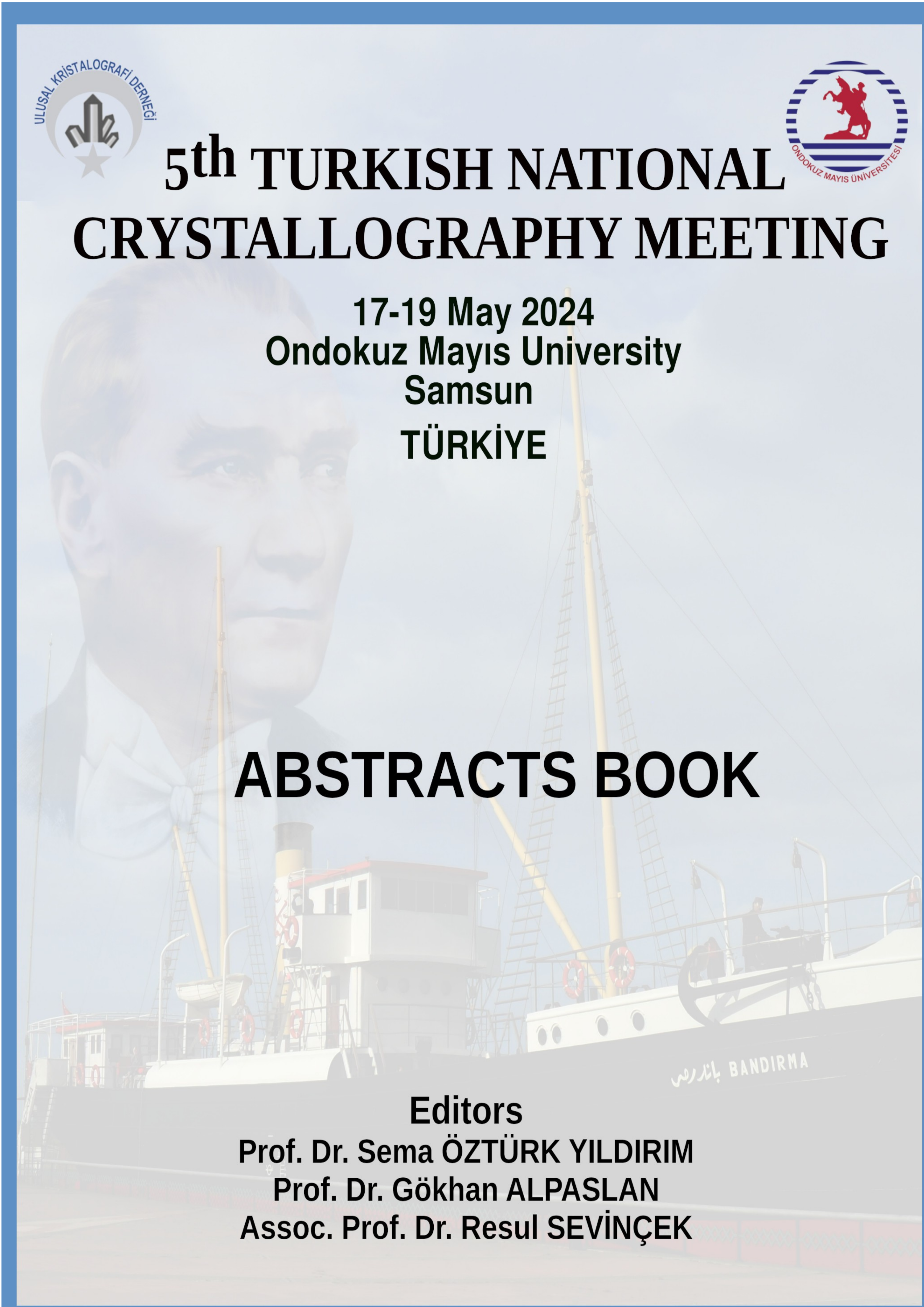


5th TURKISH NATIONAL CRYSTALLOGRAPHY MEETING

17-19 May 2024
Ondokuz Mayıs University
Samsun

TÜRKİYE

ABSTRACTS BOOK

Editors
Prof. Dr. Sema ÖZTÜRK YILDIRIM
Prof. Dr. Gökhan ALPASLAN
Assoc. Prof. Dr. Resul SEVİNÇEK

Organising Committee

Canan Kazak (President-Ondokuz Mayıs University)

Emine Berrin Poyraz (Ondokuz Mayıs University)

Gamze Turan (Ondokuz Mayıs University)

Onur Rauf Yılmaz (Sinop University)

Onur Şahin (Sinop University)

Sefa Akkoyunlu (Ondokuz Mayıs University)

Ufuk Çoruh (Ondokuz Mayıs University)

Scientific Committee

Preface

Dear colleagues,

On behalf of the Board of Directors of the National Crystallography Association, we would like to invite you to attend the 5th National Crystallography Conference to be hosted by Ondokuz Mayıs University in a face-to-face format.

The 5th National Crystallography Conference is organized by the National Crystallography Association. The association was established in 2001 within Hacettepe University in Ankara, Turkey. The aim of our association is to organize members' professional, cultural, and social activities, support education in the field of crystallography, contribute to the understanding, development, and dissemination of crystallography in Turkey, and participate in scientific activities and publications in this field. Our association is a member of the European Crystallographic Association (ECA).

During the conference, besides presentations from internationally recognized invited speakers, there will also be oral and poster presentations by participants.

We look forward to your participation in the 5th National Crystallography Conference, which will take place face-to-face from May 17th to 19th, 2024.

With respect and warm regards..

Prof. Dr. Canan Kazak
NCA Chairperson of the Board

YEŞİLYURT DEMİR ÇELİK

ULUSOYUN

Medi TRAVEL

USLU DEMİR & ÇELİK

Özön

NanoSpek
www.nanospek.com.tr

YAŞAR GROUP

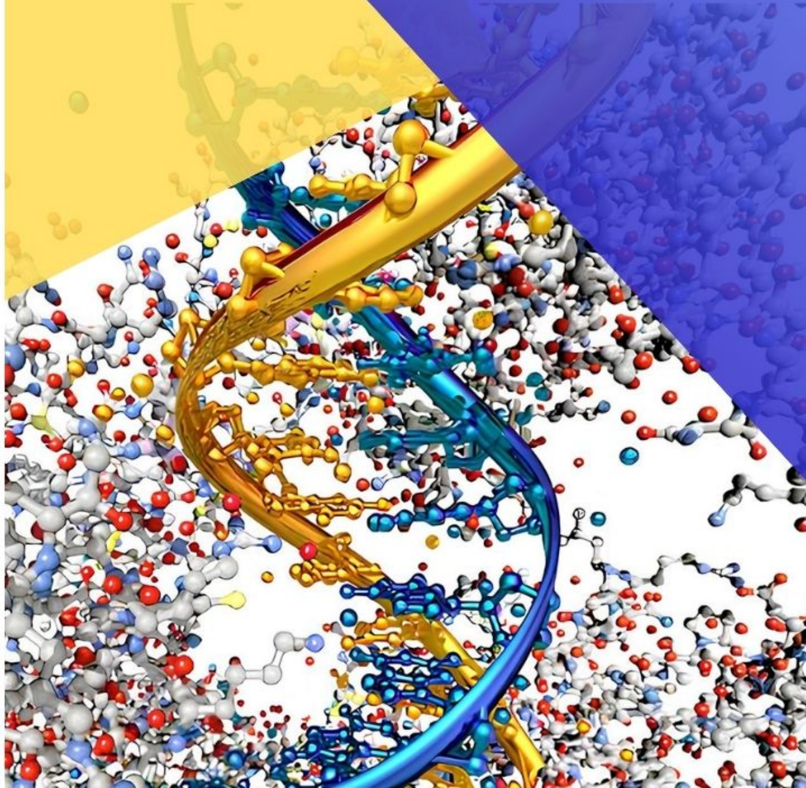
Ondokuz Mayıs Üniversitesi Kadın Girişimcilik Topluluğu

Thank you for your contributions.

www.omu.edu.tr
https://ukd.org.tr/tucr2024/
tucr.contact@gmail.com
@ulusalkristalografidernegi

5TH TURKISH NATIONAL CRYSTALLOGRAPHY MEETING

17-19 May 2024
Ondokuz Mayıs University
OMTEL Hotel
Samsun/Türkiye



INVITED SPEAKERS

Prof. Dr. Michael Richard Probert
(Newcastle University, England)

Dr. Narcis Duteanu
(Polytechnic University of Timisoara, Romania)

Prof. Dr. Peter Müller
(Massachusetts Institute of Technology, USA)

Prof. Dr. Rahime Şimşek
(Hacettepe University, Türkiye)

Prof. Dr. Santiago Garcia-Granda
(University Oviedo, Spain)

Prof. Dr. Wan Haliza Binti Abd Majit
(University of Malaya-Malaysia)

HONOR BOARD

- Prof. Dr. Yavuz Ünal (Rector- Ondokuz Mayıs University)
- Prof. Dr. Ahmet Erdönmez
- Prof. Dr. Dinçer Ülkü
- Prof. Dr. Mehmet Akkurt
- Prof. Dr. Orhan Büyükgüngör
- Prof. Dr. Rahmi Yağbasan
- Prof. Dr. Süheyla Özbey

ORGANIZING BOARD

- Prof Dr.Canan Kazak (Chairperson-Ondokuz Mayıs University)
- Research Ass. Emine Berrin Poyraz (Ondokuz Mayıs University)
- Prof. Dr. Nurdan Gamze Turan (Ondokuz Mayıs University)
- Research Ass. Onur Rauf Yılmaz (Sinop University)
- Prof. Dr. Onur Şahin (Sinop University)
- Sefa Akkoyunlu (Ondokuz Mayıs University)
- Prof. Dr. Ufuk Çoruh (Ondokuz Mayıs University)

SCIENCE BOARD

- Prof. Dr. Sema Öztürk Yıldırım (Chairperson-Erciyes University)
- Prof. Dr. Ayhan Elmalı (Ankara University)
- Prof. Dr. Betül Kaynak (Hacettepe University)
- Prof. Dr. Bilal Güneş (Gazi University)
- Prof. Dr. Çiğdem Yüksektepe Ataol (Çankırı Karatekin University)
- Prof. Dr. Gökhan Alpaslan (Giresun University)
- Prof. Dr. Hüseyin Ünver (Ankara University)
- Prof. Dr. Leyla Tatar (Hacettepe University)
- Prof. Dr. Metin Kul (Eskişehir Teknik University)
- Assoc. Dr. Muhittin Aygün (Dokuz Eylül University)
- Prof. Dr. Musa Sarı (Gazi University)
- Prof. Dr. Ömer Çelik (University of Malaya, Malasyia)
- Assoc. Dr. Resul Sevinçek (Dokuz Eylül University)

Friday, 17 May, 2024

10.00 - 12.00

Registration–Welcome–Music Concert
Opening Ceremony
Congress Opening Speeches

Prof. Dr. Canan KAZAK
Chair of the Turkish National Crystallographic Association

P

MUSIC CONCERT & VISIT TO THE STANDS & LUNCH

13.30- 14.15

SESSION I

INVITED SPEAKER

CHAIRS: Prof. Dr. Süheyla ÖZBEY & Prof. Dr. Ahmet ERDÖNMEZ

Prof. Dr. Santiago Garcia-Granda (University Oviedo, Spain)
“Design of processable polymeric carbon nitride for photo(electro) catalytic applications”

COFFEE BREAK & POSTER SESSION (14.15 - 15.15)

15.15 - 16.00

SESSION II

INVITED SPEAKER

CHAIRS: Prof. Dr. Nurdan Gamze TURAN &
Prof. Dr. Leyla YILDIRIM

Prof. Dr. Rahime ŞİMŞEK (Hacettepe University, Türkiye)
‘‘Hexahydroquinoline Derivatives as Potential Inflamatory Mediators Inhibitors’’

COFFEE BREAK & POSTER SESSION (16.00 - 16.15)

16.15 - 17.00

SESSION III

INVITED SPEAKER

CHAIRS: Prof. Dr. Ufuk ÇORUH & Prof. Dr. Sema ÖZTÜRK YILDIRIM

Wan Haliza Binti Abd Majit (University of Malaya-Malaysia)
"Optical properties of ZnO nanoparticles and thin film for OLED and sensors"

SOCIAL EVENTS (17.00 - 22.00)
SAMSUN BANDIRMA FERRY MUSEUM TRIP CITY TOUR

Saturday, 18 May, 2024

9.30 - 11.30

SESSION IV

INVITED SPEAKER

CHAIRS: Doç. Dr. Muhittin AYGÜN & Doç. Dr. Resul SEVİNÇEK

Prof. Dr. Peter MULLER (Massachusetts Institute of Technology, USA)
“Refining Disorders in Single-Crystal X-Ray Diffraction – Using Restraints the Right Way” & Workshop SHELXL Refining Disorder with SHELXL – Concepts and Examples

COFFEE BREAK & POSTER SESSION (11.30 - 11.45)

SCIENTIFIC PROGRAM – ORAL PRESENTATIONS

CHAIRS: Prof. Dr. Metin KUL & Prof. Dr. Gökhan ALPASLAN

11.45 - 12.00 (OP-1)
Burak Veli Kabasakal
Structural insights into nitrogenase complexes against oxygen damage

12.15 - 12.30 (OP-2)
Merve İzmirli, Gül Yakalı, Resul Sevinçek, Duygu Barut Celepci, Erkan Fırıncı, Rukiye Fırıncı, Muhittin Aygün
Structural Analysis and Biological Activity Predictions of Some Organometallic Compounds

12.30 - 12.45 (OP-3)
Nadihan Yolgeçti, Sema Öztürk Yıldırım, Mehmet Akkurt, Gökalp Çetin, Rahime Şimşek, Cihat Şafak, Ray J. Butcher, Ajaya Bhattarai
Tert-butyl 4-([1,1′-biphenyl]-4-yl)-2,6,6-trimethyl-5-oxo-1,4,5,6,7,8-hexa hydro quinoline-3-carboxylate Synthesis, Single Crystal X-Ray Diffraction and Density Functional Modeling Studies

12.45 - 13.00 (OP-4)
Emre Yörük, Ashwin Suresh, Petr Brázda, Małgorzata Katarzyna Cabaj, Lukáš Palatinus
Investigation of bonding in crystals using 3D electron diffraction

VISIT TO THE STANDS & LUNCH (13.00 - 13.45)

13.45 - 15.30

SESSION V

INVITED SPEAKER

CHAIRS: Prof. Dr. Orhan BÜYÜKGÜNGÖR &
Prof. Dr. Onur ŞAHİN

13.45- 14.30
Prof. Dr. Michael Richard PROBERT (Newcastle University, England)
“Beyond standard laboratory diffraction experiments”

SCIENTIFIC PROGRAM – ORAL PRESENTATIONS

CHAIRS: Prof. Dr. Yelda BİNGÖL ALPASLAN

14.30- 14.45 (OP-5)
Hanifi Özşanlı, Okan Şimşek, Onur Rauf Yılmaz, Ceren Çiçek, Erbil Ağar, Ufuk Çoruh, Ezequiel M. Vazquez-Lopez
Synthesıs, Crystal Structure, Hırshfeld Surface Analysıs, Supramolecular And Computatıonal Investıgatıon Of Compound (E)-4-Methoxy-2-(((2-Methoxy-5-(Trifluoromethyl) Phenyl)Imino) Methyl)Phenol

14.45- 15.00 (OP-6)
Onur Rauf Yılmaz, Çiğdem Albayrak Kaştaş, Canan Kazak
Comparison Of Geometrical Properties Of (E)-2-Bromo-4-Methyl-6-[(2,6-Dimethyl-Phenylimino)Methyl]Phenol And (E)-2-Bromo-4-Methyl-6-[(3,4-Dimethyl-Phenylimino)Methyl]Phenol Compounds By XRD And Hirshfeld Analysis

15.00- 15.15 (OP-7)
Güneş Süheyla Kürkçüoğlu, Seray Kekeç, Dursun Karaağaç, Onur Şahin
Crystallographic Investigation of Heteronuclear Hexacyanometalate(III) Coordination Polymers with 3-(Aminomethyl)pyridine

15.15- 15.30 (OP-8)
Seda Sahin, Seyma Kaya, Cigdem Yüksektepe, Ataol, Lütfiye Sirka
Current Applications of Artificial İntelligence and Crystals

COFFEE BREAK & POSTER SESSION (15.30 - 15.45)

SCIENTIFIC PROGRAM – ORAL PRESENTATIONS

CHAIRS: Prof. Dr. Ersin TEMEL & Prof. Dr. Gökhan KAŞTAŞ

15.45 - 16.00 (OP-9)
Dursun Karaağaç, Güneş Süheyla Kürkçüoğlu
Syntheses and crystal structures of one-dimensional [Cd(μ-4aepy)2(H2O)2][M(CN)4] [4aepy = 4-(2-aminoethylpyridine), M(II) = Ni(II) or Pd(II)] complexes

16.00 - 16.15 (OP-10)
Chaima Gharbi, Yusuf Sert, Emine Berrin Poyraz, Uwe Böhme, Necmi Dege, Chérif Ben Nasr, Lamia Khedhiri
Synthesis, Crystal Structure, Hirshfeld Surface Analysis, Molecular Docking, IR Spectroscopy and DFT Calculations of a Novel 2D Layered Hybrid Compound (C6H10N3O)2Cu2Cl6

16.15 - 16.30 (OP-11)
İlkay Yıldırım Gümüşhan
Experimental and theoretical investigation on N-(3-hydroxyphenyl)benzene sulfonamide

16.30 - 16.45 (OP-12)
Abdurrahman Suhta, Sude Saral, Ufuk Çoruh, Sevgi Karakuş, Ezequiel M. Vazquez Lopez
Synthesis, single crystal X-ray, Hirshfeld surface analysis and DFT calculation based NBO, HOMO-LUMO, MEP, ECT and molecular docking analysis of N'-[(2,6-dichlorophenyl)methylidene]-2-{[3-(trifluoromethyl)phenyl] amino} benzohydrazide

SOCIAL EVENTS 17.00-23.00
SAMSUN CITY MUSEUM TRIP
GALA DINNER

Sunday, 19 May 2024

10.00 - 12.30

CLOSING AND AWARD CEREMONY

(13.00-…) SOCIAL EVENTS

NİYAZİ KESİM RESTAURANT- BRANCH

AMAZON MUSEUM AND WEST PARK TRIP

SCHEDULE

YEŞİLYURT DEMİR ÇELİK

ULUSOYUN

Medi TRAVEL

USLU DEMİR ÇELİK

Özön

NanoSpek
www.nanospek.com.tr

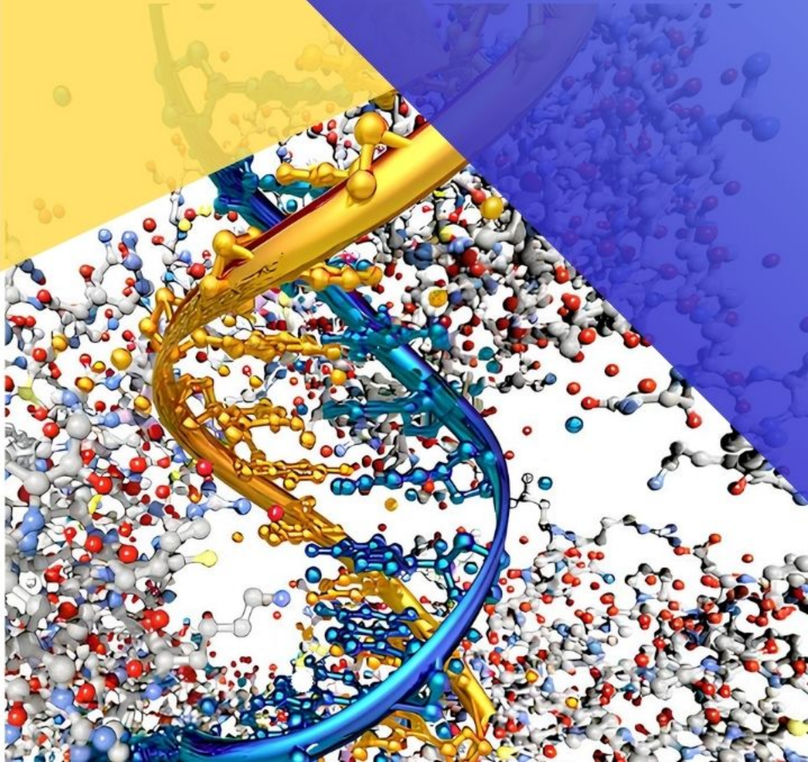
YAŞAR GROUP

Thank you for your contributions.

www.omu.edu.tr
https://ukd.org.tr/tucr2024/
tucr.contact@gmail.com
@ulusalkristalografidernegi

5TH TURKISH NATIONAL CRYSTALLOGRAPHY MEETING SCHEDULE

17-19 May 2024
Ondokuz Mayıs University
OMTEL Hotel Meeting Room
Samsun/Türkiye



Invited Speakers

Prof. Dr. Santiago Garcia-Granda (University Oviedo, Spain)

Prof. Dr. Rahime Şimşek (Hacettepe University, Türkiye)

Prof. Dr. Wan Haliza Binti Abd Majit (University of Malaya-Malaysia)

Prof. Dr. Peter Müller (Massachusetts Institute of Technology, USA)

Prof. Dr. Michael Richard Probert (Newcastle University, England)

Prof. Dr. Narcis Duteanu (Polytechnic University of Timisoara, Romania)

Design of processable polymeric carbon nitride for photo(electro)catalytic applications.

Santiago García-Granda[1]*, Igor Krivtsov*[2,3]*, Christiane Adler*[3]*, Ashish Vazirani*[3]*, Dariusz Mitoraj*[3]*, Radim Beranek*[3]
[1.] Department of Physical and Analytical Chemistry, University of Oviedo-CINN, 33006 Oviedo, Spain.
[2.] Department of Chemical and Environmental Engineering, University of Oviedo, 33006 Oviedo, Spain.
[3.] Institute of Electrochemistry Ulm University, Albert-Einstein-Allee 47, 89081 Ulm, Germany.

Polymeric carbon nitride (PCN) is a unique material in the polymer world; It is low-cost, easy to prepare and possesses outstanding thermal and chemical stability. Most importantly, however, it shows an ability to efficiently drive photocatalytic oxidation and reduction reactions under UV-blue light irradiation, which made it one of the best candidates for the role of photo(electro)catalyst for solar-fuels production. Although the material itself is not a new discovery, it has been known since times of Liebig, its photocatalytic properties were only discovered little more than a decade ago[1]. Since then, the properties of this material have been thoroughly scrutinized and a number of synthetic approaches for the preparation of PCNs with tuneable characteristics was developed. This, however, has not allowed overcoming a poor processability of bulk PCN impeding its use in advanced catalytic processes and in solar-fuel producing systems like photoelectrochemical (PEC) cells. A recent discovery of ionic PCN also known as poly(heptazine imide) (PHI) followed by the developed in our group method for water-soluble PHI synthesis[2] has made a huge step in that direction. Water-soluble PHI, apart from its high photocatalytic activity in alcohol photoxidation, also proved itself as an efficient stabilizer for ultra-small metallic nanoparticles. On the other hand, the sol-gel processing of the PHI nanoparticles enabled the first robust PCN-type photoanodes for solar alcohols reforming even under bias-free conditions[3]. It also made possible obtaining an unprecedented insight in photogenerated charge dynamics in PHI demonstrating that light-induced accumulation of electrons leads to its photodoping, resulting in a significant improvement of PEC performance[4].

[1] Wang, X.; Maeda, K.; Thomas, A.; Takanabe, K.; Xin, G.; Carlsson, J.; Domen, K.; Antonietti, M., A metal-free polymeric photocatalyst for hydrogen production from water under visible light. *Nat. Mater.* **2009,** *8* (1), 76-80.

[2] Krivtsov, I.; Mitoraj, D.; Adler, C.; Ilkaeva, M.; Sardo, M.; Mafra, L.; Neumann, C.; Turchanin, A.; Li, C. Y.; Dietzek, B.; Leiter, R.; Biskupek, J.; Kaiser, U.; Im, C.; Kirchhoff, B.; Jacob, T.; Beranek, R., Water-Soluble Polymeric Carbon Nitride Colloidal Nanoparticles for Highly Selective Quasi-Homogeneous Photocatalysis. *Angewandte Chemie-International Edition* **2020,** *59* (1), 487-495.

[3] Adler, C.; Krivtsov, I.; Mitoraj, D.; Dos Santos-Gomez, L.; Garcia-Granda, S.; Neumann, C.; Kund, J.; Kranz, C.; Mizaikoff, B.; Turchanin A., Beranek, R. *ChemSusChem* **2021**, 14, 2170-2179.

[4] Adler, C.; Selim, S.; Krivtsov, I.; Li, C. Y.; Mitoraj, D.; Dietzek, B.; Durrant, J. R.; Beranek, R., Photodoping and Fast Charge Extraction in Ionic Carbon Nitride Photoanodes. *Adv. Funct. Mater.* **2021,** *31* (45), 2105369.

We gratefully acknowledge the financial support provided by Spain´s Agencia Estatal de Investigación, PID2020-113558RB-C41.

Hexahydroquinoline Derivatives as Potential Inflamatory Mediators Inhibitors

Rahime Simsek[1], Ezgi Pehlivanlar[1], Gökalp Cetin[1], Sema Ozturk Yildirim[2,3], Pınar Erkekoglu[4], Hülya Tezel Yalcin[4], Deniz Arcak[4], Gunes Esendagli[5]

[1]Dept. of Pharmaceutical Chemistry, Faculty of Pharmacy, Hacettepe University, 06100 Sihhiye, Ankara-Turkey
[2]Dept. of Phys, Faculty of Sciences, Eskişehir Tech University, 26470 Eskişehir-Turkey
[3]Dept. of Phys, Faculty of Sciences, Erciyes University, 38039 Kayseri-Turkey
[4]Dept. of Pharmaceutical Toxicology, Faculty of Pharmacy, Hacettepe University, 06100 Sihhiye, Ankara-Turkey
[5]Dept. of Basic Oncology, Hacettepe University Cancer Institute, 06100 Sihhiye, Ankara-Turkey

Inflammation is the organism's response to an injury or infection. Various factors such as bacteria, viruses, stress, food and environmental pollution trigger inflammation. Untreated inflammation can become chronic and lead to chronic diseases such as cancer, Alzheimer's, diabetes, atherosclerosis, COVID-19, autoimmune and cardiovascular diseases. Inflammatory stimuli activate the production of inflammatory mediators by stimulating intracellular signaling pathways. Pro- and anti-inflammatory cytokines are proteins that facilitate or inhibit inflammation. Although cytokines are molecules that govern the immune response, excessive formation of inflammatory cytokines can lead to various disorders ranging from tissue damage to death. The risk of inflammation-related diseases increases as a result of chronic tissue damage and cellular dysfunction caused by inflammation mediators, and inhibition of inflammation mediators can be effective in the treatment of these diseases.

Heterocyclic rings are involved in the structure of many drug molecules. With the discovery of 1,4-Dihydropyridines (1,4-DHPs) as a heterocyclic ring, medicinal chemistry has gained an important ring system. 1,4-DHPs are biologically active compounds and currently, drug molecules carrying 1,4-DHP ring system are used in antihypertensive treatment. Recent studies have shown that 1,4-DHP derivatives used as calcium channel blockers such as nifedipine, amlodipine, nicardipine, nitrendipine, felodipine, manidipine, azelnidipine and lasidipine also have anti-inflammatory and immunosuppressive effects.

In the light of this information, since the 1,4-DHP ring is suitable for various modifications and many compounds carrying this ring system have anti-inflammatory activity, it was thought that new derivatives may also have this effect.

Based on the data that 1,4-DHP and substituted quinoline derivatives inhibit the release of inflammation mediators and the data obtained from in silico studies, it was thought that 5-oxo-1,4,5,6,7,8-hexahydroquinoline derivatives, in which the carboxylate structure at 5th position of the 1,4-DHP ring is enclosed in the ring and carrying two ring systems together, may also have this effect. For this purpose; 2-methyl-(2,6,6/2,7,7)-trimethyl-4-aryl-5-oxohexahydroquinoline-3-carboxylate derivatives containing condensed 1,4-DHP ring system were synthesized. The structure of the synthesized compounds was elucidated by IR, ^{1}H-NMR, ^{13}C-NMR, HRMS methods and X-Ray diffraction.

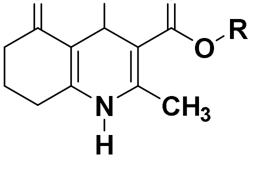


Figure 1: General structure of the synthesized compounds

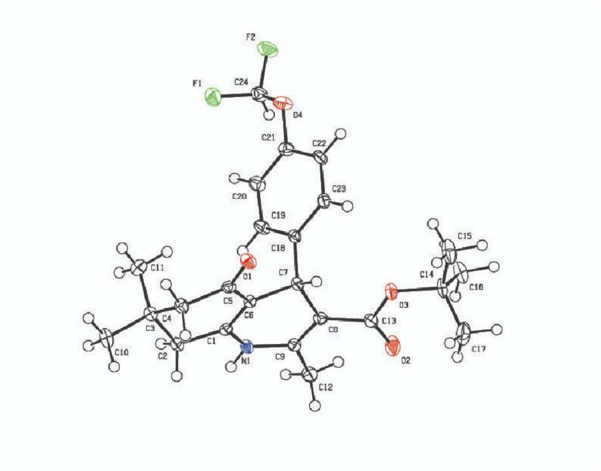


Figure 2: ORTEP diagram of t-butyl 4-(4-(difluoromethoxy)phenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate

The cytotoxicity and reactive oxygen species (ROS) generation potential of the synthesized compounds were determined and their effects on inflammation mediators were investigated. In addition, molecular modeling studies were carried out to determine the interaction of the most active derivatives with molecular targets in the protein structure.

According to the results of biological activity experiments, compounds with small substituents on phenyl at 4th position of the hexahydroquinoline ring have the ability to inhibit inflammation mediators to some extent. Compounds synthesized by placing a heterocyclic ring on phenyl at 4th position of the hexahydroquinoline ring showed TGF-β activation.

1. Meizlish ML, Franklin RA, Zhou X, Medzhitov R. Tissue homeostasis and inflammation. Annual review of immunology. 2021; 39:557-81.

2. Riley JS, Tait SW. Mitochondrial DNA in inflammation and immunity. EMBO reports. 2020; 21(4):e49799.

3. Sohal HS. A review on recent trends in synthesis and applications of 1, 4- dihydropyridines. Materials Today: Proceedings. 2022; 48:1163-70.

4. Devi L, Robert AR, Ganja H, Maddila S, Jonnalagadda SB. A rapid, sustainable and environmental friendly protocol for the catalyst-free synthesis of 2-methyl- 5-oxo-hexahydroquinoline-3-carboxylate via ultrasonic irradiation. Chemical Data Collections. 2020; 28:100432.

5. Lo MW, Woodruff TM. Complement: Bridging the innate and adaptive immune systems in sterile inflammation. Journal of Leucocyte Biology. 2020; 108(1):339-51.

6. Wooff Y, Man SM, Aggio-Bruce R, Natoli R, Fernando N. IL-1 family members mediate cell death, inflammation and angiogenesis in retinal degenerative diseases. Frontiers in immunology. 2019; 10:1618.

Structural and Optical Properties of ZnO Nanoparticles and Thin Films for OLED and Sensors

Prof Dr. Wan Haliza Abd. Majid (q3haliza@um.edu.my), Dr. Omer Celik and Dr. Mohd Arif Mohd Sarjidan

Low Dimensional Materials Research Center (LDMRC), Physics Department, Universiti Malaya,
50603 Kuala Lumpur, Malaysia.

ZnO is a II-VI oxide semiconductor with a wurtzite crystalline structure and a wide direct bandgap of 3.4 eV at room temperature. It can be used for short-wavelength optoelectronic devices and has advantages over GaN such as lower production cost and excellent radiation resistance. Therefore, ZnO nanoparticles are versatile functional materials that offer optoelectronic properties, piezoelectricity, and pyroelectricity due to the spatial distribution of the interpenetrated Zn^{2+} and O^{2-} tetrahedrons and the mixed ionic-covalent character of the Zn-O bond (with nearly equal contribution from each bonding type) which are responsible for the intrinsic polarity in the ZnO crystal along the c-axis. Despite the various morphologies, particle sizes, and structures designed for engineered ZnO nanostructures, no accurate mechanisms have been proposed to elucidate their formation during the reported procedures. Some issues such as ineffective surface passivation, interfacial charge recombination, and long-term stability have collectively led to poor electron injection efficiency. As a result, this has caused low current density and efficiency of the ZnO-based photovoltaic device, which have not been resolved. It is necessary to conduct thorough studies on the impact of facet selectivity, structure, and morphology of ZnO nanostructures on the overall efficiency of solar cells and the associated mechanism. Band positions and band gaps are dependent on particle size, which makes it challenging to create effective heterojunctions for efficient charge separation and photocatalytic activity. Furthermore, additional research is needed to carefully examine the biomedical application of ZnO NPs and their impact on biological systems. In this research, the focus is to obtain ZnO by using Zinc Acetate Dihydrate ($Zn(CH_3COOH)_2.2H_2O$), Sodium Hydroxide (NaOH), deionised water, and ethanol. Syntheses were carried out for different crystal sizes. Characterisation methods such as XRD, SEM, PL, UV-Vis, thickness measurements and capacitance response are used to obtain their structural, optical, and humidity sensing properties. The crystal sizes were calculated separately from the XRD peaks, and their averages were taken. The energy band gaps of the samples were calculated using Tauc's plot analysis. The PL emission peaks were identified from the PL spectra, and the capacitance response and response lag of the humidity sensing capabilities were evaluated on the fabricated devices. These results were used to assess the potential of the synthesized ZnO for the fabrication of organic light-emitting diodes (OLED) and humidity sensors. Table 1 shows the quantity of solution used by the designated samples in the precipitation synthesis process.

According to the XRD analysis using Scherer’s equation, the Ethanol sample has the largest crystallite size of 18.43 nm, while Water 3 has the smallest value of 13.76 nm. The crystallographic information obtained from the XRD analysis indicates that the Waste sample has the highest volume, while Water 3 has the highest defects and strains. The FESEM image of the Ethanol and Water 2 samples is shown in Figure 1, indicating that Water 2 has a smaller grain size compared to the Ethanol sample.

		ZnADiHd			NaOH			Ethanol	Mx Solution	Centrifuge	Form
		Amount (gr)	Sol (mL)	Mx Time (m)	Amount (gr)	Sol (mL)	Mx Time (m)	Amount (mL)	Mx Time (h)	4000 rpm, 15 m, Washed 2 times with Ethanol	
1	**Ethanol**	2	50 Eth.	20	0,8	50	20	100	1	x	White Powder
2	**Water 2**	2	50 DiW	20	0,8	50	20	100	1	x	White Powder
3	**Water 3**	4	100 DiW	20	1,6	50	20	100	1	x	White Shell
4	**Waste**	2	ZnADiHd was added to the waste solution consisting of Water 3.				30	100	1	x	White Powder

Table 1: Information on the synthesis process

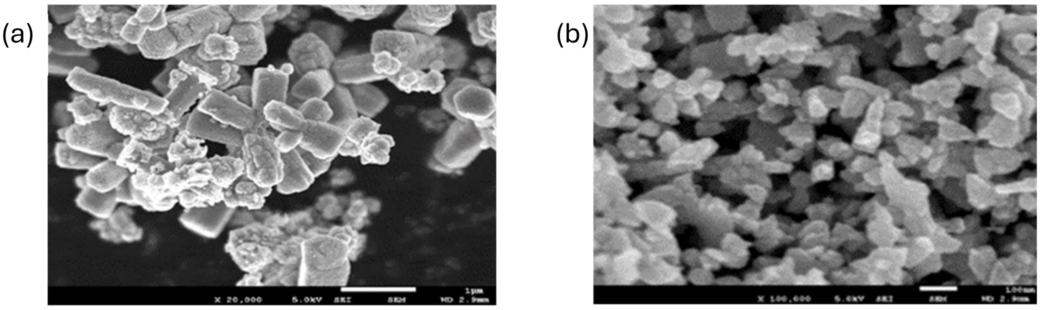


Figure 1: FESEM micrographs of (a) Ethanol (b) Water 2 samples, respectively.

The energy band gap (Eg) of the ZnO nanoparticles, calculated using Tauc's plot, is greater than 3.4 eV but falls within the range of 3.62-3.66 eV. The sample Water 2 exhibits the highest E_g of 3.66 eV, while the sample Ethanol has the smallest E_g of 3.62 eV. Two photoluminescence (PL) peaks have been identified: one related to UV-visible emissions at 2.0 eV and the other related to deep-level emissions (DLE) at 1.6 eV. Additionally, there is a PL peak at around 1.06 eV, which has not yet been reported and identified for ZnO nanoparticles. Based on the changes in the dielectric constant of the sensing film as a function of relative humidity, as shown in Figure 2, it was observed that Water 2 exhibited the highest sensitivity (2.38 pF/%RH) and the longest response lag (4.98%) among the humidity sensors operating in the 50-100% RH range. This suggests that Water 2, with its smaller grain size compared to the Ethanol sample, has a larger surface area to volume ratio, leading to better sensitivity and performance as a humidity sensor.

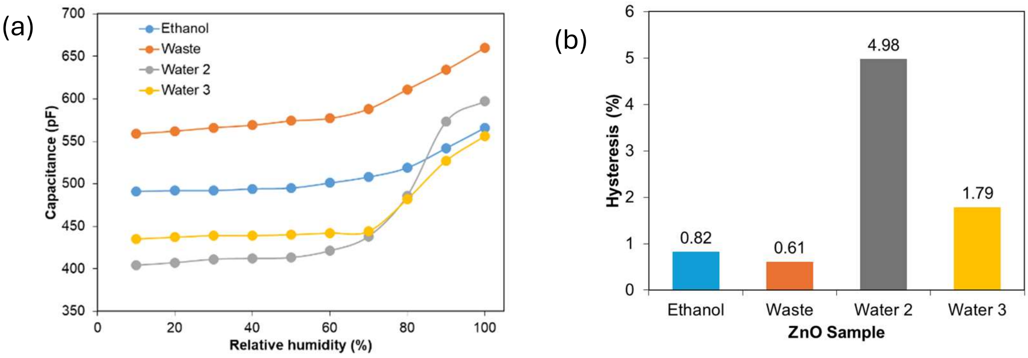


Figure 2: (a) The capacitance response of an ITO/ZnO/ITO humidity sensor with varying ZnO synthesis methods was investigated as the relative humidity increased from 10% to 100% Relative Humidity (RH) and (b) the slight response lag between dry and humid conditions.

Refining Disorders in Single-Crystal X-Ray Diffraction – Using Restraints the Right Way

Dr. Peter Müller

Massachusetts Institute of Technology 77 Massachusetts Ave, 2-325 Cambridge, MA 02139

Although widely regarded as one of the most powerful tools of three-dimensional structure elucidation, single-crystal x-ray diffraction has its limitations. The need for a high-quality single crystal is perhaps the most obvious weakness, however a more subtle yet serious issue poses the lack of understanding about the method itself. Because the final product of a crystal structure determination gives rise to a beautiful photorealistic rendering of the atomic model that looks just like a photograph of the molecule, scientist and laypersons alike tend to uncritically believe what they see, thus overestimating the powers of the method. The most fundamental misunderstanding, probably, lies in the circumstance that x-ray diffraction is not a spectroscopic method. That means one does not record individual responses from atoms or functional groups but rather the Fourier transformation of the complete electron density function in the unit cell. A crystal structure comprises the spatial and temporal average over the whole crystal and the full duration of the diffraction experiment, which gives rise to challenges such as twinning or disorder. Powerful as the method may be, crystal structure determination is complex and not usually trivial. In order to learn the most from a given diffraction experiment, one has to thoroughly understand the method and one has to carefully and skillfully perform every step of structure determination. This presentation will discuss a case where, perhaps, the wish was father to the structure more than an honest interpretation of the diffraction data; and, certainly, a better understanding of the method could have prevented the publication of a paper of dubious value.

Encapsulated Nanodroplet Crystallisation (ENaCt), arevolutionary high throughput method for small molecules

Prof Michael Richard Probert

Chemistry, School of Natural and Environmental Sciences, Newcastle University

Crystallisation is a fundamental requirement for compounds tobe exposed to the full power of analysis through diffractiontechniques. High throughput parallel approaches enable largevolumes of crystallisation space to be explored even with limitedquantities of sample. The revolutionary EncapsulatedNanodroplet Crystallisation (ENaCt) method will be introducedand placed within the crystallisation field, highlighting thebenefits of the approach. Novel results will be explored rangingfrom 'simple' structure solution of 'uncrystallisable' compoundsthrough to full polymorph screening of active pharmaceuticalingredients and drug like molecules.

Oral Presentations

Scientific Program – Oral Presentations

CHAIRS: Prof. Dr. Metin KUL & Prof. Dr. Gökhan ALPASLAN

11:45 – 12:00

(OP-1)

Burak Veli Kabasakal

Structural insights into nitrogenase complexes against oxygen damage

12:15 – 12:30

(OP-2)

Merve İzmirli, Gül Yakalı, Resul Sevinçek, Duygu Barut Celepci, Erkan Fırıncı, Rukiye Fırıncı, Muhittin Aygün

Structural Analysis and Biological Activity Predictions of Some Organometallic Compounds

12:30 – 12:45

(OP-3)

Nadihan Yolgeçti, Sema Öztürk Yıldırım, Mehmet Akkurt, Gökalp Çetin, Rahime Şimşek, Cihat Şafak, Ray J. Butcher, Ajaya Bhattarai

Tert-butyl 4-([1,1’-biphenyl]-4-yl)-2,6,6-trimethyl-5-oxo-1,4,5,6,7,8-hexa hydro quinoline-3-carboxylate Synthesis, Single Crystal X-Ray Diffraction and Density Functional Modeling Studies

12:45 – 13:00

(OP-4)

Emre Yörük, Ashwin Suresh, Petr Brázda, Małgorzata Katarzyna Cabaj, Lukáš Palatinus

Investigation of bonding in crystals using 3D electron diffraction

Scientific Program – Oral Presentations

CHAIRS: Prof. Dr. Yelda BİNGÖL ALPASLAN

14:30– 14:45

(OP-5)

Hanifi Özşanlı, Okan Şimşek, Onur Rauf Yılmaz, Ceren Çiçek, Erbil Ağar, Ufuk Çoruh, Ezequiel M. Vazquez-Lopez

Synthesıs, Crystal Structure, Hırshfeld Surface Analysıs, Supramolecular And Computatıonal Investıgatıon Of Compound (E)-4-Methoxy-2-(((2-Methoxy-5-(Trifluoromethyl) Phenyl)Imino) Methyl)Phenol

Onur Rauf Yılmaz, Çiğdem Albayrak Kaştaş, Canan Kazak

14:45– 15:00

(OP-6)

Comparison Of Geometrical Properties Of (E)-2-Bromo-4-Methyl-6-[(2,6-Dimethyl-Phenylimino)Methyl]Phenol And (E)-2-Bromo-4-Methyl-6-[(3,4-Dimethyl-Phenylimino)Methyl]Phenol Compounds By XRD And Hirshfeld Analysis

15:00– 15:15 **Güneş Süheyla Kürkçüoğlu, Seray Kekeç, Dursun Karaağaç, Onur Şahin**

(OP-7) Crystallographic Investigation of Heteronuclear Hexacyanometalate(III) Coordination Polymers with 3-(Aminomethyl)pyridine

15:15– 15:30 **Seda Sahin, Seyma Kaya, Cigdem Yüksektepe, Ataol, Lütfiye Sirka**

(OP-8) Current Applications of Artificial İntelligence and Crystals

Scientific Program – Oral Presentations

CHAIRS: Prof. Dr. Ersin TEMEL & Prof. Dr. Gökhan KAŞTAŞ

15:45 – 16:00 **Dursun Karaağaç, Güneş Süheyla Kürkçüoğlu**

(OP-9) Syntheses and crystal structures of one-dimensional [Cd(μ-4aepy)2(H2O)2][M(CN)4] [4aepy = 4-(2-aminoethylpyridine), M(II) = Ni(II) or Pd(II)] complexes

16:00 – 16:15 **Chaima Gharbi, Yusuf Sert, Emine Berrin Poyraz, Uwe Böhme, Necmi Dege, Chérif Ben Nasr, Lamia Khedhiri**

(OP-10) Synthesis, Crystal Structure, Hirshfeld Surface Analysis, Molecular Docking, IR Spectroscopy and DFT Calculations of a Novel 2D Layered Hybrid Compound (C6H10N3O)2Cu2Cl6

16:15 – 16:30 **İlkay Yıldırım Gümüşhan**

(OP-11) Experimental and theoretical investigation on N-(3-hydroxyphenyl)benzene sulfonamide

16:30 – 16:45 **Abdurrahman Suhta, Sude Saral, Ufuk Çoruh, Sevgi Karakuş, Ezequiel M. Vazquez Lopez**

(OP-12) Synthesis, single crystal X-ray, Hirshfeld surface analysis and DFT calculation based NBO, HOMO-LUMO, MEP, ECT and molecular docking analysis of N'-[(2,6-dichlorophenyl)methylidene]-2-{[3-(trifluoromethyl)phenyl] amino} benzohydrazide

Structural insights into nitrogenase complexes against oxygen damage

[1,2] Burak V. Kabasakal
[1] Imperial College London, Department of Life Sciences, London, SW7 2AZ, United Kingdom
[2] Turkish Accelerator and Radiation Laboratory, Ankara, 06830, Türkiye

* E-mail: bvkabasakal@tarla-fel.org

Abstract

Nitrogenase enzyme catalyses the conversion of atmospheric nitrogen to bio-available ammonia with its components called FeP, which is a NifH dimer and catalyzes the ATP-dependent electron transfer reaction, and MoFe protein, which has two metallocenters for electron transfer. The interaction of immature forms of MoFeP with the dispensable accessory proteins NafH, NifW, and NifZ is required for P-cluster maturation (Stappen *et al.*, 2022). The other nitrogenase catalytic component, FeP, and MgATP are also required for P-cluster maturation within MoFeP. A significant disadvantage of this system is that cytoplasmic O_2 rapidly oxidizes and degrades these cofactors. In conformational protection, FeSII (also known as Shethna Protein II) forms a complex with nitrogenase and protects the nitrogenase from oxygen damage (Shethna et al., 1968, Moshiri *et al.*, 1995). FeSII is a 13 kDa adrenodoxin type ferredoxin protein with a 2Fe-2S cluster, forming a dimer in solution. Schlesier *et al* (Schlesier et al., 2016) obtained a 2.2 Å crystal structure of FeSII in the orthorhombic crystal form. The observed FeSII crystal form has five copies in the asymmetric unit. One of them is in a “closed conformation”, forming a “closed” dimer with a crystallographic symmetry mate. It was proposed that this conformational change is induced by oxidation of the cluster, and the change renders FeSII to form the protective ternary complex with MoFe and Fe proteins. In our crystal structure of FeSII from *Azotobacter vinelandii*, which is in the same crystal form, positioning of the atoms in the unit cell is similar to the previously published one (PDB: 6YAV). However, the hypothesis is that the “open” conformation may be the product of a crystallization-induced domain swap. The 2Fe-2S cluster is not exposed to solvent, but in the crystal its interacting helix is replaced by the same helix residues from a crystal symmetry mate. The full MoFe-FeP-FeSII protein complex structure will confirm the conformation of the FeSII protein in the nitrogenase complex.

Keywords: nitrogenase, protein crystallography, protein complexes

References

Moshiri, F., Crouse, B.R., Johnson, M.K., Maier, R.J., 1995. The “nitrogenase-protective” FeSII protein of Azotobacter vinelandii: overexpression, characterization, and crystallization. 34, 12973–12982.

Schlesier, J., Rohde, M., Gerhardt, S., Einsle, O., 2016. A Conformational Switch Triggers Nitrogenase Protection from Oxygen Damage by Shethna Protein II (FeSII). . 138, 239–247

Shethna, Y.I., DerVartanian, D.V., Beinert, H., 1968. Non heme (iron-sulfur) proteins of *Azotobacter vinelandii.*31, 862–868.

Stappen, C. V., Jiménez-Vicente, E., Pérez-González, A., Yang, Z., Seefeldt, L.C., DeBeer, S., Dean, D. R., Decamps, v.L. 2022. “A Conformational Role for NifW in the Maturation of Molybdenum Nitrogenase P-Cluster”. Chemical Science 13 (12): 3489-3500.

Structural Analysis and Biological Activity Predictions of Some Organometallic Compounds

[1*]Merve İzmirli, [1]Gül Yakalı, [2]Resul Sevinçek, [2]Duygu Barut Celepci, Erkan Fırıncı, Rukiye Fırıncı
[2]Muhittin Aygün
[1] Department of Engineering Sciences, Faculty of Engineering, Izmir Katip Celebi University, Izmir 35620, Turkey
[2] Dokuz Eylül University, Faculty of Science, Department of Physics, 35160 İzmir, Türkiye

* E-mail: merve.izmirli@ikcu.edu.tr

Abstract

Barbituric acid derivatives and their organometallic compounds have long been recognized for their pharmacological potential [1-2]. There exist numerous molecular compounds in our surroundings that significantly influence human health, ranging from pharmaceuticals to environmental pollutants [3-4]. Understanding the absorption, distribution, metabolism, excretion, and toxicity (ADMET) properties of these compounds is crucial for assessing their effects on the human body. In the pursuit of developing new drugs, accurate knowledge of molecular structure is essential, achieved by X-ray diffraction techniques. In this study, two barbituric acid-based ligands, namely 1,3-dimethyl-2,4,6-trioxo-hexahydro-pyrimidine-5-(2,6-dimethylphenylamino)methylene (HL1) and 1,3-dimethyl-2,4,6-trioxo-hexahydro-pyrimidine-5-(8-quinolylamino)methylene (HL2), along with their correspond-ing organometallic compounds, were investigated. The molecular and crystal structures of these compounds were determined using X-ray diffraction techniques. The X-ray diffraction studies revealed various coordination geometries around the metal center, ranging from distorted square-planar to distorted octahedral. Additionally, non-covalent interactions were examined in detail. Furthermore, predictive biological activity studies using PASS online software suggested promising activities for these compounds, including CYP2H substrate, cell adhesion molecule inhibitor, and nicotinic receptor antagonist. This comprehensive investigation sheds light on the potential pharmacological applications of barbituric acid derivatives and their organometallic complexes, offering insights for further drug development endeavors.

Keywords: Barbituric acid, XRD, non-covalent interactions, ADME, PASS online

References

1. Barakat, A., Islam, M. S., Al-Majid, A. M., Ghabbour, H. A., Atef, S., Zarrouk, A., & Warad, I. (2018). Quantum chemical insight into the molecular structure of L-chemosensor 1,3-dimethyl-5-(thien-2-ylmethylene)-pyrimidine-2,4,6-(1H,3H,5H)-trione: Naked-eye colorimetric detection of copper(II) anions. Journal of Theoretical and Computational Chemistry, 17(01), 1850005.

2. Sharma, A., Jad, Y., Ghabbour, H., de la Torre, B., Kruger, H., Albericio, F., & El-Faham, A. (2017). Synthesis, Crystal Structure and DFT Studies of 1,3-Dimethyl-5-propionylpyrimidine-2,4,6(1H,3H,5H)-trione. Crystals, 7(1), 31.

3. Jia, C.-Y., Li, J.-Y., Hao, G.-F., & Yang, G.-F. (2019). A drug-likeness toolbox facilitates ADMET study in drug discovery. Drug Discovery Today.

4. Cheng F, Li W, Liu G, Tang Y. In silico ADMET prediction: recent advances, current challenges and future trends. Curr Top Med Chem. 2013;13(11):1273-89.

Tert-butyl 4-([1,1’-biphenyl]-4-yl)-2,6,6-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate Synthesis, Single Crystal X-Ray Diffraction and Density Functional Modeling Studies

[1]Nadihan Yolgeçti, [1,2*]Sema Öztürk Yıldırım, [1]Mehmet Akkurt, [3]Gökalp Çetin, [4]Rahime Şimşek, [5]Cihat Şafak,
[6]Ray J. Butcher, [7]Ajaya Bhattarai

[1]Erciyes University, Faculty of Science, Department of Physics 38039 Kayseri, Türkiye
[2]Eskişehir Technical University, Faculty of Science, Department of Physics, Yunus Emre Campus 26470 Eskişehir, Türkiye
[3]Erzincan Binali Yıldırım University, Faculty of Pharmacy, Department of Pharmaceutical Chemistry, 24002, Erzincan, Türkiye
[4]Hacettepe University, Faculty of Pharmacy, Department of Pharmaceutical Chemistry, 06100, Sıhhiye, Ankara, Türkiye
[5]Başkent University, Faculty of Pharmacy, Department of Pharmaceutical Chemistry, Ankara, Türkiye
[6]Howard University, Department of Chemistry, Washington DC 20059, USA
[7]Department of Chemistry, M.M.A.M.C (Tribhuvan University), Biratnagar, Nepal

*E-mail: ozturk@erciyes.edu.tr

Abstract

Calcium channels contribute to the slow depolarization phase of excitable cells such as cardiomyocytes, skeletal muscle or smooth muscle cells. Calcium channel blockers block calcium influx by stabilizing calcium channels on the membrane and are currently used to treat hypertension, cardiac arrhythmias, and angina pectoris acting on L-type channels. 1,4-dihydropyridine derivatives are widely used in antihypertensive and antiarrhythmic therapy and in the treatment of angina pectoris. In this study, *tert*-butyl 4-([1,1'-biphenyl]-4-yl)-2,6,6-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate ($C_{29}H_{33}NO_3$) was synthesized and was investigated theoretically. The molecular geometry was obtained from X-ray structure determination and optimized using the density functional theory (DFT/B3LYP) method with the 6-31G(d,p) basis set.

The geometric parameters obtained from the calculations were compared with the experimental findings and a perfect agreement was found between the two data. Molecular electrostatic potential (MEP) calculation, Mulliken population analysis and NBO analysis of the title compound were performed using optimized geometry.

Keywords: Crystal structure, DFT method, NBO analysis

References

Öztürk Yıldırım, S., Butcher, R. J., Gündüz, M. G., El-Khouly, A.,Şimşek, R. & Şafak, C. (2013). *Acta Cryst.* E**69**, 40–41.
Yıdırım, S.Ö., Büyükmumcu, Z., Butcher, R.J., Çetin, G. & Şimşek, R. (2020). J. Mol. Struc.**, 1200,** 15, 127069.

Investigation of bonding in crystals using 3D electron diffraction

[1*]Emre Yörük, [1]Ashwin Suresh, [1]Petr Brázda, [1]Małgorzata Katarzyna Cabaj, [1]Lukáš Palatinus
[1] Institute of Physics of the CAS, Na Slovance 2, Prague 8, Czechia

* E-mail: yoruk@fzu.cz

Abstract

3D electron diffraction (3D ED) is an increasingly popular alternative to x-ray diffraction, capable of *ab initio* structure determination in sub-micrometer scale [1]. Electron scattering cross-sections are typically 10^4 times larger compared to x-rays, allowing data collection from nano-sized crystals. Electron beams can be focused to diameters of tens of nanometers, making it possible to collect single crystal data from polycrystalline samples and distinguishing phases. Experiments can be carried out using transmission electron microscopes (TEM) (Fig.1) where crystals can be imaged, and spectroscopic and diffraction data collected from the same grain. Other advantages include easier localization of light atoms including hydrogens [2], direct determination of absolute structure [3], and an increased sensitivity of data to atomic charges [4]. Multiple scattering of can be taken into account during structure refinement to obtain accurate R-factors comparable to x-ray diffraction [5].
Our recent work has focused on refinement of charge transfer among atoms, including structures containing heavy atoms. This is a challenge since their smaller valence/core electron ratio leads to minute changes in electron density, requiring extremely precise diffraction data to refine bonding effects. We show that it is possible to measure 3D ED data of sufficient quality to perform these refinements using a spherical atom kappa formalism [6] where atomic contributions to the charge density remain spherical, but the population of the valence shell is refined while allowing it to expand or contract as a result of changes in electron-electron repulsion.
We present here results on multiple compounds including $CsPbBr_3$, $Lu_3Al_5O_{12}$, SiO_2, $Na_2Al_2Si_3O_{10}\cdot 2H_2O$ and $B_{18}H_{22}$. The experimentally refined charge flows agree with chemical expectations based on electronegativity (Fig.1). There are improvements in the displacement parameters and R-factors. The results are validated by DFT calculations for comparison.

Keywords: electron diffraction, charge density, quantum crystallography.

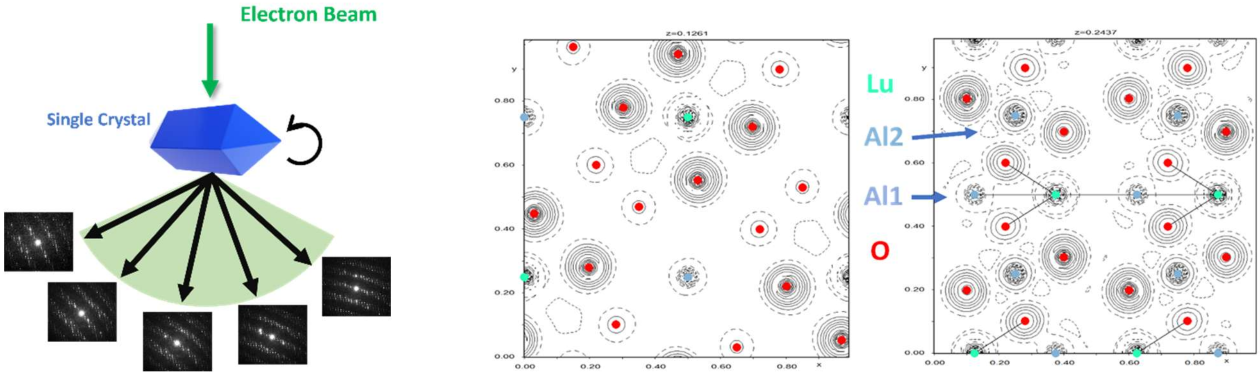


Fig. 1: Schematization of a nanocrystal being rotated while exposed to an electron beam to collect electron diffraction data (left). Static deformation maps obtained for $Lu_3Al_5O_{12}$ after charge density refinement (right).

References

[1] M. Gemmi *et al.*, "3D Electron Diffraction: The Nanocrystallography Revolution," *ACS Cent. Sci.*, vol. 5, no. 8, pp. 1315–1329, Aug. 2019, doi: 10.1021/acscentsci.9b00394.
[2] L. Palatinus *et al.*, "Hydrogen positions in single nanocrystals revealed by electron diffraction," *Science*, vol. 355, no. 6321, pp. 166–169, Jan. 2017, doi: 10.1126/science.aak9652.
[3] P. B. Klar *et al.*, "Accurate structure models and absolute configuration determination using dynamical effects in continuous-rotation 3D electron diffraction data," *Nat. Chem.*, Apr. 2023, doi: 10.1038/s41557-023-01186-1.
[4] T. Hahn, *International Tables for Crystallography*, vol. Volume C: Mathematical, Physical and Chemical Tables. New York: Springer, 2005.
[5] L. Palatinus, V. Petříček, and C. A. Corrêa, "Structure refinement using precession electron diffraction tomography and dynamical diffraction: theory and implementation," *Acta Crystallogr A Found Adv*, vol. 71, no. 2, pp. 235–244, Mar. 2015, doi: 10.1107/S2053273315001266.
[6] P. Coppens, *X-Ray Charge Densities and Chemical Bonding*. Oxford University Press, 1997. doi: 10.1093/oso/9780195098235.001.0001.

Synthesis, Crystal Structure, Hirshfeld Surface Analysis, Supramolecular And Computational Investigation Of Compound (E)-4-Methoxy-2-(((2-Methoxy-5-(Trifluoromethyl) Phenyl)Imino) Methyl)Phenol

[1]Hanifi ÖZŞANLI, [2]Okan ŞİMŞEK, [1,2]Onur Rauf YILMAZ, [3]Ceren ÇİÇEK, [3]Erbil AGAR, [1]Ufuk ÇORUH, [1]Ezequiel M. VAZQUEZ-LOPEZ

[1]Ondokuz Mayıs University, Faculty of Sciences, Department of Physics, 55200, Atakum, Samsun, Turkey
[2]Sinop University, Faculty of Sciences, Department of Physics, 57200, Sinop, Turkey
[3]Ondokuz Mayıs University, Faculty of Sciences, Department of Chemistry, 55200, Atakum, Samsun, Turkey
[4]Universidade de Vigo, Departamento de Química Inorganica, Facultade de Química, 36310, Vigo, Spain

* E-mail: 2021hanifiozsanli@gmail.com

Abstract

Crystallographic features of synthesized compound (E)-4-methoxy-2-(((2-methoxy-5-(trifluoromethyl)phenyl)imino) methyl)phenol have been investigated with Hirshfeld surface analysis and XRD method. The stability of the crystal packing primarily stemmed from N–H···O and C–H···O bonding interactions, further fortified by offset π···π stacking interactions. To delve into the supramolecular arrangement, Hirshfeld surface analysis was conducted, shedding light on the intricacies of the crystal packing. The synthesized compound's structure was determined through single crystal X-ray diffraction analysis, revealing its crystallization within the triclinic crystal system, space group P-1. Supramolecular assembly is explored by Hirshfeld surface analysis, and supramolecular geometric features of the title compound involve the compact arrangement of title molecules with each other. The properties of dispersion energy have been examined through studies on interaction energy and energy frameworks.

Keywords: Schiff base, X-ray diffraction method, Hirshfeld surface analysis, supramolecular geometric properties, interaction energy and energy frameworks

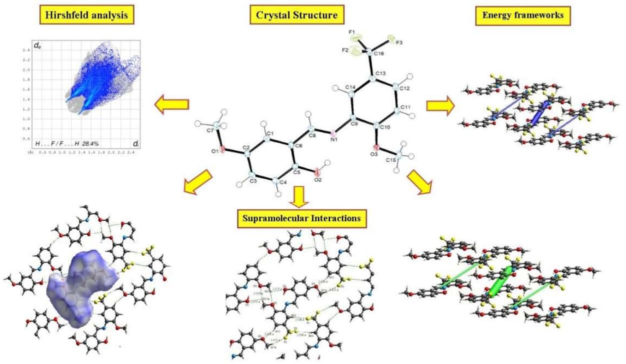


Fig. 1. Graphical abstract of title compound

References

Farrugia, L. J. (2012). WinGX and ORTEP for Windows: an update. *Journal of applied crystallography,* 45(4), 849-854.

Sheldrick, G. M. (2015). Crystal structure refinement with SHELXL. *Acta Crystallographica Section C: Structural Chemistry,* 71(1), 3-8.

Shi, Q., Chen, H., Wang, Y., Xu, J., Liu, Z. ve Zhang, C. (2022). Recent advances in drug polymorphs: Aspects of pharmaceutical properties and selective crystallization. *International journal of pharmaceutics,* 611, 121320.

Spackman, M. A. ve Jayatilaka, D. (2009). Hirshfeld surface analysis. *CrystEngComm,* 11(1), 19-32.

Turner, M. J., Thomas, S. P., Shi, M. W., Jayatilaka, D. ve Spackman, M. A. (2015). Energy frameworks: insights into interaction anisotropy and the mechanical properties of molecular crystals. *Chemical Communications,* 51(18), 3735-3738.

Yogheshwari, P., Sridhar, B. ve Anitha, K. (2022). Experimental and theoretical studies on bis (6-nitroquinoline) fumaric acid co-crystal. *Journal of Molecular Structure,* 1249, 131561.

Comparison Of Geometrical Properties Of (E)-2-Bromo-4-Methyl-6-[(2,6-Dimethyl-Phenylimino)Methyl]Phenol And (E)-2-Bromo-4-Methyl-6-[(3,4-Dimethyl-Phenylimino)Methyl]Phenol Compounds By XRD And Hirshfeld Analysis

[1]Onur Rauf YILMAZ, [1]Çiğdem ALBAYRAK KAŞTAŞ, [2]Canan KAZAK,
[1]*Sinop Üniversitesi, Fen Edebiyat Fakültesi, Fizik Bölümü, Sinop,*
[2]Ondokuz Mayıs Üniversitesi, Fen Fakültesi, Fizik Bölümü, Samsun,

* E-posta: oryilmaz@sinop.edu.tr

Abstract

We compare two new titles composed of isomer molecules of geometries, intermolecular and intramolecular interactions, spectral Uv-Vis and FT-IR analysis, strengthness and optical polarizabilities. The dihedral angles of aromatic rings of title molecules with order are 76.88° and 4.04°. Even though their plane angles drastically change, their space group are triclinic, and compatibly notable changes only appear on beta angles, with respectively 85.847 (4)° and 76.112 (2)° Furthermore, The bond distances of the intramolecular N…H-O tautomeric domain forming S(6) varied by less than the maximum of 6Å of the distances between similar bonds of two molecules.The first lemma molecules have two parallel displaced π-π interactions. In the phenol part, the distance between the plane centroid and the plane centroid is 3.594(5)Å, and the plane shift is 0.800(8) Å. On the aniline side, the plane shift is between 1.116(6) Å, and the plane centroid distance is 3.840(3) Å. The other synthesized structure's single π-π interaction has a 4.5246Å distance between aromatic benzene rings with a 2.929 Å phase shift. Associated with these interactions, we find that Hirshfeld surface analysis gives higher values of van der Waals for H-H, C-H, and H-C connection rates on the surface of the first molecule. On the other hand, Nonlinear Optics (NLO) analysis shows that the dipole moment, average isotropic polarizability, and anisotropic polarizabilities of the second structure give greater value. Moreover, NBO analysis similarly confirms that the second component has better intramolecular charge transfer. In addition, the lower Homo-Lumo gap also agrees with the results of FT-IR and Uv-Vis observation.

Keywords: Schiff Base, Hirshfeld Surface Analysis, NLO,

References

Demircioğlu, Z., Özdemir, F. A., Dayan, O., Şerbetçi, Z., & Özdemir, N. (2018). Synthesis, X-ray diffraction method, spectroscopic characterization (FT-IR, 1H and 13C NMR), antimicrobial activity, Hirshfeld surface analysis and DFT computations of novel sulfonamide derivatives. Journal of Molecular Structure, 1161, 122-137

Dolomanov, O.V.; Bourhis, L.J.; Gildea, R.J.; Howard, J.A.K.; Puschmann, H. OLEX2: a complete structure solution, refinement and analysis program, Journal of Applied Crystallography, **2009**, 42, 339-341.

Eşme, A. S. L. I., & Sağdınç, S. G. (2017). Spectroscopic (FT–IR, FT–Raman, UV–Vis) analysis, conformational, HOMO-LUMO, NBO and NLO calculations on monomeric and dimeric structures of 4–pyridazinecarboxylic acid by HF and DFT methods. *Journal of Molecular Structure*, *1147*, 322-334.

Kirk, K. L. (2006). Fluorine in medicinal chemistry: Recent therapeutic applications of fluorinated small molecules. Journal of Fluorine Chemistry, 127(8), 1013-1029.

Kundwal, M. E., & Lani, M. N. (2015). Microbial inactivation using pulsed light-A review. *Jurnal Teknologi*, *77*(13).

M.A. Spackman, D. Jayatilaka, Hirshfeld surface analysis, CrystEngComm 11, **2009**, 19–32.

M. J. Turner, S. Grabowsky, D. Jayatilaka, and M. A. Spackman. Accurate and efficient model energies for exploring intermolecular interactions in molecular crystals. J. Phys. Chem. Lett., **2014**, 5(24), 4249-4255.

Przybylski, P., Huczynski, A., Pyta, K., Brzezinski, B., & Bartl, F. (2009). Biological properties of Schiff bases and azo derivatives of phenols. *Current Organic Chemistry*, *13*(2), 124-148.

Sheldrick, G.M. (2015) Crystal Structure Refinement with SHELXL. Acta Crystallographica C, C71, 3-8.

Stanley, C., & Douglas, S. A. (2007). Principles of instrumental analysis. Thomson Brooks/Cole, Sydney, 1-1039.

Tarı, G. Ö., & Aydemir, E. (2023). Experimental and DFT study of (E)-4-bromo-2 (((3-chloro-4-(4-chlorophenoxy) phenyl) imino) methyl)-5-fluorophenol: Molecular and electronic properties in solvent media. *Journal of Molecular Structure*, *1277*, 134880.

Crystallographic Investigation of Heteronuclear Hexacyanometalate(III) Coordination Polymers with 3-(Aminomethyl)pyridine

[1*]Güneş Süheyla Kürkçüoğlu, [1]Seray Kekeç, [2]Dursun Karaağaç, [3]Onur Şahin
[1] Eskişehir Osmangazi University, Sciences Faculty, Department of Physics, TR26040, Eskişehir, Türkiye
[2] Bursa Technical University, Faculty of Engineering and Natural Sciences, Department of Physics, TR16310, Bursa, Türkiye
[3] Sinop University, School of Health, Department of Occupat Health & Safety, TR57000, Sinop, Türkiye

* E-mail: gkurkcuo@ogu.edu.tr

Abstract

Cyanide-bridged coordination polymers have been investigated for next-generation chemical designs due to their magnetic, optical, electrical, catalytic and biological properties. Besides that organic ligands can be used to enable the formation of 1D, 2D and 3D dimensional layers as well as polynuclear structures, chains and layers. In this study, three new coordination polymers with 3-(aminomethyl)pyridine (3ampy) and hexacyanometallate(III) ions ($[M(CN)_6]^{3-}$, M = Cr, Fe or Co), $[Cd_3(\mu\text{-}3ampy)_4(H_2O)_4Cr_2(\mu\text{-}CN)_8(CN)_4]_n$(**1**), $[Cd_3(\mu\text{-}3ampy)_2(H_2O)_2Fe_2(\mu\text{-}CN)_5(CN)_7]_n$ (**2**) and $[Cd_3(\mu\text{-}3ampy)_4(H_2O)_4Co_2(\mu\text{-}CN)_8(CN)_4]_n$ (**3**), were synthesized and characterized by single crystal X-ray diffraction and powder X-ray diffraction techniques. The single crystal X-ray diffraction analyses shows that coordination polymers **1** and **3** are two-dimensional structures, whereas coordination polymer **2** is a three-dimensional structure where two adjacent metal ions are linked via 3ampy and CN bridges. The coordination spheres of all coordination polymers show distorted octahedral geometries.

Keywords: Hexacyanometalatte(III) complex, 3-(Aminomethyl)pyridine Complex, Coordination polymer

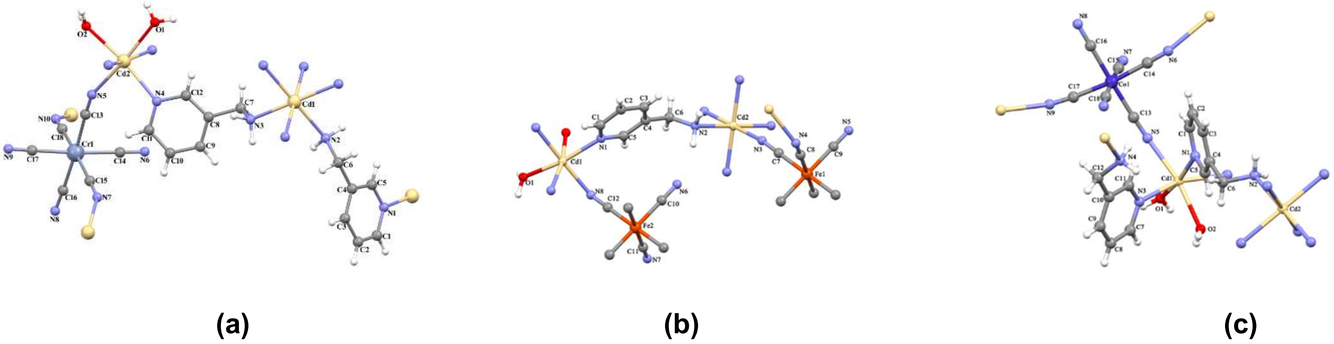


Fig. 1: The molecular structures of **1** (a), **2** (b) and **3** (c) showing the atom numbering schemes.

References

Liu M, Hu J, Wang Y. (2018) Synthesis, crystal structure and MMCT of a heterobimetallic cyanide-bridged complex trans-BrRuII $(dppe)_2(\mu\text{-}CN)$(FeIIIBr3). Polyhedron 149:79-83.

Janiak C. (2003) Engineering coordination polymers towards applications. Dalton Transactions (14):2781-804.

Kekeç, S., Kürkçüoğlu, G.S., Ünver, H., Yeşilel, O.Z., Şahin, O. (2024) Heteronuclear Hexacyanometallate(III) Coordination Polymers (Cd/Cr, Cd/Fe, Cd/Co) with 3-(Aminomethyl)pyridine: Synthesis, Characterization, and Catalytic Activities for the Peroxidative Oxidation of Benzylic Alcohols" Journal of Inorganic and Organometallic Polymers and Materials, 34:1081–1091.

Acknowledgement

This work has been financially supported by Eskişehir Osmangazi University, Scientific research Unit [grant no: 2022-2561]. The authors acknowledge Scientific and Technological Research Application and Research Center, Sinop University, Turkey, for the use of the Bruker D8 QUEST diffractometer.

Current Applications of Artificial İntelligence and Crystals

[1] Seda Sahin, [2] Seyma Kaya, [3]Cigdem Yüksektepe Ataol, [4] Lütfiye Sirka

[1]Assistant Prof. Dr., Çankırı Karatekin University, Department of Computer Engineering, Çankırı, Turkey
[2] Çankırı Karatekin University (Undergraduate Student), Department of Computer Engineering, Çankırı, Turkey
[3] Prof. Dr., Çankırı Karatekin University,Faculty of Science, Çankırı, Turkey
[4] Assistant Prof. Dr., Çankırı Karatekin University, Department of Eldivan Health Services Vocational School, Çankırı, Turkey

* E-mail: sedasahinmail@gmail.com, sedasahin@karatekin.edu.tr

Abstract

The aim of this study is to present the developments of artificial intelligence (AI) technology in the field of crystallography and to explain the relationship between crystallography and AI. Nowadays, with the use of artificial intelligence, it has become important to understand the structural properties and behaviour of crystals and also to analyse crystal structures. This study addresses how existing artificial intelligence algorithms are used in the field of crystallography and how they are effective in many areas from the synthesis of crystals to the characterisation of their properties and material design. It also discusses the role of crystals in various industrial and scientific applications and the future potential of emerging technologies together with artificial intelligence. This work serves as a guide for researchers in the field of artificial intelligence and crystallography to understand the current state and future directions.

Keywords: artificial intelligence, crystals, applications

References

Muhammad, Kennedy J., Lim C. W. (2022), Machine learning and deep learning in phononic crystals and metamaterials – A review, Materials Today Communications 33, 104606.

Kutsukake K. (2024), Review of machine learning applications for crystal growth research, Journal of Crystal Growth 630,127598.

Syntheses and crystal structures of one-dimensional $[Cd(\mu\text{-}4aepy)_2(H_2O)_2][M(CN)_4]$ [4aepy = 4-(2-aminoethylpyridine), M(II) = Ni(II) or Pd(II)] complexes

[1]Dursun KARAAĞAÇ and [2]Güneş Süheyla KÜRKÇÜOĞLU,
[1]Bursa Technical University, Faculty of Engineering and Natural Sciences, Department of Physics, TR16310, Bursa, Türkiye
[2]Eskişehir Osmangazi University, Sciences Faculty, Department of Physics, TR26040, Eskişehir, Türkiye

* E-mail: dursun.karaagac@btu.edu.tr

Abstract

Two metal-cyanide complexes given by the formula $[Cd(\mu\text{-}4aepy)_2(H_2O)_2][M(CN)_4]$ [where 4aepy = 4-(2-aminoethylpyridine), M(II) = Ni(II)(**1**) or Pd(II)(**2**)] have been synthesized, and the crystal structures of these complexes have been elucidated by single crystal X-ray diffraction technique. The structure of the complexes involves Cd(II) as the first metal, Ni(II) or Pd(II) as the second metal, and cyanide and 4-(2-aminoethylpyridine) molecules as organic ligands. It has been determined that the complexes belong to the monoclinic system and the C2/c space group using single crystal X-ray diffraction technique. The Cd(II) atom used as the first metal shows a distorted octahedral structure in coordination with the four nitrogen atoms of the 4-(2-aminoethylpyridine) molecule and the two oxygen atoms of the water molecule. In the molecular structure of the complexes, the 4-(2-aminoethylpyridine) molecule coordinates as a bridge to two cadmium atoms, but it does not coordinate to the second metal atom [Ni(II) or Pd(II)]. The atoms of the second metal, Ni(II) or Pd(II), coordinate to the four carbon atoms of the four cyanide molecules and exhibit square planar geometry. As a result of structural analysis, it has determined that the molecular structures of the complexes are similar to each other and possess a one-dimensional polymeric structure. The three-dimensional supramolecular structure of the complexes is formed by M···π and hydrogen bond (N-H···N and O-H···N) interactions. M···π interactions occur between the pyridine ring of the 4-(2-aminoethylpyridine) molecule and the M(II) metal atoms, N-H···N hydrogen bonding occurs between the NH of the 4-(2-aminoethylpyridine) molecule and the N atom of cyanide, and O-H···N hydrogen bonding occurs between the OH of the water molecule and the N atom of cyanide. Additionally, C-H···N (1) and C-H···O (2) intermolecular interactions have also been observed in the complexes.

Keywords: Tetracyanonickelate(II) complex, Tetracyanopalladate(II) complex, Cyanide complex.

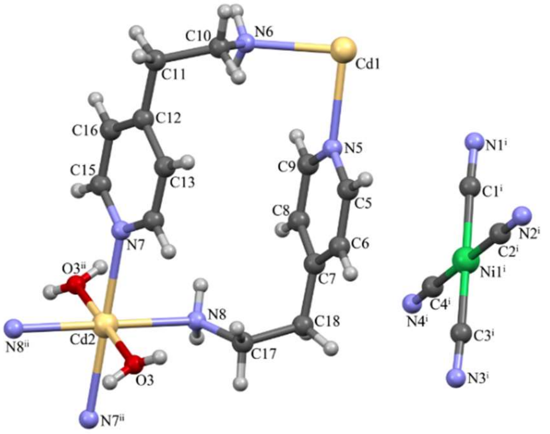


Fig. 1: The molecular structure of the complex $[Cd(\mu\text{-}4aepy)_2(H_2O)_2][Ni(CN)_4]$

References

Kürkçüoğlu, G.S., Yeşilel, O.Z., Sayın, E., Şahin, O. (2022). Nine new tetracyanometallate(II) complexes with 2-(2-aminoethyl)pyridine: synthesis, crystal structures and spectroscopic studies, Journal of Coordination Chemistry, 75, 9-10.
Kürkçüoğlu, G.S., Yeşilel, O.Z., Kekeç, S., Ünver, H., Şahin, O. (2022). Syntheses and characterizations of two-dimensional heteronuclear tetracyanonickelate(II) complexes with 4-ethylpyridine and investigation of the catalytic activity of $[Cd(4epy)_2Ni(\mu\text{-}CN)_4]_n$, Journal of Coordination Chemistry, 76, 16-24.

Karaağaç, D., Kürkçüoğlu, G.S., Şenyel, M., Hökelek, T. (2017). Syntheses, structural characterization and spectroscopic studies of cadmium(II)-metal(II) cyanide complexes with 4-(2-aminoethyl)pyridine, Journal of Molecular Structure, 1130, 80-88.

Acknowledgement

We would like to thank Prof. Dr. Tuncer Hökelek for the analysis of the crystal data of the compounds.

Synthesis, Crystal Structure, Hirshfeld Surface Analysis, Molecular Docking, IR Spectroscopy and DFT Calculations of a Novel 2D Layered Hybrid Compound (C6H10N3O)2Cu2Cl6

[1]Chaima Gharbi, [2]Yusuf Sert, [3]Emine Berrin Poyraz, [4]Uwe Böhme, [3]Necmi Dege, [1]Chérif Ben Nasr, [5]Lamia Khedhiri

[1]Laboratoire de Chimie des Matériaux, Faculté des Sciences de Bizerte, Université de Carthage, 7021, Zarzouna, Tunisia
[2]Science and Art Faculty-Department of Physics, Sorgun Vocational School, Yozgat Bozok University, Yozgat, Turkey
[3]Department of Physics, Faculty of Arts and Sciences, Ondokuz Mayis University, 55200, Samsun, Turkey
[4]Institut für Anorganische Chemie, TU Bergakademie Freiberg, Leipziger Str. 29, 09599, Freiberg, Germany
[5]Laboratoire des Matériaux Utiles, Institut National de Recherche et d'Analyse physico-chimique (INRAP), Technopole Sidi Thabet, 2020, Ariana, Tunisia

E-mail: emineberrin61@gmail.com

Abstract

The 2D hybrid compound bis(2-amino-4-methoxy-6-methylpyrimidinium) bis(μ₂-chloro)-tetrachloro-di- copper(II), $(C_6H_{10}N_3O)_2Cu_2Cl_6$, is successfully synthesized by slow solvent evaporation at room temperature. Structural properties have been investigated through single-crystal X-ray diffraction and reveal that the structure contains a centrosymmetric hexachlorodicuprate group where each Cu atom is coordinated to four Cl atoms in a slightly distorted square planar geometry. There are short contacts between neighboring $[Cu_2Cl_6]^{2-}$ dimer units. The crystalline building stability is ensured by N–H···Cl and C–H···O hydrogen bonding as well as weak C–H···π intermolecular interactions. From the infrared spectroscopy analysis, the functional groups were identified. Simultaneously, the electrical properties and Hirshfeld surface analyses were also elucidated. Furthermore, the molecular docking study of 2D hybrid compound bis(2-amino-4-methoxy-6-methylpyrimidinium) bis(2-chloro)-tetrachloro-di-copper(II) ligand with an HSP90/PDB: 5LRZ was performed by Autodock Vina. Additionally, drug-likeness and ADME properties and evaluations of the newly synthesized molecule were performed in detail. FT-IR was used to explore the modes of vibration of the different functional groups present in the studied compound.

Keywords: Crystal Structure, Hirshfeld Surface, drug-likeness, copper complex

References

F. Girardi, E. Cappelletto, J. Sandak, G. Bochicchio, B. Tessadri, S. Palanti, E. Feci, and R. D. Maggio (2014). Prog. Org. Coat. 77, 449–457.

M. Szafranski (2016). Cryst. Growth Des. 16, 3771–3776.

H. B. Duan, X. M. Ren, and Q. J. Meng (2010). Coord. Chem. Rev. 254, 1509–1522.

C. Bellitto, E. M. Bauer, and G. Righini (2015). Coord. Chem. Rev. 289–290, 123–136.

J. M. Lei, Q. X. Peng, S. P. Luo, Y. Liu, S. Z. Zhan, and C. L. Ni (2018). Mol. Catal. 448, 10–1.

Experimental and theoretical investigation on *N*-(3-hydroxyphenyl)benzenesulfonamide

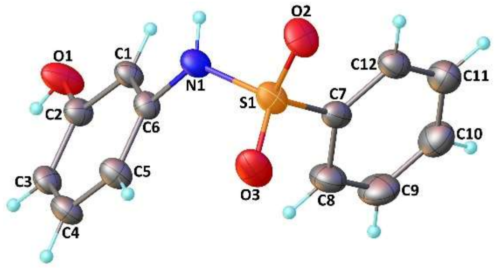
[1]İlkay Yıldırım Gümüşhan,
[1]Biruni University, Vocational School, Department of Medical Services and Techniques,
Radiotherapy Program, 34010, İstanbul, Turkey,

* E-posta: iyildirim@biruni.edu.tr

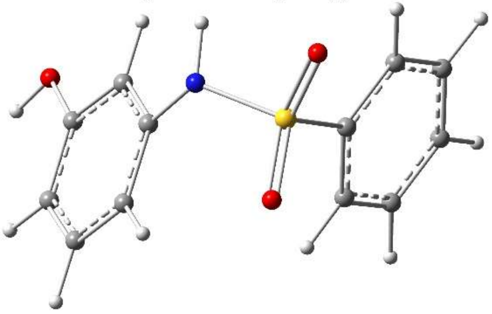
Abstract

The title compound has been characterized by single-crystal X-ray diffraction technique which crystallizes in space group *I*2/*a* with eigth molecules in the unit cell. X-ray analysis shows that intermolecular O—H···O and N—H···O hydrogen bonds stabilize the crystal structure. Quantum-chemical computations were carried out with the GaussView 5 (Dennington et al., 2009) molecular visualization program and the Gaussian 09 program package (Frisch et al., 2009). The molecular structure was optimized using HSEH1PBE density functional method (Heyd et al., 2006) at cc-pVDZ basis set (Dunning Jr., 1989). There exists a good correlation between experimental and theoretical findings.

Keywords: Crystal structure, DFT, spectroscopy.



experimental (X-ray)



theoretical (DFT)

Fig. 1: Experimental and optimized structure of N-(3-hydroxyphenyl)benzenesulfonamide

References

Dennington, R., Keith, T., Millam, J. (2009). GaussView, Version 5.0, Semichem Inc., Shawnee Mission, KS.

Dunning Jr., T.H. (1989). Gaussian basis sets for use in correlated molecular calculations. I. The atoms boron through neon and hydrogen. Journal of Chemical Physics, 90(2), 1007-1023.

Frisch, M.J., Trucks, G.W., Schlegel, H.B., et al. (2009). Gaussian 09, Revision C.01, Gaussian, Inc., Wallingford CT.

Heyd, J., Scuseria, G.E., Ernzerhof, M. (2006). Erratum: “Hybrid functionals based on a screened Coulomb potential” [J. Chem. Phys. 118, 8207 (2003)]. Journal of Chemical Physics, 124, 219906.

Synthesis, single crystal X-ray, Hirshfeld surface analysis and DFT calculation based NBO, HOMO-LUMO, MEP, ECT and molecular docking analysis of N'-[(2,6-dichlorophenyl)methylidene]-2-{[3-(trifluoromethyl)phenyl]amino}benzohydrazide

[1]Abdurrahman Suhta, [2]Sude Saral, [1]Ufuk Çoruh, [2]Sevgi Karakuş, [3]Ezequiel M. Vazquez Lopez
[1] Ondokuz Mayıs University, Faculty of Sciences, Department of Physics, Samsun, Turkey
[2] Marmara University, Faculty of Pharmacy, Department of Pharmaceutical Chemistry, İstanbul, Turkey
[3] University of Vigo, Faculty of Sciences, Department of Inorganic Chemistry, Galicia, Spain

* E-mail: a.suhta@hotmail.com

Abstract

A new Schiff base compound of N'-[(2,6-dichlorophenyl)methylidene]-2-{[3-(trifluoromethyl)phenyl]amino}benzohydrazide was synthesized and characterized through various spectroscopic techniques, including infrared, ^{1}H NMR, ^{13}C NMR spectroscopy and X–ray diffraction. Experimental results collected by XRD were compared with theoretical results obtained from Density functional theory method. Hirshfeld surface analysis was used to obtain three dimension molecular surface and two dimension fingerprint plots to illustrate the intermolecular bonding. Theoretical calculations provide valuable insights into both global and local chemical activity, as well as the properties of molecules and chemicals, including their nucleophilic and electrophilic nature. The DFT method at B3LYP/6–311++G (d,p) basis set was employed to study the optimized structure and geometric parameters, as well as to explore the frontier molecular orbitals, global reactive parameters and molecular electrostatic potential characteristics which cannot be obtained by experimental methods. Additionally, electrophilicity based charge transfer study was carried out with DNA bases to determine the direction of charge transfer. Finally, an investigation was carried out using molecular docking analysis to examine the binding energies of the title compound with PDB ID: 2QDJ protein target. The analysis yielded significant insights into the possible interactions, offering valuable findings in the process.

Keywords: Hydrazone; DFT calculations; X-ray Diffraction

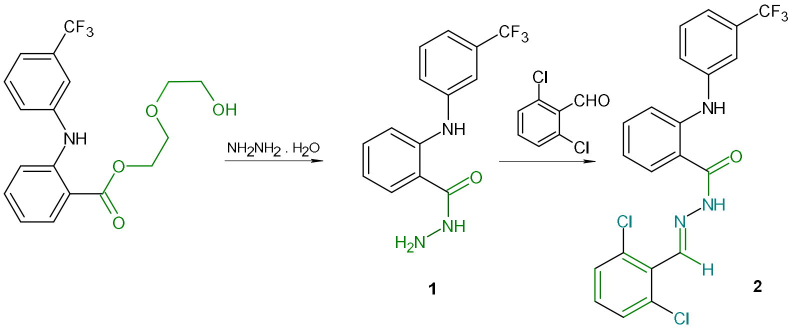


Fig. 1: Synthesis of *N*'-[(2,6-dichlorophenyl)methylidene]-2-{[3-(trifluoromethyl)phenyl]amino} benzohydrazide

References

Verma, G., Marella, A., Shaquiquzzaman, M., Akhtar, M., Ali, M. R., & Alam, M. M. (2014). A review exploring biological activities of hydrazones. Journal of Pharmacy & Bioallied Sciences, 6(2), 69. https://doi.org/10.4103/0975-7406.129170

Tatum, L. A., Su, X., & Aprahamian, I. (2014). Simple hydrazone building blocks for complicated functional materials. Accounts of Chemical Research, 47(7), 2141-2149. https://doi.org/10.1021/ar500111f

Paulus, W., Ringsdorf, H., Diele, S., & Pelzl, G. (1991). Columnar phases from semi-discoid molecules: Phase induction via hydrogen bonding and charge transfer interactions. Liquid Crystals, 9(6), 807-819. https://doi.org/10.1080/02678299108055003

Poster Presentations

	Scientific Program – Poster Presentations
(P-1)	**Onur Şahin** Sc-Xrd Analysis From Crystal Selection To Structure Solution
(P-2)	**Zarife Sibel Şahin, Zeki Kartal** Molecular characterization of a one-dimensional Ni(II) complex
(P-3)	**Gökhan Alpaslan, Halil Gökce, Mustafa Macit, Namık Özdemir** Crystal structure, Spectroscopic Analyses and DFT Studies of (E)-1-(3-((3,5-di-tert-butyl-2-hydroxybenzylidene)amino)phenyl)ethan-1-one
(P-4)	**Nadihan Yolgeçti, Mehmet Akkurt, Ezgi Pehlivanlar, Gökalp Çetin, Rahime Şimşek, Metin Kul, Sema Öztürk Yıldırım, Ray J. Butcher** Synthesis and Crystal Structure of Methyl 4-[4-(difluoromethoxy)phenyl]-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline
(P-5)	**Nefise Özçelik, Raziye Çatak Çelik, Tuncay Tunç** 2-[(2E)-2-(2-klor-4-florobenziliden)hidrazinli]piridin
(P-6)	**Nadihan Yolgeçti, Mehmet Akkurt, Gökalp Çetin, Rahime Şimşek, Sema Öztürk Yıldırım, Ray J. Butcher** Isopropyl 4-[4-(difluoro-methoxy)phenyl]-2,6,6-trimethyl-5-oxo-1,4,5,6,7,8-hexa-hydroquinoline-3-carboxylate: Synthesis and Crystal Structure
(P-7)	**İlknur Şimşek, Yelda Bingöl Alpaslan, Mustafa Macit, Namık Özdemir** The Single-Crystal X-ray Diffraction Analysis and Quantum Mechanical Calculations of (E)-2,4-di-tert-butyl-6-((3,4-dimethoxybenzylimino)methyl)phenol $(C_{24}H_{33}NO_3)$
(P-8)	**Nadihan Yolgeçti, Mehmet Akkurt, Gökalp Çetin, Rahime Şimşek, Sema Öztürk Yıldırım, Ray J. Butcher** Tertbutyl 4-[4-(difluoromethoxy)phenyl]-2,6,6-trimethyl-5-oxo-1,4,5,6,7,8-hexahydro-quinoline-3-carboxylate: Crystallographic Characterization
(P-9)	**Onur Rauf Yılmaz, Çiğdem Albayrak Kaştaş, Canan Kazak** Determination of The Structure of (E)-2-Bromo-4-Methyl-6-[(4-Bromo-Phenylimino)Methyl]Phenol by XRD, FT-IR, UV-Vis and Computational Identification

(P-10)	**Yelda Bingöl Alpaslan, İlknur Şimşek, Mustafa Macit** Single-Crystal X-ray Diffraction Analysis and Quantum Mechanical Calculations of (E)-2,4-di-tert-butyl-6-((4-iodophenylimino)methyl)phenol ($C_{21}H_{26}INO$)
(P-11)	**Duygu Barut Celepci** Understanding the Biological Activity of Malvin as an Anthocyanin Compound Using Theoretical Approaches
(P-12)	**Şenol Toprak** Quantum Mechanical Calculation Of Some Chemical Properties Of The Hypericin Molecule
(P-13)	**Çiğdem Albayrak Kaştaş, Gökhan Kaştaş** The investigation of molecular and crystal structures for (E)-2-[(4-bromo-3-methylphenylimino)methyl]-6-ethoxyphenol with experimental and computational methods
(P-14)	**Başak Koşar Kırca, Çiğdem Albayrak Kaştaş** (E)-2-((Bromophenylimino)methyl)-3,4-dichloro-6-ethoxyphenol
(P-15)	**Gökhan Kaştaş, Çiğdem Albayrak Kaştaş** Structural Investigation of bis{2-ethoxy-6-(E)-[(3-methylphenyl)imino) methyl] phenolato-κN,κO}copper(II)monohidrate
(P-16)	**Sultan Başak, Cem Cüneyt Ersanlı** Elucidation of the structure of a molecule containing a Schiff base using quantum chemical methods and investigation of its anticancer properties
(P-17)	**Erbil Dağdelen, Erbil Ağar, Canan Kazak** Crystal Structure and Molecular Docking of (E)-4-((3-chloro-4-hydroxy benzylidene)amino)-1,5-dimethyl-2-phenyl-1H-pyrazol-3(2H)-one
(P-18)	**Merve İzmirli, Hande Karabıyık, Resul Sevinçek, Hasan Karabıyık, Duygu Barut Celepci, Muhittin Aygün** Crystal Structure and Hirshfeld Surface Analyses of two novel benzimidazole bromide compounds
(P-19)	**New Benzimidazolium Salts Bearing Chloro-/Fluorobenzyl-Substituted: Synthesis and Crystal Structures** Betül ŞEN YÜKSEL, Resul Sevinçek Aydın AKTAŞ, Yetkin GÖK, Muhittin AYGÜN

Sc-Xrd Analysis From Crystal Selection To Structure Solution

[1*]Onur ŞAHİN

[1] Sinop University, Faculty of Health Sciences, Department of Occupational Health & Safety, Sinop, Türkiye

* E-mail: onurs@sinop.edu.tr

Abstract

Single crystal X-ray diffraction analysis is an effective and accurate analysis used in structure determination. The purpose of this analysis process is to determine the structure of crystals in single crystal form at the atomic scale. In this study, I aim to provide a detailed explanation of the single crystal analysis process, which is an intensively used field, so that it can be better understood by all users. In this regard, it aims to make the operations easier to understand by supporting the explanation with pictures. Single crystal XRD analysis is explained step by step for all application steps, starting from the first step, crystal selection. Data reduction was performed with APEX 3. Data were corrected for absorption effects using the multi-scan method (SADABS). The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm.

Keywords: SC-XRD, APEX 3.

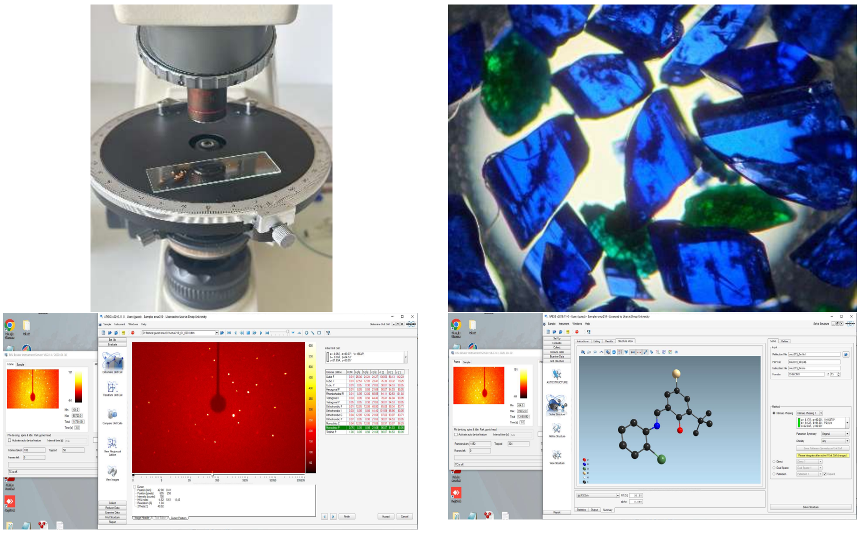


Fig. 1: Processes from crystal selection to data collection.

References

APEX 3, Bruker AXS Inc. Madison Wisconsin USA (2013).

SADABS, Bruker AXS Inc. Madison Wisconsin USA (2012).

SAINT, Bruker AXS Inc. Madison Wisconsin USA (2013).

Molecular characterization of a one-dimensional Ni(II) complex

[1*]Zarife Sibel ŞAHİN, [2]Zeki KARTAL
[1] Sinop University, Faculty of Engineering and Architecture, Department of Energy Systems Engineering, Sinop, Türkiye
[2] Retired Professor, Kütahya, Türkiye

* E-mail: zarifesibel@sinop.edu.tr

Abstract

The X-ray single crystal study shows that the complex **1** has 1D coordination polymer. The Ni(II) ion is coordinated by three nitrogen atoms from 3-aminopyridine ligands, two nitrogen atoms from thiocyanate molecules, one oxygen atom from aqua ligand, thus showing a octahedral coordination geometry. The Ni(II) ions are bridged by amino groups to form a 1D coordination polymer which is running parallel to the [010] direction. Adjacent these 1D coordination polymers are joined by N-H···O, O-H···N and N-H···S hydrogen bonds to generate 3D supramolecular network.

The structure was solved by direct methods using SHELXS-2013 [1] and refined by full-matrix least-squares methods on F^2 using SHELXL-2013 [2]. The following procedures were implemented in our analysis: program used for molecular graphics were as follow: MERCURY programs [3]; GUI for other software related to structure solution: WinGX [4].

Keywords: SC-XRD, coordination polymer, hydrogen bonds.

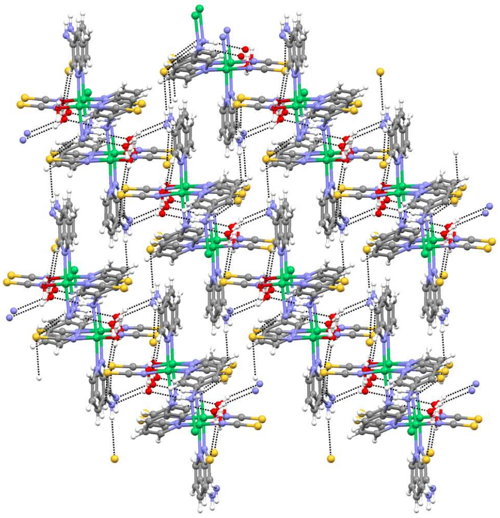


Fig. 1: The 3D supramolecular network

References

[1] Sheldrick, G.M. Acta Cryst. 2008, A64, 112.
[2] Sheldrick, G. M. Acta Cryst. 2015, C71, 3.
[3] Macrae, C. F., Sovago, I., Cottrell, S. J., Galek, P. T. A., McCabe, P., Pidcock, E., Platings, M., Shields, G. P., Stevens, J. S., Towler, M. & Wood, P. A. (2020). J. Appl. Cryst. 53, 226-235.
[4] Farrugia, L. J. (2012). J. Appl. Cryst. 45, 849–854.

Crystal structure, Spectroscopic Analyses and DFT Studies of (*E*)-1-(3-((3,5-di-tert-butyl-2-hydroxybenzylidene)amino)phenyl)ethan-1-one

[1*]Gökhan Alpaslan, [1]Halil Gökce, [2]Mustafa Macit, [3]Namık Özdemir

[1]Giresun University, Vocational High School of Health Services, Department of Medical Services and Techniques, Giresun, Turkey
[2]Ondokuz Mayıs University, Faculty of Arts & Science, Department of Chemistry, Samsun, Turkey
[3] Ondokuz Mayıs University, Faculty of Arts & Science, Department of Physic, Samsun, Turkey

* E-mail: gokhan.alpaslan@giresun.edu.tr

Abstract

The molecular structure of the title compound, $C_{23}H_{29}NO_2$, was determined by X-ray single crystal diffraction technique. The compound crystallizes in the monoclinic, space group $P2_1/c$ with unit cell dimensions a=19.2539(19) Å, b= 7.1440(7) Å, c= 16.7712(16) Å, β=111.265(7)° and Z=4. X–ray diffraction investigation shows that the title compound in phenol–imine form with O−H···N intramolecular hydrogen bond. Detailed investigations of the presence and nature of the intermolecular contacts within solid state crystal packing form of title compound were examined by Hirshfeld surface analysis. The optimized molecular geometry and vibrational wavenumbers of the compound have been calculated using the density functional method (DFT) in the ground state and compared with the experimental data. In addition, DFT calculations of the compound, molecular electrostatic potential (MEP) and frontier molecular orbital calculations were performed at B3LYP/6-311++G(d,p) level of theory.

Keywords: Crystal Structure, Hirshfeld, DFT.

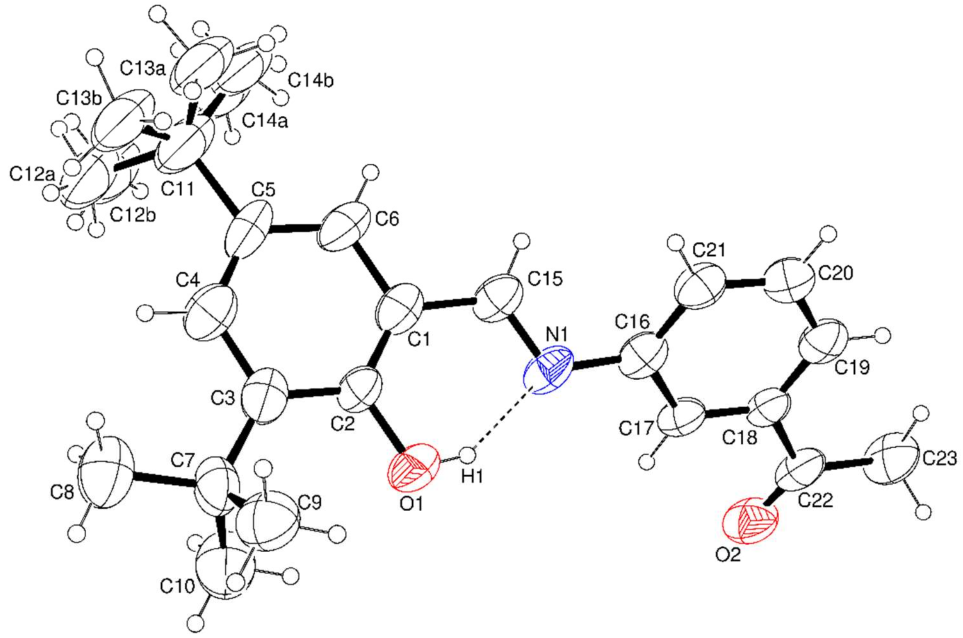


Fig. 1: ORTEP-3 structure of title compound

Synthesis and Crystal Structure of Methyl 4-[4-(difluoromethoxy)phenyl]-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline

[1]Nadihan Yolgeçti, [1]Mehmet Akkurt, [2]Ezgi Pehlivanlar, [3]Gökalp Çetin, [2]Rahime Şimşek, [4]Metin Kul,
[1.4]Sema Öztürk Yıldırım, [5]Ray J. Butcher

[1]Erciyes University, Faculty of Science, Department of Physics 38039 Kayseri, Türkiye
[2]Hacettepe University, Faculty of Pharmacy, Department of Pharmaceutical Chemistry 06100 Sıhhiye-Ankara, Türkiye
[3]Erzincan Binali Yıldırım University, Faculty of Pharmacy, Department of Pharmaceutical Chemistry, 24002, Erzincan, Türkiye
[4]Eskişehir Technical University, Faculty of Science, Department of Physics, 26470 Eskişehir, Türkiye
[5]Howard University Department of Chemistry, Washington DC 20059, USA

*E-mail: nadihanyolgecti@hotmail.com and ozturk@erciyes.edu.tr

Abstract

Methyl 4-[4-(difluoromethoxy)phenyl]-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline crystallizes with Z = 8 in the C 2/c monoclinic space group. In the crystal structure, molecules are linked by N—H…O and C—H…O interactions, forming a periodic network in three dimensions. The cohesion of the molecular packing is ensured by van der Waals forces between these layers. The 1,4-dihydropyridine ring (N1/C1/C6–C9) of the compound as shown in Figure 1 adopts a distorted boat conformation [puckering parameters (Cremer & Pople, 1975) are Q_T = 0.196 Å, θ = 72.2° and φ = 185.8°], while the cyclohexane ring (C1– C6) has a distorted half-chair conformation. The atoms of the 4-difluoromethoxyphenyl group in the compound are disordered over two sites with refined occupancy factors of 0.647 and 0.353. Disorder 4-[4-(difluoromethoxy]phenyl ring major (C15–C20) and minor (C15A–C20A) components are separated by the mean plane of the quinoline ring system [N1/C1– C9; maximum deviation = 0.382 (2) Å] by 80 Å, respectively.

Keywords: Crystal structure, 1,4-dihydropyridine ring.

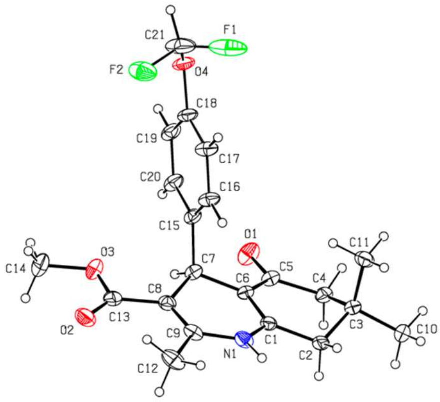


Figure 1. Molecular Structure of the Compound.

References

Cremer, D. & Pople, J. A. (1975). *J. Am. Chem. Soc.* **97**, 1354–1358.
Pehlivanlar, E., Yıldırım, S.Ö, Simşek R., Akkurt, M., Butcher, R. J. & Bhattarai, A. (2023). *Acta Cryst.* E**79**, 664–668.
Yıldırım, S.Ö., Akkurt, M., Pehlivanlar, E., Çetin, G., Şimşek, R., Butcher, R. J. & Bhattarai, A. (2023). *Acta Cryst.* E**80**, 1-8.

2-[(*2E*)-2-(2-klor-4-florobenziliden)hidrazinli]piridin

[1*]Nefise Özçelik, [2]Raziye Çatak Çelik, [3]Tuncay Tunç
[1,2] Aksaray Üniversity, Arts and Sciences Faculty, Physics Department, Aksaray, TURKEY
[3] Aksaray Üniversity, Education Faculty, Science Education Department, Aksaray, TURKEY

* E-mail: nefised@gmail.com

Abstract

The condensation product of a hydrazine with aldehydes or ketones is called hydrazone. Hydrazones are ligands which can be synthesized in a very simple way and are good crystallizing compounds with sharp melting points. Hydrazones are also very 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-4-fluorobenzylidene)hydrazinyl]pyridine schiff base molecule has been synthesized and characterized by single crystal X-ray determination (Fig. 1) . Intensity data were collected with a 16 Megapixel Bruker APEX-II CCD detector on the Bruker Smart Breeze three circles diffractometer at the Aksaray University, Science and Technology Application and Research Center. Unit cell was determined with 5825 reflections. According to the data found, it was seen that the monoclinic system in the P $2_1/c$ space group crystallized. The collected data were applied the multi-scan absorption correction. The crystal structure was directly solved using the SHELXS-97 program [8] in the WinGX program [9], which was found in 2465 independent reflection out of 17626 total reflections. According to the criteria determined in the refinement process, the refinement was carried out by the least squares method using the SHELXL-2018 program [8], taking into account 155 parameters for 1551 reflections. As a result of the refinement, bond lengths, bond angles, torsion angles, atomic coordinates and temperature parameters of the structure were obtained. It was determined that there was an N-H…N hydrogen bond between the molecules in the crystal.

Keywords: Hydrazone, Crystal, X-Ray.

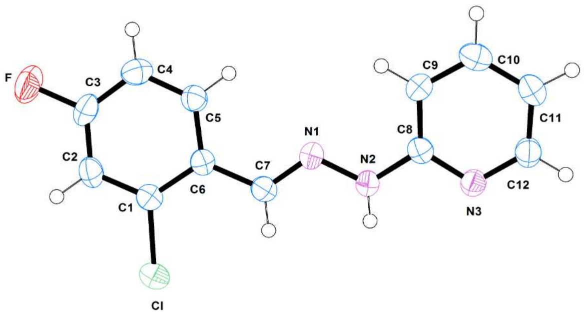


Fig. 1: An ORTEP-III drawing of title compound.

References

1. Tunç, T., Tezcan, H., Sari, M. , Büyükgüngör, O., Yağbasan, R. (2003). N-(4-nitrobenzylidene)-N'-phenylhydrazine. Acta Cryst., C59: o528-o529.
2. Fun, H. K., Sujith,K.V., Patil, P.S., Kalluraya, B., Chantrapromma,S. (2008). N′-[(*E*)-1-Phenyl-ethyl--idene]benzo-hydrazide. Acta Cryst., E64: o1961-o1962.
3. Koçyiğit Kaymakçıoğlu, B., Oruç, E., Unsalan, S., Kandemirli, F., Shvets, N., Rollas, S., Anatholy, D. (2006). Synthesis and characterization of novel hydrazide–hydrazones and the study of their structure–antituberculosis activity. Eur. J. Med. Chem., 41(11): 1253-1261.
4. Küçükgüzel, S. G., Rollas, S., Küçükgüzel, I., Kiraz, M. (1999). Synthesis and antimycobacterial activity of some coupling products from 4-aminobenzoic acid hydrazones. Eur. J. Med. Chem., 34(12): 1093-1100.
5. Maccari,R., Ottana, R., Vigorita, M.G. (2005). In vitro advanced antimycobacterial screening of isoniazid-related hydrazones, hydrazides and cyanoboranes: Part 14. Bioorg. Med. Chem. Lett., 15(10): 2509-2513.
6. Raparti, V., Chitre, T., Bothara, K., Kumar, V., Dangre, S., Khachane, C., Gore, S., Deshmane, B. (2009). Novel 4-(morpholin-4-yl)-N′-(arylidene)benzohydrazides: Synthesis, antimycobacterial activity and QSAR investigations. Eur. J. Med. Chem., 44(10): 3954-3960.
7. Easmon, J., Purstinger, G., Thies, K.S., Heinisch, G., Hofmann, J. (2006). Synthesis, Structure−Activity Relationships, and Antitumor Studies of 2-Benzoxazolyl Hydrazones Derived from Alpha-(N)-acyl Heteroaromatics. J. Med. Chem., 49(21): 6343-6350.
8. Sheldrick, G. M. (2008). A short history of SHELX. Acta Cryst., A64(1): 112-122.
9. Farrugia, L. (1999). WinGX suite for small-molecule single-crystal crystallography. J. Appl. Cryst., 32(4): 837-838.

Isopropyl 4-[4-(difluoro-methoxy)phenyl]-2,6,6-trimethyl-5-oxo-1,4,5,6,7,8-hexa-hydroquinoline-3-carboxylate: Synthesis and Crystal Structure

[1]Nadihan Yolgeçti, [1]Mehmet Akkurt, [2]Gökalp Çetin, [3]Rahime Şimşek, [1,4]Sema Öztürk Yıldırım, [5]Ray J. Butcher

[1]Erciyes University, Faculty of Science, Department of Physics 38039 Kayseri, Türkiye
[2]Erzincan Binali Yıldırım University, Faculty of Pharmacy, Department of Pharmaceutical Chemistry, 24002, Erzincan, Türkiye
[3]Hacettepe University, Faculty of Pharmacy, Department of Pharmaceutical Chemistry 06100 Sıhhiye-Ankara, Türkiye
[4]Eskişehir Technical University, Faculty of Science, Department of Physics, Yunus Emre Campus 26470 Eskişehir, Türkiye
[5]Howard University Department of Chemistry, Washington DC 20059, USA

*E-mail: nadihanyolgecti@hotmail.com and ozturk@erciyes.edu.tr

Abstract

Isopropyl 4-[4-(difluoro-methoxy)phenyl]-2,6,6-trimethyl-5-oxo-1,4,5,6,7,8-hexa-hydroquinoline-3-carboxylate orthorhombic P bca It crystallizes in the space group with Z = 8. In the crystal, molecules are bonded by N—H…O, C—H…F and C—H… π interactions, forming layers parallel to the (002) plane. The stability of molecular packing is provided by van der Waals forces between these layers. The 1,4-Dihydropyridine (N1/C1/C6–C9) and cyclohexane (C1—C6) rings both have the distorted boot conformation (Figure 1) [for the 1,4-dihydropyridine ring, shrinkage parameters: Q_T = 0.3187 (9) Å, θ = 105.86 (16)°, φ = 359.72 (17)° and for the cyclohexane ring: Q_T= 0.4332(11) Å θ = 131.14(13)°, φ= 301.37 (17)°]. The 4-[4-(Difluoromethoxy]phenyl ring (C17–C22) has a dihedral of 86.39 (4)° with the mean plane of the quinoline ring system (N1/C1–C9; maximum deviation = 0.421 (1)) Å]. makes an angle.

Keywords: crystal structure, cyclohexane ring; van der Waals interactions.

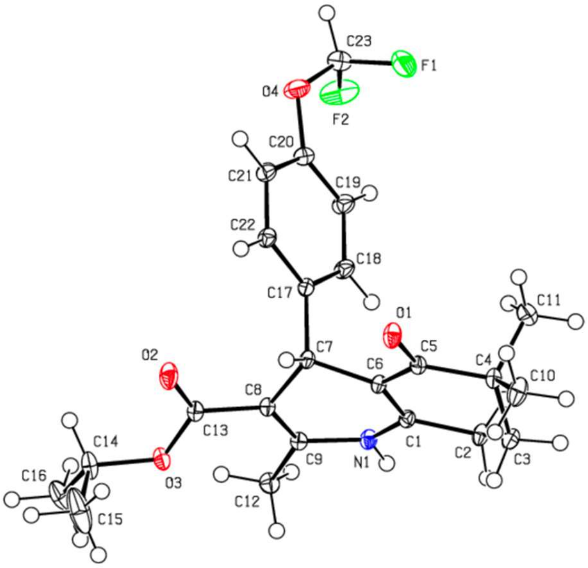


Figure 1. Moleculer Structure

References

Yıldırım, S.Ö, Akkurt, M.,Çetin, G., Şimşek, R., Butcher, R. J. & Bhattarai, A. (2022). *Acta Cryst.* E**78**, 798–803.
Yıldırım, S.Ö., Akkurt, M., Pehlivanlar, E., Çetin, G., Şimşek, R., Butcher, R. J. & Bhattarai, A. (2023). *Acta Cryst.* E**80**, 1-8.

The Single-Crystal X-ray Diffraction Analysis and Quantum Mechanical Calculations of (*E*)-2,4-di-tert-butyl-6-((3,4-dimethoxybenzylimino)methyl)phenol *($C_{24}H_{33}NO_3$)*

[1*]**İlknur Şimşek**, [1]**Yelda Bingöl Alpaslan**, [2]**Mustafa Macit**, [3]**Namık Özdemir**

[1]Giresun University, Faculty of Arts & Science, Department of Physic, Giresun, Turkey
[2]Ondokuz Mayıs University, Faculty of Arts & Science, Department of Chemistry, Samsun, Turkey
[3] Ondokuz Mayıs University, Faculty of Arts & Science, Department of Physic, Samsun, Turkey

* E-mail: ilknursimsek28.is@gmail.com

Abstract

The molecular structure of the title compound, $C_{24}H_{33}NO_3$, was determined by X-ray single crystal diffraction technique. The compound crystallizes in the monoclinic, space group $P2_1/n$ with unit cell dimensions a=8.7461(8) Å, b= 35.213(3) Å, c= 7.3723(8) Å, β=95.525(8)° and Z=4. X–ray diffraction investigation shows that the title compound in phenol–imine form with O−H···N intramolecular hydrogen bond. The quantum mechanical calculations of crystals were carried out with Gaussian 09W [1] package program using Density Functional Theory (DFT) in order to compare the obtained experimental data with theoretical data and to determine some molecular properties that cannot be determined by the X-ray single crystal diffraction method. Firstly, the optimized molecular geometry of the compound have been calculated using B3LYP/6-311++G(d,p) level of theory. Additionally, Mulliken atomic charges distribution, Molecular Electrostatic Potential (MEP) and Frontier Molecular Orbitals (FMOs) calculations were at the same methods.

Keywords: Schiff Base, X-ray diffraction, Quantum Chemical Methods, Density Functional Theory

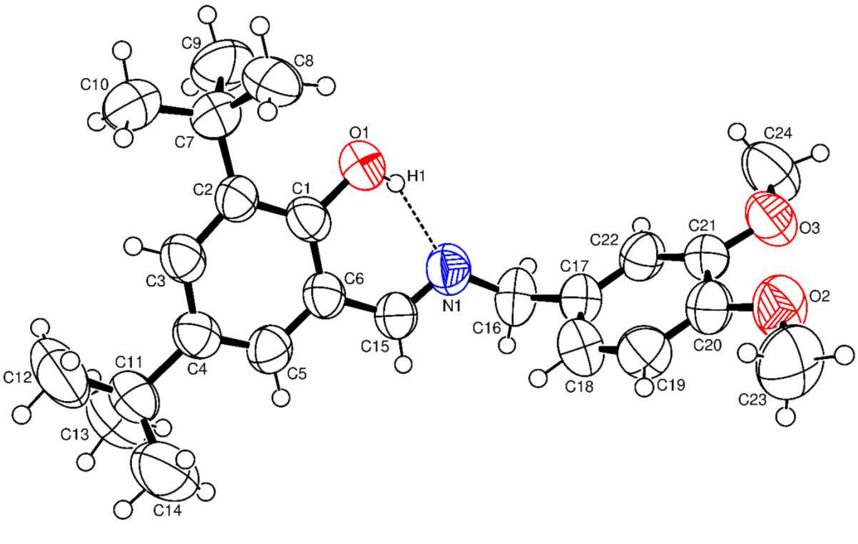


Fig. 1: ORTEP-3 structure of title compound

Kaynaklar

[1] M. J. Frisch, G. Trucks, H. Schlegel, G. Scuseria, M. Robb, J. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G.Petersson, Gaussian 09, Revision D. 01, Gaussian, Inc., Wallingford, 20, CT, 2009.

Tertbutyl 4-[4-(difluoromethoxy)phenyl]-2,6,6-trimethyl-5-oxo-1,4,5,6,7,8-hexahydro-quinoline-3-carboxylate: Crystallographic Characterization

[1]Nadihan Yolgeçti, [1]Mehmet Akkurt, [2]Gökalp Çetin, [3]Rahime Şimşek, [1.4]Sema Öztürk Yıldırım,
[5]Ray J. Butcher

[1]Erciyes University, Faculty of Science, Department of Physics 38039 Kayseri, Türkiye
[2]Erzincan Binali Yıldırım University, Faculty of Pharmacy, Department of Pharmaceutical Chemistry, 24002, Erzincan, Türkiye
[3]Hacettepe University, Faculty of Pharmacy, Department of Pharmaceutical Chemistry 06100 Sıhhiye-Ankara, Türkiye
[4]Eskişehir Technical University, Faculty of Science, Department of Physics, Yunus Emre Campus 26470 Eskişehir, Türkiye
[5]Howard University Department of Chemistry, Washington DC 20059, USA

*E-mail: nadihanyolgecti@hotmail.com and ozturk@erciyes.edu.tr

Abstract

The compound crystallizes in the orthorhombic P bca space group with Z = 8. The 1,4-Dihydropyridine ring (N1/C1 – C4/C9) and the cyclohexane ring (C4 – C9) both have a distorted boat structure [shrinkage parameters for the 1,4-dihydropyridine ring: Q_T = 0.3403 Å, ϴ = 73.4°, φ = 180.4° and for the cyclohexane ring: Q_T = 0.420 Å, ϴ = 131.7 (6)°, φ = 356.2°]. The 4-[4-(Difluoromethoxy] phenyl ring (C18 – C23) is a component of the major and minor disordered components of the quinoline ring system with their mean planes dihedral angles of 84.47 (4) and 88.71 (5)°, respectively, in the cyclohexane ring of the quinoline ring system (Figure 1).

The two carbon atoms (C7/C7A and C8/C8A), the atoms of the dimethyl group attached to the cyclohexane ring, and the two carbon atoms of the cyclohexane ring are disordered in the crystal over two regions in the ratio of 0.646 (3):0.354 (3). They form layers parallel to the (0 0 2) plane by bonding with C—H…F and C—H…p interactions.

Keywords: Crystal structure, quinoline ring system, disorder.

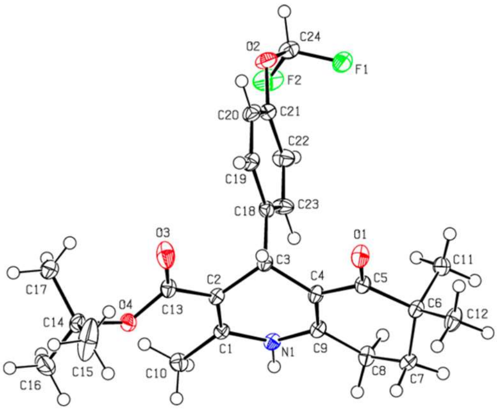


Figure 1. Moleculer Structure

References

Yıldırım, S.Ö, Akkurt, M., Çetin, G., Şimşek, R., Butcher, R. J. & Bhattarai, A. (2022). *Acta Cryst.* E**78**, 798–803.
Yıldırım, S.Ö., Akkurt, M., Pehlivanlar, E., Çetin, G., Şimşek, R., Butcher, R. J. & Bhattarai, A. (2023). *Acta Cryst.* E**80**, 1-8.

Determination of The Structure of (E)-2-Bromo-4-Methyl-6-[(4-Bromo-Phenylimino)Methyl]Phenol by XRD, FT-IR, UV-Vis and Computational Identification

[1*]Onur Rauf YILMAZ, [2]Çiğdem ALBAYRAK KAŞTAŞ, [3]Canan KAZAK,
[1] Sinop University, Faculty of Arts and Science, Physics Department, Sinop,
[2] Sinop University, Faculty of Arts and Science, Chemistry Department, Sinop,
[3] Ondokuz Mayis University, Faculty of Sciences, Physics Department, Samsun,

* E-mail: oryilmaz@sinop.edu.tr

Abstract

We examine the structure of (E)-2-Bromo-4-methyl-6-[(4-bromo-phenylimino)methyl]phenol geometrical features with XRD. The title compound has a triclinic crystal system with $\bar{P}1$ space groups (no.2). We illustrate molecular orbital features of vibration and lowest molecular translation energy levels via FT-IR and Uv-Vis. Spectroscopic results are compatible with our computational HOMO-LUMO, IR, and UV-Vis results. Two-dimensional fingerprint plots and Hirshfield surface analysis were used to elaborate intermolecular and intramolecular interactions. The main induced dipole effect appears between hydrogen and hydrogen at 47% percentage. Related to center of inversion symmetry, the second practical intermolecular molecular van der Walls effect is the Br-H with 15.2%.
NLO analysis shows that the dipole moment is 1.5 au, the average isotropic polarizability is 252.4 au, and the anisotropic polarizability is 252.03 au. That result clarifies that the title molecule is stable and less polarizable than literatüre. NBO analysis gives that molecular charge transfer mainly occurs on intramolecular tautomeric ring S(6). In the literature, the title molecule is more stable than related to similar structures.

Keywords: Hirshfeld Surface Analysis, NBO, NLO

References

Spackman, M.A., Jayatilaka,(2009) D., Hirshfeld surface analysis, CrystEngComm 11, 19–32.

Stanley, C., & Douglas, S. A. (2007). Principles of instrumental analysis. Thomson Brooks/Cole, Sydney, 1-1039.

Tarı, G. Ö., & Aydemir, E. (2023). Experimental and DFT study of (E)-4-bromo-2 (((3-chloro-4-(4-chlorophenoxy) phenyl) imino) methyl)-5-fluorophenol: Molecular and electronic properties in solvent media. *Journal of Molecular Structure*, *1277*, 134880.

Single-Crystal X-ray Diffraction Analysis and Quantum Mechanical Calculations of (*E*)-2,4-di-tert-butyl-6-((4-iodophenylimino)methyl)phenol *($C_{21}H_{26}INO$)*

[1*]<u>Yelda Bingöl Alpaslan</u>, [1]İlknur Şimşek, [2]Mustafa Macit

[1]Giresun University, Faculty of Arts & Science, Department of Physic, Giresun, Turkey
[2]Ondokuz Mayıs University, Faculty of Arts & Science, Department of Chemistry, Samsun, Turkey

* E-mail: yelda.alpaslan@giresun.edu.tr

Abstract

The molecular structure of the title compound, $C_{21}H_{26}INO$, was determined by X-ray single crystal diffraction technique. The compound crystallizes in the monoclinic, space group $P2_1/c$ with unit cell dimensions a=18.2550(7) Å, b= 10.7749(6) Å, c= 10.3253(5) Å, β=93.143(4)° and Z=4. X–ray diffraction investigation shows that the title compound in phenol–imine form with O−H···N intramolecular hydrogen bond. The quantum mechanical calculations of crystals were carried out with Gaussian 09W [1] package program using Density Functional Theory (DFT) in order to compare the obtained experimental data with theoretical data and to determine some molecular properties that cannot be determined by the X-ray single crystal diffraction method. Firstly, the optimized molecular geometry of the compound have been calculated using B3LYP/6-311++G(d,p) level of theory. Additionally, Mulliken atomic charges distribution, Molecular Electrostatic Potential (MEP) and Frontier Molecular Orbitals (FMOs) calculations were at the same methods.

Keywords: Schiff Base, X-ray diffraction, Quantum Mechanical Methods, MEP, FMOs

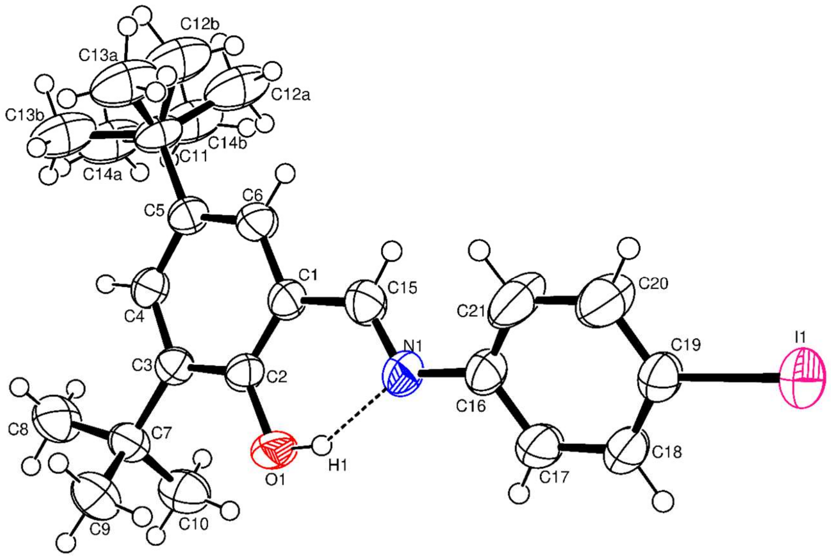


Fig. 1: ORTEP-3 structure of title compound

Kaynaklar

[1] M. J. Frisch, G. Trucks, H. Schlegel, G. Scuseria, M. Robb, J. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G.Petersson, Gaussian 09, Revision D. 01, Gaussian, Inc., Wallingford, 20, CT, 2009.

Understanding the Biological Activity of Malvin as an Anthocyanin Compound Using Theoretical Approaches

[1*]Duygu Barut Celepci
[1] Dokuz Eylül University, Faculty of Science, Department of Physics, 35160 İzmir, Türkiye

* E-mail: duygu.barut@deu.edu.tr

Abstract

Colorful fruits and vegetables have been linked to improved health and lifespan, as well as a lower risk of some chronic diseases. Many studies have focused on the properties of polyphenolic chemicals, a wide family of compounds found in plants. Inside this family, flavonoids are abundant in foods like fruits and vegetables. The most prominent class of flavonoids is anthocyanins. Anthocyanins have received significant attention in pharmaceutical research due to their vibrant color, excellent water solubility, and beneficial biological effects. In their glycoside form, which is bound to sugar molecules, is more stable and less sensitive to degradation caused by light, pH changes, and heat. In this presentation, the biological activity and the potential inhibition properties of malvin (malvidin-3,5-diglucoside) molecule on SARS-CoV-2 protein will be discussed in detail. The results of the theoretical studies such as the geometry of the molecule, its electronic structure, and vibrational and topological analysis will be shown. Also, the outcomes of inhibition studies and biological activity predictions that are carried out by Molecular Docking and ADME will be given, and compared to one of the most effective drugs that has been used during the Covid-19 pandemic.

Keywords: Anthocyanin, malvidin-3,5-diglucoside, DFT, molecular docking

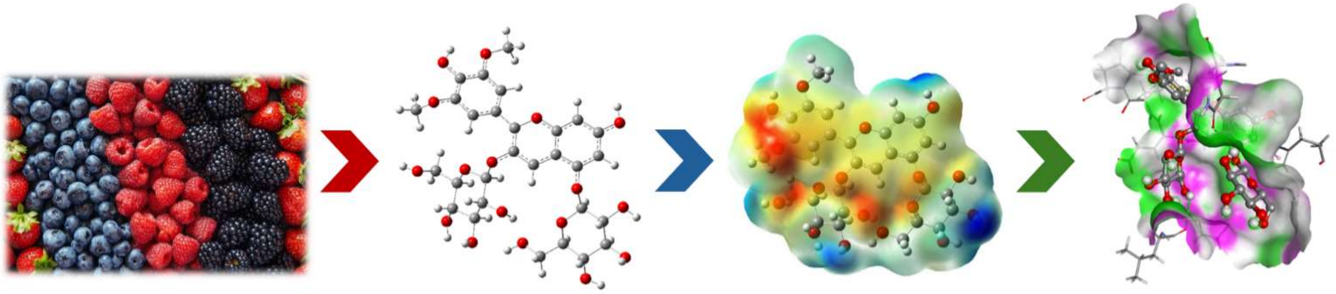


Fig. 1: Scheme of the theoretical analysis of malvin as an anthocyanin.
(First image: https://www.britannica.com/science/anthocyanin)

References

Frisch, M.J., Trucks, G.W., Schlegel, H.B., Scuseria, G.E., Robb M.A. et al. (2013). Gaussian 09, Revision D.01. Gaussian, Inc., Wallingford CT.

Eberhardt, J., Santos-Martins, D., Tillack, A.F., Forli, S. (2021). AutoDock Vina 1.2.0: New Docking Methods, Expanded Force Field, and Python Bindings, J. Chem. Inf. Model. 61 3891-3898.

E.F. Pettersen, T.D. Goddard, C.C. Huang, G.S. Couch, D.M., Meng, E.C., Ferrin, T.E. (2004). UCSF Chimera--a visualization system for exploratory research and analysis, J Comput Chem. 25 1605-1612

Daina, A., Michielin, O., Zoete, V. (2017). SwissADME: a free web tool to evaluate pharmacokinetics, drug-likeness and medicinal chemistry friendliness of small molecules. Scientific Reports, 7 (1): 42717.

Quantum Mechanical Calculation Of Some Chemical Properties Of The Hypericin Molecule

Şenol TOPRAK

Amasya University, Vocational School of Technical Sciences, Department of Electronics and Automation, Amasya, Turkey,

* E-mail: senol.toprak@amasya.edu.tr

Abstract

Hypericin is a naturally occurring compound found in St. John's wort (Hypericum perforatum) and some other plants in the Hypericaceae family. The chemical formula of hypericin is $C_{30}H_{16}O_8$, it has a red dye and is one of the main active ingredients responsible for the medicinal properties of St. John's wort. Hypericin has generally been studied for its potential antidepressant, antiviral, and anticancer properties and continues to be studied today.

Hypericin is a medicinal herb commonly used to treat mild to moderate depression, anxiety, and sleep disorders. Its homeland is Europe, but it can also be found in other parts of the world with a temperate climate. There is evidence that the active compounds in St. John's wort, including hypericin, hyperforin and flavonoids, have antidepressant and anxiolytic properties by affecting neurotransmitters such as serotonin, dopamine and norepinephrine in the brain. Hypericin can be obtained from St. John's wort through a maceration process that takes about 55-60 days to produce tinctures or extracts for medicinal purposes. Maceration refers to a process in herbal therapy or pharmacology in which herbal material is soaked in a liquid (usually a solvent such as alcohol or oil) to extract its active ingredients. Obtaining this red plant essence is a long process. We obtained the St. John's wort plant by exposing it to sunlight in a glass jar with extra virgin olive oil.

Since the hypericin molecule has found such a wide field of research in folk medicine and other scientific circles, it is believed that this plant extract deserves further research. In this study, we aimed to perform quantum mechanical calculations of the hypericin molecule to better understand the structure of this molecule and shed light on future studies.

Keywords: Hypericin, Maceration, St. John's wort.

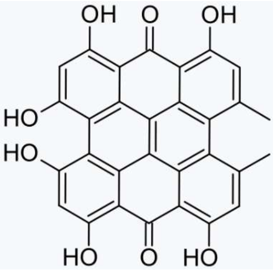


Fig. 1: Hypericin molecule

References

Schmidt, Mathias, and Veronika Butterweck (2015). "The mechanisms of action of St. John's wort: an update." Wiener Medizinische Wochenschrift 165.11-12: 229-235.

Ulicny, J., Leulliot, N., Grajcar, L., Baron, M. H., Jobic, H., & Ghomi, M. (1999). NIS, IR and Raman spectra with quantum mechanical calculations for analyzing the force field of hypericin model compounds. In AIP Conference Proceedings (Vol. 479, No. 1, pp. 183-186). American Institute of Physics.

The investigation of molecular and crystal structures for (*E*)-2-[(4-bromo-3-methylphenylimino)methyl]-6-ethoxyphenol with experimental and computational methods

[1*]Çiğdem Albayrak Kaştaş, [2]Gökhan Kaştaş
[1]Sinop University, Faculty of Arts and Sciences, Department of Chemistry, Sinop, Türkiye
[2]University of Samsun, Özdemir Bayraktar Faculty of Aeronautics and Astronautics, Department of Aerospace Engineering, Samsun, Türkiye

* E-posta: calbayrak@sinop.edu.tr

Abstract

A new Schiff base, (*E*)-2-[(4-bromo-3-methylphenylimino)methyl]-6-ethoxyphenol, was synthesized (Fig 1). It has been investigated experimentally (XRD and UV-vis) and computationally (DFT and HOMA). It is known that there are two tautomeric forms of an o-hydroxy Schiff base in the solid state named phenol-imine form and keto-amine form. The most important differences between the phenol-imine and keto-amine forms are the location of the tautomeric proton, the changes in the bond lengths of the aromatic ring, and the C-N, C-O bond lengths associated with the tautomerism [1, 2]. According to the XRD studies, the tautomeric proton (H1) is located on the oxygen atom (O1) in the compound. Namely, compound exists in phenol-imine form in solid state. The dihedral angle between the aromatic rings is 26.60°, which shows significant deviation from the planarity. In order to reveal tautomerism-related-changes in the molecular structures, we have also used the DFT method as an alternative approach. The calculated values proved that the C-O and C-N bonds possess single and double bond characters, respectively. The phenol-imine form was found to be preferred by the compound. We have applied Harmonic Oscillator Model of Aromaticity (HOMA) [3]. The HOMA indices of the rings R(C1-C6) and R(C8-C13) in the compound have been calculated as 0.973 and 0.979, respectively. Therefore, it can be proposed that the rings in the compound have almost pure aromatic characters and high π-electron delocalization. The results of PES scan process have been also used to calculate the activation energy for the transition from phenol form to the keto-amine form. The activation energies have been obtained as 6.16 kcal/mol.UV-vis spectra of the compound have recorded in two solvents with different dielectric constants. Regarding the spectra, we can say that the compound exists only in the phenol-imine form.

Keywords: Schiff Base, XRD, DFT.

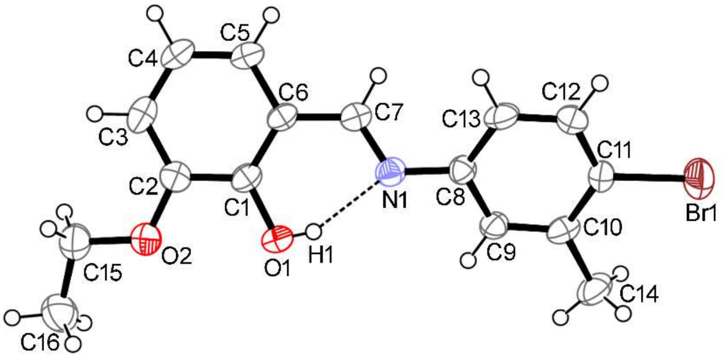


Fig. 1: The molecular structure of compound.

References

[1] Filarowski, A. Kochel, A. Kluba M. and Kamounah, F. S. (2008). J. Phys. Org. Chem. 21, 939–944.

[2] Diziembowska, T., Jagodzinska, E., Rozwadowski, Z., Kotfica, M. (2001). J. Mol. Struct. 598, 229-234.

[3] Krygowski, T.M., Zachara, J.E., Moszynski, R. (2005) J. Chem. Inf. Model., 45 (6), 1837–1841.

(*E*)-2-((Bromophenylimino)methyl)-3,4-dichloro-6-ethoxyphenol

[1]Başak KOŞAR KIRCA, [2]Çiğdem ALBAYRAK KAŞTAŞ

[1] Sinop Üniversitesi, Eğitim Fakültesi, Matematik ve Fen Bilimleri Eğitimi Bölümü, SİNOP

[2] Sinop Üniversitesi, Fen-Edebiyat Fakültesi, Kimya Bölümü, SİNOP

* E-posta: bkosar@sinop.edu.tr

Abstract

Schiff bases are compounds having C=N double bond and formed by reaction of a primary amine and an aldehyde. The most commonly studied class of compounds are *o*-hydroxy Schiff base derivatives. *o*-Hydroxy Schiff bases have attracted the interest of chemists and physicist because of their photochromic and thermochromic features in the solid state. They have widely used as ligands in the field of coordination chemistry, for the design of various molecular electronic devices and in the synthesis of important drugs [1].

o-Hydroxy Schiff bases exist as enol, keto or zwitterionic form in solid state. Depending on their forms, three types of strong intramolecular hydrogen bonds are possible in ohydroxy Schiff bases: O–H…N in enol-imine, N–H…O in keto-amine tautomers and N^{+}–H· · ·O^{-} in zwitterionic forms [2]. The title compound, (E)-2-((Bromophenylimino)methyl)-3,4-dichloro-6-ethoxyphenol adopts a keto-amine tautomeric form and displays a strong intramolecular N-H…O hydrogen bond between atoms N1 and O1. In this study, we examined and illustrated the molecular structure and non-covalent interactions for the o-hydroxy Schiff base compound (E)-2-((Bromophenylimino)methyl)-3,4-dichloro-6-ethoxyphenol based on X-ray diffraction data.

Keywords: Crystallography, Non-Covalent Interactions, Hirshfeld Surfaces.

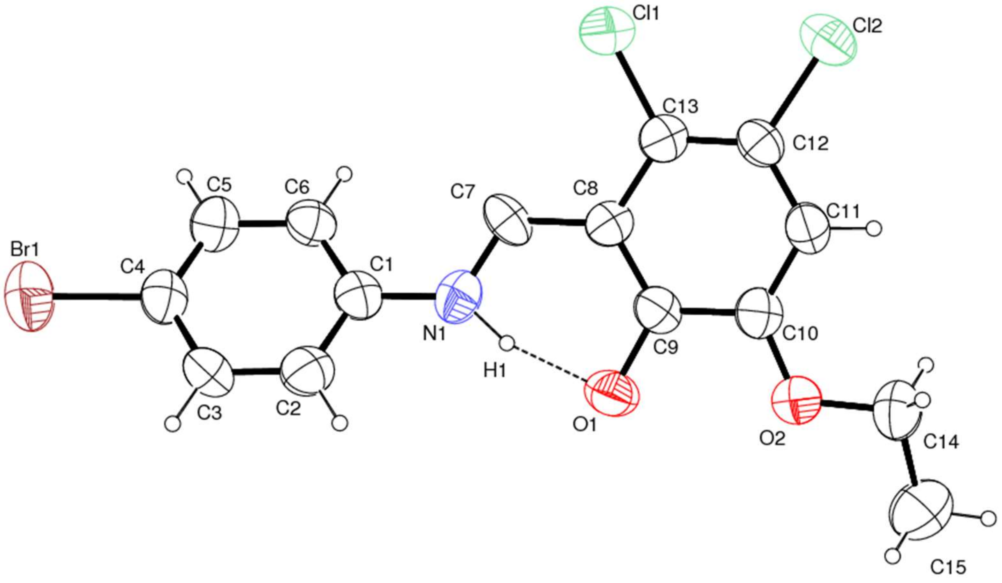


Fig. 1: Molecular structure of (E)-2-((Bromophenylimino)methyl)-3,4-dichloro-6-ethoxyphenol

Kaynaklar

[1] B. Kosar, C. Albayrak. Spectrochimica Acta Part A 78 (2011) 160–167.

[2] H. Petek, C. Albayrak, N. Ocak Iskeleli, E. Ağar, I. Şenel. J. Chem. Crystallogr. 37 (2007) 285–290.

Structural Investigation of bis{2-ethoxy-6-(*E*)-[(3-methylphenyl)imino)methyl]phenolato-κN,κO}copper(II)monohidrate

[1*]Gökhan KAŞTAŞ, [2]Çiğdem ALBAYRAK KAŞTAŞ

[1]University of Samsun, Özdemir Bayraktar Faculty of Aeronautics and Astronautics, Department of Aerospace Engineering, Samsun, Türkiye
[2]Sinop University, Faculty of Arts and Sciences, Department of Chemistry, Sinop, Türkiye

*E-posta: gokhan.kastas@samsun.edu.tr

Abstract

In this study*, the copper complex of a Schiff base, bis{2-ethoxy-6-(*E*)-[(3-methylphenyl)imino)methyl]phenolato-κN,κO}copper(II)monohidrate has been synthesized (Fig. 1). Its molecular and crystal structures have been investigated using X-ray diffraction technique (XRD), FT-IR, and UV-vis spectroscopy. It was found that the Schiff bases behave as bidentate ligands chelating the Cu(II) ion through two imine N atoms and two phenolic O atoms in a *cis* configuration. The two phenyl rings in the same ligand have different aromaticies from each other. This is also the case for corresponding rings of two ligands. The Cu(II) ion has a slightly distorted square-planar coordination geometry. In the crystal packing of the complex, the aromatic C-H···C interactions forms the 1D structure of the network. The dimensionality increases to 2D via C-H···Cg interactions between the aliphatic C-H groups and aromatic rings. The 2D structure extends in the plane (010) topologically forming a common rectangular, also named as (4,4) or (44)-net.

Keywords: Schiff base, copper complex, XRD.

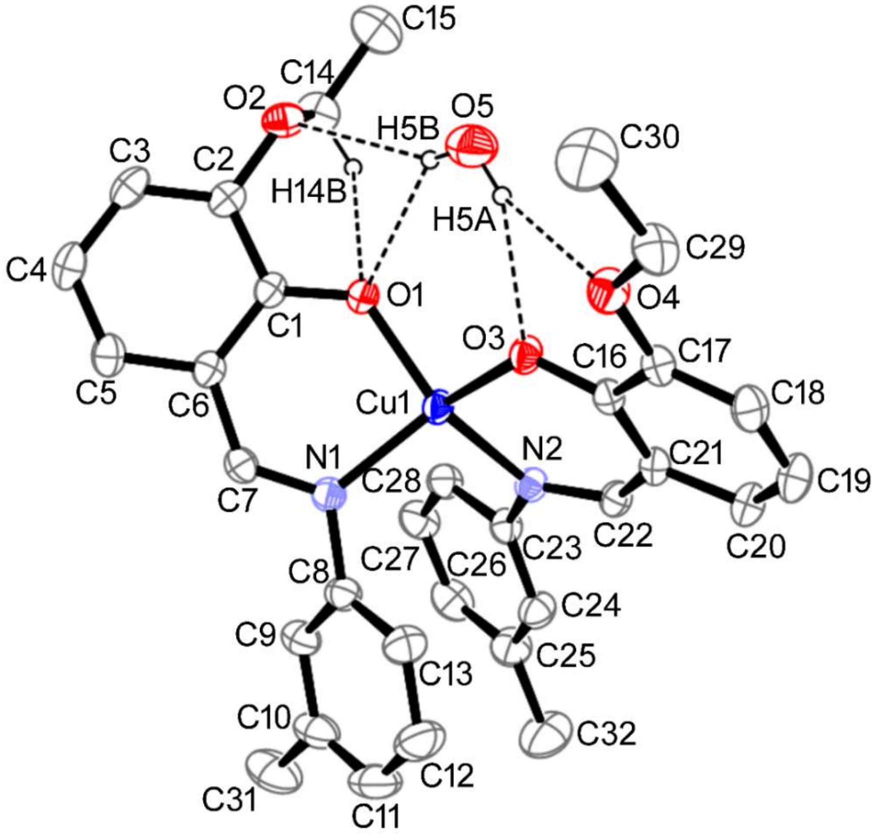


Fig. 1: The molecular structure of bis{2-ethoxy-6-(E)-[(3-methylphenyl)imino)methyl]phenolato-κN,κO}copper(II)monohydrate

---

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

Elucidation of the structure of a molecule containing a Schiff base using quantum chemical methods and investigation of its anticancer properties

[1*]Sultan Başak, [1] Cem Cüneyt Ersanlı
[1] Sinop University, Faculty of Arts and Sciences, Department of Physics, Sinop

* E-mail: sultaan.basaak@gmail.com

Abstract

Schiff bases, named after German chemist Hugo Schiff, are compounds with a central functional group containing an imine or azomethine (-C=N-) linkage. They have been extensively studied in various fields such as organic synthesis, coordination chemistry, and medicinal chemistry due to their diverse properties and wide range of applications. Schiff bases have been extensively utilized in scientific research since their discovery due to their multifaceted properties. The intense focus on Schiff bases in the literature stems from their versatile characteristics. This study aims to elucidate the theoretical physical and chemical properties of a compound containing a Schiff base,(*Z*)-4-(2,6-dichlorophenyldiazenyl)-6-{[1,3-dihydroxy-2-(hydroxymethyl)propan-2-ylamino]methyl}-2-methoxycyclohexa-2,4-dienone, whose structure was previously experimentally elucidated by X-ray diffraction. GaussView 4.1.2 and Gaussian 03W were employed to determine the compound's physical and chemical properties, while AutoDock Vina 1.5.7 was used for protein-ligand docking simulation. Based on experimental and theoretical geometric parameters, the compound was observed to possess a keto-amine tautomeric form and exhibit high aromaticity, as evidenced by computational HOMA indices. The compound's electrophilic and nucleophilic regions were illuminated based on identified frontier molecular orbitals and electronic parameters derived from these orbitals, indicating its stability. These findings were supported by molecular electrostatic potential (MEP) maps, revealing electrophilic and nucleophilic attack regions on the structure. Polarizability anisotropy ($\Delta\alpha$) and hyperpolarizability (β) values were calculated as 73.3003Å^3 and 5.46547x10^{-29}, respectively, indicating the structure's high polarizability feature. Natural bond orbital (NBO) analysis elucidated the nature of intramolecular hydrogen bonding and delocalization between electron-donor and acceptor-type orbitals. Mulliken charge analysis supported electrophilic and nucleophilic binding regions within the structure. Finally, docking simulation with BRAF V600E mutant protein yielded a binding affinity value of -8.2 kcal/mol, indicating stable binding geometry and strong protein-ligand interaction.

Keywords: Schiff bases, molecular modelling, molecular docking.

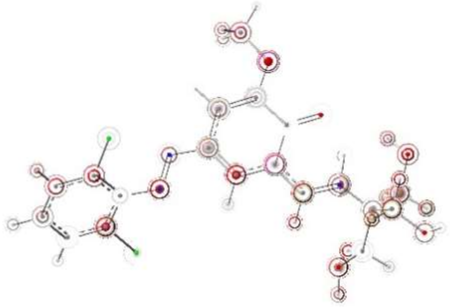


Fig. 1: Geometry optimization of the compound.

References

Challacombe, M., Gill, P. M. W., Johnson, B., Chen, W., Wong, M. W., Gonzalez, C. and Pople, J. A. 2004. Gaussian 03W, Revision E.01. Gaussian, Inc , Wallingford CT.

Howsaui, H. B., Basaleh, A. S., Abdellattif M. H., Hassan W. M., Hussien M. A., (2021). Synthesis, structural investigations, molecular docking, and anticancer activity of some novel Schiff bases and their uranyl complexes. *Biomolecules 11*(8): 1138. doi: 10.3390/biom11081138.

Ritterhouse, L. L., Barletta, J. A. (2015). BRAF V600E mutation-specific antibody: A review. *Semin Diagn Pathol*. *32*(5): 400-8. doi: 10.1053/j.semdp.2015.02.010.

Schiff, H., (1869). Untersuchungen über salicinderivate. *Justus Liebigs Annalen der Chemie*. *150*(2), 193-200.

Trott, O., and Olson A. J. (2010). AutoDock Vina: improving the speed and accuracy of docking with a new scoring function, efficient optimization and multithreading. *Journal of Computational Chemistry 31*(2), 455-461. doi: 10.1002/jcc.21334.

(E)-4-((3-chloro-4-hydroxybenzylidene)amino)-1,5-dimethyl-2-phenyl-1H-pyrazol-3(2H)-one Crystal Structure and Molecular Docking

[1*]Erbil Dağdelen, [2]Erbil Ağar, [1]Canan Kazak
[1] Ondokuz Mayıs University, Faculty of Arts and Sciences, Department of Physics, 55139, Samsun
[2] Ondokuz Mayıs University, Faculty of Arts and Sciences, Department of Chemistry, 55139, Samsun

* E-posta: ferhat.dadelen@hotmail.com

Abstract

The ortep drawing showing the molecular structure of the $C_{18}H_{16}ClN_3O_2$ crystal is given in Figure 1. The crystal system of the molecule in question is monoclinic and the space group is $P2_1/c$. The number of molecules (Z) in the unit cell of the [$C_{18}H_{16}ClN_3O_2$] crystal is four. The [$C_{18}H_{16}ClN_3O_2$] crystal is non-planar and the angle between the two benzene rings is 60.588^0. At the same time, the angle between the C1/C6 ring and the C9/C10N1N2 ring is 59.906^0, while the angle between the C13/C18 ring and the C9/C10N1N2 ring is 9.918^0. The molecules are arranged in parallel in a chain, $O2—H2A\cdots O1^i$, $C12—H12\cdots O2^{ii}$ and $C7—H7C\cdots O1^{iii}$ by intermolecular hydrogen bonding. In addition, in the crystal, the molecules are connected by weak π-π interaction to form a three-dimensional supramolecular structure. The size of the π-π interaction is Cg1•••Cg3i = 3,6619 Å; Cg1 and Cg3 are the centers of the C1–C6 and C13–C18 rings, respectively. Here i is the symmetry code: [2-x, 1-y, 1-z]. The N2─N1 bond length of the crystal is 1.389 (2) Å, the N3─C10 bond length is 1.397 (2) Å and the O2─C16 bond length is 1.344 (2) Å, showing a single bond character. O1─C11 bond length of 1,253 (2) Å and N3─C12 bond length of 1,272 (2) Å show double bond character. The interaction of $C_{18}H_{16}ClN_3O_2$ crystal with the target protein was investigated with AutoDockTools programme and the binding energy between the crystal and the protein was determined. The drug potential of the crystal was evaluated in ADMETLAB database. Using the observed reflections, the structure was solved using direct methods with SHELXT [2] structure analysis software in WinGX [1].

Keywords: Single Crystal, X-Ray Analysis, XRD, molecular docking

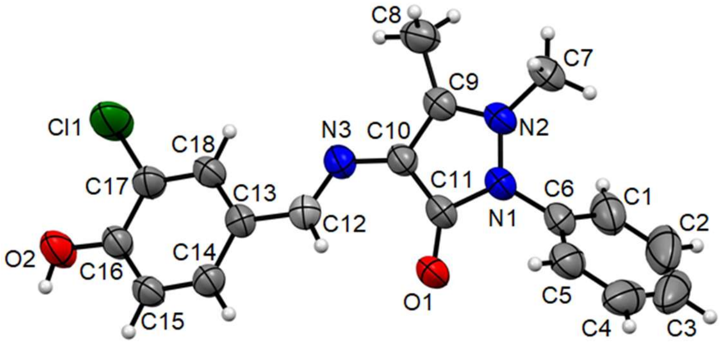


Figure 1. Ortep image of asymmetric unit of [$C_{18}H_{16}ClN_3O_2$] crystal drawn with 50% probability thermal ellipsoids

References

[1] L. J. Farrugia, J. Appl. Cryst. 32 (1999) 837.

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

Crystal Structure and Hirshfeld Surface Analyses of two novel benzimidazole bromide compounds

[1*]Merve İzmirli, [2]Hande Karabıyık, [2]Resul Sevinçek, [2]Hasan Karabıyık, [2]Duygu Barut Celepci, [2]Muhittin Aygün

[1]Department of Engineering Sciences, Faculty of Engineering, Izmir Katip Celebi University, Izmir 35620, Turkey
[2] Dokuz Eylül University, Faculty of Science, Department of Physics, 35160 İzmir, Türkiye

* E-mail: merve.izmirli@ikcu.edu.tr

Abstract

Benzimidazolium salts derived from benzimidazole are also known as N-heterocyclic carbene (NHC) precursors. These compounds have a wide range of applications from chemical to medical applications (Erdoğan et al, 2018; Johnson & Southern, 2017). Recently, some benzimidazolium bromide salts have been found in enzyme inhibition studies for the designation of their inhibition efficacy (Behçet et al, 2018; Erdemir et al, 2018). In this study, two new benzimidazole bromide salts were examined. The molecular and crystal structures of these compounds were determined using single crystal X-ray diffraction technique. C-H···Br type weak hydrogen bonds and parallel-displaced (offset) type $\pi\cdots\pi$ stacking interactions observed in both crystal structures were also investigated by means of Hirshfeld Surface Analysis.

Keywords: Benzimidazolium salts, XRD, Hirshfeld Surface Analysis

Acknowledgment: Thanks to Assoc. Prof. Dr. Aydın Aktaş and Yetkin Gök from İnönü University, who carried out the synthesis studies of the compounds.

References

Erdoğan, H., Aktaş¸ A., Gök, Y., Sarı, Y. N-Propylphthalimide-substituted bis-(NHC)PdX2 complexes: synthesis, characterization and catalytic activity in direct arylation reactions, Transit. Met. Chem. 43 (2018) 31-37.

Johnson, N.A., Southerland, M.R. J. Wiley, Youngs, Molecules 22 (2017) 1263.

Behçet, A., Çağlılar, T., Barut Celepci, D., Aktaş¸ A., Taslimi, P., Gök, Y., Aygün, M., Kaya, R., Gülçin, İ. Synthesis, characterization and crystal structure of 2-(4-hydroxyphenyl)ethyl and 2-(4-nitrophenyl)ethyl Substituted Benzimidazole Bromide Salts: Their inhibitory properties against carbonic anhydrase and acetylcholinesterase, J Mol Struct. 1170 (2018) 160-169.

Erdemir, F., Barut Celepci, D., Aktaş, A., Taslimi, P., Gök, Y., Karabıyık, H., Gülçin, İ. 2-Hydroxyethyl substituted NHC precursors: Synthesis, characterization, crystal structure and carbonic anhydrase, α-glycosidase, butyrylcholinesterase, and acetylcholinesterase inhibitory properties, , J Mol Struct. 1155 (2018) 797-806.

New Benzimidazolium Salts Bearing Chloro-/Fluorobenzyl-Substituted: Synthesis and Crystal Structures

[1] Betül ŞEN YÜKSEL, [1]Resul Sevinçek [2]Aydın AKTAŞ, [2]Yetkin GÖK, [1]Muhittin AYGÜN
[1] Dokuz Eylül University, Faculty of Science, Department of Physics, 35160-Buca, İzmir, Turkey

[2] Inonu University, Faculty of Science and Arts, Department of Chemistry, 44280, Malatya, Turkey

* E-posta: betul.sen@deu.edu.tr

Abstract

NHC precursors are known to be quite important ligands in organic and organometallic chemistry [1]. Among many NHC compounds, imidazole and benzimidazole derivatives are vastly known to have excellent therapeutic assets [2].Chloro-/fluorobenzyl-substituted benzimidazolium salts were synthesized from the reaction of 4-fluorobenzyl/2-chloro-4-fluorobenzyl-substituted benzimidazole and chlorinated aromatic hydrocarbons. The crystal structures of the complexes **I-V** were determined by single-crystal X-ray diffraction methods. These compounds were crystallized in the triclinic crystal system with a P-1 space group. The crystal packing of all complexes is dominated by O–H···Cl hydrogen bonds, which link the water molecules and chloride anions, forming a chloride–water tetrameric cluster.Static disorder was observed and modeled in compounds **I**, **III**, and **V** due to two-fold molecular symmetry. In compound **V**, quite large residual electron densities were observed at the equivalent places of Cl and F atoms in two-fold symmetry. Firstly, small and large components of both atoms were repeatedly refined with free s.o.f. values. Then, evaluating the results obtained the s.o.f. values of the components of the F and Cl atoms were fixed as 0.82/0.18. As a result of the refinements, the largest peaks and the deepest holes in the Fourier difference map were obtained quite well as 0.30/-0.38(eÅ^{-3}). In compounds **I** and **III**, it was observed that only the F atom has a static disorder. With the same method, after the refinement processes, the s.o.f. values of the components of the F atom were fixed respectively to be 0.7/0.3 for **I** and 0.8/0.2 for **III**. The largest peaks and the deepest holes in the Fourier difference map for these compounds were obtained as 0.17/-0.14 and 0.66/-0.38 (eÅ^{-3}), respectively. A very strong dynamical disorder was observed in all atoms of one of the phenyl groups of molecule **II.**

Keywords: benzimidazolium salts, static disorder, crystal structure.

References

[1] Gök, Y., Aktaş, A., Erdogan, H., Sarı, Y. (2018). Inorganica Chimica Acta: New 4-vinylbenzyl-substituted bis(NHC)-Pd(II) complexes: Synthesis, characterization and the catalytic activity in the direct arylation reaction. 471–735–740.

[2] Shalini, K., Sharma, P.K., Kumar, N. (2010). Der Chemica Sinica Imidazole and its biological activities: A review. 1–36–47

Index of Participants

Affiliation	**Name - Surname**	**Email address**	**Registration type**
Prof. Dr.	Michael Richard Probert	michael.probert@ncl.ac.uk	Invited Speaker
Prof. Dr.	Narcis Duteanu	narcis.duteanu@upt.ro	Invited Speaker
Prof. Dr.	Peter Müller	pmueller@mit.edu	Invited Speaker
Prof. Dr.	Rahime Şimşek	rsimsek@hacettepe.edu.tr	Invited Speaker
Prof. Dr.	Santiago Garcia-Granda	sgg@uniovi.es	Invited Speaker
Prof. Dr.	Wan Haliza Binti Abd Majit	q3haliza@um.edu.my	Invited Speaker
PhD Student	Abdurrahman Suhta	a.suhta@hotmail.com	Oral Presentation
Dr.	Burak V. Kabasakal	bvkabasakal@tarla-fel.org	Oral Presentation
Assoc. Prof. Dr.	Dursun Karaağaç	dursun.karaagac@btu.edu.tr	Oral Presentation
Assoc. Prof. Dr.	Duygu Barut Celepci	duygu.barut@deu.edu.tr	Oral Presentation
Dr.	Emre Yörük	yoruk@fzu.cz	Oral Presentation
Prof. Dr.	Güneş Süheyla Kürkçüoğlu	gkurkcuo@ogu.edu.tr	Oral Presentation
PhD Student	Hanifi Özşanlı	2021hanifiozsanli@gmail.com	Oral Presentation
Assoc. Prof. Dr.	İlkay Yıldırım Gümüşhan	iyildirim@biruni.edu.tr	Oral Presentation
Dr.	Merve İzmirli	merve.izmirli@ikcu.edu.tr	Oral Presentation
PhD Student	Nadihan Yolgeçti	nadihanyolgecti@hotmail.com	Oral Presentation
Assoc. Prof. Dr.	Ömer Çelik	celiko21@yahoo.com	Oral Presentation
PhD Student	Onur Rauf Yılmaz	y.onur86@gmail.com	Oral Presentation
Assist. Prof. Dr	Seda Şahin	sedasahin@karatekin.edu.tr	Oral Presentation
Prof. Dr.	Sema Öztürk Yıldırım	semaozturkyildirim@yahoo.com	Oral Presentation
Prof. Dr.	Çiğdem Albayrak Kaştaş	calbayrak@sinop.edu.tr	Poster Presentation
Other	Erbil Dağdelen	ferhat.dagdelen@hotmail.com	Poster Presentation
Prof. Dr.	Gökhan Alpaslan	gokhan.alpaslan@giresun.edu.tr	Poster Presentation
Prof. Dr.	Gökhan Kaştaş	gokhan.kastas@samsun.edu.tr	Poster Presentation
MSc Student	İlknur Şimşek	ilknursimsek28.is@gmail.com	Poster Presentation
Prof. Dr.	Metin Kul	mkul@eskisehir.edu.tr	Poster Presentation
Assoc. Prof. Dr.	Muhittin Aygün	muhittin.aygun@deu.edu.tr	Poster Presentation
Prof. Dr.	Nefise Özçeli̇k	nefised@gmail.com	Poster Presentation
PhD Student	Nour Eddine Benharkat	n.benharkat@univ-chlef.dz	Poster Presentation
Prof. Dr.	Onur Şahi̇n	onurs@sinop.edu.tr	Poster Presentation
Assoc. Prof. Dr.	Resul Sevinçek	rsevincek@gmail.com	Poster Presentation
Assist. Prof. Dr	Şenol Toprak	senol.toprak@amasya.edu.tr	Poster Presentation
Other	Sultan Başak	sultaan.basaak@gmail.com	Poster Presentation
Prof. Dr.	Yelda Bi̇ngöl Alpaslan	yelda.alpaslan@giresun.edu.tr	Poster Presentation
Prof. Dr.	Leyla Tatar Yıldırım	tatar@hacettepe.edu.tr	Poster Presentation
Prof. Dr.	Zarife Sibel Şahin	zarifesibel@sinop.edu.tr	Poster Presentation
BSc Student	Ahmed Elhamdo	ahmetoglak111@gmail.com	Attendance
Prof. Dr.	Ahmet Erdönmez	ahmeterdonmez52@gmail.com	Attendance
Prof. Dr.	Ahmet Köroğlu	kahmet@omu.edu.tr	Attendance
BSc Student	Ahmet kula	ahmetkula1903@gamil.com	Attendance
Assoc. Prof. Dr.	Anıl Sazak Çamaş	anilsazak@gmail.com	Attendance
PhD Student	Ayda Kaltehei	ayda.kaltehei@gmail.com	Attendance
BSc Student	Ayşenur Arslan	aysenurrarslann1@gmail.com	Attendance
BSc Student	Aysima Berber	22130129@stu.edu.omu.tr	Attendance
BSc Student	Bengü Baş	bengubas14@gmail.com	Attendance
BSc Student	Beyza Tantoğlu	beyzatantoglu@gmail.com	Attendance
BSc Student	Beyzanur Kızıl	20160577@stu.omu.edu.tr	Attendance
Other	Burcu Durmaz	burcu.dur7@gmail.com	Attendance
Prof. Dr.	Canan Kazak	ckazak68@gmail.com	Attendance
BSc Student	Diyar Berşan Özer	diyarbersan3636@gmail.com	Attendance
PhD Student	Emine Berrin Poyraz	emineberrin@omu.edu.tr	Attendance
Other	ENES Di̇lmen	nsdilmen@gmail.com	Attendance
PhD Student	Enis Güzel	enisguzel2@gmail.com	Attendance
BSc Student	Ergün Gözlü	ergungozlu0@gmail.com	Attendance
Assoc. Prof. Dr.	Erhan Yıldırım	erhanyildirim65@gmail.com	Attendance
Prof. Dr.	Ersin Temel	ersin.temel@giresun.edu.tr	Attendance
PhD Student	Ezgi Yeşil	yesil_ezgi@hotmail.com	Attendance

Prof. Dr.	Filiz Betül Kaynak	gulsen@hacettepe.edu.tr	Attendance
Assoc. Prof. Dr.	Filiz Öztürk	filiz.ozturk@omu.edu.tr	Attendance
Assoc. Prof. Dr.	Fulya Aydın Temel	fulya.temel@giresun.edu.tr	Attendance
MSc Student	Gökhan Demirelli	demirelligokhan@gmail.com	Attendance
Assoc. Prof. Dr.	Gonca Özdemir Tarı	gozdemir@omu.edu.tr	Attendance
Other	Gül Öden Odabaş	gulgulnurodabas@gmail.com	Attendance
Dr.	Hakan Bülbül	hakanbulbul55@gmail.com	Attendance
Prof. Dr.	Hanife Büyükgüngör	hbuyukg@omu.edu.tr	Attendance
Assist. Prof. Dr	Huriye Demir Kabaş	huriye.demirkabas@omu.edu.tr	Attendance
Dr.	Işıl Yılmaz	isilylmaz@gmail.com	Attendance
BSc Student	Kadir Gedik	19020144@stu.omu.edu.tr	Attendance
Prof. Dr.	Mehmet Akkurt	akkurt@erciyes.edu.tr	Attendance
BSc Student	Mehmet Sait Turhan	mehmetturhanx19@gmail.com	Attendance
BSc Student	Melike Nur Deniz	melikenurdenizz27@gmail.com	Attendance
MSc Student	Mert Çaylı	mert.cayli@meb.gov.tr	Attendance
Prof. Dr.	Metin Yavuz	myavuz@omu.edu.tr	Attendance
BSc Student	Murat Özcan	murat46360@gmail.com	Attendance
BSc Student	Mustafa Solanlar	23130167@stu.omu.edu.tr	Attendance
Prof. Dr.	Nurda Gamze Turan	gturan@omu.edu.tr	Attendance
BSc Student	Ömer Ayhan	18020119@stu.omu.edu.tr	Attendance
Prof. Dr.	Orhan Büyükgüngör	orhanb@omu.edu.tr	Attendance
MSc Student	Özlem Öztürk	yeniarasozlem@gmail.com	Attendance
Prof. Dr.	Gülçin Sağdıçoğlu Cele	gulcin.celep@gmail.com	Attendance
BSc Student	Rabia Han	23130158@stu.omu.edu.tr	Attendance
Assoc. Prof. Dr.	Rukiye Demir	rukiye.demir@samsun.edu.tr	Attendance
Prof. Dr.	Sedat Gümüş	sedatg@omu.edu.tr	Attendance
Assoc. Prof. Dr.	Şehriman Atalay	atalays@stu.omu.edu.tr	Attendance
BSc Student	Semih Şencan	marbles.55_@hotmail.com	Attendance
Assoc. Prof. Dr.	Serap Uzun	serap.uzun@samsun.edu.tr	Attendance
BSc Student	Şevval İşgörür	23130160@stu.omu.edu.tr	Attendance
Prof. Dr.	Süheyla Özbey	sozbey@hacettepe.edu.tr	Attendance
Assoc. Prof. Dr.	Süheyla Yüce Emre	syuce@omu.edu.tr	Attendance
BSc Student	Sümeyye Kaymak	23060446@stu.omu.edu.tr	Attendance
Assoc. Prof. Dr.	Tuğba Aycan	taycan@sinop.edu.tr	Attendance
Prof. Dr.	Ufuk Çoruh	ucoruh@gmail.com	Attendance
Prof. Dr.	Ümit Ceylan	umit.ceylan@giresun.edu.tr	Attendance
PhD Student	Wahidullah Enayat	wahidullah.enayt123@gmail.com	Attendance
Prof. Dr.	Yavuz Köysal	yavuzk@omu.edu.tr	Attendance

Ulusal Kristalografi Derneği

https://ukd.org.tr/tucr2024/home-2/

Turkish Crystallographic Association

https://ukd.org.tr/home/

5. Ulusal Kristalografi Toplantısı

https://ukd.org.tr/tucr2024/

5th National Crystallography Meeting

https://ukd.org.tr/tucr2024/home-2/#about

Ulusal Kristalografi Derneği (youtube)

https://www.youtube.com/@UlusalKristalografiDernegi

Ulusal Kristalografi Derneği (facebook)

https://www.facebook.com/UlusalKristalografiDernegi?locale=tr_TR

Sponsors

ONDOKUZ MAYIS ÜNİVERSİTESİ

YEŞİLYURT
DEMİR ÇELİK

ULUSOYUN

USLU
DEMİR ÇELİK

Medi TRAVEL

CUPRA SEAT
Özön

SAMSUN BÜYÜKŞEHİR BELEDİYESİ

Ondokuz Mayıs Üniversitesi – Kadın Girişimcilik Topluluğu –

NanoSpek
www.nanospek.com.tr

YAŞAR
GROUP

https://ukd.org.tr/

https://ukd.org.tr/tucr2024