid Hesaplama Merkezi'nde (TRUBA kaynaklarında) gerçekleştirilmiştir.

P-14: Detailed examination of 4-[(4-Ethyl-5-phenyl-4H-1,2,4-triazol-3-yl)sulfanyl]phthalonitrile crystal packing, Hirshfeld surface analysis, and 2D fingerprint map

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Abstract

In this study, the crystal packing and intermolecular interactions of 4-[(4-ethyl-5-phenyl-4H-1,2,4-triazol-3-yl)sulfanyl] phthalonitrile (EtPh-Tz-SPN), whose structure was previously determined by single-crystal X-ray diffraction (XRD), were investigated in detail using Hirshfeld surface analysis and two-dimensional fingerprint plots. The analyses were carried out using CrystalExplorer software, and the .cif (crystallographic information file) of the compound was directly used as the input file. The results indicate that the crystal structure is mainly stabilized by weak C–H···N hydrogen bonds and van der Waals (vdW) interactions. Fingerprint analyses revealed that N···H (34.6%), H···H (27.6%), and C···H (16.4%) interactions are dominant. The obtained findings are consistent with similar triazole derivatives reported in the literature.

Key Words: Hirshfeld, Fingerprint, 1,2,4-triazole, phthalonitrile

P-15: Investigation of the Crystal Structure of a 4,5-Dicyanobenzene Derivative via Hirshfeld Surface Analysis and Energy Frameworks Method

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Abstract

In this study, the intermolecular environment and crystal packing of 4,5-Dicyano-1,2-bis(2-dimethylaminoethy lsulfanyl)benzene ($C16H22N_4S_2$) were comprehensively investigated using modern computational methods. The Hirshfeld Surface Area of the data, which was originally synthesized and its XRD data were reported by U. Çoruh et al. in 2003, has been studied. The title compound crystallizes in the orthorhombic system. Its molecular structure features a dicyanobenzene ring and two 2-dimethylaminoethylsulfanyl substituents that exhibit a twist conformation.Intermolecular interactions were visualized and quantified using CrystalExplorer software. The Hirshfeld surfaces were mapped over d_{norm}, curvedness, and shape index to identify the contact regions. Quantitative analysis of the 2D fingerprint plots revealed that the crystal packing is dominated by H···H (40.0%), N···H/H···N (29.2%), and C···H/H···C (18.3%) interactions, which are the primary contributors to the total Hirshfeld surface area. The contacts, appearing as characteristic spikes, correspond to hydrogen bonds, while secondary stabilization is provided by other weak forces. Minor contributions from S···H (8.6%) and S···C (3.5%) contacts were also identified. Furthermore, crystal voids and energy frameworks were calculated to evaluate the packing efficiency and lattice energy. The hydrogen bonding network and ORTEP displacement ellipsoid visualizations were generated using the Olex2 program to complement the structural analysis. This research provides a detailed computational re-evaluation of the synergy of multiple weak intermolecular forces that maintain the crystal stability of this phthalonitrile derivative.

Key Words: Hirshfeld Surface, Fingerprint Plots, CrystalExplorer, Phthalonitrile, Crystal Structure, Energy Frames

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P-16: Charge Mobility Analysis of Phenanthroline Derivatives via Density Functional Theory: Role of Reorganization Energy and Charge Transfer Integrals

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Abstract Molecular packing and noncovalent interactions strongly affect charge transport in organic electronic devices such as OLEDs, OPVs, and OFETs. In this study, the electronic properties of phenanthroline derivatives were investigated using density functional theory (DFT) and Marcus charge transfer theory. The calculated electron mobilities for molecules 1 and 2 were 21.13 and 18.00 $cm^2\ V^{-1}\ s^{-1}$, respectively, mainly due to strong J-type $\pi \cdots \pi$ stacking interactions with short intermolecular distances. Both compounds exhibited lower electron reorganization energies than hole reorganization energies, indicating n-type semiconductor behavior. Charge transfer integrals showed a strong dependence on intermolecular stacking distance, where high transfer integrals and low reorganization energies resulted in enhanced charge mobility. In addition, band gap, ionization potential, and charge injection barriers were analyzed, revealing low LUMO energies and small electron injection barriers. Overall, both molecules appear to be promising n-type organic semiconductors with high charge mobility.

Key Words: DFT, charge mobility, reorganization energy

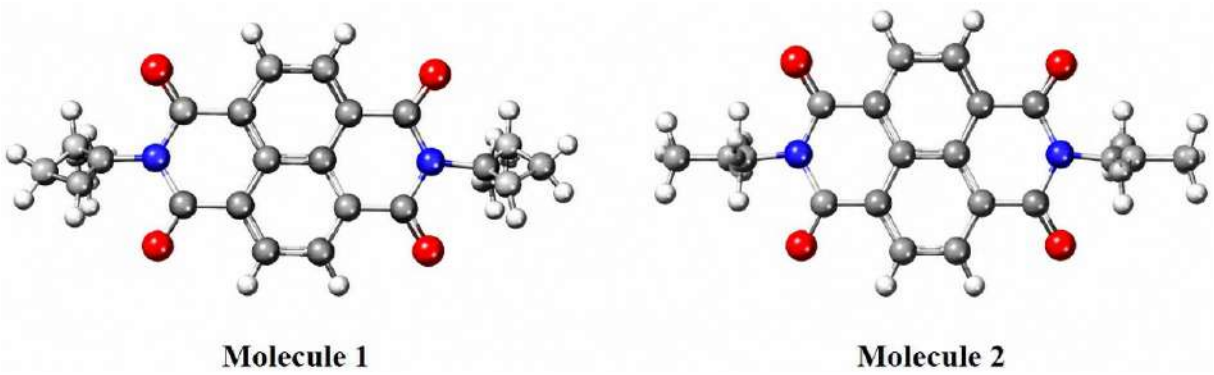

Fig. 1: The optimized geometry of the studied molecules.

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P-17: Crystal Structure and Hirshfeld Surface Analyses of some PEPPSI Type Pd(II)NHC Complexes

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Abstract N-heterocyclic carbene (NHC) complexes are well established in organometallic chemistry. In particular, palladium–NHC complexes, especially PEPPSI-type derivatives, are widely used in cross-coupling catalysis and have recently attracted attention in medicinal chemistry. In this study, three new PEPPSI-type (NHC)$PdBr_2$(Py) complexes were examined. The single crystals of the complexes were elucidated using the XRD method. Analysis confirmed a slightly distorted square planar geometry around the Pd(II) center. C–H$\cdots$O and C–H$\cdots$Br type weak hydrogen bonds, as well as C–H$\cdots\pi$ and $\pi\cdots\pi$ stacking interactions observed in the crystal structures, were also investigated using Hirshfeld Surface Analysis.

Key Words: NHC, XRD, Hirshfeld Surface Analysis

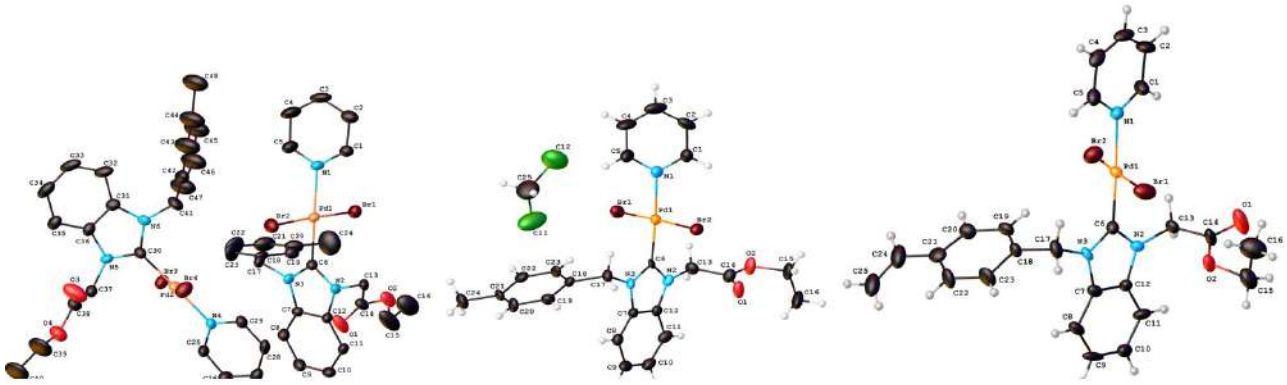

Fig. 1: Molecular structures of PEPPSI-Pd-NHC complexes in this study.

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