# ANCON 2017

# INTERNATIONAL CONGRESS ON CHEMISTRY AND MATERIALS SCIENCE

**EDITORS**

Prof. Dr. Selen BİLGE KOÇAK
Assoc. Prof. Dr. Zafer ÜSTÜNDAĞ

ANKARA-TURKEY
October 5-7

BOOK OF
abstract

# ANCON 2017

## INTERNATIONAL CONGRESS ON CHEMISTRY AND MATERIALS SCIENCE

## BOOK OF Abstract

**October 5-7, 2017**
**ANKARA-TURKEY**

**EDITORS**
**Prof. Dr. Selen BİLGE KOÇAK**
**Assoc. Prof. Dr. Zafer ÜSTÜNDAĞ**

**ISBN**
**978-605-245-971-3**

**First Edition**
**November 2017, Ankara**

# WELCOME LETTER

Dear Participants,

We are proud to present you the Abstract Book of ''the Ancon 2017-International Congress on Chemistry and Materials Science'' which is held on 5 - 7 October 2017, in the Best Western Hotel 2000, Ankara-TURKEY. This fruitful Congress aims at forming a platform where eminent scientists present and discuss recent advances in chemistry and materials science.

We have 300 participants from 20 countries (Algeria, Belgium, Bosnia and Herzegovina, Denmark, Iran, Italy, Japan, Jordan, Korea, Kyrgyzstan, Malaysia, Mongolia, Pakistan, Romenia, Slovakia, Sweden, Turkey, Turkish Republic of Northerm Cyprus, Ukraine and USA). We have 7 Plenary and 13 Invited Speakers. We also have 140 oral and 156 poster presentations covering a broad range of subjects related to chemistry and materials science. The Congress topics may be grouped under eleven major areas: Analysis, Archaeological Chemistry, Bioscience & Biotechnology, Computational & Theoretical Chemistry, Electrochemistry, Energy, Enviromental & Green Chemistry, Food Chemistry, Materials Science, Nanotechnology and Synthesis & Characterization. This congress provides us with a wealth of information, a platform to exchange scientific ideas, many opportunities for discussions, new contacts for closer co-operation, inspire new research, and plans for the future on the exciting fields of chemistry and materials science.

I hope that you will return two years later with more colleagues for the 2nd ANCON Congress, the ANCON 2019, which will have a broader scope and more participants.

Best regards,

Selen Bilge

Prof. Dr. Selen BİLGE KOÇAK
President, Organizing Committee
Ancon 2017-International Congress on Chemistry and Materials Science

## SPONSORS

*We wish to express to our thanks to the institutions listed below for their sponsorship*

**GÜVEN HASTANESİ**

**SATE–SATE GIDA ve KİMYA SANAYİ ve TİCARET LTD. ŞTİ.**

**BEYPAZARI BELEDİYESİ**

**TARMAY KİMYA–TARIMSAL MAKİNA, KİMYEVİ ve GIDA MADDELERİ İTHALAT, İHRACAT ve TİCARET LTD. ŞTİ.**

**KİMETSAN–KİMETSAN KİMYA MADEN METALURJİ NDÜSTRİLERİ, İÇ VE DIŞ TİCARET, MÜŞAVİRLİK, MÜHENDİSLİK LTD. ŞTİ.**

**SEM–LABORATUAR CİHAZLARI PAZARLAMA SANAYİ VE TİCARET A.Ş.**

**STENKİM–STENKİM YAPI KİMYASALLARI**

**CKS–COŞKUN KAUÇUK SANAYİ VE TİCARET A.Ş.**

**ONGEN–ONGEN MEDİKAL**

**ÇINARLAR MADENCİLİK SANAYİ VE TİCARET A.Ş.**

**REFERANS KİMYA**

**PROTHERM FURNACES**

**BETAREKS–BETAREKS METALİZE İPLİK VE AMBALAJ SANAYİ A.Ş.**

**UNICONISTANBUL**

**BİNOM–ULUSLARARASI EĞİTİM SAĞLIK TURİZM ve ORGANİZASYON LTD. ŞTİ.**

**BEST WESTERN HOTEL 2000**

**KING HOTEL GÜVENLİK**

**SİSTEM TEKNİK–SİSTEM TEKNİK ENDÜSTRİYEL FIRINLAR LTD. ŞTİ.**

**KURUKAHVECİ MEHMET EFENDİ**

**ANKARA LIFE**

**İLDAM–İLDAM KİMYA KİMYEVİ MADDELER LABORATUVAR MALZEMELERİ SANAYİ ve TİCARET LTD. ŞTİ.**

## SPONSORS

*We wish to express to our thanks to the institutions listed below for their sponsorship*

GÜVEN
Sate
BEYPAZARI BELEDİYESİ 1883

TARMAY KİMYA
KİMETSAN

sem
stenkim yapı kimyasalları

CKS COŞKUN KAUÇUK SANAYİ VE TİCARET ANONİM ŞİRKETİ
ONGEN Bilimsel ihtiyaçlariniz için doğru yer
ÇINARLAR MADENCİLİK SAN. TİC.A.Ş.

REFERANS KİMYA
protherm FURNACES
Betareks

UNICONİSTANBUL
Binom

BW Best Western Hotels & Resorts
King | HOTEL GÜVENLİK

ST sistem teknik ENDÜSTRİYEL FIRINLAR
KURUKAHVECİ MEHMET EFENDİ
ankara Life BU DERGİNİN İÇİNDE HAYAT VAR
İLDAM

## COMMITTEES

### HONORARY PRESIDENT

***Erkan İBİŞ**, Rector, Ankara University, Turkey*

### PRESIDENT

***Selen BİLGE KOÇAK**, Department of Chemistry, Ankara University, Turkey*

### ORGANISING COMMITTEE

***Selen BİLGE KOÇAK**, Department of Chemistry, Ankara University, Turkey*
***Zafer ÜSTÜNDAĞ**, Department of Chemistry, Dumlupınar University, Turkey*
***Aliye KÖMEZ**, Department of Chemistry, Ankara University, Turkey*
***Aslı ERKAL**, Alanya Alaaddin Keykubat University, Antalya, Turkey*
***Aysel KOÇ DEMİR**, Department of Chemistry, Ankara University, Turkey*
***Aytuğ OKUMUŞ**, Department of Chemistry, Ankara University, Turkey*
***Büşra DOĞANAY**, Department of Chemistry, Ankara University, Turkey*
***Emel YILDIZ**, Department of Chemistry, Çukurova University, Turkey*
***Gamze ELMAS**, Department of Chemistry, Ankara University, Turkey*
***Gözde AYDOĞDU TIĞ**, Department of Chemistry, Ankara University, Turkey*
***Gönül DOĞANÖZ**, Public Relations Specialist, Ankara, Turkey*
***Hatice ERCAN**, Department of Chemistry, Ankara University, Turkey*
***İhsan AŞIK**, Department of Pharmacy Services, Mehmet Akif Ersoy University, Turkey*
***Kübra KARAAĞAÇ**, Department of Chemistry, Ankara University, Turkey*
***Mehmet Selçuk ERDOĞAN**, Department of Chemistry, Dumlupınar University, Turkey*
***Mehtap ÖZGÜR**, Department of Chemistry, Ankara University, Turkey*
***Pınar ACAR BOZKURT**, Department of Chemistry, Ankara University, Turkey*
***Serap DURKUT**, Department of Chemistry, Ankara University, Turkey*

### SCIENTIFIC COMMITTEE

***Abdurrahman ŞENGÜL**, Department of Chemistry, Bülent Ecevit University, Turkey*
***Alaa El-Din Ali EL-SHAFEİ**, Department of Chemistry, Mansoura University, Egypt*
***Ali KARADUMAN**, Department of Chemical Engineering, Ankara University, Turkey*
***Alina Adriana MİNEA**, Industrial and Materials Engineering, Gheorghe Asachi Technical University of Iasi, Romania*
***Alper Tolga ÇOLAK**, Department of Chemistry, Dumlupınar University, Turkey*
***Arife YURDAKUL**, Department of Metallurgical and Materials Science Engineering, Alanya Alaaddin Keykubat University, Turkey*
***Arturs VİKSNA**, Department of Analytical Chemistry, University of Latvia, Latvia*
***Ashutosh TİWARİ**, Linkoping University, Linkoping, Sweden*

***Aybüke TURAN***, *General Directorate of Mineral Research And Explorations, Turkey*

***Bolormaa OYUTSETSEG***, *Department of Chemistry, National University of Mongolia, Mongolia*

***Burak ÇOBAN***, *Department of Chemistry, Bülent Ecevit University, Turkey*

***Burhanettin İNEM***, *Department of Metallurgical and Materials Engineering, Gazi University, Turkey*

***Cecilia ARSENE***, *Department of Chemistry, Alexandru Ioan Cuza University, Romania*

***Celal Tuğrul ZEYREK***, *Ankara Nuclear Research and Training Center, Turkish Atomic Energy Authority, Turkey*

***Cemal ÇARBOĞA***, *Department of Metallurgical & Materials Science Engineering, Nevşehir Hacıbektaş Veli University, Turkey*

***Corby ANDERSON***, *Department of Metallurgical & Materials Engineering, Colorado School of Mines, USA*

***Danilo SUVOROV***, *Department of Advanced Materials, Institute of Joseph Stefan, Slovenia*

***Emel YILDIZ***, *Department of Chemistry, Çukurova University, Turkey*

***Emine KARAKUŞ***, *Department of Chemistry, Yıldız Technical University, Turkey*

***Emine YAĞMUR***, *Department of Chemical Engineering, Ankara University, Turkey*

***Erdal ÇELİK***, *Department of Metallurgical and Materials Engineering, Dokuz Eylül University, Turkey*

***Erdal DİNÇ***, *Department of Analytical Chemistry, Ankara University, Turkey*

***Ertugrul Gazi SAĞLAM***, *Department of Chemistry, Bozok University, Turkey*

***Fae'q A. A. RADWAN***, *Faculty of Engineering, Near East University, KKTC*

***Fatih APAYDIN***, *Department of Metallurgical and Materials Engineering, Bileşik Şeyh Edebali University, Turkey*

***Fatih Mehmet EMEN***, *Department of Chemistry, Mehmet Akif Ersoy University, Turkey*

***Fatma Nil ERTAŞ***, *Department of Chemistry, Ege University, Turkey*

***Gaida Maruta SEDMALE***, *Faculty of Material Sciences and Applied Chemistry, Riga Technical University, Latvia*

***Ghulam Hussain BHATTİ***, *Cadet College Hasan Abdal, Pakistan*

***Gülüzar Duygu SEMİZ***, *Department of Farm Structures and Irrigation, Ankara University, Turkey*

***Haslet EKŞİ KOÇAK***, *Department of Biomedical Engineering, Istanbul Aydın University, Turkey*

***Hua Chun ZENG***, *Department of Chemical and Biomolecular Engineering, National University of Singapore, Singapore*

***Irena MİHAİLOVA***, *Faculty of Metallurgy and Material Science, University of Chemical Technology and Metallurgy, Bulgaria*

***Irina KARADJOVA***, *Department of Chemistry, Sofia University, Bulgaria*

***Iveta VASKOVA***, *Department of Metallurgical Engineering, Technical University of Kosice, Slovakia*

***İbrahim Ender MÜLAZIMOĞLU***, *Department of Chemistry, Necmettin Erbakan University, Turkey*

***Jaroslaw W. DRELICH***, *Department of Materials Science and Engineering, Michigan Technological University, USA*

***Lokman UZUN***, *Department of Chemistry, Hacettepe University, Turkey*

***Mariana-Dana DAMACEANU***, *Petru Poni Institute of Macromolecular Chemistry, Romania*

***Mehmet YILMAZ***, *Department of Chemistry, Kocaeli University, Turkey*

***Metin GÜRÜ***, *Department of Chemical Engineering, Gazi University, Turkey*

***Michael L. FREE***, *Department of Metallurgical Engineering, University of Utah, USA*

***Mikolaj SZAFRAN***, *Faculty of Chemistry, Warsaw University of Technology, Poland*

***Milind H. JOSHİPURA***, *Department of Chemical Engineering, Nirma University, India*

***Munawar Saeed QURESHİ***, *Department of Basic Sciences & Humanties, Khwaja Fareed University of Engineering & Information Technology, Pakistan*

***Mustafa Oğuzhan ÇAĞLAYAN***, *Department of Nanotechnology Engineering, Cumhuriyet University, Turkey*

***Müşerref ÖNAL***, *Department of Chemistry, Ankara University, Turkey*

***Özcan YALÇINKAYA***, *Department of Chemistry, Gazi University, Turkey*

***Paul MUNROE***, *Department of Materials Science and Engineering, University of New South Wales, Australia*

***Salvatore DANİELE***, *Department of Molecular Sciences and Nanosystems, Ca' Foscari University of Venice, Italy*

***Sammia SHAHİD***, *Department of Chemistry, University of Management and Technology, Pakistan*

***Selen BİLGE KOÇAK***, *Department of Chemistry, Ankara University, Turkey*

***Sibel AKAR***, *Department of Chemistry, Eskişehir Osmangazi University, Turkey*

***Tülay BAL DEMİRCİ***, *Department of Chemistry, İstanbul University, Turkey*

***Ülkü BAYHAN***, *Department of Physics, Mehmet Akif Ersoy University, Turkey*

***Vladimir Vasilyevich PANKOV***, *Department of Physical Chemistry, Belarussian State University, Belarus*

***Yee-wen YEN***, *Department of Materials Science and Engineering, National Taiwan University of Science and Technology, Taipei, Taiwan*

***Yusuf DİLGİN***, *Department of Chemistry, Çanakkale Onsekiz Mart University, Turkey*

***Yutaka KAGAWA***, *Department of Materials Engineering, University of Tokyo, Japan*

***Zafer ÜSTÜNDAĞ***, *Department of Chemistry, Dumlupınar University, Turkey*

***Zehra YAZAN***, *Department of Chemistry, Ankara University, Turkey*

***Zeliha KAYAALTI***, *Society of Forensic Toxicology, Ankara, Turkey*

## ADVISORY COMMITTEE

***Adem KILIÇ***, *Department of Chemistry, Gebze Technical University, Turkey*

***Ali Osman SOLAK***, *Dean, Kyrgyz Turkish Manas University, Kyrgyzstan*

***Ali Rehber TÜRKER***, *Department of Chemistry, Gazi University, Turkey*

***Atilla GÜNGÖR***, *Department of Chemistry, Marmara University, Turkey*

***Atilla ÖKTEMER***, *Department of Chemistry, Ankara University, Turkey*

***Ayşen DEMİR MÜLAZIMOĞLU***, *Department of Chemistry, Necmettin Erbakan University, Turkey*

***Bekir ÇETİNKAYA***, *Department of Chemistry, Ege University, Turkey*

***Emine KILIÇ***, *Department of Chemistry, Ankara University, Turkey*

***Esma KILIÇ***, *Department of Chemistry, Ankara University, Turkey*

***Figen KADIRGAN***, *Department of Chemistry, İstanbul Technical University, Turkey*

***İsmail ÖZDEMİR***, *Department of Chemistry, İnönü University, Turkey*

***Meral KARAKIŞLA ŞAHİN***, *Department of Chemistry, Ankara University, Turkey*

***Metin OBALI***, *Department of Chemistry, Ankara University, Turkey*

***Muammer CANEL**, Department of Chemistry, Ankara University, Turkey*

***Mürvet VOLKAN**, Department of Chemistry, Middle East Technical University, Turkey*

***Nevin ERK**, Department of Analytical Chemistry, Ankara University, Turkey*

***Nurşen SARI**, Department of Chemistry, Gazi University, Turkey*

***Okan Zafer YEŞİLEL**, Department of Chemistry, Eskişehir Osmangazi University, Turkey*

***Saim ÖZKAR**, Department of Chemistry, Middle East Technical University, Turkey*

***Şeref GÜÇER**, Department of Chemistry, Uludağ University, Turkey*

***Şule PEKYARDIMCI**, Department of Chemistry, Ankara University, Turkey*

***Tarık PEKEL**, Department of Chemistry, Ankara University, Turkey*

***Zeki AKTAŞ**, Department of Chemical Engineering, Ankara University, Turkey*

***Zeynel KILIÇ**, Department of Chemistry, Ankara University, Turkey*

# GRAND HALL

# ABSTRACTS OF PLENARY LECTURES

# Progress of Multi Functional Properties of Organic-Inorganic Hybrid System, A[Fe(II)Fe(III)$X_3$] (A = $(C_nH_{2n+1})_4N$, Spiropyran; X = $C_2O_2S_2$, $C_2O_3S$)

**Norimichi Kojima***

Toyota Physical and Chemical Research Institute, Aichi, Japan

*E-mail: Kojima@toyotariken.jp*

In the case of mixed-valence systems whose spin states are situated in the spin crossover region, new types of conjugated phenomena coupled with spin and charge are expected. From this viewpoint, we have investigated the multifunctional properties coupled with spin, charge and photon for the organic-inorganic hybrid system, A[Fe(II)Fe(III)$X_3$] (A = $(C_nH_{2n+1})_4N$, spiropyran; X = dto ($C_2O_2S_2$), mto ($C_2O_3S$)). A[Fe(II)Fe(III)$(dto)_3$] undergoes the ferromagnetic phase transitions, while A[Fe(II)Fe(III)$(mto)_3$] undergoes the ferrimagnetic transitions [1,2]. In $(C_nH_{2n+1})_4N$[Fe(II)Fe(III)$(dto)_3$] (n = 3,4), a new type of phase transition called charge transfer phase transition (CTPT) takes place at around 120 K, where the thermally induced charge transfer between Fe(II) and Fe(III) occurs reversibly. At the CTPT, the iron valence state dynamically fluctuated with a frequency of about 0.1 MHz, which was confirmed by means of muon spin relaxation. The CTPT and the ferromagnetic transition for $(C_nH_{2n+1})_4N$[Fe(II)Fe(III)$(dto)_3$] remarkably depend on the size of intercalated cation [3-6]. In the case of (SP)[Fe(II)Fe(III)$(dto)_3$] (SP = spiropyran), the photoinduced isomerization of SP under UV irradiation induces the CTPT in the [Fe(II)Fe(III)$(dto)_3$] layer and the remarkable change of the ferromagnetic transition temperature. In the case of $(C_nH_{2n+1})_4N$[Fe(II)Fe(III)$(mto)_3$], a rapid spin equilibrium between the high-spin state ($S$ = 5/2) and the low-spin state ($S$ = 1/2) at the Fe(III)$O_3S_3$ site takes place in a wide temperature range, which induces the valence fluctuation of the $FeS_3O_3$ and $FeO_6$ sites through the ferromagnetic coupling between the low spin state ($S$ = 1/2) of the FeIIIS3O3 site and the high spin state ($S$ = 2) of the Fe(II)$O_6$ site [7-9].

## References

[1] N. Kojima, W. Aoki, M. Itoi, Y. Ono, M. Seto, Y. Kobayashi, Yu. Maeda, Solid State Commun., 120 (2001) 165-170.
[2] T. Nakamoto, Y. Miyazaki, M. Itoi, Y. Ono, N. Kojima, M. Sorai, Angew. Chem. Int. Ed., 40 (2001) 4716-4719.
[3] M. Itoi, Y. Ono, N. Kojima, K. Kato, K. Osaka, M. Takata, Eur. J. Inorg. Chem., 2006, 1198-1207
[4] N. Kida, M. Enomoto, I. Watanabe, T. Suzuki, N. Kojima, Phys. Rev. B, 77 (2008) 144427-1-5.
[5] N. Kida, M. Itoi, M. Enomoto, N. Kojima, et al, J. Am. Chem. Soc., 131 (2009) 212-220.
[6] N. Kojima, M. Enomoto, N. Kida and K. Kagesawa, Materials, 3 (2010) 3141-3187.
[7] H. Ida, A. Okazawa, N. Kojima, R. Shimizu, Y. Yamada, M. Enomoto, Inorg. Chem., 51 (2012) 8989-8996.
[8] N. Kojima, M. Itoi, Y. Miyazaki, Current Inorg. Chem., 4 (2014) 85-99.
[9] M. Enomoto, I. Watanabe, N. Kojima, Current Inorg. Chem. 6 (2016) 49-60

---

* Corresponding author, *E-mail: Kojima@toyotariken.jp*

PL-2

# Synthesis, Recovery, Properties and Applications of Polyhydroxyalkanoate – Biodegradable Plastics from Microbes

**Kumar Sudesh***

School of Biological Sciences, Universiti Sains Malaysia, 11800 Penang, Malaysia

*E-mail: ksudesh@usm.my*

Polyhydroxyalkanoates (PHA) are microbial storage polyesters accumulated as water insoluble granules. Upon extraction and purification from the bacterial cells, PHAs show thermoplastic properties similar to polypropylene and low-density polyethylene. Unlike petrochemical plastics, PHAs are 100% biodegradable in various natural environments. The renewable nature of PHAs makes them attractive as potential substitutes for some non-biodegradable single use commodity plastics. In addition, PHAs are also biocompatible and have much potential as a biomaterial for medical applications. The PHAs are synthesized and kept in the form of granules by the bacterial cells. PHA synthase [1,2] is the enzyme that polymerizes various types of PHAs. The synthesized and accumulated PHAs have to be recovered from the cells by breaking the cell wall. The PHA granules are surrounded by various proteins that are involved in their metabolism, such as the PHA synthase, phasins and depolymerases. These proteins form a layer on the surface of the PHA granules. In order to obtain pure PHA, it is necessary to remove all these proteins. The best and most commonly used method by researchers to obtain very pure PHA is by chloroform extraction and subsequent precipitation in methanol. Other methods involve the use of detergents and chemicals. Here, a biological recovery method is proposed whereby the cells containing the PHA granules are fed to animals [2]. The animals' digestive system is able to partially digest the cell material, but not the PHA granules which are excreted in the form of whitish fecal pellets [3]. Upon washing with water and small amounts of detergents the purity of the recovered PHA can be improved to more than 95% [4]. The biologically recovered PHA granules were also subjected to various characterizations and were found to have essentially the same properties as the chloroform extracted PHA [3,4]. The method reported here is relatively simple and eliminates the need for solvents and strong chemicals [5]. The resulting PHA is applicable for agricultural applications such as for the controlled release of fertilizers.

**References**

[1] M.F. Chek, S.-Y. Kim, T. Mori, H. Arsad, M.R. Samian, K. Sudesh and T. Hakoshima, Scientific Reports, 7 (2017) 5312.
[2] K. Bhubalan, J.-A. Chuah, F. Shozui, C.J. Brigham, S. Taguchi, A.J. Sinskey, C. Rha and K. Sudesh, Applied and Environmental Microbiology, 77 (2011) 2926-2933.
[3] B. Kunasundari, V. Murugaiyah, G. Kaur, F.H.J. Maurer and K. Sudesh, PLoS ONE, 8 (2013) e78528.
[4] P. Murugan, L. Han, C.Y. Gan, F.H.J. Maurer and K. Sudesh, Journal of Biotechnology, 239 (2016) 98-105.
[5] B. Kunasundari, C.R. Arza, F.H.J. Maurer, V. Murugaiyah, G. Kaur and K. Sudesh, Separation and Purification Technology, 172 (2017) 1-6.

---

* Corresponding author, *E-mail: ksudesh@usm.my*

# 3D Printers in Medicine

**Osman Eroğul***

TOBB University of Economics and Technology, Biomedical Engineering Department, Ankara, Turkey

*E-mail: erogul@etu.edu.tr*

Three Dimensional (3D) printers can be used in a wide variety of applications in medicine. The implant can be defined as organic and inorganic substance that is placed in an appropriate place inside the body in order to support the organs. In many countries, due to traffic accidents and terror attacks, brain injuries and organ damages are frequently observed. Therefore, in the process of cranial trauma repair and reconstruction, custom made skull implants are needed [1,2]. Benefits and features of custom made implants can summarized as; satisfying esthetic results, better anatomic fit versus conventional fixation/reconstruction methods, reduced operating time compared to traditional reconstruction methods that require extensive contouring and impact and facture resistant for protection of underlying structures [3,4]. 3D printing methods are used in the creation of the implants and Ti6Al4V is selected as an implant material. This study summarizes how to design and produce implants that are custom-designed for each individual patient. Various tests and analyses performed before the implementation of implants are discussed and the results are evaluated in details.

**References**

[1] A.L. Jardini, M.A. Larosa, R.M. Filho, C.A. de Caryalho Zayaglia, L.F. Bernardes, C.S. Lambert, D.R. Calderoni and P. Kharmandayan, Journal of Cranio-Maxillo-Facial Surgery, 42(8) (2014) 1877-1884.
[2] S.T. Chen, C.J. Chang, W.C. Su, L.W. Chanq, I.H. Chu and M.S. Lin, Injury, 46(1) (2015) 80-85.
[3] Y Safi, S. Hohenberger, C. Robbenmenk, F. Banki, e. al., Investigation of the failure behavior of a cranial implant-skull model under different load conditions using FEM 2010 SIMULIA Customer Conference.
[4] B.W Huang, H.K. Kung, K.Y. Chang, P.K. Hsu and J.-G. Tseng, Life Science Journal, 6(4) (2009) 15-22.

---

* Corresponding author, *E-mail: erogul@etu.edu.tr*

# Technical and Economic Aspects of the Use the Flue Gas Desulphurization Gypsum

**Azra Jaganjac***

University of Sarajevo, Faculty of Science, Department of Chemistry, 71000 Sarajevo, Bosnia and Herzegovina

*Email: ElizabethB1943@hotmail.com*

Industrial processing of the FGD gypsum, generated during Flue Gas Desulphurization to make gypsum building materials, is one of the most significant examples of overcoming an industrial waste problem [2]. This paper records the progress of FGD gypsum from waste to the secondary raw material. Description leads from the legislative measures to limit the emission of SO2 to 200 mg/m$^3$ from large combustion systems, via comparison of the characteristics and assessment of FGD gypsum with those of natural gypsum, to the development of new chemical processes and products. The practical differences between FGD gypsum and natural one are explained (Table1) [1]. It is given an indication of the growing importance of utilizing FGD gypsum from coal-derived TPPs of Bosnian lignite mining area and the new states in the region [3]. Removal of FGD gypsum from the European Waste Catalogue and its acceptance as a product from a high point in the efforts to put FGD gypsum on an equal footing with natural one as a raw material [4].

**Table 1.** Characteristic Chemical Composition of FGD Gypsum (VKR Scholven in Germany) and Natural Gypsum (Rigips) Compared with the Target Values for FGD Gypsum [1]

| Properties + Composition | Units | FGD Gypsum | Natural Gypsum | Target Values for FGD Gypsum |
|---|---|---|---|---|
| Purity | % | 97 | 85 | 95 |
| pH value | % | 7.4 | 7.0 | 5-8 |
| $Na_2O$ | % | 0.002 | 0.005 | 0.06 |
| Cl, water soluble | % | 0.008 | 0.003 | 0.010 |
| $CaSO_3$ x ½ $H_2O$ | % | 0.02 | n.n. | 0.50 |
| $Fe_2O_3$ | % | 0.12 | 0.20 | 0.15 |
| $CaCO_3 + MgCO_3$ | % | 1.5 | 12.0 | 1.5 |

## References

[1] Hrustanović, S. (2013): Chemical Characteristics of Natural Gypsum of some Mines in B&H as a Criteria for Use in Production α-Hemihydrates, Doctoral Thesis, University of Sarajevo, Faculty of Science.
[2] Jaganjac, A. and S.Hrustanović (2004): Gypsum Binder Production from FGD-Gypsum, European Conference on Raw Building Materials and Coal: New Perspectives, Sarajevo. May20-21.

---

* Corresponding author, *E-mail: ElizabethB1943@hotmail.com*

PL-5

# Chelating Agents for Metal Intoxication

**Guido Crisponi***

University of Cagliari, Department of Chemical and Geological Sciences, Cittadella Universitaria, I-09042 Cagliari, Italy

*E-mail: crisponi@unica.it*

Exposure to metal ions is ever increasing in the present industrial society, despite the increasing awareness of their toxic effects for humans, and the increasing prevention measures for occupational and environmental safety. Metal ions enter in everyday life: metal compounds are used in medicine, in food industries, in water purification plants, in cosmetics, in painting, and so on [1]. Three different types of metal toxicity can be distinguished:

- Acute ingestion of toxic metal ions, accidental or voluntary;
- Chronic intoxication, which may depend on environmental, occupational or iatrogenic causes;
- Metal overload related to genetic diseases.

This first row classification is of primary importance in establishing the required treatments, spanning from an immediate clinical powerful treatment for acute toxicity, to a lifelong treatment for genetic diseases. One of the principal ways to counteract metal toxicity in humans involves the treatment with metal chelators with the aim of eliminating a toxic metal ion from the organism, or of attenuating its toxicity [2]. In the years, the requisites of a chelating agent have been better and better defined:

- lack of toxicity of the chelating agent and of the formed complexes;
- stability of the formed complexes;
- selectivity toward the target metal ion;
- slow biochemical metabolism of the chelating agent into the body;
- good absorption and bioavailability;
- fast kinetic of exchange with endogenous ligands;
- easy excretion of the formed complexes.

The relevance of metal chelators in medicine has increased in recent years, not only to treat metal intoxication, but also to cure different diseases, as cancer, diabetes, and neurodegeneration, and in diagnostic medicine. Despite the considerable effort devoted by the scientific community to have proper metal chelators the results have been limited. The failure can be ascribed in some cases to difficulties related to the biological, chemical and clinical restraints, but above all to two main causes:

- the low utilization of these drugs, that prevents strong research investments by pharmaceutical industries;
- The scarce interaction between chemical and biomedical research, which leads to a wasting of efforts and resources.

I hope that the dialogue among chemists and clinicians will be able to achieve the common target of ameliorating the possible pertinent treatment for any metal intoxication.

## References

[1]G. Crisponi and V.M. Nurchi, Metal Ion Toxicity, in Encyclopedia of Inorganic and Bioinorganic Chemistry, © 2015 John Wiley & Sons, Ltd.
[2] J. Aaseth, G. Crisponi and O.Andersen (Eds.), Chelation Therapy in the Treatment of Metal Intoxication, Academic Press, 2016.

---

* Corresponding author, *E-mail: crisponi@unica.it*

# Designing Precursors for the Deposition of Inorganic Nanostructures

**Lisa McElwee-White***

University of Florida, Department of Chemistry, Gainesville, Florida 32608 USA

*E-mail: lmwhite@chem.ufl.edu*

Nanostructures can be deposited from organometallic and inorganic precursors by a variety of techniques including chemical vapor deposition (CVD), surface plasmon mediated chemical solution deposition (SPMCSD) and electron beam induced deposition (EBID). Precursor choice requires consideration of the reaction conditions and possible decomposition mechanisms for the particular method. Mechanism-based design of precursors for CVD and SPMCSD will be presented in case studies for contrast with strategies for design of EBID precursors. The examples for CVD will be low temperature deposition of tungsten carbonitride ($WN_xC_y$) or tungsten oxide ($WO_x$) films and nanoparticles [1,2]. For SPMCSD, the illustration will be growth of Au nanoparticles from $CH_3AuPPh_3$ upon excitation of the SPR of a Ag film on nanosphere (AgFON) substrate by irradiation with visible light [3]. In contrast, the conditions for EBID (Figure 1) are surface reactions under high electron flux, necessitating different precursor design rules [4]. Strategies for adapting selected CVD precursor types for EBID and efforts to identify privileged ligand classes and optimal coordination spheres for EBID precursors will be discussed in the context of studies on ($\eta^3$-allyl)$Ru(CO)_3Cl$, $Pt(CO)_2Cl_2$ and related complexes [5].

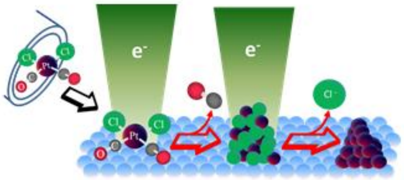


**Figure 1.** Representation of the EBID process

## References

[1] K.R. McClain, C. O'Donohue, A. Koley, R.O. Bonsu, K.A. Abboud, J.C. Revelli, T.J. Anderson, L. McElwee-White, J. Am. Chem. Soc., 136 (2014) 1650-1662.
[2] R.O. Bonsu, H. Kim, C. O'Donohue, R.Y. Korotkov, K.A. Abboud, T.J. Anderson, L. McElwee-White, Inorg. Chem., 54 (2015) 7536-7547.
[3] J. Qiu, Y.-C. Wu, Y.-C. Wang, M.H. Engelhard, L. McElwee-White, W.D. Wei, J. Am. Chem. Soc., 135 (2013) 38-41.
[4] J. Spencer, S. Rosenberg, M. Barclay, Y.-C. Wu, L. McElwee-White, D.H. Fairbrother, Appl. Phys. A: Mater. Sci. Process., 117 (2014) 1631-1644.
[5] J.A. Spencer, Y.C. Wu, L. McElwee-White, D.H. Fairbrother, J. Am. Chem. Soc., 138 (2016) 9172-9182.

---

* Corresponding author, *E-mail: lmwhite@chem.ufl.edu*

# Electrochemical Synthesis of VI-B Metals Borides and Silicides in Molten Salts

**Victor Malyshev***

National Academy of Science of Ukraine, V.I. Vernadsky Institute of General and Inorganic Chemistry, Kyiv, Ukraine.
University "Ukraine", Institute of Engineering and Technology, Kyiv, Ukraine

*E-mail: viktor.malyshev.igic@gmail.com*

The analysis of the current state of the problem of high-temperature electrochemical synthesis (HTES) of silicides and borides shows that the further development of the method is possible only on the basis of clarifying the mechanism of, and of the development of principles for the implementation and management of, multi-electron electrode reactions of electrodepostion of chromium, molybdenum, tungsten, silicon, and boron. As a prerequisite for the electrodeposition of compounds is the proximity of the potentials of deposition of components, it is necessary to develop ways to bring them together and to find the conditions for the alignment of the potentials of various component deposition processes.

Equilibrium potentials of compound decomposition were calculated from the standard Gibbs free energy for the decomposition reaction. Combinations of the anodic reaction with various realizations of cathodic reduction give chemical reactions. From the values of decomposition voltage, it follows that process of immediate deposition of boron and silicon should be energetically more favorable. From the results of calculations, it can be seen that the deposition potentials for Cr, Mo and W metals and silicon (boron) are significantly different. Therefore, HTES of their silicides and borides is possible only in a kinetic mode. Thermodynamic analysis of the decomposition voltage of similar compounds of boron, silicon, chromium, tungsten, and molybdenum has shown that these metals are more electropositive than boron and silicon for 0.5-0.7 V. Values of depolarization of boron and silicon deposition onto tungsten and molybdenum are no more than 200 mV [1,2].

From the current-voltage dependences for chloride-cryolite melt with the co-presence of sodium tungstate and oxides of silicon and boron. As expected, there are two waves. The first wave corresponds to the process of electroreduction of oxyfluoride complex of tungsten to metal tungsten, and the second - to the electroreduction of oxyfluoride complexes of silicon (boron) to free silicon (boron). The difference of half-wave potentials is 0.7-0.8 V. A similar pattern is observed in the presence of sodium molybdate or chromate, with the only difference being that the potential of electroreduction of oxyfluoride complexes of molybdenum and chromium, for 150-200 and 250-300 mV higher than that of tungsten, respectively. In order to optimize obtaining process of chromium silicides, high-temperature electrochemical synthesis was carried out in the $KCl-KF-K_2SiF_6-K_2CrO_4$ system. Depending on the electrolyte composition and electrolysis parameters, both individual phases $Cr_2O3$, $Cr_3Si$, and $CrSi_2$ and mixtures of these phases with low silicon content were obtained.

**References**

[1] A. I. Hab, Materials Science, 43 (2007) 383-397.
[2] V.V. Malyshev, H.B. Kushkov and V.I. Shapoval, Journal of Applied Electrochemistry, 32 (2002) 573-579.

---

* Corresponding author, *E-mail: viktor.malyshev.igic@gmail.com*

# GRAND HALL

# ABSTRACTS OF INVITED LECTURES

# The Story of KIMETSAN Chem Group

**Erol Özensoy***

KIMETSAN Chemicals, Mining and Metallurgical Industries International, Trade Consulting and Engineeing Co. Ltd. Ankara, Turkey

*E-mail: erolozensoy@kimetsan.com*

Kimetsan Chem Group have 8 companies with 2 plants in Turkey. 3 of the group companies located in the United Kingdom. The first company Kimetsan Chem. Met. Min. Industries Ltd. established in 1986. The group is very active in Chemical, Metallurgical and Mining Industries. Metalllurgical part is mainly manufacturers of industrial corrosion inhibitors and vapor pahse corrosion inhibitors (called as VCI). Mining section is active manufacturing drilling and mining chemicals and too many inorganics from the ores/minerals. The group Ankara Plant is a multipurpose chemical plant making around 1300 chemicals/products. This plant is one of the biggest plant in Turkey and Middle East for manufacturing fine and performance chemicals. This plant also makes analytical and R&D Chemicals. This section was the core of research and development at laboratory scale initially and later Pilot Plants operated and scaled up for industrial stage manufacturing units. All of the products know- how developed by Kimetsan Chemists and Chemical Engineers. Fine and R&D chemicals, organic/inorganic chemicals, performance chemicals, specialty chemicals, photographic chemicals, metal surface treatment chemicals, industrial cleaning materials, custom synthesis. Kimetsan Chemists, Chemical Engineers and Metallurgical Engineers were developed environmentally friendly water borne nano (mean diameter 40-45 nm) binder at industrial scale in 1988. This development followed the military aerospace coatings. Kimetsan signed a contract with the Turkish Government to develop 2-18 GHz range stealth coating in 2006. This product was qualified in 2012 as the World first nano tecnological stealth coating. After that night vision NIR camouflage (700-1400 nm), thermal camouflage (Mid and and FAR IR) qualified by the Turkish Military and NATO. The visable range (300-700 nm) camouflage gives less than 0.1 % reflections in any type militray coatings.

Success of Kimetsan may be summarised in very simple wording. All decission makers are chemical/metallurgical engineers and chemists. R&D in laboratory scale and pilot plants with the industrial scaling up all made in the group.

Currently Kimetsan have 14 manufacturing groups and exports to 38 countries.

---

* Corresponding author, *E-mail: erolozensoy@kimetsan.com*

I-2

# Tailoring Polymeric Interfaces for Diagnostics and Delivery

**Amitav Sanyal***

Bogazici University, Department of Chemistry, 34342, Istanbul, Turkey

*E-mail: amitav.sanyal@boun.edu.tr*

Functional polymeric interfaces are crucial for enabling many of the applications related to diagnostics and delivery. In particular, these soft interfaces act as a bridge between the material and biological world. These applications entail design of polymeric materials that can interact with the underlying platform and display biological ligands for processes like sensing and directed delivery. While robust nature of such interfaces is important to withstand the challenging biological milieu, properties such as selective interaction with targeted biological entities like proteins or oligonucleotides or cells are a must. Ideally, such interfaces should be anti-biofouling i.e. not prone toward non-specific binding of biological materials, but should be efficient in interacting through the biological cues present at the interface. In recent years, we have developed a novel class of thiol-reactive polymers that allow facile conjugation of (bio)molecules [1]. These materials are designed to afford functionalizable coatings on planar [2,3] and nanoparticle surfaces (Figure 1) [4,5]. The talk will outline the design and synthesis of such materials and highlight their application in cellular targeting and sensing.

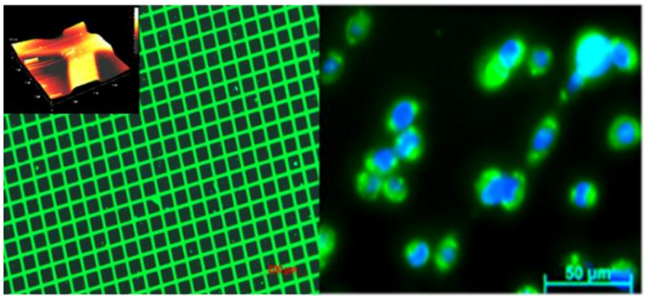


**Figure 1.** Planar and nanoparticle interfaces interacting with proteins and cells

**References**
[1] O. Gok, I. Kosif, T. Dispinar, T. N. Gevrek, R. Sanyal and A. Sanyal, Bioconjugate Chemistry, 26 (2015) 1550-1560.
[2] T. N. Gevrek, I. Kosif and A. Sanyal, ACS Applied Materials and Interfaces, 9 (2017) 27946–27954.
[3] M. Dubner, V. J. Cadarso, T. N. Gevrek, A. Sanyal, N. D. Spencer and C. Padeste, ACS Applied Materials & Interfaces, 9 (2017) 9245-9249.
[4] M. Arslan, T. N. Gevrek, J. Lyskawa, S. Szunerits, R. Boukherroub, R. Sanyal, P. Woisel and A. Sanyal, Macromolecules, 47 (2014) 5124-5134.
[5] Y. Oz, M. Arslan, T. N. Gevrek, R. Sanyal and A. Sanyal, ACS Applied Materials & Interfaces, 8 (2016) 19813-19826.

---

* Corresponding author, *E-mail: amitav.sanyal@boun.edu.tr*

I-3

# Functionalized Conjugated Polymers: Synthesis and Application

**Atilla Cihaner***

Atılım University, Faculty of Engineering, Department of Chemical Engineering and Applied Chemistry, 06836, Ankara, Turkey

*E-mail: atilla.cihaner@atilim.edu.tr*

Since the discovery of polyacetylene [1], conjugated electrically conducting polymers have attracted the interest of many scientists. Today, conjugated polymers are promising candidates for use in organic light-emitting diodes, organic photovoltaic devices, electrochromic displays and devices, smart windows, chemical sensors, transistors, and the like. For example, conjugated polymers have the ability of changing their optical properties (color) as persistent and reversible response by the application of a voltage pulse. Conjugated polymers continue to fascinate many scientists due to their several advantages; e.g., low cost, processability, high optical contrast ratio, multi-colors with the same material, high stability and long cycle life with low response time. Conjugated polymers as electrochromic materials have the ability of changing their optical properties as persistent and reversible response by the application of a voltage pulse. There are some factors that influence electrochromism: Coloration efficiency, high contrast, injected/ejected charge, stability, continuously variable color intensity and structural flexibility (the ability to easily modify the monomer's structure to obtain desired properties). This study presents an overview of new derivatives of polythiophenes, polyselenophenes, donor–acceptor-donor type polymers, etc (Figure 1). The design, synthesis, and applications of the functionalized polymers are discussed in detail and compared with the corresponding features of the corresponding analogues. The electrochemical and electrochromic properties and the band gaps of the polymers are also discussed in relation to their chemical structures. Furthermore, some applications like electrochromic devices and sensors will be discussed in detail.

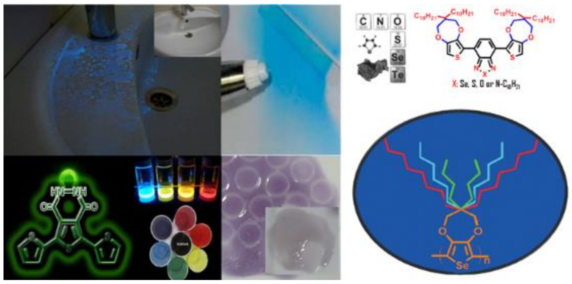


**Figure 1.** Some conjugated polymers and their applications

**References**

[1] H. Shirakawa, E.J. Lewis, A.G. MacDiarmid, C.K. Chiang and A.J. Heeger, J. Chem. Soc., Chem. Commun., (1977) 578-580.

---

* Corresponding author, *E-mail: atilla.cihaner@atilim.edu.tr*

# Molecular Engineering Approaches to High-Performance Organic Materials for Optoelectronics

**Hakan Usta***

Abdullah Gül University, Faculty of Engineering, Department of Materials Science
and Nanotechnology Engineering, 38080, Kayseri, Turkey

*E-mail: hakan.usta@agu.edu.tr*

π-Conjugated functional organic materials have attracted significant scientific and technological attention over the last three decades as electro-active materials for the development of low-cost, printable and flexible optoelectronic devices. They are envisioned as essential components of next-generation optoelectronic devices such as flexible displays, low-cost solar panels, electronic papers, printable RFID tags, and sensors. These new technologies are expected to revolutionize the role of electronics in our daily lives and compliment current inorganic-based optoelectronic devices, which has greatly impacted our society starting from the second half of the 20th century. To this end, the theoretical design and synthetic tailoring of π-conjugated architectures have been very crucial to optimize the physicochemical and optoelectronic properties of organic materials for any particular application. In this study, we show that thin-films prepared by properly designed organic semiconductors can form favorable nanostructures, which can be used for a variety of organic optoelectronic applications ranging from light-emitting transistors (OLETs) to bulk-heterojunction organic photovoltaics (OPVs). [1-7]

**References**

[1] M. Yilmaz, E. Babur, M. Özdemir, R. L. Gieseking, Y. Dede, U. Tamer, G. C. Schatz, A. Facchetti, H. Usta and G. Demirel, Nature Materials (Nature) (2017) In Press.
[2] R. Ozdemir, D. Choi, M. Ozdemir, G. Kwon, H. Kim, U. Sen, C. Kim and H. Usta, Journal of Materials Chemistry C (RSC), 5 (2017) 2368-2379.
[3] M. Yilmaz, M. Erkartal, M. Özdemir, Ü. Şen, H. Usta and G. Demirel, ACS Applied Materials & Interfaces (ACS), 9 (2017) 18199–18206.
[4] M. Ozdemir, D. Choi, Y. Zorlu, B. Cosut, H. Kim, C. Kim and H. Usta, New Journal of Chemistry (RSC), (2017) In Press.
[5] R. Ozdemir, D. Choi, M. Ozdemir, H. Kim, S. T. Kostakoğlu, M. Erkartal, H. Kim, C. Kim and H. Usta, ChemPhysChem (Wiley), 18 (2017), 850–861.
[6] M. Ozdemir, D. Choi, G. Kwon, Y. Zorlu, B. Cosut, H. Kim, A. Facchetti, C. Kim and H. Usta, ACS Applied Materials & Interfaces (ACS), 8 (2016) 14077–14087.
[7] H. Usta, C. Sheets, M. Denti, G. Generali, R. Capelli, S. Lu, X. Yu, M. Muccini and A. Facchetti, Chem. Mater. (ACS), 26 (2014), 6542–6556.

---

* Corresponding author, *E-mail: hakan.usta@agu.edu.tr*

I-5

# Functional Nanomaterials for Catalysis, Synthetic Fuels and Chemical Energy Conversion

**Khurram Saleem Joya***

Department of Energy Conversion and Storage, Technical University of Denmark
(DTU), Frederiksborgvej 399, 4000 Roskilde, Denmark
Department of Chemistry, University of Engineering and Technology, GT Road
54890 Lahore, Punjab, Pakistan

*E-mail: khurramdtu@gmail.com*

Functionalized nanomaterials are becoming increasingly significant for many important applications in industry, for essential catalytic processes and for solar & chemical energy conversion schemes [1-3]. In this pursuit, developing robust and high activity electrocatalytic materials for water oxidation and $CO_2$ conversion, and their synergistic interfacing with competent light-harvesting modules is very important to progress the construction of solar to fuel conversion system [4] during last 10 years, we have exploited various functional nanoscale materials for catalytic water splitting, $CO_2$ reduction, and recently for biomass catalysis and solar energy conversion [4,5]. We implemented several molecular, inorganic nanomaterials and metal-oxides displaying great potential to be used in electrocatalysis [5,6]. Their effective interfacing with semiconductor photo-responsive materials and/or $CO_2$ reduction systems can provide a potential scheme to make renewable energy supplies [7,8]. Further we are also exploring catalysis for biomass conversion into chemicals and synthetic fuels opening new ventures for chemicals and energy conversion.

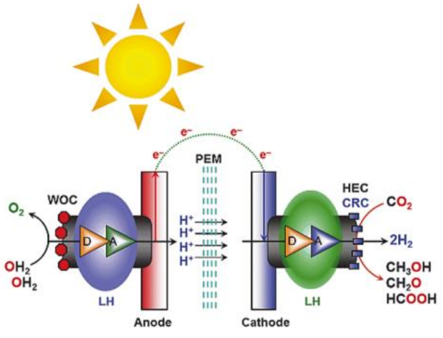


**Figure 1.** Proposed solar-driven water splitting scheme

### References

[1] K.S. Joya, Y.F. Joya, K. Ocakoglu and R. van de Krol, Angew. Chem., 125 (2013) 10618-10630.
[2] K.S. Joya, Y.F. Joya, K. Ocakoglu and R. van de Krol, Angew. Chem. Int. Ed., 52 (2013) 10426-10437.
[3] K.S. Joya, Y.F. Joya and H.J.M. de Groot, Adv. Energy Mater., 4 (2014) 1301929.
[4] M. de Respinis, K.S. Joya, H.J.M. De Groot, F. D’Souza, W.A. Smith, R. van de Krol and B. Dam, J. Phys. Chem. C, 119 (2015) 7275-7281.
[5] K.S. Joya and H.J.M. de Groot, ACS Catal., 6 (2016) 1768-1771.
[6] K.S. Joya, N.K. Subbaiyan, F. D'Souza and H.J.M. de Groot, Angew. Chem. Int. Ed., 51 (2012) 9601-9605.
[7] K.S. Joya, N. Morlanés, E. Maloney, V. Rodionov and K. Takanabe, Chem. Commun., 51 (2015) 13481-13484.
[8] K.S. Joya, Z. Ahmad, Y.F. Joya, A. Garcia and H.J.M. de Groot, Nanoscale, 8 (2016) 15033-15040.

---

* Corresponding author, *E-mail: khurramdtu@gmail.com*

# Evaluation of Chestnut Honey Quality Based on Their Physico-Chemical Parameters and Mineral Content Using Multivariate Techniques

**Vildana Alibabić***

University of Bihać, Biotechnical faculty, Department of Food Technology, 77000 Bihać, Bosnia and Herzegovina

*E-mail:vildana.btf@gmail.com*

The study aimed to assess the relation between the physico-chemical parameters [1] and the contents of minerals (K, Na, Mg, Zn, Fe, Mn, Al) and some heavy hazardous metals (Cd, Pb, As) of chestnut honey originated in northwestern part of Bosnia and Herzegovina. The differences in sucrose, electrical conductivity, invertase activity and Al content reached significance ($P < 0.05$) between geographical distributions of 43 samples. A significant positive correlation ($p<0.05$) was found between the reduced sugars and content of Fe, ash and K, Na, Al, Zn and Fe, activity values of invertase and Zn, and between HMF and Na. The predominant mineral was potassium, with a concentration that ranged from 680.4 to 634.7 mg/kg. By applying PCA [2] method were found that chestnut honey have positive PC1 values with content of Na, Mg, Pb, Cd and positive PC2 values with content of Fe, water and invertase activity.

**Table 1.**The significant ($p<0.05$) Pearson correlation between physico-chemical parameters and mineral content

| **Parameter** | **Range** | **Correlation coefficient ($R^2$) ($p<0.05$)** |
|---|---|---|
| Water (%) | 18.01- 18.76 | -0.609 (K) |
| Reducing sugars (%) | 70.77-71.88 | 0.606 (Fe) |
| Sucrose (%) | 1.49-1.32 | |
| Ash (%) | 0.97-0.95 | 0.987 (K), 0.601 (Al),0.559 (Zn), 0.538 (Na), 0.522 (Fe) |
| Electrical conductivity (mS/cm) | 0.97-0.95 | |
| Acidity (mmol/kg) | 12.19-19.22 | -0.579 (Na) |
| Diastase activity (DN) | 27.56-23.84 | |
| Invertase activity (IN) | 26.59-29.26 | 0.674 (Zn) |
| HMF (mg/kg) | 14.88-14.67 | -0.505 (Mg),0.599 (Na) |
| Proline (mg/kg) | 616.51-699.57 | -0.616 (Al) |
| Optical rotation (°) | -1.66- -1.96 | |

## References

[1] S.A. El Sohaimy, S.H.D.Masry and M.G.Shehata, Annals of Agricultural Science, 60 (2015) 279-287E.
[2] Kivima, A. Seiman, R. Pall, E. Sarapuu, K. Martverk and K. Laos, Proceedings of the Estonian Academy of Sciences, 63 (2014) 183-192.

---

* Corresponding author, *E-mail: vildana.btf@gmail.com*

I-7

# High Pressure Carbon Dioxide Assisted Nebulization-Electrodeposition (CAN-ED) as One-Step Synthesis Process of Nano- and Micro-Powder Structures: Preparation and Application

**Ruken Esra Demirdöğen***

Çankırı Karatekin University, Faculty of Science, Department of Chemistry,
TR18100, Çankırı, Turkey

*E-mail: esrademirdogen@karatekin.edu.tr*

Advent of nano and and micro-powders opened new horizons both in application and research in a great variety of fields such as energy, materials science, catalysis, medicine, medical devices, tissue engineering, jet printing to pattern bioactive molecules and cells, cell carriers and drug delivery. The ultra-small building units which they are composed of have high surface/volume ratio. This confers special mechanical, magnetic and opto-electronic properties to them [1]. The global market share of nanoparticles is growing at a high pace such as with annual growth of rate of 20% and is expected to reach $79.8 billion by 2019 in life sciences [2]. This indicates that as their designs improve their functionality, application areas and market shares would also increase. The better knowledge of their synthesis would enable their design to become better, but yet there is still much to explore in both their synthesis and application and there are many challenges to overcome. Since the current process methods (i.e., CVD, CVC, CCVC, HPPD) are not eco-friendly, new methods, which allow performance of mass production in a relatively easy and "green" way but yielding similar quality final products, is a great need. Electrochemical deposition or electrodeposition, which deposits a large variety of nanomaterials in many different forms in big quantities from various solutions [3], is exploited for producing micro- and nano-scale particles (electrospraying) composed of polymers, ceramics or composites [4]. However, since liquids with surface tension higher than $50 \times 10^{-3}$ $N.m^{-1}$ cannot be atomized in air by electric forces [5] organic solvents have become preference of choice in electrospraying. Nevertheless, detrimental effectf os organic solvents had to be overcome. Thus carbon dioxide came into play as benign alternative. Therefore, interest in electrodeposition in presence of supercritical fluids is increasing each day. Currently there is no electrospraying device working in combination with supercritical fluids. Successful designs may be developed via using high pressure carbon dioxide for producing nano and micro-powdered structures in one step synthesis [6]. In this presentation the motive, advantages and challenges of design, preparation and application of high pressure carbon dioxide assisted nebulization-electrodeposition (CAN-ED) as one-step synthesis process of nano- and micro-powder structures will be outlined.

## References

[1] R.W. Seigel, Nanophase materials assembled from atom clusters, Mater Sci Engin: B, 19(1-2) (1993) 37-43.
[2]http://www.drug-dev.com/Main/Back-Issues/NANOTECHNOLOGY-MARKET-Nanotechnology-Markets-in-He-803.aspx).
[3] https://goldbook.iupac.org/html/E/E01955.html)
[4] J. Du, Y.Q. Wu and K.L. Choy, Thin Solid Films, 497(1-2) (2006) 42-47.
[5] D.P.H. Smith, IEEE Trans. Ind Appl., 22(3) (1986) 527-535.
[6] R.E. Demirdöğen, F.M. Emen, K. Ocakoglu, P. Murugan, K. Sudesh and G. Avsar, Journal of Biological Macromolecules, (2017) in press.

## Acknowledgement

This research has been financially supported by The Higher Education Commission of Turkey.

---

* Corresponding author, *E-mail: esrademirdogen@karatekin.edu.tr*

# Organic Photovoltaics with different fabrication processes

**Şule Erten Ela***

Ege University, Solar Energy Institute, 35100 Bornova Izmir, Turkey

*E-mail:* suleerten@yahoo.com

Solar energy conversion using organic or hybrid organic-inorganic solar cells is an emerging area of interest that has rapidly evolved in recent years and with its technology constitutes the most promising low-cost alternative to traditional silicon photovoltaic cells. The most advanced and most promising among these new light conversion devices are organic photovoltaics (OPV). Dye sensitized solar cells, heterojunctions solar cells and perovskite solar cells are all photovoltaic technologies [1,2]. Dye sensitized solar cells consists of a counter electrode covered with a thin layer of Pt, an electrolyte containing an iodide/triiodide redox mediator, a working electrode including a wide band gap metal oxide coated over a transparent conducting substrate in a sandwich geometry. In dye sensitized solar cells, the photon incident on the dye excites the dye molecules. An excited dye molecule, electron will be released into the conduction band of the titania or any other metaloxide semiconductor material. Then, the electron flow through the porous $TiO_2$ film to the transparent conductive oxide, then move through an external circuit and reach the counter electrode. The oxidized dye molecules regenerated when the dye receives electrons from a redox mediator. Metal oxide synthesis and characterizations in the dye sensitized solar cells are crucial. Metal oxide materials synthesis and characterizations were developed for photovoltaic technologies in this study. Organic solar cell was achieved using poly (3-hexylthiophene) (P3HT) as a hole transporting polymer. In the main research in organic photovoltaics is to develop electron acceptor material. Mostly, PCBM material is used in organic solar cell. PCBM is an expensive material. Novel strategy for this type of solar cell is to develop novel fullerene material instead of PCBM. Novel fullerene materials were synthesized and characterized for organic photovoltaics. All type organic photovoltaics will be presented and discussed with different fabrication processes.

**References**

[1] Graetzel M, Nature 414 (2001) 338.
[2] Sule Erten Ela et al., New Journal of Chemistry (RSC) 39 (2015) 4086.

---

*Corresponding author, *E-mail:* sule.erten@ege.edu.tr

# Biomimetic Approaches in Nanostructured Architectures for Solar Fuel Production

**Kasım Ocakoğlu***

Mersin University, Tarsus Faculty of Technology, Department of Energy Systems Engineering, 33480 Mersin, Turkey
Mersin University, Advanced Technology Research and Application Center, Çiftlikköy Campus, TR33343, Yenişehir, Mersin, Turkey.

*E-mail: kasimocakoglu@gmail.com*

The creation of new materials based on biological systems comprises much more than simply copying structures observed in nature [1-4]. Firstly, building principles used in their construction should be comprehended by researchers. This is also essential for an exact understanding of the relationship between structure and function. Natural photosynthesis is a primary energy converter: every year, global photosynthesis converts solar energy into biomass corresponding to nearly 50 times the total human energy consumption per year [5]. Direct conversion of solar energy into a fuel is of particular interest as it gives a storable product. In this way, the produced solar fuel could be molecular hydrogen, small alcohols or other carbon-based products from $CO_2$ reduction. Research on artificial photosynthesis is aimed not only comprise fundamental studies to understand the processes and principles by use of biomimetic systems and models and also comprise potential applications which required novel designs [2-4]. There is currently no solar fuel technology based on artificial photosynthesis [5]. On the other hand, ambitious research efforts may lead to development of practical systems for direct solar fuel production. Successful designs may be integrated with natural or artificial components into novel systems for the production of solar fuels.

This talk will outline challenges and advantages of design, preparation and implementation of biohybrid electrodes bearing extremely stable natural photosynthetic complexes for solar fuel production.

## References

[1] C. Ortiz and M. C. Boyce, Science, 319 (2008) 1053-1054.
[2] K. Ocakoglu, K.S. Joya, E. Harputlu, A. Tarnowska and D.T. Gryko, Nanoscale, 6 (2014) 9625-9631.
[3] K.S. Joya, Y.F. Joya, K. Ocakoglu and R. van de Krol, Angew. Chem. Int. Ed., 52 (2013) 10426-10437.
[4] K. Ocakoglu, T. Krupnik, B. van den Bosch, Harputlu, M.P. Gullo, J.D.J. Olmos, S. Yildirimcan, R.K. Gupta, F. Yakuphanoğlu, A. Barbieri, J.N.H. Reek and J. Kargul, Adv. Funct. Mater., 24 (2014) 7467-7477.
[5] L. Hammarström and M. R. Wasielewski, Energy Environ. Sci., 4 (2011) 2339-2339.

## Acknowledgement

This research has been financially supported by The Scientific and Technological Research Council of Turkey, TUBITAK (Grant: 215M389).

---

* Corresponding author, *E-mail: kasimocakoglu@gmail.com*

I-10

# Nanocatalysts in a Wide-Range Application Spectrum: From Energy Storage to Organic Synthesis

**Önder Metin***

Department of Chemistry, Faculty of Science, Atatürk University, 25240, Erzurum, Turkey

*E-mail: ometin@atauni.edu.tr*

Transition metal nanoparticles (TMNPs) are widely used in a variety of fields owing to their distinct physical and chemical properties compared to those of bulk metals. TMNPs have rather large surface area and catalytically more active surface atoms than bulk metals, which is one of the most important reasons behind their widely usage. Therefore, they have been preferentially used as catalysts in various catalytic reactions and show advantageous catalytic properties compared to those of homogeneous and heterogeneous analogues [1]. Therefore, the new term, "*Nanocatalysis*", is raised and growing fast. Up to date, nanoparticles of all catalytically active transition metals have been synthesized by using different methods and their catalysis were studied in various reactions. However, the interest in the use of bimetallic nanoparticles instead of monometallic ones has been increased daily because the bimetallic TMNPs either in alloy or core-shell form show higher activity, selectivity and stability compared to the monometallic counterparts owing to the "*Synergistic*" effects formed between two distinct metal atoms. In particular, economical catalysts could be developed by the preparation of bimetallic alloy or core-shell nanoparticles of noble metals with a non-noble metal, which is considered to be very advantageous for the catalytic reactions using noble metals as catalyst. However, the composition control over the bimetallic nanoparticles is very important for the design of most efficient catalysts in different catalytic applications. In this presentation, after giving a brief introduction to the nanoparticles and catalysis, I am going to talk about our recent research activities on the synthesis of monodisperse monometallic and bimetallic nanoparticles, their structural characterization and their various catalytic applications comprising the organic, inorganic and electrochemistry. Among the monometallic NPs, monodisperse Pd and Au nanoparticles will be covered while **M**-Pd (**M:** Co, Ni, Cu, Ag, Au) and **M**-Pt (**M:** Co, Ni, Cu) alloy NPs, and **M**@Pd (**M:** Ni, Ag and Au) core@shell NPs as examples to the bimetallic nanoparticles would be mentioned. These NPs were supported either on commercially available high-surface area carbon materials or 2D materials including reduced graphene oxide (rGO) or mesoporous graphitic carbon nitride (mpg-$C_3N_4$) before their catalytic use. As the catalytic reactions; the dehydrogenation of ammonia borane ($H_3NBH_3$, AB) as a chemical hydrogen storage platform, the transfer hydrogenations using AB as the hydrogen source, the C-C cross-coupling reactions, the electrochemical reduction of $CO_2$ and the high-performance electrocatalysts for the rechargeable Li-air batteries will be covered. More importantly, our attempt towards to commercialization of rGO-$Ni_{30}Pd_{70}$ nanocatalysts will be mentioned.

**References**

[1] M. Zahmakıran and S. Özkar, Nanoscale, 3 (2011) 3462-3481.

---

* Corresponding author, *E-mail: ometin@atauni.edu.tr*

# Nanostructured Functional Thin Films through Vapor Phase Deposition

**Gökhan Demirel***

Gazi University, Faculty of Science, Department of Chemistry, 06500, Ankara, Turkey

*E-mail: gdemirel@gazi.edu.tr*

The ability to control the physicochemical properties of surfaces is important for many areas such as biomedical or optical coatings, sensors, and catalyst supports. We have been developing nanostructured polymeric, metallic, biologic, and semiconductor thin films based on oblique angle deposition (OAP) method for these applications without using any lithography techniques or template materials (Figure 1). These films posses' novel anisotropic (directional) properties which could be potentially manipulated based on the growth conditions and the deposition parameters. The surface-to-volume ratio of structured films is very high and the available surface area increases by more than two orders of magnitude in relation to the bulk film. We are studying nucleation, crystallinity and growth as well as pore size and geometries of nanostructured thin films [1]. Our technique opens a new wealth of applications to assemble many possible combinations of monomers or metallic precursors that have desired functional groups or plasmonic features for creating novel thin films [2,3]. In this presentation, we will describe our process for creating nanostructured thin films and present results concerning their applications.

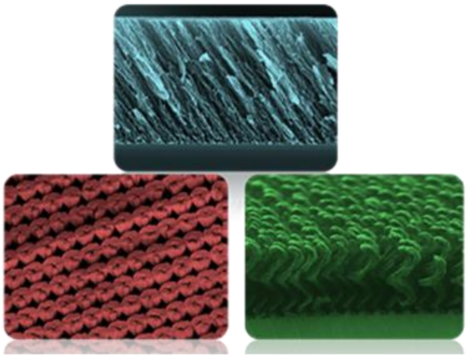


**Figure 1.** SEM images of nanostructured polymeric films

**References**

[1] M. Yilmaz, E. Babur, M. Ozdemir, R.L. Gieseking, Y. Dede, U. Tamer, G.C. Schatz, A. Facchetti, H. Usta and G. Demirel, Nature Materials,16 (2017) 918-924.
[2] M. Yilmaz, M. Ozdemir, H. Erdogan, U. Tamer, U. Sen, A. Facchetti, H. Usta and G. Demirel, Advanced Functional Materials, 25 (2015) 5669-5676.
[3] M. Yilmaz, H.B. Kuloglu, H. Erdogan, S.S. Cetin, M.S. Yavuz, G.O. Ince and G. Demirel, Advanced Materials Interfaces, 2 (2015) 1-5.

---

* Corresponding author, *E-mail: gdemirel@gazi.edu.tr*

I-12

# Aryl C-N Bond Formation Using Organometallic Reagents

**Tahir Daşkapan***

Ankara University, Faculty of Science, Department of Chemistry,
06100, Ankara, Turkey

*E-mail: daskapan@science.ankara.edu.tr*

Aromatic amines are important building blocks in the synthesis of various important organic compounds such as pharmaceuticals, agrochemicals, polymers, dyes, xerographic and photographic materials. Therefore, the development of methods allowing the synthesis of arylamines in high yields is of great importance. Among modern amination methods, electrophilic amination of an easily available organometallic reagent has been found to be a viable alternative method for the formation of aryl C–N bonds and continues to be an active area for research in synthetic organic chemistry [1].

To date various type of aminating reagents have been used in the electrophilic amination of organomagnesium, -zinc, -copper, and -lithium reagents for the introduction of free or protected amino moieties, such as haloamines, substituted hydroxylamines, imines, oxaziridines, oximes, diazonium salts, azodicarboxylates, azides, and metal amides. We focused on the use of ketoximes as aminating reagents in the electrophilic amination of organomagnesium, -zinc, -copper and -cadmium reagents and we developed methods for formation of primary aryl C-N bonds using organometallic reagents that mentioned [2-6].

**References**

[1] T. Daskapan, Arkivoc, v (2011) 230-262.
[2] T. Daskapan, Tetrahedron Lett., 47 (2006) 2879-2881.
[3] T. Daskapan, F. Yeşilbağ and S. Koca, Appl. Organometal. Chem., 23 (2009) 213-218.
[4] T. Daskapan and S. Koca, Appl. Organometal. Chem., 24 (2010) 12-16.
[5] T. Daskapan and A. Korkmaz, Synthetic Communications, 46(9) (2016) 813-817.
[6] T. Daskapan and S. Çiçek, Synthetic Communications, 47(9) (2017) 899-906.

**Acknowledgement**

Financial supports from Ankara University Research Fund is greatly acknowledged by the author.

---

* Corresponding author, *E-mail: daskapan@science.ankara.edu.tr*

# Monitoring Element Compositions and Source Apportionment of Aerosol in Ulaanbaatar, Mongolia

**Amgalan Natsagdorj***

School of Arts and Science, Department of Chemistry, National University of Mongolia, 24100, Ulaanbaatar, Mongolia

*E-mail: n_amgalan@num.edu.mn*

The interest in atmospheric aerosol is high because of its impact on human health and its possible role in climate change. It has also a distinctive effect on visibility and contributes to soiling of monuments. Many epidemiological studies have shown the association between health effects and particulate matter (PM) in ambient air. Health effects of PM are likely to depend on several factors, however, ambient concentrations, size and composition of the particles belong to the most important ones [1].

This study focused on the contents of the air particulate matter pollution of Ulaanbaatar and also determined the chemical composition of air borne samples and the source of those particles. By today, 11 air quality monitoring station have been used to observe an air pollution within Ulaanbaatar. Samples of fine and coarse fractions of particulate matter were collected using a “Gent” stacked filter unit in two fractions of 0-2.2 μm and 2.2-10 μm sizes in two semi-residential areas from September 2012 to August 2016. Multi-elemental analysis was determined by Roentgen Fluorescence Analysis (RFA) using SPESTRO XEPOS spectrometer. This net contribution to soil contamination near the lower value (5%) that arise around the vacuum environment in substantial amounts (14%), where is open around the buildings and residential areas, the soil is considered to be due to the construction. But the data points to the highway in the distance, where is 9% of contaminated of all vehicles smoke, exhaust is similar to the data collected in Ulaanbaatar. Since the analysis was done on a sample-by-sample basis, it is possible to estimate the daily contributions of pollution sources and provide useful information based on a The mass concentration ranged from 25.3 to 148.5 μg/m$^3$, with an annual average of 37.9 μg/m$^3$ for $PM_{10}$. The mass concentration of $PM_{2.5}$ ranged from 21.2 to 106.1 μg/m$^3$ with an annual average of 14.1 μg/m.

Enrichment factors (EF) for elements in $PM_{10}$ and $PM_{2.5}$ were calculated and indicate that elements from anthropogenic origins such as Zn, Pb, Cu, Cr and Cd were highly enriched with respect to crustal elements Al, Fe and Ca.

**References**

[1] P.K. Davy, G. Gunchin, A. Matkwitz, S. Lodoysamba et al., 2011: Air Particulate Matter Pollution in Ulaanbaatar, Mongolia: Determination of Compositions, Source Contributions and Locations, in: Atmospheric Pollution Research 2 (2011) 126-137.

---

* Corresponding author, *E-mail: n_amgalan@num.edu.mn*

# YAKUT HALL

# ABSTRACTS OF ORAL PRESENTATIONS

# Analysis

O-1

# Effect of Suspended Limestone on $SO_2$ Absorption

**Hayrunnisa Mazlumoğlu*** and M. Şahin Gülaboğlu

Ataturk University, Faculty of Engineering, Department of Chemistry, 25000, Erzurum, Turkey

*E-mail: h.mazlumoglu@atauni.edu.tr*

Wet flue desulfurization methods are commonly used to absorb sulfur oxides produced by burning in large coal-fired power stations. The action between aquatic suspensions containing appropriate absorbents and the sulfur oxides in the flue gas forms the basis of these methods. One of the wet flue gas desulfurization methods uses suspended limestone as an absorbent. With this method, $SO_2$ is first physically absorbed within water and then with the aid of the reactive material used is bound with chemical absorption [1,2]. This ore used in the experiments was determined to have appropriate pore distribution and high porosity during research into gas-solid reactions. Linked to these properties this ore had a high $SO_2$ adsorption efficiency rarely seen in the literature [3-7]. In this study with the aim of investigating the effects of limestone on $SO_2$ absorption, experiments were completed in a reactor operating with a three-phase continuous system. The absorption process was first completed in water and then in suspensions with different concentration values and the variation in molar flow of $SO_2$ was investigated. In conclusion phosphate rock, with appropriate characteristics identified in previous studies, may be said to easily enter a reaction with $SO_2$ with high efficiency under conditions appropriate to wet flue gas desulfurization. Furthermore, in light of the data obtained, as the sludge concentration increased, the molar flow was observed to increase.

## References

[1] H. Çavuşoğlu, M.Ş and Gülaboğlu, Mühendislik Bilimler Dergisi, 19(4) (2013) 187-194.
[2] T. Takashina, S. Honjo, N. Ukawa and T. Oishi, Journal Chemical Engineering of Japan. 34 (2001) 810-818.
[3] J. Naktiyok, H. Bayrakçeken, A.K. Özer A and M.Ş. Gülaboğlu, Energy and Fuels. 27 (2013) 1466-1472.
[4] M. Sınırkaya, H. Bayrakçeken, A.K. Özer and M.Ş. Gülaboğlu, Fuel, 87 (2008) 3200-3206.
[5] A.K. Özer, M.Ş. Gülaboğlu and S. Bayrakçeken, Ind. Eng. Chem. Res., 39 (2000) 679-683.
[6] A.K. Özer, M.Ş. Gülaboğlu, S. Bayrakçeken and W. Weisweiler, Fuel, 81 (2002) 41-49.
[7] A.K. Özer, M.Ş. Gülaboğlu, S. Bayrakçeken and W. Weisweiler, Advanced Powder Technol., 17(5) (2006) 481-94.

---

* Corresponding author, *h.mazlumoglu@atauni.edu.tr*

# Antimicrobial and Cytotoxic Activities, and DNA Interactions of Vanillinato Substituted NN or NO Spirocyclic Monoferrocenyl Cyclotriphosphazenes

**Yasemin Tümer*, Nuran Asmafiliz, Zeynel Kılıç, L. Yasemin Koç, Leyla Açık and Hossien Soltanzade**

Karabük University, Department of Chemistry, 78050, Karabük, Turkey

*yasemintumer@karabuk.edu.tr*

In this study, tetrachlorocyclotriphosphazenes containing pendant NN or NO monoferrocenyl groups (**1–5**) were synthesized as starting materials. These compounds have four replaceable Cl atoms with the substituents. Thus, this study focuses on the successive substitution reactions of **1–5** with potassium vanillinate with the aim of investigating the antimicrobial and cytotoxic activities, and the DNA interactions of the mono- (**1a–5a**), geminal and non-geminal *cis/trans* (**1b–5b**), tri- (**1c–5c**) and tetra-substituted monoferrocenylphosphazenes (**1d–5d**) [1]. The compounds **5d** and **cis-5b** have cytotoxic effects on HeLa cell lines in a time dependent fashion (Figure 1). The twelve phosphazenes obtained in this study were screened against G(+) and G(−) bacteria and fungus, *C. albicans*. The compounds **3c**, **3d**, **4c** and **4d** were active against *B. subtilis*. Taking the MIC values into account, **3c** was very effective against *S. aureus* at the very low concentration. Moreover, interactions between the phosphazenes and pBR322 plasmid DNA were observed.

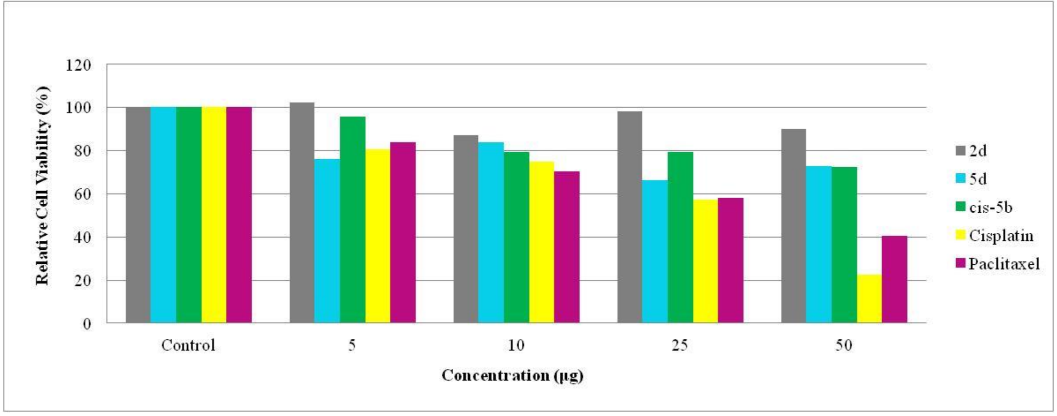


**Figure 1.** Relative cell viability (%) of HeLa cells following exposure of various concentration of compounds **2d**, **5d**, **cis-5b**, cis-platin and paclitaxel between 5 and 50 µg/mL and untreated control cell for 24 h

## References

[1] Y. Tumer, L. Y. Koc, N. Asmafiliz, Z. Kılıc, T. Hokelek, H. Soltanzade, L. Acık, M.L. Yola and A.O. Solak, J. Biol. Inorg. Chem., 20 (2015) 165-178.

## Acknowledgement

The authors acknowledge the “Scientific and Technical Research Council of Turkey” Grant No.112T043.

---

* Corresponding author, *E-mail: yasemintumer@karabuk.edu.tr*

# Square Wave Voltammetric Determination of Cefpodoxime Proxetil by using Pencil Graphite Electrode

**Sevcan Erden*** and **Zehra Yazan**

Ankara University, Faculty of Science, Department of Chemistry, 06100, Ankara, Turkey

*E-mail: sevcanerden@hotmail.com*

Cefpodoxime proxetil (CP) is one of the important semi-synthetic beta-lactam antibiotic belonging to the third generation cephalosporin. It has also been reported as an oral prodrug for the extended spectrum of the bactericidal antibiotic cefpodoxime. Chemically, it is (RS)-1-(isopropoxycarbonyloxy)-ethyl(+)-(6R,7R)-7-[2-(2-amino-4-thiazolyl)-2-{(Z)-methoxy-imino} acetamido]-3methoxymethyl-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylate. The structural formula of CP is represented in Figure 1 [1,2].

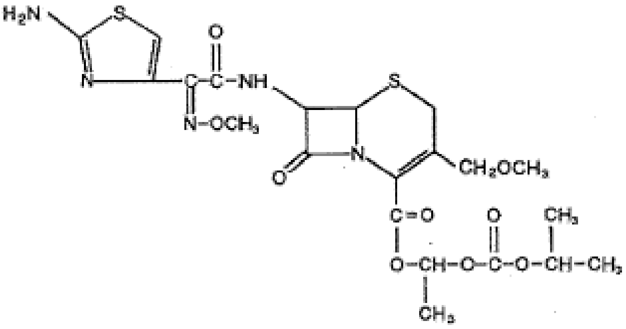


**Figure 1.** The structural formula of CP

In this study, a pencil graphite electrode was used as the electrode for direct electrochemical quantification of cefpodoxime proxetil by using square wave anodic adsorptive stripping voltammetric method. The optimum experimental conditions (pH medium, accumulation time and accumulation potential) and the analytical parameters such as linear working range and detection limit were determined. pH 3.0, accumulation time 15 s and accumulation potential 0.0 V were found. Linear working range was $1.0\times10^{-8} – 6.0\times10^{-7}$ $\mathrm{molL^{-1}}$ and limit of detection (LOD) and limit of quantification (LOQ) were calculated as $2.7\times10^{-9}$ and $9.0\times10^{-9}$, respectively. The procedure was applied successfully to the determination of CP assay in pharmaceutics.

## References

[1] B. Ogorevc, A. Krasna, V. Hudnik and A. Gomiscek, Microchim. Acta, 1 (1991) 131-144.
[2] The Merck Index, an Encyclopedia of Chemicals, Drugs and Biologicals, 13th Edition, Merck & Co., INC New York (2001).

---

* Corresponding author, *E-mail: sevcanerden@hotmail.com*

O-4

# Determination of $H_2O_2$ by High Spin Peroksocomplex

**Tuğba Yavuz** and Levent Pelit*

Ege University, Faculty of Science, Department of Chemistry, 35100, İzmir, Turkey

*E-mail: yavuztugba@yandex.com*

$H_2O_2$ is a reactive oxygen species, which has a great importance in chemistry, biochemistry, and in the field of life sciences. $H_2O_2$, which is an unstable compound cause radical formation in some cases and may have carcinogenic effects to human. For example, 0.1%-0.4% compositions which is administered in the drinking water are found to cause cancer in the mouse duodenum [1]. Because of the rapid degradation of $H_2O_2$, monitoring and identification of it with a fast technique is so important analytical problem. Many methods in the literature including titrimetric, gravimetric, fluorimetric [2], chemiluminescence [3], electrochemical [4] and liquid chromatography [5] were used for the determination of $H_2O_2$. However, most do not have access to adequate sensitivity and these are time consuming methods. In this study, it was aimed to determine $H_2O_2$ in a quickly, reliable and sensitive way for real water samples by spectrophotometrically. The method is based on the complexation of hydrogen peroxide with the Fe(III)-EDTA complex in the alkaline medium. A purple color of low stable peroxo-iron(III)-EDTA complex was formed in this study (Figure 1).

**Figure 1.** The color of a) Fe(III)-EDTA-$NH_3$ and b) Fe(III)-EDTA-$NH_3$-$H_2O_2$ complex

The method was applied to spectrophotometric analysis at 525 nm. Limit of detection and limit of quantification was found as $2.5x10^{-6}$ and $8.5x10^{-6}$mol/L. Intraday and interday relative standard deviation of the proposed method for $2.0x10^{-4}$mol/L of $H_2O_2$ were found as 1.5% and 6.1% respectively. The proposed method was successfully applied to real water samples namely drinking water, tap water and seawater with acceptable recovery value between 90% and 118%.

**References**
[1] J.M. Desesso, A.L. Lavin, S.M. Hsia and R.D. Mavis, Food and Chemical Toxicology, 38 (2000) 1021-1041.
[2] M.E. Abbas, W. Luo, L. Zhu, J. Zou and H. Tang, Food Chemistry, 120 (2010) 327-331.
[3] S. Lu, J. Song and L. Campbell-Palmer, Scientia Horticulturae, 120 (2009) 336-341.
[4] J.V.B. Kozan, R.P. Silva, S.H.P. Serrano, A.W.O. Lima and L. Angnes, Analytica Chimica Acta 591 (2007) 200-207.
[5] S. Effkemann, U. Pinkernell and U. Karst, Analytica Chimica Acta, 363 (1998) 97-103.

---

* Correspondingauthor, *E-mail:levent.pelit@ee.edu.tr*

# Adsorptive Stripping Voltammetric Determination of the Anti-Cancer Agent Dasatinib Using Disposable Pencil-Graphite Electrode

**Dilek Eskiköy Bayraktepe*, Zehra Yazan and Kamran Polat**

Ankara University, Faculty of Science, Department of Chemistry, 06560, Ankara, Turkey

*E-mail: dilekeskikoy@gmail.com*

Dasatinib (DST), N-(2-chloro-6-methylphenyl)-2-[[6-[4-(2-hydroxyethyl)-1-piperazinyl]-2-methyl-4-pyrimidinyl]amino]-5-thiazole, Figure 1, is a multitarget tyrosine kinase inhibitor, effective against the proliferation of cells expressing mutant kinases. It is synthesized from a 2-aminothiazole derivative which is considered the novel Src family kinase inhibitor template [1]. Drug is under investigation for the treatment of chronic, accelerated or blast-phase myeloid leukaemia resistant or intolerant to prior therapy [2-4]. It is also on stage of clinical trials for the treatment of nonHodgkin's lymphoma, metastatic breast cancer and prostate cancer. In this study, electrochemical oxidation behavior and voltammetric anodic adsorptive stripping determination of DST was studied by using a disposable pencil graphite as the electrode (PGE). Cyclic voltammetry (CV) on the PGE was chosen to study the electrochemical redox properties of DST. The CV studies show that DST has an irreversible oxidation signal at about +1.0 V in acidic media. Furthermore, adsorptive stripping anodic square wave voltammetric technique was developed to determine DST in real samples. The anodic peak current of DST varies linearly in the concentration range 0.0092-1.0 µmol $L^{-1}$. Detection and quantification limits (LOD and LOQ) were calculated as 0.0028 µmol $L^{-1}$ and 0.0092 µmol $L^{-1}$. The voltammetric technique devised was applied to the DST analysis in human urine.

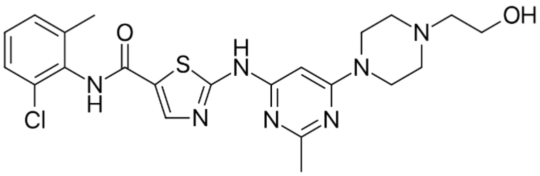


**Figure 1.** Chemical structure of DS

**References**

[1] J. Das, P. Chen, D. Norris, R. Padmanabha, J. Lin, R.V. Moquin, Z. Shen, L.S. Cook, A.M. Doweyko, S. Pitt, S. Pang, D.R. Shen, Q. Fang, H.F. De Fex, K.W. McIntyre, D.J. Shuster, K.M. Gillooly, K. Behnia, G.L. Schieven, J. Wityak and J.C. Barrish, J. Med. Chem., 49 (2006) 6819-6832.
[2] J.C. Montero, S. Seoane, A. Ocaña and A. Pandiella, Clin. Cancer Res.,17 (2011) 5546-5552.
[3] M. Steinberg, Clin. Ther., 29 (2007) 2289-2308.
[4] J.S. Tokarski, J.A. Newitt, C.Y.J. Chang, J.D. Cheng, M. Wittekind, S.E. Kiefer, K. Kish, F.Y.F. Lee, R. Borzillerri, L.J. Lombardo, D. Xie, Y. Zhang and H.E. Klei, Cancer Res., 66 (2006) 5790-5797.

---

* Corresponding author, *E-mail: dilekeskikoy@gmail.com*

O-6

# Synthesis and DSSC Applications of New Ruthenium Complexes Bearing Benzimidazole Type Ligands

**Melek Tercan** and Osman Dayan*

Çanakkale Onsekiz Mart University, Faculty of Science and Arts, Department of Chemistry, 17100, Çanakkale, Turkey

*E-mail: melek-tercan@hotmail.com*

In recent years, DSSC design has become very important as an alternative to silicon based solar cells. Many different classes of dyes are used in DSSS's, but in the literature the best photovoltaic performance and longest stability have obtained by $ML_2(X)_2$ type complexes (M: Ru, L: 2,2'-bipyridyl-4,4'-dicarboxylic acid ligand, X: halogen, Cyanide, thiocyanate, acetyl acetonate, water) [1]. Pyridinyl ligands affect charge transfer transition energy from metal to ligand significantly. Also, it is possible to adjust the redox properties of the metal center by selecting the appropriate ligand [2,3]. In this study, 7 different polypyridyl ligands (derivatives of 2-(6-methylpyridine-2-yl)-1H-benzimidazole) and their Ru complexes were synthesized and characterized (Figure 1). Electrochemical and dye sensitized solar cell properties of the complexes were investigated and the results are given in Table 1.

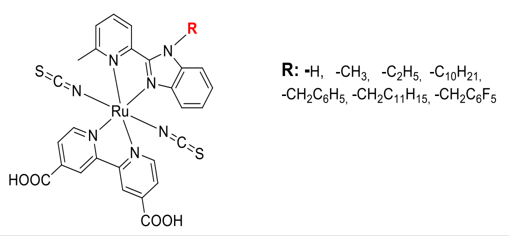


**Figure 1.** Synthesized Ru-polypyridyl complexes

**Table 1.** Photovoltaic characteristics of the complexes

| Complex | $V_{oc}$ (V) | $I_{sc}$ (mA/cm$^2$) | ff | % η | % η* |
|---|---|---|---|---|---|
| MT-47 | 0.448 | 0.87 | 0.3586 | 0.141 | 0.85 |
| MT-48 | 0.499 | 0.32 | 0.4747 | 0.076 | 0.46 |
| MT-49 | 0.499 | 0.65 | 0.5756 | 0.187 | 1.12 |
| MT-50 | 0.409 | 0.30 | 0.4340 | 0.053 | 0.32 |
| MT-51 | 0.339 | 0.08 | 0.4650 | 0.013 | 0.08 |
| MT-52 | 0.559 | 1.53 | 0.5940 | **0.509** | **3.05** |
| MT-53 | 0.439 | 0.39 | 0.5780 | 0.090 | 0.54 |
| Reference | 0.649 | 2.75 | 0.5710 | **1.020** | **≈6** |

## References

[1] L.L. Li and E.W.G. Diau, Chem. Soc. Rev., 42 (2013) 291-304.
[2] H.N. Yi, J.A. Crayston and J.T.S. Irvine, Dalton Trans., 4 (2003) 685-691.
[3] D.B. Kuang, C. Klein, S. Ito, J.E. Moser, R. Humphry-Baker, S.M. Zakeeruddin, M. Gratzel, Adv Funct Mater, 17 (2007) 154-160.

---

* Corresponding author, *E-mail: osmandayan@hotmail.com & osmandayan@comu.edu.tr*

O-7

# Potential Bioactive 1,4-Naphthoquinone Derivatives

**Ayşecik Kaçmaz***

Istanbul University, Faculty of Engineering, Department of Chemistry, 34320,
Istanbul, Turkey

*E-mail: ayse_kacmaz@yahoo.com*

Naphthoquinones are of considerable interest, which is associated with their biological activities [1] such as molluscicidal, cyclotoxic, antibiotic, antiviral, anti-tumor, antibacterial, antifungal, anti-inflammatory, antiproliferative, antipyretic, antimicrobial, antiparasitic activities and other uses such as synthetic intermediates, photosensitizer and dyes. Also, plants including naphthoquinone are used in the traditional medicines. Quinone's pharmacological activities are related to their oxide/reduction properties.

In this study, it is described that the synthesis of some NH- substituted-1,4-naphtoquinone derivatives with the reactions of 2,3-dibromo-1,4-naphtoquinone (or 2-bromo-1,4-naphthoquinone) and some amines. Aminonaphthoquinones are formed by nucleophilic displaced of halogen of naphthoquinones. The formation of novel quinone derivatives was carried out in the presence of organic solvents such as chloroform, ethanol and methanol at room or reflux temperature. All the synthesized compounds were purified by column chromatography with solvents (chloroform or n-hexane). These synthesized compounds were characterized by mass spectrometry, UV-Vis, IR, $^{1}$H-NMR, NMR ($^{13}$C/APT), ESI-MS techniques. The novel synthesized naphthoquinone derivatives are promising compounds for using in pharmacological field.

**Reference**

[1] P. Babula, V. Adam, L. Havel and R. Kizek, Current Pharmaceutical Analysis, 5 (2009) 47-68.

---

* Corresponding author, *E-mail: ayse_kacmaz@yahoo.com*

# Water Soluble Silicon Phthalocyanines, Naphthalocyanines and Investigation of their DNA Binding, DNA Photocleavage, Topoisomerase I Inhibition

**Ayşenur Sofuoğlu[1], Zekeriya Bıyıklıoğlu[1]*, Burak Barut[2] and Arzu Özel[2]**

[1]Karadeniz Technical University, Faculty of Science, Department of Chemistry, 61080, Trabzon, Turkey
[2]Karadeniz Technical University, Faculty of Pharmacy, Department of Biochemistry, 61080, Trabzon, Turkey

*E-mail: aysenur_sofuoglu@hotmail.com*

Cancer is one of the deadliest diseases in the world. Although there are several methods for treatment of this disease such as chemotherapy, radiation therapy and surgery, these methods have important side effects such as haematopoietic, neurologic disorders, cardiotoxicity and hyperpigmentation [1]. Photodynamic therapy (PDT) is an alternative method for cancer treatment because of minimal toxicity and selectively abolishing of a malignant tumor generation of reactive oxygen species [2]. Phthalocyanines (Pcs) are used as photosensitizer for PDT due to photo-stabilities, high singlet oxygen production abilities their strong absorption in the phototherapeutic window. The water soluble photosensitizers are important compounds in the cellular uptake and photodynamic efficacy in PDT [3]. In this study, new water soluble axially disubstituted silicon phthalocyanine and naphthalocyanines were synthesized for the first time (Figure 1). The binding modes of the Pcs with calf thymus-DNA (CT-DNA) were carried out using UV-Vis absorption titration, competitive ethidium bromide and thermal denaturation experiments. In addition, DNA-cleavage activities (hydrolytic, photoinduced, oxidative) of water soluble phthalocyanines were investigated using supercoiled pBR322 plasmid DNA on agarose gel electrophoresis. Also, the topoisomerase I inhibitory properties of these compounds were investigated using agarose gel electrophoresis.

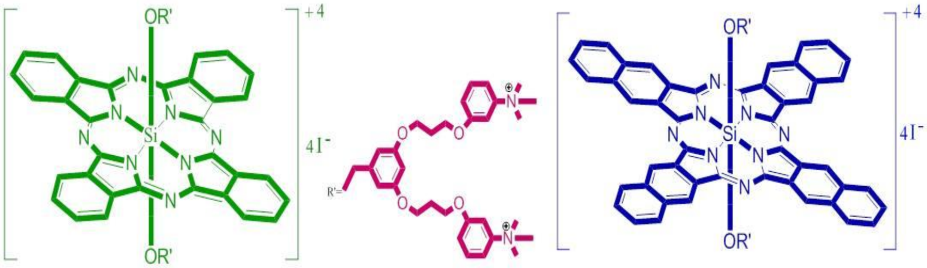


**Figure 1.** Water soluble silicon phthalocyanine and naphthalocyanine

**References**
[1] T. Keleş, B. Barut, Z. Biyiklioglu and A. Özel, Dyes and Pigments, 139 (2017) 575-586.
[2] S. Çolak, M. Durmuş and S.Z. Yıldız, Polyhedron, 113 (2016) 115-122.
[3] S. Çolak, M. Durmuş and S.Z. Yıldız, J. Photochem. Photobiol. A: Chem., 325 (2016) 125-134.

**Acknowlegement**
This study was supported by The Scientific & Technological Research Council of Turkey (TÜBİTAK, project no: 116Z364).

---

* Corresponding author, *E-mail: zekeriyab@ktu.edu.tr*

# Comparative Study of New Spectrophotometric Techniques for the Simultaneous Determination of Ezetimibe and Rosuvastatin in Binary Mixtures

**Gizem Tırıs[1] and Nevin Erk[2]***

[1]Bezmialem Vakıf University, Faculty of Pharmacy, Department of Analytical Chemistry, İstanbul, Turkey
[2]Ankara University, Faculty of Pharmacy, Department of Analytical Chemistry, 06100, Ankara, Turkey

*E-mail: gizem.tiris@gmail.com*

Two highly accurate and rapid new spectrophotometric techniques were presented as convenient and useful alternatives for simultaneous determination of Ezetimibe (EZ) and Rosuvastatin (RO) in binary mixtures. The simultaneous ratio difference spectrophotometry, the difference amplitudes in the ratio spectra at 227.3-254.6 nm and at 241.8-253.9 nm were selected to determine EZ and RO in the binary mixture. The mean percentage recoveries were calculated to be 100.8 % for EZ and 98.7 % for RO, respectively. The other method depends on the application simultaneous ratio subtraction spectrophotometry to resolve the interference due to spectral overlapping [1]. The simultaneous ratio subtraction spectrophotometry was based on the ratio $\lambda_{max}$ absorbances in the ratio spectra obtained by measurements of the signals at 227.3 for EZ and 241.8 nm for RO, respectively [2]. The developed methods were rectilinear in the concentration ranges 6.0-36.0 ug/mL for EZ and 6.0-40.0 ug/mL for RO, respectively. The results of the simultaneous determination of EZ and RO in laboratory synthetic prepared mixtures with the use of the simultaneous ratio subtraction spectrophotometry was showed good precision and recovery when the calibration graphs were estimated using classical regression equation: $y = 0.1213x-0.2073$ ($R^2$: 0.9989) (where y is analytical signals in the ratio $\lambda_{max}$ absorbances spectra in ratio spectra , and C is the concentration) at 227.3 nm and $y = 0.0974\ x - 0.0549$ ($R^2$: 0.9981) at 241.8 nm for EZ and RO, respectively. Regarding the precision of the presented spectrophotometric methods a statistical comparasion of the results of was performed using Student's t-test and F-test at the 95 % confidence limits.

**References**

[1] H.M. Lotfy and M.A.M. Hegazy, Spectrochim. Acta A, 113 (2013) 107-114.
[2] H.M. Lotfy and M.A.M. Hegazy, Spectrochim. Acta A, 96 (2012) 259-270.

---

* Corresponding author, *E-mail: erk@pharmacy.ankara.edu.tr*

# Novel Spectrophotometric Methods for the Determination of Zofenopril and Lercanidipine in Binary Mixtures

**Nevin Erk* and Berk Toker**

Ankara University, Faculty of Pharmacy, Department of Analytical Chemistry, 06100, Ankara, Turkey

*E-mail: berktoker*@me.com

Ratio difference and Derivative UV spectrophotometric methods are presented for the simultaneous determination of antihypertensive binary mixture namely Zofenopril (ZO)-Lercanidipine (LE). A new ratio difference UV spectrophotometric method [1] is based on the signal difference between two wavelengths in the ratio spectra. Using ratio difference UV spectrophotometry, the amplitudes in the ratio spectra at 271.9 – 289.6 nm and 241.3 – 271.5 nm are selected to simultaneous determine ZO and LE in the binary mixture. The linearity range and percentage recovery for ZO and LE are 3.0–35.0, 5.0–35.0 μg.ml$^{-1}$ and 99.47 ± 1.23, 100.09 ± 1.38, respectively. The other method, zero-crossing derivative UV spectrophotometry [2], is based on recording the first derivative curves and determining each component using zero-crossing method. The first derivative spectrophotometry, the signals in the first derivative UV spectra at 229.5 and 241.5 nm are selected to simultaneous determination ZO and LE in the binary mixture. The linear regression of derivative absorbance signals on concentration gave the equation; y = -0.0142 x – 0.0181 (R$^2$: 0.9931) (where y is analytical signals in the first derivative spectra, and C is the concentration) at 229.7 nm and y = -0.0013 x - 0.0009 (R$^2$: 0.9981) at 241.5 nm for ZO and LE, respectively. Lambert-Beer law is obeyed in the concentration range of 3.0–35.0 μg.ml$^{-1}$ for ZO and 5.0–35.0 μg.ml$^{-1}$ for LE, respectively. The percentage assay of ZO and LE are 100.4 ± 1.34 and 101.3 ± 0.55, respectively. The novel spectrophotometric methods, which give thoroughly comparable data, are simple, fast, require no preliminary separation steps, can reliably be used for routine analysis of ZO and LE in bulk drug and laboratory prepared binary mixtures.

**References**

[1] P. Leveıllıan and D. Fompeydıe, Anal., 14 (1986) 1-8.
[2] H.M. Lotfy and M.A.M. Hegazy, Spectrochim. Acta A, 113 (2013) 107-114.

---

* Corresponding author, *E-mail: erk@pharmacy.ankara.edu.tr*

# Archaeological Chemistry

O-11

# Advantages and Disadvantages of Raman Spectroscopy to the EPMA in the Determination of Mineral Composition of the Rocks

**Yusuf Kağan Kadıoğlu***

Department of Geological Eng., Ankara University, Golbasi, Ankara, Turkey
Earth Sciences Application and Research Center of Ankara University, Ankara, Turkey

*E-mail: kadi@ankara.edu.tr*

The element varieties of the rock minerals depend on the source of the liquid of the main magma source with the equilibrium conditions, cooling and re-equilibration of the components within the system. The detail elemental compositions may reflect the nature and crystallization history of the minerals in the whole system of the rock unit. Electron microprobe (EPMA) is one of the most useful methods in the determination of the detail element composition for the nomenclature of minerals within the rock units. Confocal Raman spectrometry (CRS) is one of the useful methods in the nomenclature of the minerals using their shift in the wavelength of the elastically scattered radiation providing from the chemical and structural of the minerals [1]. CRS is one of the useful technique that can be used for mineralogical researches, since it has high spatial resolution and non-destructive properties [2]. This spectrometry can provide data with high spatial resolution of < 1μm when coupled to confocal microscopy of the system. In addition, on-site analysis can be performed using mobile systems and remote sampling accessories even in the field studies. The Raman Shift spectrum of the different classes of the minerals provides instant identification of the specific class. The high bending modes or the constant value of Raman Shift of the minerals reveals an important value in the nomenclature of each type of the minerals. EPMA Perform chemical microanalyses of the minerals for all types of the rock units. The contributions of the EPMA to the characterization of minerals, both igneous, metamorphic and sedimentary, and to other significant geological studies, such as light element analysis, trace element analysis, rare earth element analysis and even element mapping, is quite easy and capable. Although EPMA is one of the useful methods in the determination of the mineral chemistry, however the alterations to their products within the minerals may lead to dismiss of the understanding the source of the magma during the crystallization. CRS has most advantage to the EPMA in the determinations of the type and reason of the alteration in the obtaining the Raman shift value during the measurement. Detail EPMA analysis may use in the calculation of the crystal thermometry and barometry however the CRS Raman Shift may not able to obtain the crystallization condition of the whole magma. Many examples can be given to the advantages and disadvantages of the both spectroscopy during the applications.

**References**

[1] B. Güllü and Y.K. Kadıoğlu, Spectrochimica Acta Part A, 183 (2017) 68-74.
[2] İ. Üstündağ, Z. Üstündağ, O.M. Kalfa, Y.K. Kadıoğlu, Nuclear Instruments and Methods in Physics Research B, 254 (2007) 153–159.

---

* Corresponding author, *E-mail: kadi@ankara.edu.tr*

# Archaeometric Analyses of Medieval Period Ceramics from Hasankeyf Archaeological Area

**Ali Akın Akyol[1]*, Nurşen Özkul Fındık[2] and Nurşen Sarı[3]**

[1]Gazi University, Faculty of Fine Arts, Department of Conservation and Restoration of Cultural Properties, 06830, Ankara-Turkey
[2]Gazi University, Faculty of Arts, Dept. of History of Art, 06500, Ankara-Turkey
[3]Gazi University, Faculty of Science, Dept. of Chemistry, 06500, Ankara-Turkey

*E-mail: aliakinakyol@gmail.com*

Today, people give a special attention on historical events and ancient materials. It is very obvious that the historical movements and archaeological findings are the mirror for human to see their past and to find their cultural roots. Ceramics are the most preferred materials to reach historical and cultural knowledge (especially for the prehistoric), so they are accepted as one of the main materials creating a communication bridge among the communities socially. In other words, scientifically c*eramic* is an inorganic, non-metallic, solid material comprising metal, non-metal or metalloid atoms primarily held in ionic and covalent bonds. In this sense, commonly used methods are archaeometric studies which include physical, chemical, mineralogical, spectroscopic, thermal and microscopic characterizations of ancient relics recovered in archaeological excavations. In this study, ceramic samples obtained from the Hasankeyf (Batman, Turkey) archaeological site were investigated. Hasankeyf is a significant medieval settlement area over the Batman-Mardin and Batman-Şırnak highways 37 km from the city center of Batman located in the Southeastern Anatolia Region. The city, which has been a residential area since the prehistoric times, served as a strategically significant fortress during the reign of the Roman Empire (2nd century AD). Starting with the 7th century AD, the sovereignty of the Umayyad, Abbasid, Hamdani and Mervani in order was lived in Hasankeyf. The Hasankeyf medieval period ceramic samples were primarily evaluated visually and then coded and photographed within the scope of documentation work. Accordingly the physical properties (their color and thickness) and the dynamic characteristics of the samples were determined by means of an ultrasonic velocity (SV) measurement tests. The petrographic characteristics of the samples were determined by thin-section optical microscopy analysis and the chemical structures were determined by XRF, SEM-EDS and TGA analyses [1].

**Figure 1.** Medieval period ceramic samples from Hasankeyf Archaeological Area

## Reference

[1] N. Özkul Fındık, A.A. Akyol and N. Sarı, Journal of Mediterranean Archaeology & Archaeometry, 14 (2014) 261-271.

---

* Corresponding author, *E-mail: aliakyol@gazi.edu.tr*

# Bioscience & Biotechnology

# Microfluidic Biosensor Integrated Organ-an-a-Chip System for Drug Discovery

**Hüseyin Avcı***

Eskisehir Osmangazi University, Metallurgical and Materials Engineering Department, 26040, Eskisehir, Turkey

*E-mail: havciesogu@gmail.com*

The significant development in the construction of microscale cell culture platforms and interest in bioanalytical analysis to recapitulate the important cellular biological and physiological activities have resulted emerging a new concept of 'organ-on-a-chip' system [1,2]. Organ-on-a-chip is a new three-dimensional (3D) *in vitro* microfabricated unit that contains a multichannel microfluidic cell culture unit. They are a viable platform for personalized medicine and drug screening. These models are demonstrating biomimetic compositions, architectures, and functions. It is highly expected to be replaced with the conventional planar, static cell cultures and the more accurate results bridging the current gap between main clinical complaints. As shown in Figure 1, a novel aptamer-based electrochemical biosensor which was integrated to an organ-on-a-chip platform with enhanced sensitivity for measurements of very small amounts of cardiac injury biomarker of CK-MB has been developed recently [3]. Successful demonstration of capturing trace amounts of CK-MB secreted by the cardiac organoids after treatment with a common drug in a dose-dependent manner, thereby allowing continuous *in situ* detection of biomarkers of interest. The result was also confirmed to have a significant relationship with the changes in the beating rates and cellular viability assessments.

It is strongly believed that these novel platforms that are capable of automated and continual detection will be used for long-term recording and analyzing of human tissues and organoids during the drug development and treatments.

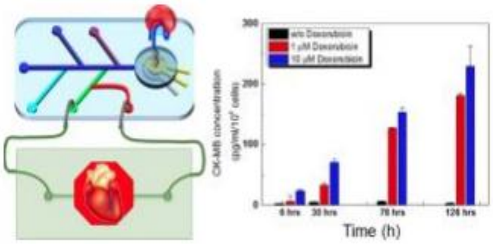


**Figure 1.** Schematic representation of heart-on-a-chip connected to the electrochemical biosensor and CK-MB concentrations versus time

**References**

[1] H. Avci, F.D. Guzel, S. Erol and A. Akpek, Turkish Journal of Chemistry (2017) (Just accepted).

[2] Y.S. Zhang, J. Aleman, S.R. Shin, T. Kilic, D. Kim, S.A.M. Shaegh, S. Massa, R. Riahi, S. Chae, N. Hu, H. Avci, W. Zhang, A. Silvestri, A.S. Nezhad, A. Manbohi, F. De Ferrari, A. Polini, G. Calzone, N. Shaikh, P. Alerasool, E. Budina, J. Kang, N. Bhise, J. Ribas, A. Pourmand, A. Skardal, T. Shupe, C.E. Bishop, M.R. Dokmeci, A. Atala and Ali Khademhosseini, PNAS (2017) 201612906.

[3] S.R. Shin, Y.S. Zhang, D.J. Kim, A. Manbohi and H. Avci, Analytical Chemistry, 88 (2016) 10019-10027.

---

* Corresponding author, *E-mail: havciesogu@gmail.com*

O-14

# An Effective Natural Approach to Synthesize Magnetic Nanoparticles

**Hamed Ghorbanpoor**[1], **Hüseyin Avcı**[2]* **and Macid Nurbaş**[3]

[1]Eskisehir Osmangazi University, Department of Polymer Science and Technology, 26040, Eskişehir, Turkey
[2]Eskisehir Osmangazi University, Metallurgical and Materials Engineering Department, 26040, Eskişehir, Turkey
[3]Eskisehir Osmangazi University, Chemical Engineering Department, 26040, Eskişehir, Turkey

*Email:hamedeghorbanpoor@gmail.com*

Nowadays, different plant materials are utilized for bio-based synthesis of nanoparticles by using green technology mainly due to having no any harmful chemicals. Biosynthesis methods demonstrate many advantages over many traditional procedures in the terms of the availability of more biological entities and eco-friendly approach. The rich biodiversity and easy reach of the plant entities reasoned that the considerable research has been devoted to the syntheses of the nanomaterials [1]. The purpose of this study was to improve the synthesis method for obtaining magnetic nanoparticles ($Fe_3O_4$) by using ferric chloride hexa-hydrate, ferrous chloride tetra-hydrate and by extraction of *Platanus* leaves without any stabilizers, distributors and oxidants. By this way, an easy, economic and environmentally friendly synthesis was aimed without using organic solvents and physical steps with surface active materials. In our research, the $Fe_3O_4$ magnetite nanoparticles were successfully obtained as demonstrated by one remarkable peak at 553 $cm^{-1}$ in the spectra of the synthesized magnetite nanoparticles [2]. This peak is assigned to the Fe–O stretching band of the bulk magnetite. The metal-oxygen band at 553 $cm^{-1}$ can be contributed to intrinsic stretching vibrations of metal at the tetrahedral site [3]. The geometry of the most nanoparticles was quasi-spherical like structures with the average diameters of 7.69 ± 1.55 nm. Other particles possess the average diameter of 39.70 ± 2.76 nm as shown in Figure 1. The reason of the variety of the size distribution of the nanoparticles probably because of the mixture of various derived components with different reducing mechanisms in *Platanus* leaf extract. As a result, our eco-friendly approach for synthesizing the nanoparticles is simple and cost effective by using non-toxic components. Hence, it has a high potential to use in many different applications from the wastewater treatment to the biomedical uses with further investigations.

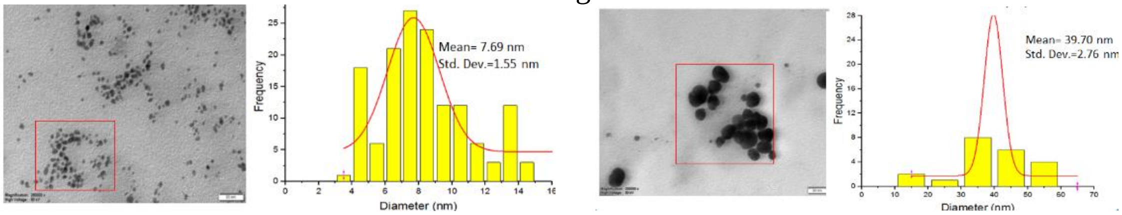


**Figure 1.** TEM images and size distributions of magnetite iron oxide nanoparticles

## References

[1] M. Johannsen, U. Gneveckow and *et al*. International Journal of Hyperthermia, 23 (2007) 315-323.
[2] Y.P. Yew, K. Shameli, M. Miyake, N. Kuwano and *et al*., Nanoscale Research Letters, 11 (2016) 276.
[3] A. Demir, R. Topkaya and A. Baykal, Polyhedron, 65 (2013) 282-287.

---

* Corresponding author, *E-mail: havciesogu@gmail.com*

O-15

# The Effect of Synthesis Conditions on Formation of Protein-Inorganic Hybrid Nanoflowers (hNFs)

**Nalan Özdemir***, **Cevahir Altınkaynak and İsmail Yılmaz**

Erciyes University, Faculty of Science, Department of Chemistry, 38039 Kayseri, Turkey

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

In 2012, firstly Dr. Zare and co-workers reported protein-inorganic hybrid nanoflowers using some proteins [1]. Over the past five years, as a new hybrid material, flower-like protein-inorganic hybrid nanomaterials (nanoflowers) have aroused tremendous interests. These flower-like nanomaterials possess large surface-to-volume ratio compared with that of bulk materials and combine with the advantages of organic and inorganic components [2-4].

In this work, we synthesized flower-like protein-$Cu_3(PO_4)_2.3H_2O$ nanoflowers and studied some important features (structure, encapsulation yield, weight percentage, etc.) of these hybrid materials as a function of synthesis conditions (metal ion and enzyme concentrations, the pH of the buffer solution, synthesis volume etc.). Synthesized hybrid materials were characterized by SEM, FTIR, XRD, EDX, and UV-Vis. It was found that synthesis conditions significantly influence the properties of these hybrid nanoflowers.

## References

[1] J., Ge, J. Lei and R. N. Zare, Nature Nanotechnology, 7 (2012) 428-432.
[2] B. Somtürk, M. Hancer, I. Ocsoy and N. Özdemir, Dalton Transactions, 44 (31) (2015) 13845-13852
[3] C. Altinkaynak, S. Tavlasoglu, N. Özdemir and I. Ocsoy, Enzyme Microbial Technology, 93-94 (2016) 105-112.
[4] Z. Lin, Y. Xiao, Y. Yin, W. Hu, W. Liu and H. Yang, ACS Applied Materials Interfaces, 6 (13) (2014) 10775-10782.

## Acknowledgement

This study is supported by a grant (Project Number: FYL-2016-6582) from Scientific Research Projects Committee of Erciyes University.

---

* Corresponding author, *E-mail: ozdemirn@erciyes.edu.tr*

# Nanopores as Single Molecule Sensing Tools

**Fatma Doğan Güzel***

Department of Biomedical Engineering, Ankara Yıldırım Beyazıt University, Ankara 06010, Turkey

*E-mail: fdogan@ybu.edu.tr*

Nanopores, both solid-state and biological ones, are excellent tools to detect single molecules with high precision. They are being utilized in many applications so far including DNA-RNA sensing, epigenetics, DNA-protein interactions and even antibiotic resistance [1,2]. Detection using nanopores has numerous advantages over conventional techniques (e.g. gel electrophoresis) and these are label-free detection, use of low sample volumes and the ability to extract single molecule information. A nanopore can be either biological or fabricated on a solid-state microchip. Biological nanopores exists naturally and can be experimentally inserted into artificially created lipid bilayers, allowing the electrophysiological study of the ionic current across. As for solid-state nanopores, many non-porous semiconducting and insulating material (e.g. Si, $SiO_2$, graphene, polymers) can be employed for nanopore chip fabrication. Here, we present compact nanopore-integrated microfluidic devices with single molecule detection capability. Both solid-state and biological nanopores (single one of them) are integrated into a single microfluidic channel for the detection of single DNA molecules in flow and the investigation of antibiotic permeability, respectively (Figure 1). The detection concept is simple: upon the application of the electric field, an ionic pathway is created from the channel to the back side of the device through a single nanopore. As shown in 1c, this is recorded as a stable current trace due to the passage of the electrolyte ions. Once DNA is added to the channel, DNA blocks the pore for a certain amount of time and current blockage events are observed, referring to individual DNA translocations. In conclusion, these studies demonstrate that nanopore-integrated microfluidic sensors can be used for single molecule detection in flow, successfully.

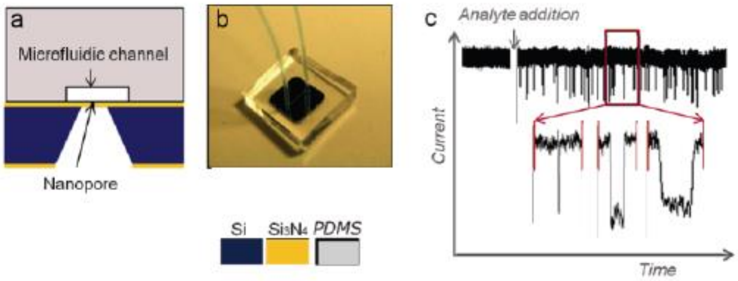


**Figure 1.** Schematic of the device, a photography image and representative data for detection signal

**References**
[1] B.N. Miles, et al. Chemical Society Reviews, 2012.
[2] C. Dekker, Nat. Nano., 2(4) (2007) 209-215.

---

* Corresponding author, *E-mail: fdogan@ybu.edu.tr*

# Design of Medium Conditions by Plackett Burman Method for Microbial Production of cis,cis-Muconic Acid

**F. Elif Uzun, Rahime Songür and Emine Bayraktar***

Ankara University, Faculty of Engineering, Department of Chemical Engineering,
06100, Ankara, Turkey

*E-mail: elf.uzun@gmail.com*

Muconic acid, one of the unsaturated dicarboxylic acid (2,4-hexadienedioic acid), has industrial significance because of their double bond and two carboxylic groups and therefore it can be polymerized to produce synthetic resins and biodegradable polymers. There are three isomers of muconic acid designated *cis,cis*-muconic acid, *cis,trans*-muconic acid, and *trans,trans*-muconic acid. By means of having three isomers, muconic acid is used as precursors in many areas of industry. Adipic acid, terephthalic acid and trimellitic acid are obtained from these three isomers and they are widely used in the production of commercially important chemical substances. A number of products might be generated that has industrial importance with those chemical compounds obtained from the isomers of muconic acid such as; nylon-6,6, polytrimethylene terephthalate, polyethylene terephthalate, dimethyl terephthalate, trimellitic anhydride, industrial plastics, resins, polyester polyols, food ingredients, pharmaceuticals, plasticizers, cosmetics, and engineering polymers. *cis,cis*-Muconic acid is produced by aromatic compounds (benzene, benzoate, toluene and catechol) are degraded by several microbial species such as *Pseudomonas*, *Arthrobacter*, *Corynebacterium* and *Sphingobacterium* and it is called β-ketoadipate (orto-cleavage) pathway [1].

The aim of this study is microbial production of *cis,cis*-muconic acid by *Pseudomonas putida* KT2440 cells with using sodium benzoate and design the medium conditions with the Plackett Burman method. For this purpose, design of the levels of sodium benzoate and glucose concentration, pH, temperature, $Na_2HPO_4$, $KH_2PO_4$, NaCl, $(NH_4)_2SO_4$, $MgSO_4$, $CaCl_2$ and $FeSO_4$ components wes performed by the Design Expert (10.0) and conditions for product concentration were determined.

**References**

[1] N. Z. Xie, H. Liang, R. B. Huang and P. Xu, Biotechnology Advances, 32 (2014) 615-622.

**Acknowlegement**

This study is supported by the project of Ankara University Scientific Research Projects number of 17L0443004.

---

* Corresponding author, *E-mail: bayrakta@eng.ankara.edu.tr*

# An Electrochemical Biosensor for the Development of an Antibiotic Permeability Assay

**Hilal Yıldırım[1], Abdellatif Baraket[2], Nadia Zine[2], Abdelhamid Errachid[2] and Fatma Doğan Güzel[1]***

[1]Department of Biomedical Engineering, Ankara Yıldırım Beyazıt University, Ankara 06010, Turkey
[2]Université de Lyon, Institut des Sciences Analytiques, UMR 5280, 69100 France

*E-mail: hlalyildirim@gmail.com*

The efficacy of antibiotics mainly depends on their ability to pass through the lipid membrane of the bacterial cell wall. The development of highly sensitive quick tests to directly monitor the membrane transport processes however has been an experimental challenge. In this work we report the development of a highly sensitive electrochemical biosensor to characterize antibiotic uptake (e.g; norfloxacin (NF). The biosensor platform contains 4 working gold micrelectrodes (WEs), integrated reference and counter microelectrodes (Figure 1B). The detection of the antibiotic was carried out by using electrochemical impedance spectroscopy (EIS) and a competitive assay. Therefore, a specific biomarker SA2BSA was immobilized onto gold working electrodes using diazunium salt. These biomarkers are detectable by anti-Norfloxacine antibodies (ANF). Afterward, the biosensor was incubated in a solution of ANF at fixed concentration and NF antibiotics (Figure 1). Here the ANF were in a state of competition to detect either SA2BSA or NF. In case this latter is present at high concentration, all the antibodies ANF will be saturated and there will be no detection onto the gold WEs (Figure 1A). In case of the medium concentration of NF, the antibodies will be detected at the same time with NF and SA2BSA attached onto the modified gold WE. This will be highlighted by an increase in impedance in Nyquist plot (Figure 1B). Finally, in case of the absence of NF, all the antibodies will detect the SA2BSA which also increase the impedance in Nyquist plot (Figure 1C).

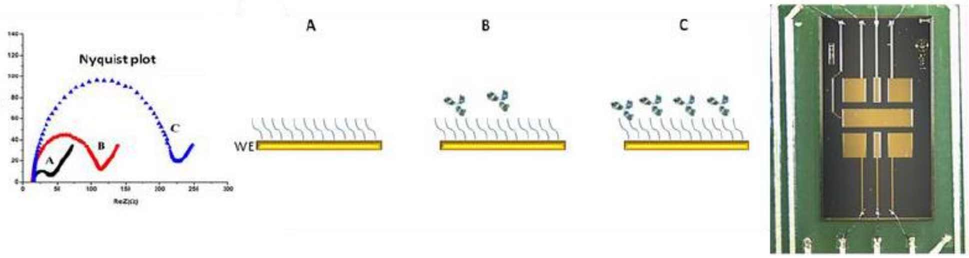


**Figure 1.** Schematic illustration of antibiotic detection using 4 WE biofunctionlised with the corresponding antibiotic. The measurements will be performed with EIS technique. The impedance will be increased as function of the detected concentration of the antibiotics

Such electrochemical characterization of antibiotics is a very promising way for rapid measurement of capacitive behavior of the electrodes functioned on electrodes [1]. It is hoped that this detection scheme will give the way for the development of on-chip antibiotic permeability assay.

## References

[1] A. Baraket, M. Lee, N. Zine, M. Sigaud, J. Bausells and A. Errachid, Biosensors and Bioelectronics, 93 (2016) 170-175.

## Acknowlegement

The Authors would like to acknowledge funding from Erasmus+ Traineeship Student Mobility.

---

* Corresponding author, *E-mail: fdogan@ybu.edu.tr*

O-19

# Therapeutic and Prophylactic Effects of Silymarin in Sodium Fluoride-Induced Hepatotoxicity and Oxidative Stress in Rats

**Efe Kurtdede***, **Mert Pekcan and Hilal Karagül**

Ankara University, Faculy of Veterinary, Department of Biochemistry, TR-06110 Dışkapı, Ankara, Turkey

*E-mail: efekurtdede@gmail.com*

In our country, especially in the Eastern part of Turkey despite the long work done over the years, some of the effects of fluoride on the body is still not fully explained. Fluorine is a highly reactive chemical element and a member of the halogen family. Fluorides entry into the organism and cells that increases the production of superoxide. Fluoride compounds continue to be widespread, fluoride release during the use of fluoride-containing raw materials used in the industry, and the formation of the fluorosis. As shown in the literature [1], oral sodium fluoride will be demonstrated as an experimental fluorosis model with the use of 300 ppm/day for 30 days. The changes at the activities in some enzymes such as, ALT, AST, SOD, MDA and glutathione peroxidase were evaluated both as the hepatotoxic and oxidative effects of sodium fluoride, and as the prophylactic and therapeutic effects of silymarin against these adverse effects.

In this study, 45 wistar rats were used. In the first group of 9 rats, were given sodium fluoride, at the dose of 300 ppm/day in drinking water for a month. In the second group of 9 rats, sodium fluoride was given at the dose of 300 ppm/day in drinking water, together with it, the silymarin at the dose of 200 ppm/day orally for one month. In the third group of 9 rats, after completion of the administration of sodium fluoride at the dose of 300 ppm/day for a month, the rats were begun to give the silymarine at the dose of 200 ppm/day for one week. In the fourth group of 9 rats were given only tap water for a forty days. In the fifth group of 9 rats were given only silymarin at the dose of 200 ppm/day for thirty days.

Significant correlation was found, between the mean AST value in rats given sodium fluoride and in rats fed fluoride and silymarin together and in rats given only tap water ($p<0.001$). There was no statistically significant difference in blood serum ALT values between the rats in the study groups. The mean SOD value determined in the rats in the first group was significantly different from the values in groups 4th and 5th ($p<0.01$). The mean MDA value determined in the rats in the first group was significantly different from the values in the other groups ($p<0.05$). The mean value of Glutation Peroxidase determined in the rats in the first group was significantly different from the values in groups 4th and 5th ($p<0.001$).

There was a significant difference in liver weights between the rats in the first group and the liver weight values obtained from the second, fourth and fifth groups ($p<0.001$). In the rats in the first group, degeneration in the remark cords was more severe than the materials obtained in the third and fifth groups. Significant infiltrating changes were determined in liver tissue in the first group rats when compared to the materials obtained in the 2nd, 3rd and 5th group rats.

## References

[1] A. Mendoza-Shulz, C. Solano-Agama, L. Arreola-Mendoza, B. Reyes-Marquez, O. Barbier, L.M. Del Razo and M.E. Mendoza-Garrido, Toxicol. Lett., 190 (2009) 179-186.

---

* Corresponding author, *E-mail: efekurtdede@gmail.com*

O-20

# Effect of Metal Ion Types on Morphology and Activity of Laccase Hybrid Nanoflowers (LhNFs)

Cevahir Altınkaynak*, Firdevs Geçili, Merve Türk and Nalan Özdemir

Erciyes University, Faculty of Science, Department of Chemistry, Kayseri, Turkey

*E-mail: akcevahir@gmail.com*

The synthesis of hybrid nanostructures is improving biological functions of proteins and expanding potential applications. Various metal ions as an inorganic component and enzymes as an organic component have generally been used to form hybrid nanostructures [1-3]. Disadvantages of enzyme embedded hybrid nanostructures generally present lower enzymatic activities in comparison with free forms if conventional immobilization techniques are applied [4]. In 2012, unlike the traditional immobilization technique, Zare and co-workers reported a novel approach in immobilization by constructing flower-like hybrid nanostructure formed of protein and copper ions ($Cu^{2+}$) with enhanced catalytic activity and stability [5]. However, the enzyme-inorganic hybrid nanoflowers (hNFs) have not been enoughly investigated, particularly the relation between enzymes, which are included cofactor and different metal ions as inorganic components.

In this study, laccase hybrid nanoflowers (LhNFs) were synthesized by using laccase as organic compound and different metal ions ($Ni^{2+}$, $Co^{2+}$, $Zn^{2+}$, $Cu^{2+}$, $Mn^{2+}$) as inorganic compound. These hybrid nanostructures were characterized by SEM, FTIR and XRD. Then, the role of different metal ions as an activator for morphology and enzymatic activity was evaluated. Furthermore, the enhanced enzyme activity of laccase hybrid nanoflowers and reusability was also demonstrated.

**References**

[1] R. Wang, Y. Zhang, D. Lu, J. Ge, Z. Liu and R.N.Zare, WIREs Nanomed Nanobiotechnol., 5 (2013) 320-328.
[2] C. Altinkaynak, S. Tavlasoglu, N. Özdemir and I. Ocsoy, Enzyme Microb Technol., 93-94, (2016) 105-112.
[3] C. Altinkaynak, I. Yilmaz, Z. Koksal, H. Özdemir, I. Ocsoy and N. Özdemir, Int. J. Biol. Macromolec., 84 (2016) 402-409.
[4] Z. Lin, Y. Xiao, Y. Yin, W. Hu, W. Liu and H. Yang, ACS Appl. Mater. Interfaces, 6(13) (2014) 10775-10782.
[5] J. Ge, J. Lei and R.N. Zare, Nature Nanotechnology, 7 (2012) 428-432.

---

* Corresponding author, *E-mail: akcevahir@gmail.com*

O -21

# Preparation and Characterization of Cellulose Acetate Membranes Containing Laccase Hybrid Nanoflowers

**Merve Türk**[1]*, **Elif Kaba**[2], **Cevahir Altınkaynak**[1], **Nalan Özdemir**[1] **and Kemal Sarıoğlu**[2]

[1]Erciyes University, Faculty of Science, Department of Chemistry, 38039 Kayseri, Turkey
[2]Erciyes University, Faculty of Engineering, Department of Food Engineering, 38039 Kayseri, Turkey

*E-mail: merve_durmus88@hotmail.com*

Cellulose acetate is a polymeric membrane material used unique for aqueous base separation [1]. This membrane has good toughness, high hydrophilicity, good desalting, high potential flux, and relatively low cost, thus they have been widely used for reverse osmosis, ultrafiltration, microfiltration, and gas separation [1]. And several components can be incorporated into the cellulose structure to allow the development of membranes for different applications. Recently, Zare and co-workers reported an elegant approach for the synthesis of immobilized enzymes in the form of nanoflower with highly enhanced catalytic activity and stability [2]. These flower-like hybrid nanostructures are developed and used for various applications.

The objective of this study is to investigate the preparation and characterization of cellulose acetate membranes containing laccase hybrid nanoflowers (CAM-hNFs). First, laccase-$Cu^{2+}$ hybrid nanoflowers were prepared using a descriptive method before [2,3] and some characteristics of them were confirmed by SEM and EDX. In addition, these prepared nanoflowers were incorporated into cellulose acetate membrane with different concentrations. The CAM-hNFs was characterized by SEM, XRD and FTIR compared with raw membrane. The catalytic activity of (CAM-hNFs) also were evaluated. The SEM images of CAM-hNFs confirmed that the laccase hybrid nanoflowers (hNFs) were successfully immobilized into the celluloso acetate membrane (CAM). We think that the synthesized CAM-hNFs has potential to be used in the dye decolorization.

**References**

[1] D. Koseoglu-Imer, N. Dizge and I. Koyuncu, Colloids and Surfaces B: Biointerfaces 92 (2012) 334-339.
[2] J. Ge, J. Lei and R.N. Zare, Nature Nanotechnology 7 (2012) 428–432.
[3] C. Altinkaynak, I. Yilmaz, Z. Köksal, H. Özdemir, I. Ocsoy and N. Özdemir, International Journal of Biological Macromolecules, 84 (2016) 402-409.

---

* Corresponding author, *E-mail: merve_durmus88@hotmail.com*

# Computational & Theoretical Chemistry

O-22

# Koçak's Nonlinear Least Squares Workbench Fits Standard Linear Solids Models Used in Characterization of Viscoelastic Materials by Nanoindentation

**Mehmet Çetin Koçak**[1]* and **Nahil Sobh**[2]

[1]Ankara University, Faculty of Engineering, Department of Chemical Engineering,
06100, Ankara, Turkey
[2]Beckman Institute, University of Illinois, Urbana-Champaign, IL 61801, USA

*E-mail: mckocak@ankara.edu.tr*

The Standard Linear Solid (SLS) model comprises ***one spring*** and ***n*** so-called ***Kelvin-Voigt units*** in series. Each Kelvin-Voigt unit has a spring and a dashpot connected in parallel. Each spring (dashpot) represents an elastic (viscous) component. Based on certain assumptions, this model generates the following ramp-hold response in spherical nanoindentation [1]:

$$h^{3/2} = K\begin{cases} x_0\, t - \sum_{i=1}^{n} x_i\, T_i\,(1 - e^{-t/T_i}) & 0 \le t \le t_r \\ x_0\, t_r + \sum_{i=1}^{n} x_i\, T_i\, e^{-t/T_i}\,(1 - e^{t_r/T_i}) & t_r \le t \end{cases}, \qquad K = 3(1 - v)P_{max} / (4 t_r \sqrt{r})\,.$$

Characteristic properties are estimated from fitted T and x parameters. The fit problem is nonlinear (linear) with respect to time constants T (coefficients x) in the model. T has n elements; x has n+1. ***The challenge*** is that the ***equations*** associated with ***least squares*** can be ***ill-conditioned*** which means that their solutions can be highly sensitive to little changes in the coefficients. ***Koçak's nonlinear least squares workbench*** has been successfully applied to virtual data to optimize ***n***, ***T***, and ***x*** parameters and hence obtain ***estimates the characteristic properties***. There is no need to initialize the parameters; once activated, the fit starts with n=1 incrementing it by one at a time up to the optimum. Coded in Matlab, the workbench has two wings to link to solvers; one is for direct calls, one is for calls via nested variable projection function. The currently offered solvers are fminsearch, fminunc, fmincon, nlinfit, lsqcurvefit, and lsqnonlin. Together, these solvers offer over ten algorithms. Some of them can harness analytic Jacobians or their approximations. This work calculated analytical derivatives for the SLS models. The workbench docks applications as a nested Matlab function, say Nest, housing two user blocks. The first block is the main function Nest which defines the experimental points, weights, bounds, and tolerances, initializes the parameters, calls the selected solver, and processes the results. The second block is the objective or model function that is called by the solver. The triggered solver tries to minimize the sum of the squares of the residues until it encounters a convergence or failure condition. The points may be assigned unequal weights if some of them are more important or more accurate than others. In addition, there may be constraints. The user supplies the models and utilities as ***child*** functions.

## References

[1] M.L. Oyen, Ph.D Thesis, Ultrastructural Characterization of Time-Dependent, Inhomogeneous Materials and Tissues, University of Minnesota (2005).

---

* Corresponding author, *E-mail: mckocak@ankara.edu.tr*

O-23

# A Computational Study on βC Alkaloids: Solvent Effect, Quantum Chemical Descriptors, FMO Analysis

**Goncagül Serdaroğlu***

Cumhuriyet University, Department of Mathematics and Science Education, Sivas, Turkey

*E-mail: Goncagul.serdaroglu@gmail.com*

βC alkaloids have an important role in the many of research fields such as pharmacology, biochemistry, medicinal chemistry, physical chemistry because of their invaluable pharmaceutical and photophysical properties [1]. All DFT calculations have been done by using the Gaussian 09W [2] software package. Geometry optimization and frequency calculations have been employed at the B3LYP level of the theory [3,4] in the different solvent media besides the gas phase. The IPCM have been used to get both the solvation free energy and to get quantum chemical identifiers of the all studied βC alkaloids. The solvent effect on the chemical reactivity behavior and on the chemical stability of the βC alkaloids has been evaluated. Figure 1 shows the Solvation free energy as a function of the solvent dielectric constant. It can be suggested that the derivative **D** is the most stabilized structure because it has the most polarizable substituent group (6-methoxy naphthalene-2-yl) on the C1 position of the basic structural unit. One of the important results is that the stabilization energy for these derivatives strongly depends on the solvent media as well as the basis set used in this work.

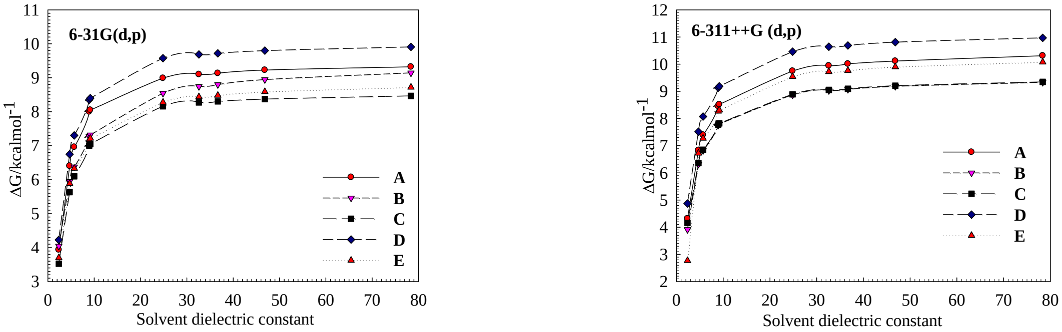


**Figure 1.** Solvation Free Energies as a function of solvent dielectric constant for non-substituted βC Alkaloids

## References

[1] M.C. Biondic, R. Erra-Balsells, J. Chem. Soc., Perkin Trans. 2 (1997), 1323-1327.
[2] M. J. Frisch, et al. (2013) Gaussian 09 D.01. Gaussian, Inc, Wallingford CT.
[3] A.D Becke, J. Chem. Phys. 98 (1993) 1372-1377.
[4] C. Lee, W. Yang, R.G. Parr, Phys. Rev., B37 (1988) 785-789.

## Acknowledgement

The author thanks to Scientific Research Projects of Cumhuriyet University (Project No: EĞT-066). The all calculations have been conducted at TUBITAK ULAKBIM, High Performance and Grid Computing Center.

---

* Corresponding author, *E-mail: Goncagul.serdaroglu@gmail.com*

O-24

# A preliminary Process Model for Lithium-ion Batteries

**Salim Erol***

Department of Chemical Engineering, Eskisehir Osmangazi University, Eskişehir 26040, Turkey

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

A mathematical model was developed that was based on the reactions and mass transport proposed to take place at the anode and cathode of Lithium-ion batteries. The resulting model can be expressed as

$$Z = Z_{\mathrm{a}} + R_{\mathrm{e}} + Z_{\mathrm{c}} \tag{1}$$

where $R_{\mathrm{e}}$ is the electrolyte resistance, $Z_{\mathrm{a}}$ and $Z_{\mathrm{c}}$ are the equivalent impedances of the negative and positive electrodes, respectively, and are expressed as

$$Z_{\mathrm{a}} = R_{\mathrm{f,a}} / (1 + \mathrm{j}\omega C_{\mathrm{f,a}} R_{\mathrm{f,a}}) + [(R_{\mathrm{t,a}} + Z_{\mathrm{d}})^{-1} + \mathrm{j}\omega C_{\mathrm{d,a}}]^{-1} \tag{2}$$

and

$$Z_{\mathrm{c}} = R_{\mathrm{f,c}} / (1 + \mathrm{j}\omega C_{\mathrm{f,c}} R_{\mathrm{f,c}}) + [(R_{\mathrm{t,c}} + Z_{\mathrm{d}})^{-1} + \mathrm{j}\omega C_{\mathrm{d,c}}]^{-1} \tag{3}$$

where $R_{\mathrm{f}}$ refers to the solid-electrolyte interphase (SEI) film resistance, $R_{\mathrm{t}}$ refers to the charge transfer resistances for the intercalation and de-intercalation reactions, $C_{\mathrm{f}}$ refers to the SEI capacitance, $C_{\mathrm{d}}$ is the double-layer capacitance, and $Z_{\mathrm{d}}$ is the diffusion impedance. Diffusion may play a role in the proposed process across the SEI, through the solution phase in the electrode, and through the solid phase of the electrode. Each of these may be treated explicitly. For the present preliminary model, only a simplified treatment is assumed in which diffusion takes place through a stagnant layer, i.e.,

$$Z_{\mathrm{d}} = Z_{\mathrm{d}}(0) \coth\left(\sqrt{\mathrm{j}K}\right)\left(\sqrt{\mathrm{j}K}\right)^{-1} \tag{4}$$

where $Z_{\mathrm{d}}(0)$ is the diffusion impedance at zero frequency and $K$ is the dimensionless frequency given as

$$K = \omega \delta^2 \left(D_{\mathrm{Li}^+}\right)^{-1} \tag{5}$$

where $\delta$ is the diffusion layer thickness and $D_{\mathrm{Li}^+}$ is the diffusion coefficient of $\mathrm{Li}^+$ ions.
The preliminary model of the battery was developed considering aspects of theories by Doyle et al. [1] and Aurbach [2].

## References

[1] M. Doyle, J.P. Meyers and J. Newman, J. Electrochemical Soc., 147 (2000) 99-110.
[2] D. Aurbach, J. Power Sources, 89 (2000) 206-218.

---

* Corresponding author, *E-mail: esalim@ogu.edu.tr*

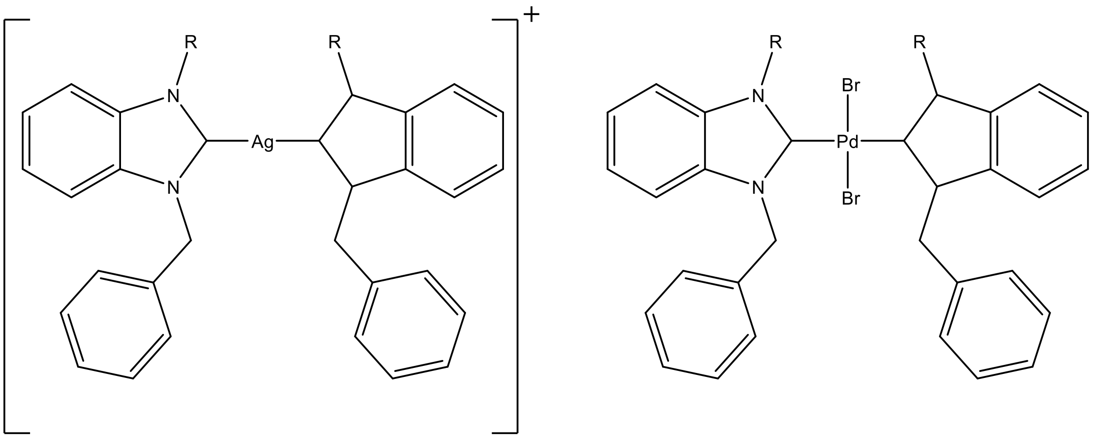
# Computational Investigation of Ag(I) and Pd(II) Complexes with N-Heterocyclic Carbene Ligand: A DFT Studies

**Koray Sayın***

Cumhuriyet University, Faculty of Science, Department of Chemistry, 58140, Sivas, Turkey

*E-mail: krysayin@gmail.com*

Structural, spectral and biological properties of Ag(I) and Pd(II) complexes with N-heterocyclic carbene ligand will be investigated by computational chemistry methods. In this study, B3LYP method is used in all calculations. In addition to this method, LANL2DZ basis set is used for metal atoms and 6-31+G(d,p) basis set is used for the rest atoms. Studied complexes have been synthesized by Ghdhayeb et al. in 2017 [1]. There is no X-ray data belong to them in their paper. Structural and spectral (IR, UV-VIS and NMR) analyses are performed in detail. Additionally, the interaction between B-DNA dodecamer (PDB Code: 1BNA) and studied complexes are investigated by docking calculations. Schematic diagrams of studied complexes are represented in Figure 1.



Complex **1**: R=allyl
Complex **2**: R=allyl

Complex **3**: R=allyl
Complex **4**: R=allyl

**Figure 1.** Schematic representation of related complexes

## Reference

[1] M.Z. Ghdhayeb, R.A. Haque, S. Budagumpi, M.B.K. Ahamed, A.M.S. Abdul Majid, Polyhedron,121 (2017) 222-230.

---

* Corresponding author, *E-mail: krysayin@gmail.com*

# Metallic $Ca_{72}Zn_{28}$ Glass from First Principle Molecular Dynamics Simulations

**Duygu Tahaoğlu and Murat Durandurdu***

Abdullah Gül University, Faculty of Engineering, Department of Materials Science
and Nanotechnology Engineering, 38100, Kayseri, Turkey

*E-mail: duygu.tahaoglu@agu.edu.tr*

We investigate the rapid solidification of $Ca_{72}Zn_{28}$ from its liquid state using a first principle molecular dynamics technique within a generalized gradient technique and expose its structural characteristics in details. The $Ca_{72}Zn_{28}$ metallic glass exhibits a phase separation due to the aggregation of Zn atoms. Consequently, this material can be categorized as a metallic *nanoglass*. The average coordination numbers of Ca and Zn atoms are 13.87 and 10.59, respectively. The bond pair analysis shows that the model predominantly has the perfect and defective icosahedral bonding environments (60 %). The Voronoi tessellation analysis reveals that the perfect and defective icosahedrons are the most dominated clusters around Zn atoms. Ca atoms, on the other hand, favor to structure in higher coordinated polyhedrons.

**Reference**

[1] H. Gleiter. "*Nanoglasses: A New Kind of Noncrystalline Material and the Way to an Age of New Technologies?*", Small 2016, 12, No. 16, 2225-2233.

---

* Corresponding author, *E-mail: murat.durandurdu@agu.edu.tr*

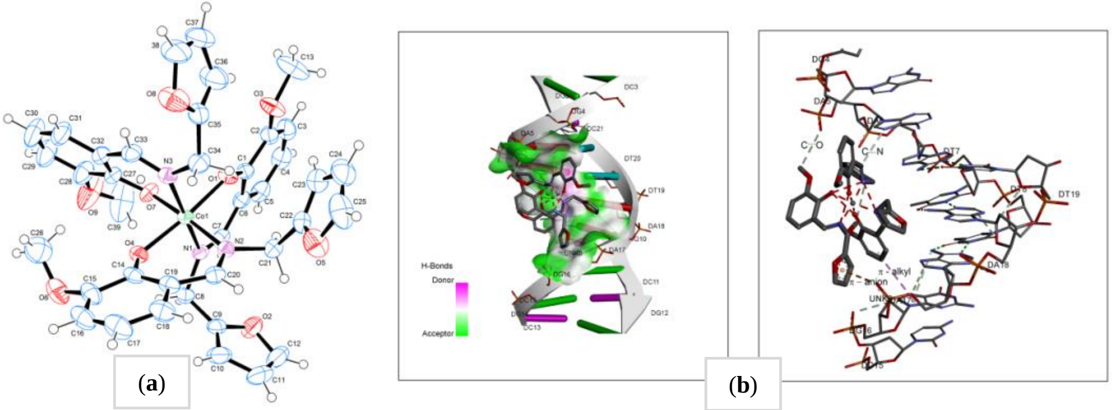
# Crystal Structure, Density Functional Modelling and Molecular Docking Studies of Tris[N-(2-furylmethyl)-3-methoxy-salicylidenaminato]cobalt(III)

Celal Tuğrul Zeyrek[1]*, Zeliha Hayvalı[2], Hüseyin Ünver[3] and Ayhan Elmalı[4]

[1]Ankara Nuclear Research and Training Center, Turkish Atomic Energy Authority, 06100 Beşevler, Ankara, Turkey
[2]Ankara University, Science Faculty, Department of Chemistry, 06100 Beşevler, Ankara, Turkey
[3]Ankara University, Science Faculty, Department of Physics, 06100 Beşevler, Ankara, Turkey
[4]Ankara University, Faculty of Engineering, Department of Physics Engineering 06100 Beşevler, Ankara, Turkey

*E-mail: ctzeyrek@gmail.com*

Transition metal complexes of Schiff base ligands have been investigated for various purposes. In this regard, Schiff base complexes of cobalt(III) have attracted great interest. Cobalt(III) Schiff base complexes have been extensively studied for their biological and catalytic activities [1,2]. Particularly, cobalt complexes have effective urease inhibitory activities [2]. In this study, Tris[N-(2-furylmethyl)-3-methoxy-salicylidenaminato]cobalt(III) complex was synthesized and characterized by X-ray single crystal analysis (Figure 1a). The cationic part of the complex is comprised of a dianionic $N_2O_2$ type Schiff base ligand occupying the six equatorial positions of an octahedron around the Co(III) ion. Quantum mechanical studies of the complex have been reported by using density functional theory (DFT) with the functional B3LYP using the LANL2DZ basis set. The experimental structure and calculated geometric structure of the complex have been compared. The DFT optimized structures of the complexes agreed well with the corresponding X-ray structure. Molecular docking studies of the investigated complex have also been reported to identify the interaction of the Co(III) complex with DNA (Figure 1b).



(a)

(b)

**Figure 1.** (a) Crytstal structure of the title compound and (b) Docked poses of Co(III) complex and binding interactions with B-DNA at the active site residues

## References

[1] A.H. Kianfar, W.A.K. Mahmood, M. Dinari, M.H. Azarian and F.Z. Khafri, Spectrochim. Acta A**,** 127 (2014) 422-428.
[2] C.L. Jing, C.F. Wang, K. Yan, K.D. Zhao, G.H. Sheng, D. Qu, F. Niu, H.L. Zhu and Z.L.You, Bioorganic Med. Chem., 24(2) (2016) 270-276.

---

* Corresponding author, *E-mail: ctzeyrek@gmail.com*

# An Experimental and Theoretical Study on the Interaction of DNA with New Trinuclear Boron Complexes

**Kübra Karaağaç[1], Celal Tuğrul Zeyrek[2], Özge Can Daysalılar[1], Selen Bilge Koçak[1]*, Burak Çoban[3] and Ufuk Yıldız[3]**

[1]Ankara University, Faculty of Science, Department of Chemistry, 06100, Ankara, Turkey
[1]Ankara Nuclear Research and Training Center, Turkish Atomic Energy Authority, 06100, Beşevler, Ankara, Turkey
[3]Bülent Ecevit University, Faculty of Arts and Sciences, Department of Chemistry, 67100, Zonguldak, Turkey

*E-mail: karaagac@ankara.edu.tr*

Recently, there has been a considerable interest in the synthesis, characterization and study of boron complexes, due to a great variety of applications derived from these complexes in medicinal chemistry, as anticancer agents in boron neutron capture therapy, and as bioactive materials [1]. In this study, the DNA cleavage activity of the trinuclear boron complexes (**I** and **II**) was studied on double-stranded pBR322 DNA using gel electrophoresis experiments. It was found that **I** and **II** caused the high level of DNA damage even at low ratios of R, and the 8-membered O-B-N-$(CH_2)_3$-N-B ring, with or without the CHO group in the phenyl ring, had a significant effect on the ability of **I** and **II** to damage the plasmid DNA. The interactions of **I** and **II** with calf thymus DNA were also investigated using absorption spectrometry. The isosbestic points observed in the UV-vis absorption spectra of trinuclear boron complexes (**I** and **II**) showed that the complexes covalently linked to the DNA. The molecular docking was also performed to identify the interaction of the complexes (**I** and **II**) with DNA. Molecular docking calculations for **I** and **II** were performed on AutoDock Vina software and AutoDockTools (ADT) was used for creating docking data entry files. The crystal data of CT-DNA were obtained from Protein Data Bank (PDB) identifier 1BNA for B-DNA. Trinuclear boron complexes (**I** and **II**) bind at the active site of the B-DNA by weak non-covalent interactions most prominent of which are H-bonding and π-donor (Figure 1). The relative binding energy of docked **I**-B-DNA and **II**-B-DNA were found to be -8.4 and -8.6 kcal/mol, respectively. The molecular docking results suggest that **I** and **II** exhibit binding effect against DNA; however further tests should be done to validate the computational predictions. The findings of this study may thus benefit the development of effective applications in medicine such as cancer therapy or prove valuable in the future design of new anticancer drugs.

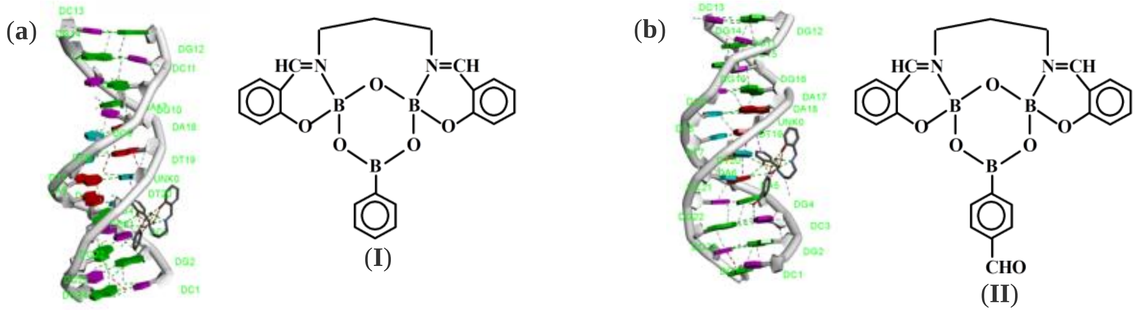


**Figure 1.** Binding interactions of the compounds (a) **I** with B-DNA and (b) **II** with B-DNA

## References

[1] M.F. Hawthorne and M.W. Lee, J. Neuro-Oncol., 62 (2003) 33-45.

---

* Corresponding author, *E-mail: sbilge@science.ankara.edu.tr*

# Experimental and Molecular Docking Investigation on DNA Interaction of Novel Dinuclear Boron Complexes

Aliye Kömez[1], Celal Tuğrul Zeyrek[2], Özge Can Daysalılar[1],
Selen Bilge Koçak[1]*, Burak Çoban[3] and Ufuk Yıldız[3]

[1]Ankara University, Faculty of Science, Department of Chemistry, 06100, Ankara, Turkey
[2]Ankara Nuclear Research and Training Center, Turkish Atomic Energy Authority, 06100, Beşevler, Ankara, Turkey
[3]Bülent Ecevit University, Faculty of Arts and Sciences, Department of Chemistry, 67100, Zonguldak, Turkey

*E-mail: komez@ankara.edu.tr*

In the last years there has been great interest in the study of boron compounds due to the great number of applications found, for example, in medicinal chemistry, as anticancer agents directly applied in the technique known as boron neutron capture therapy used for the treatment of certain brain tumors [1]. Some boron compounds also present cytotoxic activity [2]. In this study, the DNA binding propensity of the dinuclear boron complexes (**I** and **II**) was studied. It was found that **I** and **II** caused the high level of DNA damage even at low ratios of R, and the propane diimine moiety, with or without the CHO group in the phenyl ring, had a significant effect on the ability of **I** and **II** to damage the plasmid DNA. A decrease in absorbance at around 400 nm in the UV-vis absorption spectra of **I** and **II** explained that the complexes bind to DNA by intercalation. Molecular docking calculations using AutoDock Vina software were carried out to predict the mode of interaction of the compounds with DNA. The DNA sequence (CGCGAATTCGCG)2 dodecamer (PDB ID: 1BNA) was obtained from the Protein Data Bank. The complexes (**I** and **II**) bind at the active site of the B-DNA by weak non-covalent interactions. The molecular docking results suggest that dinuclear boron complexes **I** and **II** exhibit inhibitory activity against DNA and however further tests should be done to validate the computational predictions. The findings of this study may thus benefit the development of effective applications in medicine and biochemistry.

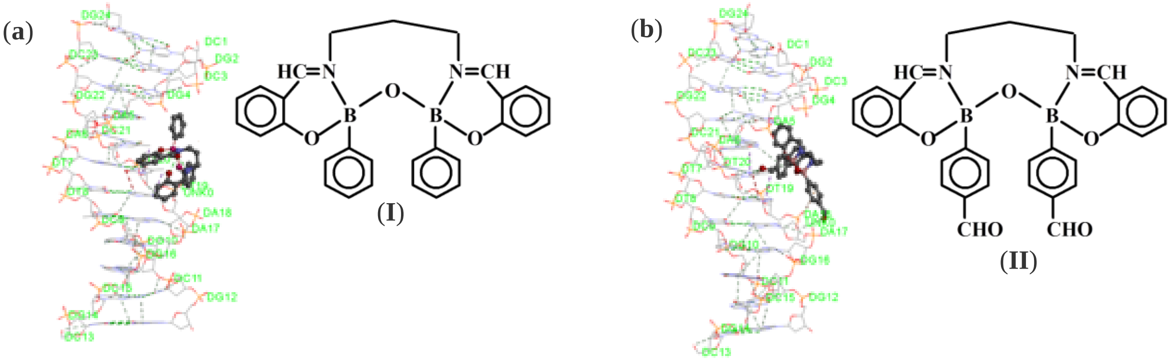


**Figure 1.** Binding interactions of the compounds (a) **I** with B-DNA and (b) **II** with B-DNA

## References

[1] S. Miyatake, S. Kawabata, R. Hiramatsu, T. Kuroiwa, M. Suzuki, N. Kondo and K. Ono, Neurol. Med. Chir. (Tokyo), 56(7) (2016) 361-371.
[2] M. Ibarra-Rodríguez, B.M. Muñoz-Flores, H.V.R. Dias, M. Sánchez, A. Gomez-Treviño, R. Santillan, N. Farfán and V.M. Jiménez-Pérez, J. Org. Chem., 2017, 82(5) (2017) 2375-2385.

---

* Corresponding author, *E-mail: sbilge@science.ankara.edu.tr*

# Electrochemistry

# Determination of Serotonin in the Presence of Dopamine and Ascorbic Acid on $MnO_2$ doped Pseudo Carbonaceous Fiber Electrode

**İlknur Üstündağ* and Hatice Çakmak**

Dumlupınar University, Faculty of Arts and Science, Department of Physics, Kutahya, Turkey

*E-mail: iozkirim@gmail.com*

5-hydroxytryptamine (Serotonin, 5-HT) is a vital molecule in physiological systems. 5-HT is plays a vital role in the regulation of mood and sleep. It is also involved in some cognitive functions, including memory and learning. Thus, concentration of 5-HT in a biological system is very important [1].

In this study, glass fiber (GF) was covered with coal tar pitch (CTP). The carbonization was carried out by heating under flowing inert nitrogen at 1000 °C at a heating ramp of 10 °C/min for a hold period of 1 h. The $MnO_2$ doped carbonaceous material was prepared with sol-gel oxidation under heat treatment [2]. The materials were denoted as GF-CTP-$MnO_2$. The carbonized material GF-CTP-$MnO_2$ was ground into fine powder in a planetary ball mill PM-100 (Retcsch, Germany). The carbonaceous material was characterized by IR, XPS, SEM and electrochemical methods. The GF-CTP-$MnO_2$ suspension was dropped on the GC electrode. The electrode was used for the determination of 5-HT in the presence of 100 µM dopamine (DA) and 1 mM ascorbic acid (AA) by differential pulse voltammetry (DPV). It exhibits a linear response to 5-HT in the range of 0.1–250 µM. The detection limit (S/N=3) for 5-HT is 3.1 nM. This work provides a simple and easy approach to selective detection of 5-HT in the presence of AA and DA. Finally, the fabricated sensor was used successfully for electroanalytical determination of 5HT in human serum.

## References

[1] H.S. Han, H.K. Lee, J.-M. You, H. Jeong and S. Jeon, Sensors and Actuators B, 190 (2014) 886–895.
[2] A. Erkal, İ. Üstündağ, S. Yavuz and Z. Üstündağ, Journal of the Electrochemical Society, 162(4) (2015) H213-H219.

---

* Corresponding author, *E-mail: iozkirim@gmail.com*

O-31

# Carbon Nanotube Supported Carbonaceous Electrode for Sensitive Determination of Dopamine and Uric Acid in Presence of Ascorbic Acid

**Mohammad Shamsuddin Ahmed**[1], **Seungwon Jeon**[1] **and**
**Zafer Üstündağ**[2]*

[1]Chonnam National University, Department of Chemistry and Institute of Basic Science,
Gwangju 500-757, Korea
[2]Dumlupınar University, Faculty of Arts and Science, Department of Chemistry, Kütahya,
Turkey

*E-mail: suddin_bcsir@yahoo.com*

Carbon-rich materials such as fullerenes, carbon nanotubes, graphene and its derivatives are experiencing the golden age today. They have attracted chemical and physical properties such as thermal conductivity, mechanical resistance, and electrical conductivity [1,2]. The carbonaceous materials are used as sensors template, electronic device element, next-generation electronic materials, battery materials, biomaterials, heat exchangers, thermal insulations, and electrode materials [3,4].

In this study, the carbonaceous electrode material was prepared from multi-walled carbon nanotube (MWCNTs) doped coal tar pitch ((m% of MWCNTs: 1%, 3%, 5% and 10%) in the tube furnace at 1000 °C under nitrogen atmosphere [3]. The material was characterized with cyclic voltammetry, electrochemical impedance spectroscopy (EIS), Infrared (IR) spectroscopy, and X-ray diffraction (XRD), scanning electron microscopy (SEM) and X-ray photoelectron spectroscopy (XPS). Electrochemically enhanced carbonaceous material was modified on glassy carbon electrode and used as dopamine and uric acid sensor in the presence of ascorbic acid by using differential pulse voltammetry (DPV) [3]. The electrode exhibits linear responses to DA and UA in the ranges of 1 μM-100 μM in the presence of 250 μM of L-ascorbic acid (AA). The detection limits (S/N=3) for DA and UA are 4,3 nM (R=0,9741) and 6,8 nM (R=0,9854), respectively [5-7].

## References

[1] M. Wang, C. Wang, T. Li and Z. Hu, Carbon, 46 (2008) 84-91.
[2] R. Narasimman and K. Prabhakaran, Carbon, 50 (2012) 1999-2009.
[3] A. Erkal, İ. Aşık, S. Yavuz, A. Kariper, Z. Üstündağ, Journal of the Electrochemical Society, 163 (2016) H269-H277.
[4] H. Liu, T. Li, X. Wang, W. Zhang and T. Zhao, Journal of Analytical and Applied Pyrolysis, 110 (2014) 442-447.
[5] S.H. Huang, H.H. Liao and D.H. Chen, Biosensors and Bioelectronics, 25 (2010) 2351-2355.
[6] B. Habibi and M.H. Pournaghi-Azar, Electrochimica Acta, 55 (2010) 5492-5498.
[7] C. Xiao, X. Chu, Y. Yang, X. Li, X. Zhang and J. Chen, Biosensors and Bioelectronics, 26 (2011) 2934-2939.

---

* Corresponding author, *E-mail: zustundag@gmail.com*

O-32

# Fipronil Sensitive Molecularly Imprinted Polymer Electrode

**Ashutosh Tiwari**[1], **Zafer Üstündağ**[2] **and Lokman Uzun**[3]*

[1]Linköping University, Biosensors and Bioelectronics Centre, IFM, Linköping, Sweden
[2]Dumlupınar University, Faculty of Arts and Science, Department of Chemistry, Kütahya, Turkey
[3]Hacettepe University, Faculty of Science, Department of Chemistry, Ankara, Turkey

*E-mail: ashutosh.tiwari@liu.se*

Fipronil (5-amino-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]–4-[(trifluoromethyl)sulfinyl]-1H-pyrazole-3-carbonitrile) is an insecticide from the phenyl pyrazole family that targets the gamma-amino butyric acid (GABA) receptor [1]. In this study, the graphene nanoribbons enhanced coal tar pitch carbonaceous based on molecularly imprinted polypyrrole was prepared for the determination of fipronil. Graphene nanoribbon was synthesized with longitudinal unzipping of carbon nanotubes by wet chemical oxidation method [2]. Graphene nanoribbons doped coal tar pitch was carbonized in a tube furnace under $N_2$-atmosphere with a heating rate of 10 °C/min to reach 1000 °C. The carbonized solid was ground into fine powder in a planetary ball mill. A very small amount of *Cedrus libani* A. Rich. The resin was sprayed in 2 g of the powder. The moistened powders were pressed into pellets of 10 mm diameter. The disk electrodes were dried in an oven at 75 °C under vacuum. The electrodes were packed into the cavity of a Teflon tube. The developed electrode was prepared by incorporation of a template fipronil molecule during the electrooxidation of pyrrole on the carbonaceous disk electrode in aqueous solution using cyclic voltammetry. The electrochemical performance of the imprinted and bare electrodes was evaluated by differential pulse stripping voltammetry (DPSV). The polymerization conditions were investigated and optimized. The carbonaceous electrode was used in the determination of fipronil by DPSV in a 0.10 mol/L Britton-Robinson buffer solution under pH 8.0 with accumulation potential and time of 0.50 V and 120 s, respectively. The limits of detection and quantification were 0.80 and 2.67µg/L, respectively. The electrode exhibits linear responses to fipronil in the ranges of 0.1 µM–5 µM. The detection limits (S/N=3) for fipronil is 0.27 µg/L. Recovery tests were performed in five tap water samples with values ranging from 97.1 to 102.7%.

## References

[1] F. Okumura, R.B. Amaral, E. Orestes, A.B.F. Silva and L.H. Mazo, J. Braz, Chem. Soc., 27 (2016) 925-932.
[2] D.V. Kosynkin, A.L. Higginbotham, A. Sinitskii, J.R. Lomeda, A. Dimiev, B.K. Price and J.M. Tour, Nature, 458 (2009) 872-877.

---

* Corresponding author, *E-mail: lokman@hacettepe.edu.tr*

# Determination of DNA arrays on Carbonaceous Electrode by Electrochemical Impedance Spectroscopy

**Munawar Saeed Qureshi[1]*, Ali Osman Solak[2] and Zafer Üstündağ[3]**

[1]Khwaja Fareed Engineering University and Information Technology, Department of Basic Sciences and Humanties, Rahimyar Khan 64200, Pakistan
[2]Kyrgyz-Turkish Manas University Faculty of Engineering, Department of Chemical Engineering, Bishkek, Kyrgyzstan
[3]Dumlupınar University, Faculty of Arts and Science, Department of Chemistry, Kütahya, Turkey

E-mail: *saeed.munawar9@gmail.com*

Carbon materials, CMs, such as coal tar pitch, fullerenes, carbon nanotubes (CNT), graphene and its derivatives, graphene nanoribbons (GNR), polymers and their composites, coal tar pitch (CTP), and carbonaceous materials have become very important materials. They have very special different physical and chemical properties.

In this study, carbonaceous pencil electrode was prepared from coal tar pitch covered pencil electrode. The electrode was characterized with cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS), spectroscopic methods (XPS and IR) and microscopy technique (SEM). A novel sensitive sensitive method for determination of DNA hybridization was developed via impedimetry [1,2]. The carbonaceous pencil electrode was modified with 4-aminobenzene by electroreduction of diazonium salt. The nanofilm was terminated via AuNps. The single-stranded probe: 5'-[CCG AAT CTA CGT TTA]-T3-C2-SH-3' was modified with the electrode. The immobilized and hybridized electrode was studied by cyclic voltammetry (CV), and impedance spectroscopy (EIS). The target and non-complementary sequences were used in order to determine sensor performance. The limit of detection was 11.2 pM with a detection range of 10-750 nM.

**Reference**

[1] X. Han X. Fang, A. Shi, J. Wang and Y. Zhang, Analytical Biochemistry, 443 (2013) 117-123.
[2] A. Shi, J. Wang, X. Han, X. Fang and Y. Zhang, Sensors and Actuators B: Chemical, 200 (2014) 206-212.

---

* Corresponding author, *E-mail: saeed.munawar9@gmail.com*

# Biosensor Performance of Carbonaceous Electrodes

**Munawar Saed Qureshi[1], Haslet Ekşi-Koçak[2]* and Zafer Üstündağ[3]**

[1]Khwaja Fareed Engineering University and Information Technology, Department of Basic Sciences and Humanties, Rahimyar Khan 64200, Pakistan
[2]İstanbul Aydın University, Faculty of Engineering, Department of Biomedical Engineering, İstanbul, Turkey
[3]Dumlupınar University, Faculty of Arts and Science, Department of Chemistry, Kütahya, Turkey

E-mail: *saeed.munawar9@gmail.com*

A novel carbonaceous material was prepared from single-walled carbon nanotubes (SWCNTs) doped coal tar pitch (CTP) with tube furnace at 1000°C under a nitrogen atmosphere at a heating ramp of 10 °C/min for a hold period of 1 h. It was used as disk electrode after mixing of the material with an organic resin binder [1]. The electrode was characterized with X-ray photoelectron spectroscopy (XPS), X-ray diffraction (XRD), scanning electron microscopy (SEM) and Raman spectroscopy. The prepared electrode was characterized by electrochemical techniques such as cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS). The carbonaceous electrode was used for determination of dopamine (DA), uric acid (UA) and Folic acid (FA) by differential pulse voltammetry (DPV). The linear range was calculated as 0.5 μM to 60 μM for DA and UA; 1 μM to 40 μM for FA. The detection limits (S/N=3) for DA, UA and FA are 8.1 nM, 13.7 nM and 21.3 nM, respectively. Precision and accuracy results of the method were studied. The method was applied to human serum sample. Analytical recovery of DA, UA and FA added to urine samples was calculated as ≤ 103.7%. The influences of some ions and important molecules such as glucose, ascorbic acid, oligonucleotide array, on the peak currents of 1 μM UA, DA and FA, in 0.1 M PBS (pH 7.0) were studied. The values of signal change are approximately ≤4.07% and ≥-3.75%.

## References

[1] İ. Üstündağ and A. Erkal, Sensors and Materials, 29 (2017) 85-94.
[2] E.G. de Araújo, N.S. Fernandes, L.G. da S.-Solon, C.F. S. Aragão and C.A. M.-Huitle, Electroanalysis, 27 (2015) 398-405.

---

* Corresponding author, *E-mail: hsleksi@gmail.com*

# Passivation Properties of Noble and Refractory Metals as Determination Factor of Their Electrochemical in Low-Temperature Ionic Melts

**Svetlana Kochetova**[1], **Victor Malyshev**[1,2]* **and Dimitrii Shakhnin**[2]

[1]National Academy of Science of Ukraine, V.I. Vernadsky Institute of General and Inorganic Chemistry, Kyiv, Ukraine
[2]University “Ukraine”, Institute of Engineering and Technology, Kyiv, Ukraine

*E-mail: svetaasya@mail.ru*

It was found that low-temperature melts based on urea, acetamide, imidazole, and tetraalkylammonium chlorides are stable and having a low melting point (<100°C). In the presence of alkali metals, ammonium, and aluminum chlorides, these melts have good electrical conductivity, are good solvents for noble and refractory metals salts, and can serve as a background for electrochemical studies [1].

On the base of the study results of the electrochemical behavior of noble and refractory metals in these melts, relationship between the passivation properties of these metals and their electrochemical behavior was established. Metals which are not passivated (Ag, Cu, Pt, and Pd) are deposited on the cathode in the form of powder or galvanic coating. Galvanic coatings of Pt (from urea), Pd (from acetamide), Cu, Ag (from urea, acetamide, and imidazole) of different thickness were deposited with good adhesion to the substrate. Pd powders were deposited from urea having spherical and needle structure. Electropolishing of such metals is unprofitable due to high consumption of metal during unimpeded dissolution. Metals which are poorly passivated (Ru, Rh, Ir, Ti, Mo, and W) are deposited on the cathode in the form of metal or metal-like deposit containing mainly oxihalide complexes and a small amount of pure metals. In the case of metals which are well passivated (Nb and Ta), cathode deposit obtaining is not possible. Metals which are passivated are suitable for electropolishing. The lower is the passivation degree of metal, the higher is the efficiency of the process (polishing conditions - time, current density, and surface quality).With a weak passivation of metal, metal-like deposit is deposited on the cathode (containing small amount of metal and mainly its unsoluble compounds). Obtained relationships allow to predict the possibility of applied solutions realization, i.e. obtaining of cathodic deposit and its purity, and also the efficiency of anodic surface treatment of metals.

## References

[1] V. Malyshev, A. Gab, D. Shaknin, A.-M. Popescu, V. Constantin and M. Olteanu, Rev. Roum. Chim., 55 (2010) 233-238.

---

* Corresponding author, *E-mail: victor_malyshev@mail.ru*

# Theoretical Background and Practical Realization of Refractory and Noble Metals Electrodeposition from Low- and Medium-Temperature Melts

**Svetlana Kochetova[1], Angelina Gab[2], Dmitrii Shakhnin[2] and Victor Malyshev[1,2]***

[1]National Academy of Science of Ukraine, V.I. Vernadsky Institute of General and Inorganic Chemistry, Kyiv, Ukraine
[2]University "Ukraine", Institute of Engineering and Technology, Kyiv, Ukraine

*E-mail: shakhnin@ukr.net*

Industrial applications of noble and refractory metals and non-metals and their compounds define further development and improvement of existing technologies and development of new and more effective ones, more effective and ecologically safe. The use of molten ionic electrolytes as reaction medium can solve these problems. To achieve the objectives stated, the following points are necessary: a) electrolyte suitable for this purpose; b) corresponding electrochemical properties of metals and non-metals; c) targeted scientifically substantiated approach to the implementation and control of the mechanism and kinetics of electrode processes [1].

Relevance of the topic is due to its importance for modern melts electrochemistry. From a theoretical point of view, of importance are the following issues: 1) Mechanism and kinetics of electrode processes of noble and refractory metals and non-metals in low-temperature melts; 2) Study of the melt state after anodic dissolution of metal (ions oxidation state, complexation etc.); 3) Theoretical study of anodic dissolution of metals in multicomponent electrolytes with complexation; 4) Investigation of processes occurring at the interface metal/melt (passivation, adsorption etc.) in steady state and during polarization; 5) Investigation of the mechanism and kinetics of codeposition of refractory metals with other metals and non-metals in the medium-temperature melts.

From a practical point of view, the following is important:

- Electrodeposition of metals and metal alloys from ionic melts.
- Possibility to control a form of cathodic deposits (powders, galvanic coatings etc.).
- Electrochemical synthesis of binary and ternary compounds of refractory metals with nonmetals.
- Possibility of separation of metals during processing of their joint raw materials.
- Electrochemical processing and polishing of the surface of refractory metals.

**References**

[1] V. Malyshev, A. Gab, D. Shaknin, A.-M. Popescu, V. Constantin and M. Olteanu, Rev. Roum. Chim., 55 (2010) 233-238.

---

* Corresponding author, *E-mail: victor_malyshev@mail.ru*

O-37

# Carbonaceous Electrode Fabrication from Pyrolyzed Coal Tar Pitch

**Alla Sushchenko[1], Viktor Malyshev[1], Mustafa Oğuzhan Çağlayan[2] and İbrahim Ender Mülazımoğlu[3]***

[1]University "Ukraine", 23 Lvivska St., Kyiv 03115, Ukraine
[2]Cumhuriyet University, Faculty of Engineering, Department of Nanotechnology Engineering, Sivas, Turkey
[3]Necmettin Erbakan University, Faculty of Education, Department of Chemistry, 42090, Konya, Turkey

*E-mail: alla.suschenko@gmail.com*

Pyrolysis of some polymers is a relatively preparation of carbon materials containing nitrogen substituted for carbon atoms. Limitations in the practical application of the process are, however, a high cost of the precursors and, with few exceptions, a low thermal stability of nitrogen functionalities and a low yield and unsuitable morphology of the solid residue [1]. Pitch is the most important component in the production of many modern carbon materials, such as carbon fiber, graphite electrodes, carbon composites and activated and modified carbonaceous materials. Much attention has been paid to the properties of pitch and improvement in pitch properties. The characteristics of the final product depend on the initial material and the type of treatment and also on parameters such as the duration of treatment, the heating rate and the pressure [2]. Coal tar pitch (CTP) is composed of hundreds of polycyclic aromatic hydrocarbons, which confer binder properties to pitch and the potential of being transformed into graphitizable carbon by pyrolysis. For these reasons, coal-tar pitch is widely used in the preparation of carbon anodes for the aluminum industry and graphite electrodes for electric arc furnaces. However, the use of coal-tar pitch has some drawbacks in relation with the emission of polycyclic aromatic hydrocarbons during pyrolysis [3]. The modification can be very attractive for application of carbonaceous materials in catalysis, adsorption and electroanalytical chemistry. The drawbacks of the method are relatively high cost of reagents, especially when frequently associated with low yields of solid residue, its unsuitable morphology and loss of a considerable part of introducing nitrogen on subsequent thermal treatment. As a way to overcome, at least in part, the drawbacks the co-pyrolysis of nitrogen containing polymers within CTP matrix is proposed in the work. CTP is one of the most common aromatic precursors used for manufacturing of conventional and advanced carbonaceous materials. The reason is the unique thermal behaviour of constituting aromatic and heteroaromatic compounds. The thermally induced reactions of radical condensation, which start to occur when the temperature is in excess of 350 °C, result in high yield of solid carbon of suitable morphology and structural ordering [4]. CTP composite was carbonized in a nitrogen atmosphere tube furnace with a heating rate of 10 °C/min to reach 1000 °C. This was followed by the annealing of the materials at 1000 °C in nitrogen atmosphere for 1 h. The black material transformed into metallic grey. The carbonized solid was ground into fine powder in a planetary ball mill. In addition, a pure CTP electrode was synthesized under the same conditions for comparison with the CTP electrode.

## References

[1] B. Grzyb, J. Machnikowski and J.V. Weber, J. Anal. Appl. Pyrolysis, 72 (2004) 121-130.
[2] A.P. Petrovykh, A.L. Abaturov, I.V. Moskalev, D.M. Kiselkov, S.A. Astafeva and A.I. Vinokurov, Coke Chem., 60 (2017) 75-79.
[3] M. Perez, M. Granda, R. Santamarıa, T. Morgan and R. Menendez, Fuel, 83 (2004) 1257-1265.
[4] B. Grzyb, J. Machnikowski, J.V. Weber, A. Koch and O. Heintz, J. Anal. Appl. Pyrolysis, 67 (2003) 77-93.

---

* Corresponding author, *E-mail: iemulazimoglu@konya.edu.tr*

O-38

# Analysis of Serum Copper and Zinc Concentrations in Healthy Adults Living in West Algeria

**Tarik Attar**[1,2]* and **Lahcène Larabi**[3]

[1]Highschool of applied sciences, Tlemcen, Algeria
[2]Laboratory of Toxicomed, Faculty of Medical Sciences, Abou-Bekr Belkaïd University, Algeria
[3]Laboratory of Electrochemistry and Analytical Chemistry, Abou-Bekr Belkaïd University, Algeria

*E-mail: att.tarik@gmail.com*

The biological role of trace metals, especially serum zinc (Zn) and serum copper (Cu), in different physiologic and pathologic conditions, has been extensively investigated in recent years [1]. Copper and zinc are essential trace elements in people, is required for functional activity of several enzyme systems. The present study aimed to evaluate copper (Cu) and zinc (Zn) status in a healthy population from west of Algeria. A total of one hundred eleven-five subjects (52 males and 63 females) of healthy adults. The mean levels of Cu and Zn were 105.26±19.63 µgdL$^{-1}$ and 79.44±10.28 µg.dL$^{-1}$, respectively. The serum copper and zinc concentrations were determined by differential pulse anodic stripping voltammetry on a hanging mercury drop electrode (Table 1).

**Table 1.** Gives the results of means copper and zinc concentrations, S.D.s, range, and 95% confidence intervals for the mean present at serum samples of one hundred five healthy

| | Copper | Zinc |
|---|---|---|
| Mean ± SD (µg.dL$^{-1}$) | 105.26 ± 19.63 | 79.44 ± 10.28 |
| Confidence 95% | 98.80 - 111.74 | 77.59 - 81.36 |
| Range (µg.dL$^{-1}$) | 72.13 - 155.27 | 53.70 - 121.65 |

**References**
[1] S. Turgut, S. Hacıoğlu, G. Emmungil, G. Turgut and A. Keskin, Polish J. of Environ. Stud., 18 (2009) 273-277.

---

* Corresponding author, *E-mail: att.tarik@gmail.com*

# Energy

# Development of a Novel Dye with Bi-Anchoring Pattern

**Mariana-Dana Damaceanu**[1]*, **Catalin-Paul Constantin**[1], **Mihai Mihaila**[2], **Mihaela Kusko**[2] and **Razvan Pascu**[2]

[1]"Petru Poni" Institute of Macromolecular Chemistry, Aleea Grigore Ghica Voda 41A, Iasi, 700487, Romania
[2]National Institute for Research and Development in Microtechnologies (IMT), 126A, Erou Iancu Nicolae Street, 077190, Bucharest, Romania

*E-mail: damaceanu@icmpp.ro*

Among 3rd generation solar cells, dye-sensitized solar cells (DSSCs) have emerged as a prospective alternative to conventional silicon-based photovoltaic devices, mainly due to their low cost and versatility. The most important part of a DSSC is the photosensitizer since it harvests sunlight and generates photo-excited electrons at the dye-semiconductor interface. For high performance, the sensitizer must fulfill several requirements, such as to contain a chemical group to anchor on the semiconductor material, appropriate LUMO and HOMO levels for effective charge injection into $TiO_2$ and dye regeneration by electrolyte, high molar extinction coefficients in the visible and NIR region for light-harvesting, good photostability and solubility [1]. One of the major issues which lead to low conversion efficiency and stability of DSSCs is the binding strength of the dye on the $TiO_2$ surface. Strong binding of the dye on $TiO_2$ not only improves adsorption, but also causes an efficient charge injection [2]. The incorporation of only one anchoring group could be the reason for the lower performance of the metal-free organic sensitizers compared to Ru(II) sensitizers, where 1 to 4 anchoring groups are used for an efficient electron transfer [3]. By far the most common architecture of organic sensitizers is the D–$\pi$–A system, where an electron-rich moiety (D) is linked to an electron-acceptor (A) endgroup through a $\pi$ spacer. The acceptor moiety carries an anchoring group, typically a carboxylic acid, for electronic coupling with $TiO_2$ surface. Keeping in mind the demands for a strong binding ability of the organic sensitizer on $TiO_2$ surface and for the reduced tendency towards aggregation, it was appeared challenging for us to design and develop a novel dye with phenoxazine and triphenylamine core and bi-anchoring groups. We thoroughly investigated the structure-properties relationships with a special concern on the photophysical, electrochemical and DSSC performance.

## References

[1] S. Zhang, X.Yang, Y. Numata and L. Han, Energy Environ. Sci., 6 (2013) 1443-1464
[2] A. Hagfeldt and M. Grätzel, Accounts Chem. Res., 33 (2000) 269-277.
[3] C.H. Yang, H.L. Chen, Y.Y. Chuang, C.G. Wu, C.P. Chen, S.H. Liao and T.L. Wang, J. Power Sources,188 (2009) 627-634.

## Acknowledgement

This work was financially supported by UEFISCDI Romania through the Project PN-III-P2-2.1-PED-2016-0510, contract no. 59PED/2017.

---

* Corresponding author, *E-mail: damaceanu@.icmpp.ro*

O-40

# Molecular Design and DSSC Performance of a Novel D-D-π-A Dye

**Catalin-Paul Constantin**[1]*, **Mariana-Dana Damaceanu**[1],
**Andra-Elena Stroia**[1], **Mihai Mihaila**[2], **Mihaela Kusko**[2] **and Razvan Pascu**[2]

[1]"Petru Poni" Institute of Macromolecular Chemistry, Aleea Grigore Ghica Voda
41A, Iasi, 700487, Romania
[2]National Institute for Research and Development in Microtechnologies (IMT),
126A, Erou Iancu Nicolae Street, 077190, Bucharest, Romania

*E-mail: constantin.catalin@icmpp.ro*

Solar energy is one of the fastest growing renewable energy sources due to the increase in fossil energy costs and the related global warming problems [1]. Among 3rd generation solar cells, dye-sensitized solar cells (DSSCs) appear the most promising for commercial use. Among various sensitizers used in DSSCs, a special attention has been paid to metal-free organic dyes due to their high molar-extinction coefficients, easy synthesis and structural modification. Particularly interesting aromatic structures are phenoxazine (POZ) and triphenylamine (TFA), two strong electron donor moieties largely used in DSSCs [2]. An important feature of phenoxazine is the easy structural modification to tune the properties of the dye incorporating it. Moreover, the butterfly conformation of POZ can sufficiently inhibit molecular aggregation and excimers formation [3]. On the other hand, TFA is known for their reversible oxidation process and generation of stable radical cations. Moreover, the oxidation potentials of TFA can be modulated by coupling them to aromatics of different electron richness [4]. Thus, the rational design of the terminal electron donor very recently led to a consecutive efficiency increase of POZ dyes. Herein, we report on the synthesis and characterization of a novel POZ sensitizer with D–D–π–A structure. To this dye, hexyloxy units were incorporated to enable the modulation of the HOMO/LUMO levels and charge recombination. The effect of electron double donor structure of the optical, electrochemical and the photovoltaic properties was systematically investigated. The detailed analyses of the photo-physical behavior proved the existence of the intramolecular charge-transfer transition from the donor to the acceptor units. The novel dye has more negative HOMO energy than the $I^-/I_3^-$ redox couple, leading to a fast regeneration of the oxidized dye and a more positive LUMO energy relative to the conduction band of $TiO_2$ to ensure an effective injection of excited electrons. Preliminary tests of this new sensitizer in DSSC showed an efficiency of about 3.11, without coadsorbant and optimization.

## References

[1] B.O'Regan and M. Grätzel, Nature, 353 (1991) 737-740.
[2] S. Wang, R. Yang, J. Guo and G. Li, Synth. Met., 215 (2016) 184-193.
[3] M.D. Damaceanu, M. Mihaila, C.P. Constantin, S. Chisca, B.C. Serban, C. Diaconu, O. Buiu, E.M. Pavelescu and M. Kusko, RSC Adv., 5 (2015) 53687-53699.
[4] T. Manifar and S. Rohani, Can. J. Chem. Eng., 82 (2004) 323-334.

## Acknowledgement

This work was financially supported by UEFISCDI Romania through the Project PN-III-P2-2.1-PED-2016-0510, contract no. 59PED/2017.

---

* Corresponding author, *E-mail: constantin.catalin@icmpp.ro*

# Rational Design of a Double Donor Core-based Dye for DSSC

**<u>Andra-Elena Stroia</u>[1], Catalin-Paul Constantin[1], Mariana-Dana Damaceanu[1]*, Mihai Mihaila[2], Mihaela Kusko[2] and Razvan Pascu[2]**

[1]"Petru Poni" Institute of Macromolecular Chemistry, Aleea Grigore Ghica Voda 41A, Iasi, 700487, Romania
[2]National Institute for Research and Development in Microtechnologies (IMT), 126A, Erou Iancu Nicolae Street, 077190, Bucharest, Romania

*E-mail: stroia.andra@icmpp.ro*

Since their discovery, dye-sensitized solar cells (DSSCs) have been intensively explored as alternatives to conventional silicon-based solar cells due to the possibility of low-cost production and fabrication on flexible substrates and high power conversion efficiency. The organic donor-acceptor system - the dye anchored on the $TiO_2$ surface which acts as a light absorber is one of the key components in DSSCs, having a strong influence on the solar cell efficiency. Metal-free organic sensitizers with donor-π bridge-acceptor (D-π-A) were intensively used in DSSCs due to their well-known advantages: high molar extinction coefficients, versatile and relatively cheap synthesis, attainable structural tuning and less environmental issues [1]. Various donor groups have been investigated as building blocks in the sensitized dye, including carbazole, coumarin, anthraquinone, indoline, triarylamine, phenoxazine, phenothiazine etc., while cyanoacrylic acid and rhodamine-3-acetic acid were by far the most commonly used anchoring and electron acceptor units. The π-conjugated bridge structural motif can be easily tuned and comprise functional units as phenylenevinylene, benzothiadiazole, thiophene, dithienothiophene, EDOT, selenophene, and so on [2]. The phenothiazine-based dyes comprise a large proportion and have the unique advantages due to the phenothiazine non-planar butterfly conformation that may prevent molecular aggregation and excimer formation on the $TiO_2$ surface, and due to the strong electron donor ability settled by electron-rich sulfur and nitrogen heteroatoms, among others [3]. On the other hand, the triphenylamine donor core based dyes, holding the record for validating efficiency over 10.3%, are promising candidates for highly efficient DSSCs [4]. Herein, a novel organic dye based on phenothiazine-substituted triarylamine moiety was designed, synthesized, and fully characterized for use in DSSCs. The relationship between the dye structure, photophysical behavior and electrochemical properties were thoroughly investigated to predict the DSSC performance. Systematic comparisons of the energy levels, light absorption, and interfacial charge transfer dynamics was made to understand the influence of the electron donor structural motif on the DSSC performance. Investigation of the photovoltaic performances of this dye under irradiation with simulated solar light was carried out.

## References

[1] B. Basheer, D. Mathew, B. K. George and C. P. R. Nair, Sol. Energy, 108 (2014) 479-507.
[2] J. Liu, X. Yang, J. Zhao and L. Sun, RSC Adv., 3 (2013) 15734-15743.
[3] L. Jun-Sheng, W. Zhong-Quan and J. Chun-Yang, Chinise Chemical Letters, 27 (2016) 1304-1318.
[4] A. Mahmood, Sol. Energy, 123 (2016) 127-144.

## Acknowledgement

This work was financially supported by UEFISCDI Romania through the Project PN-III-P2-2.1-PED-2016-0510, project no. 59PED/2017.

---

* Corresponding author, *E-mail: damaceanu@icmpp.ro*

O-42

# A Comparative Study on Uranium Recovery from Central Anatolia Region Uranium Ores

**Aybüke A. İsbir Turan*, Kamer Derin and Erol Üçgül**

MTA Mineral Research & Exploration General Directorate, Department of Mining Analysis and Technologies, Ankara, 06800, Turkey

*E-mail: aybuke.turan@mta.gov.tr*

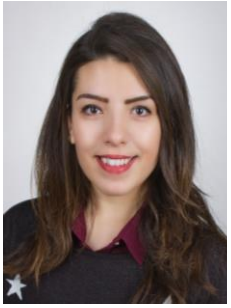
In this study, alkaline and acidic agitation leaching of Central Anatolia Region uranium containing ores were studied. The bottle roll test procedure is conducted to recover of uranium from the composite core samples include 600 mg U/kg ore. Sulfuric acid ($H_2SO_4$) solutions were used for the acidic leaching, while solid sodium bicarbonate ($NaHCO_3$) and hydrogen peroxide ($H_2O_2$) solutions were utilized for the alkaline leaching [1-3]. After the agitation leaching step, liquid-solid separation is conducted by using a high speed centrifugal installation. The obtained solid and pregnant solutions are weighted. Uranium containing pregnant solution is stocked and sent to the chemical analysis step. The comparisons of % uranium resource recovery from heads grade and from tails plus leach were investigated. At the end of the alkaline leaching tests by using 2 g/L $NaHCO_3$ and 0.2 g/L $H_2O_2$ 92.46 % of uranium recovery was achieved in 12 days leaching duration. The maximum uranium recovers values were calculated as 98.78 % in the acidic leaching tests by using 2.0 M $H_2SO_4$ during 54 hours.

## References

[1] T.R. Guiliger, R.S. Schechter, L.W. Lake, J.G. Price and P. Bobeck, "Factors Influencing Production Rates in Solution Mining of Uranium Using Basic Lixiviants", *Minerals and Metallurgical Processing*, 278 (1985) 60-67.
[2] P.S. Sundar, "In-Situ Leaching Simulation Studies Of Uranium Ores", *1978 AIME Annual Meeting*, 78-AS-102, Society of Mining Engineers of AIME, Colorado, USA (1978).
[3] S.W. Robertson and P.J. Van Staden, "The Progression of Metallurgical Testwork during Heap Leach Design", *Hydrometallurgical Conference 2009*, 31-42, The Southern African Institute of Mining and Metallurgy, Cape Town, South Africa (2009).

---

* Corresponding author, *E-mail: aybuke.turan@mta.gov.tr*



# Titania Supported Rhodium(0) Nanoparticles As Highly Active Catalyst in Dehydrogenation of Dimethylamine Borane

**Seda Tanyıldızı Karaboğa**[1]*, **İzzet Morkan**[1] **and Saim Özkâr**[2]

[1]Abant İzzet Baysal University, Faculty of Science, Department of Chemistry, 14280, Bolu, Turkey
[2]Middle East Technical University, Faculty of Science, Department of Chemistry, 06800, Ankara, Turkey

*Email: tanyildizi_s@ibu.edu.tr*

Hydrogen ($H_2$) is one of the sustainable and environmentally benign energy carriers [1]. The lack of safe, effective and cost-effective hydrogen storage sources for transportable and stationary applications is one of the main obstacles to overcome for the application of the hydrogen economy. Among the amine boranes [2], which have been considered as solid hydrogen storage materials because of their stability, high hydrogen content and nontoxicity [3], dimethylamine borane (DMAB, $Me_2NHBH_3$) has attracted particular interest as it can release equivalent 1 $H_2$ in the presence of a suitable catalyst under mild conditions (eq. 1) [4].

$$2Me_2NH.BH_3 \xrightarrow{catalyst} (Me_2N.BH_2)_2 + 2H_2 \qquad (1)$$

In this work, rodium(II) hexanoate was used as a precursor for the formation of rhodium(0) nanoparticles, Rh(0)/nano$TiO_2$ during the dehydrogenation of dimethylamine borane at 60.0 ± 0.5°C. The results of characterization by using XRD, SEM, SEM-EDX, TEM, UV-vis, XPS techniques reveal the formation of highly dispersed rhodium(0) nanoparticles with average particle size of 3.17 ± 0.52 nm on the surface of titania nanopowders. They provide 9700 turnovers in hydrogen generation from the dehydrogenation of DMAB over 27 h before deactivation and a record initial TOF value of 2900 $h^{-1}$ in $H_2$ generation at 60.0 ± 0.5°C, which is the highest TOF value ever reported for dehydrogenation of dimethylamine borane using homogeneous or heterogeneous catalyst. Rh(0)/nano$TiO_2$ is also a quite reusable catalyst preserving 57% of the initial catalytic activity even after the fourth run of dehydrogenation reaction. This study also includes the results of a kinetic study on the catalytic dehydrogenation of dimethylamine borane depending on the temperature and catalyst concentration.

## References

[1] L. Schlapbach and A. Zuttel, Nature 414 (2001) 353-358.
[2] H.W. Langmi and G.S. McGrady, Coord. Chem. Rev., 35 (2007) 251-925.
[3] M.C. Denney, V. Pons, T.J. Hebden, D.M. Heinekey and K.I. Goldberg, J. Am. Chem. Soc., 128 (206) 12048-12049.
[4] C.A. Jaska, K. Temple, A.J. Lough and I. Manners, Chem. Commun., 11 (2001) 962-963.

---

* Corresponding author, *Email: tanyildizi_s@ibu.edu.tr*

# Co-pyrolysis of Microalgae with Plastic Wastes over ZSM-5

**Gamze Özçakır and Ali Karaduman***

Ankara University, Faculty of Engineering, Department of Chemical Engineering, 06100, Ankara, Turkey

*E-mail: gamze_ozcakir@windowslive.com*

*Spirulina* is a kind of microalgae. There have been so many researches that produced liquid bio-oil and chemicals from these microalgae using several methods. Plastic wastes like low-density polyethylene (LDPE) and polystyrene (PS), are another energy source, have been studied for producing oil and chemicals. It is important that pyrolysis can be used to recycle these two energy sources. Pyrolysis products of biomass are bio-oil, char and non-condensed gas. Products of co-pyrolysis of *Spirulina* and LDPE/PS which zeolite catalysts are used in are wondered.

In this research, catalytic and non-catalytic experiments occurred at 420-460-500˚C. Catalytic experiments are based on CoZSM5 catalyst with 15:1 WHSV. Firstly co-pyrolysis of plastic wastes were made with LDPE:PS (4:1) ratio. Secondly *Spirulina*/plastic wastes (1:1 and 4:1) were made. Lastly yields of products were calculated and aromatic compounds in liquid product (benzene, toluene, styrene) are found with GC-MS analysis.

**Figure 1.** Figure of experimental set up

**Table 1.** Researches about algal biomass pyrolysis

| **Researchers** | **Findings** |
|---|---|
| Lorenzetti vd. (2016) | Bio-oil obtained from catalytic pyrolysis with ZSM-5 catalyst includes a huge amount of aromatic compounds and low amount of oxygenic compounds |
| Anand vd. (2016) | Benzene, toluene, naphthalene and methyl naphthalane are founded by catalytic pyrolysis at 600 ˚C with ZSM-5 |

**References**
[1] C. Lorenzetti, R. Conti, D. Fabbri and J. Yanik, Fuel, 166 (2016) 446-452.
[2] V. Anand, V. Sunjeev and R. Vinu, Journal of Analytical and Applied Pyrolysis, 118 (2016), 298-307.

---

* Corresponding author, *E-mail: ali.karaduman@ankara.edu.tr*

# Enviromental & Green Chemistry

# Application of Activated Carbon to the Removal of Methylene Blue in Drinking Water

**Sadaf Adhami**[1], **Hamed Ghorbanpor**[2], **Macid Nurbaş**[3] **and Hüseyin Avcı**[4]*

[1,3]Eskisehir Osmangazi University, Chemical Engineering Department, 26040, Eskişehir, Turkey
[2]Eskisehir Osmangazi University, Department of Polymer Science and Technology, 26040, Eskişehir, Turkey
[4]Eskisehir Osmangazi University, Metallurgical and Materials Engineering Department, 26040, Eskişehir, Turkey

*E-mail: sadaf.adhami92@gmail.com*

The lack of clean and fresh water with the growing demand is becoming a more profound problem worldwide. Many people suffer from malnutrition, sickness, and even die due to the lack of access to potable water [1]. It is highly expected, in the near future, it will be struggled to maintain access to the drinking water because of the population growth, improved living standards, agricultural with industrial activities, and so on [2]. In this research, we have conducted to remove methylene blue in the contaminated water by using activated carbon which was obtained by a lignocellulosic material of the apricot kernel shell. Activated carbon has more efficient adsorbent due to a high degree of surface reactivity, variable characteristics of surface chemistry, large surface area that can reach 3000 $m^2/g$ and sophisticated porosity development [3]. In addition, apricot kernel shell has low-cost and can be found abundantly in Turkey [4]. Activated carbon which was received from Dr. Onal's research group from Inonu University was investigated based on its adsorption performance of methylene blue and reusability capacity.

As a result of the analysis with UV-Vis spectrophotometer, more than 95% dye removal was obtained within the first half hour (Figure 1). Even if it is strongly believed that the cycle of reusability of the activated carbon which was obtained by using an apricot kernel shell is higher due to a very high surface area, the experiment was terminated after the third cycle. It can be concluded that our country, which is the first in the world for the apricot production, can supply the apricot kernel shell with a very low cost can have a great potential for clean water to combat one of the most important problems of our lives.

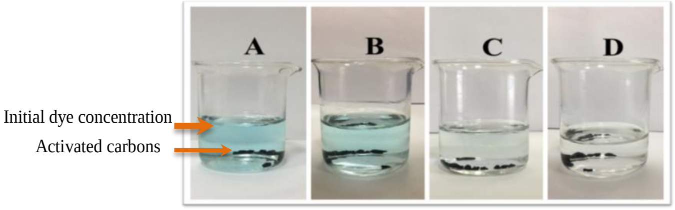


**Figure 1.** Images of methylene blue at the beginning (A), after 30 min (B), 60 min (C), and 90 min (D) treatment with the activated carbon

## References

[1] M.A. Shannon, P.W. Bohn, M. Elimelech, J.G. Georgiadis, B.J. Marinas and A.M. Mayes, Nature 452 (2008) 301-310.
[2] H.W. Liang, X. Cao, W.J. Zhang, H.T. Lin, Y. Yang, L.-T. Song, X. Wang and S.-H. Yu, Advanced Functional Materials 21 (2011) 3851-3858.
[3] G. Rajalekshmi, T. Mrithaa and S.V. Ch, Journal of Industrial Pollution Control 32 (2016).
[4] T. Depci, Y. Onal and K.A. Prisbrey, Journal of the Taiwan Institute of Chemical Engineers 45 (2014) 2511-2517.

---

* Corresponding author, *E-mail: havciesogu@gmail.com*

O-46

# Determination of Polycyclic Aromatic Hydrocarbons with Novel SPME Fiber in Sea Water and Tap Water

**Paniz Tashakkori**[1], **Pelin Erdem**[2], **Serap Seyhan Bozkurt**[2]* **and Melek Merdivan**[2]

[1] Dokuz Eylul University, The Graduate School of Natural and Applied Sciences, 35160, Izmir, Turkey
[2]Dokuz Eylul University, Faculty of Science, Chemistry Department, 35160, Izmir, Turkey

*E-mail: paniztashakkori@yahoo.com*

Polycyclic aromatic hydrocarbons (PAHs) are widely present environmental pollutants and they have cancerogenic and toxic effects or hazardous for human health and the environment. They are found in the atmosphere as well as in environmental water sources. Very small amounts of these substances in tap water to find may cause toxic and carcinogenic effects in the human body. In nature over 100 PAH compounds have been determined, but only 16 of them have been proven their higher toxicity [1]. In environmental samples PAHs presence of very low levels so sample preparation methods involving clean-up and enrichment steps are often required prior to the chromatographic analysis. The detection of PAHs in environmental water sources involves the use of solid-phase extraction method. Nowadays, solid-phase micro extraction procedures, with environmentally friendly advantages, are preferred [2]. It is necessary to discover new fiber with fixed substrate and selective coating according to the properties of the target analytes in order to obtain remarkable extraction efficiency due to the extractions requirement of different trace environmental pollutants [3]. In this study, determining PAHs in tap water and sea water with novel SPME fibers was carried out using stainless steel wire as support and grahpene-oxide modified with ionic liquids [1-(3-aminopropyl)-3-vinyllimidazolium bis(trifluoromethylsulfonyl)imide and 1-(3-aminopropyl)-3-benzyllimidazolium bis(trifluoromethylsulfonyl)imide] as coating material by GC-MS. Thus, graphene-oxide-ionic liquid based SPME fibers were prepared using the sol-gel method. The structures of sorbents were investigated by FTIR and XRD. Thermal behaviours were determined by TGA curves. PAHs were separated from tap water and sea water with the SPME method by means of prepared graphene fibers and analyzed using gas chromatography-mass spectrometer (GC-MS). The analytical parameters were studied for each with the fibers (dynamic range, precision, limit of detection, selectivity, recovery, accuracy). Also, the prepared fibers were compared to commercial SPME fibers PDMS and DVB/CAR/PDMS.

## References

[1] H.I. Abdel-Shafy, M.S.M. Mansour, Egyptian Journal of Petroleum, 25 (2015) 107-123.
[2] M. Merdivan, V. Pino, J.L. Anderson, Environmental Technology, 2016, DOI: 10.1080/09593330.2016.1240242, 1479-1487.
[3] X. Hou, Y. Guo, X. Liang, X. Wang, L. Wang, X. Liu, Talanta, 153 (2016) 392-400.

## Acknowledgement

The authors would also like to thank Scientific and Technological Research Council of Turkey (TUBITAK) financially supported by project 215Z212.

---

* Corresponding author, *E-mail: serap.seyhan@deu.edu.tr*

O-47

# Water Quality Survey of Transboundary Selenge River Basin and Lake Baikal

**Bayartsetseg Batbayar[1], Ganchimeg Batbold[1], Batdulam Battulga[2], Bolormaa Oyuntsetseg[1]*, Masayuki Kawahigashi[2], Viacheslav Victorovich Khakhinov[3], Takayuki Kobayashi[4] and Nobuhide Fujitake[5]**

[1]Department of Chemistry, National University of Mongolia, Ulaanbaatar, Mongolia
[2]Department of Geography, Tokyo Metropolitan University, Tokyo, Japan
[3]Department of Biology, Buryat State University, Buryatia, Russia
[4]College of Bioresource Science, Nihon University, Tokyo, Japan
[5]Graduate School, Agricultural Science, Kobe University, Kobe, Japan

*E-mail:bolormuis@gmail.com*

The Selenge River basin is a transnational mega-ecosystem, the largest water basin of Mongolia and Russia. The Selenge River is a transboundary water system, which rises in the Khanghai Mountains in Mongolia and flows into the Lake Baikal in the Republic of Buryatia. Lake Baikal is the deepest and largest fresh water reservoir on the Earth, and has a unique ecosystem [1-3].

The current study was carried out to determine hydro chemical parameters, to monitor water quality in the transboundary river system and to identify the self-purification process.

Fifty water samples were collected from two regions, including Mongolia and Russia during 2013-2015. In the field study, the water physico-chemical parameters were measured using HI 9828 Multiparameter (Hanna instruments, USA). The water major ions and loss on ignitions were analyzed by conventional methods. The biogenic elements ($NH_4^+$, $NO_3^-$ and $NO_2^-$) were detected using a spectrophotometric method. The water microelements were investigated by inductively coupled plasma atomic emission spectroscopy (ICP-AES). From the results, river and lake water were determined low alkalinity (7.6-8.5, pH) and dominant ion was bicarbonate (42.7-75.7%, $HCO_3^-$) in the study areas. The most of water samples were very soft (0.9-3.0 mg-eq/l) by O.A.Alekin's water hardness classification and the water mineralization (64.95 mg/l to 519.36) included low mineralized water by A.M.Ovchinnicov's classification. The contents of Cd (0.0258-0.1970 mg/l) and Zn (0.261-0.434 mg/l) were determined higher than Mongolian National Standard (MNS 4586:1998, Cd: 0.005 mg/l, Zn: 0.01 mg/l)'s acceptable concentration of water quality. Chemical composition of waters can be affected by various factors which include: chemical composition of rock and soils, size and shape of the catchment, weather condition, vegetation and human activities. It is shown that surface water in the transboundary Selenge river affected by rainfall, soil erosion and anthropogenic activity in the study areas. The physico-chemical parameters of water in Lake Gusinoe and Buir River, which tributaries of Selenge River, were higher than other sampling sites due to androgenic activity and low flowrate. Therefore, when comparing with other researcher's results, there were no significant differences in the natural water system through the water quality in the transboundary Selenge river.

## References

[1] A. Munguntsetseg, Hydrochemistry of River "Selenge", (2006) 13-16, 22-35.
[2] M. Orgilbold, M. Kawahigashi, O. Bolormaa and N. Fujitake, Environ Earth Sci (2017) 76:346.
[3] B. Batdulam, O. Bolormaa, V.V. Khakhinov and M. Kawahigashi, Proceedings of the Mongolian Academy of Sciences, 56(01) (2016) 65-79.

---

* Corresponding author, *E-mail: bolormuis@gmail.com*

O-48

# Chemical Composition Study of Lake Oigon, Western Mongolia

**Bayanmunkh Baatar[1], Buyan Chuluun[1], Narangarvuu Dashdondog[2], Sen-Lin Tang[3], Ochirkhuyag Bayanjargal[4] and Bolormaa Oyuntsetseg[1]***

[1]Department of Chemistry, School of Arts and Sciences, National University of Mongolia (NUM), Ulaanbaatar 14201, Mongolia
[2]Department of Biology, School of Arts and Sciences, NUM, Ulaanbaatar 14201, Mongolia
[3]Biodiversity Research Center, Academia Sinica, Taipei, Taiwan
[4]Department of Chemical and Biological Engineering, School of Engineering and Applied Sciences, NUM, Ulaanbaatar 14201, Mongolia

*E-mail: b_chuluun@yahoo.com*

As defined by Bayly & Williams meromictic lakes are lakes in which some water remains partially or wholly unmixed with the main mass of water at the normal circulation periods [1]. 80% of meromictic lakes in the world occur only in Antarctica. Despite rare occurrence of meromictic lakes they are salt lakes deeper than 5 m. Meromictic lakes in Eurasian landmass can be found at the point farthest from any ocean where Southern Siberia, Russia and Western Mongolia are located. Water and sediment samples were collected from the Lake Oigon in the Zavkhan province, one of five provinces in Western Mongolia. Physico-chemical parameters, macro ions and micro elements were determined and correlation between water and sediment was analyzed. Lake Oigon (mean of 25.7 g per L) was classified as a mesosaline lake by salinity level. According to Kurnakov-Valyashko's hydrochemical classification, Lake Oigon was chloride lake. In Lake Oigon, chemical composition had a clear vertical separation between surface (oxic) and bottom (anoxic) waters. Vertical distribution of chemical compositions in Lake Oigon was generally similar to those of other stratified lakes in terms of trophic characteristics [2-4]. Salinity, dissolved oxygen and $H_2S$ profiles in deep water of Lake Oigon were very constant due to thermal stratification within the oxic surface (0 to 7 m) and anoxic deep water (7.75 to 9 m). The vertical profile of hardness, sulfate and chloride ions, and electrical conductivity variations were directly reflected by salinity gradients, each with increasing depth. Overall, results were consistent with other permanent stratified lakes, including sulfur cyclical processes in anoxic deep water [3,4]. Lake Oigon clearly has high diversity and uniqueness of bacterial communities between water layers within the lake [5]. Our results of a chemical composition study suggested that Lake Oigon was the first meromictic lake ever reported in Mongolia.

## References

[1] R.M. Hand and H.R. Burton, Hydrobiologia, 81 (1981) 363-374.
[2] B. Boehrer and M. Schultze, Rev Geophys, 46 (2008).
[3] A.G. Degermendzhy, E.S. Zadereev, D.Y. Rogozin, I.G. Prokopkin, Y.V. Barkhatov, A.P. Tolomeev, E.B. Khromechek, J.H. Janse, W.M. Mooij and R.D. Gulati, Aquat Ecol, 44 (2010) 619-632.
[4] D.Y. Rogozin, V.V. Zykov, M.Y. Chernetsky, A.G. Degermendzhy and R.D. Gulati, Aquat Ecol, 43 (2009) 661-672.
[5] B. Baatar, P.W. Chiang, D.Y. Rogozin, Y.T. Wu, C.H. Tseng, C.Y. Yang, H.H. Chiu, B. Oyuntsetseg, A.G. Degermendzhy and S.L. Tang, PloS One 11 (2016), doi:10.1371/journal.pone.0150847.

---

* Corresponding author, *E-mail: bolormuis@gmail.com*

O-49

# The Effect of Ionic Liquids on Laboratory Made Polypyrrole SPME Fibers

**Tuğberk Nail Dizdaş, Levent Pelit*, Füsun Okçu Pelit, Hasan Ertaş and F. Nil Ertaş**

Ege University, Faculty of Science, Department of Chemistry, 35100, İzmir, Turkey

*E-mail: tugberkdizdas@gmail.com*

Solid-phase microextraction (SPME) technique which is an efficient, solvent-free, sample preparation method was first introduced by Arthur and Pawliszyn in 1990 [1]. Although different types of commercially available polymer materials such as PDMS, CAR, PEG have been widely used as sorbent in SPME, they suffer from short lifetime and high cost. Consequently, recent studies have been focused on fabricating low cost, simple, robust and long-life fiber with enhanced selectivity for the target analyte by introducing novel materials as functional coatings. Conducting polymers (CP) meet these requirements due to their mechanical and chemical stability and high porosity with increased surface area, the use of conducting organic polymers as a sorbent material in SPME has been very popular [2]. Physical and chemical properties of CP are directly related to preparation condition of conducting polymer. Ions in supporting electrolyte are used as a charge transfer agent (dopant) which is doped during the electro polymerization proses affects both oxidation and physical properties of the polymers.

Preparation conditions of polypyrrole (PPy) which is the most popular conducting polymer were investigated in this study. PPy fibers were coated on 316 type stainless steel wire in different supporting electrolyte containing medium (ie. sodium dodecyl sulphate, tartrate and alkyimidazolium type ionic liquids with different alkyl chain) by electrochemical technique (ie. cyclic voltammetry). Their thermal stability, surface and chemical properties were investigated by thermogravimetric, XPS and FTIR respectively. Prepared SPME fibers were applied for the determination of some endocrine disruptor pesticides in water by the head space SPME method. Their fiber performances were also compared with commercial SPME fibers.

**References**

[1] C.L. Arthur and J. Pawliszyn, Analytical Chemistry, 62 (1990) 2145-2148.
[2] F.O. Pelit, L. Pelit, T.N. Dizdaş, C. Aftafa, H. Ertaş, E.E. Yalçınkaya, H. Türkmen and F.N. Ertaş, Analytica Chimica Acta, 859(15) (2015) 37-45.

**Acknowledgement**

Authors would like to thank TUBITAK (Project numbers: 113Z672 and 114Z394) and Ege University Research projects (2013 FEN 065, 2010 FEN 033).

---

* Corresponding author, *E-mail: levent.pelit@ege.edu.tr*

O-50

# Uranium and Hydrochemical Study of Ground and Drinking Waters in Ulaanbaatar City, Mongolia

**Tegshbayar Norov[1], Ankhnybayar Batdelger[2], Batdulam Battulga[3], Bolormaa Oyuntsetseg[4]* and Tsookhuu Khinayat[1]**

[1]Department of Physics, School of Arts and Sciences, National University of Mongolia, Ulaanbaatar-14201, Mongolia
[2]Central Geological Laboratory, Ulaanbaatar-18080, Mongolia
[3]Department of Geography, Tokyo Metropolitan University, Tokyo, Japan
[4]Department of Chemistry, School of Arts and Sciences, National University of Mongolia, Ulaanbaatar-14201, Mongolia

*Email: tegshbayart@yahoo.com*

An assessment of the radioactive uranium and physicochemical characterization of the drinking water resources in the Ulaanbaatar city area was carried out in this study. The quality of ground and drinking water is of paramount importance issue, not only in Mongolia but also in the world. Groundwater is essential drinking water resource of Ulaanbaatar city.
In this study, we aimed to determine and evaluate the uranium concentration in ground and drinking water and to assess hydrochemical characterizations and micro-elements in Ulaanbaatar city, Mongolia. Totally 143 ground and drinking water samples were collected from Ulaanbaatar city. Chemical characterizations were determined by appropriate methods according to Water Quality Assessments of World Health Organizations. The uranium and micro-elemental analysis was carried out with filtered (0.45 μm membrane filter) and acidified (2 M nitric acid) water samples using Inductivity Coupled Plasma Mass Spectrophotometry (ICP-MS) at the Central Geological Laboratory (CGL) in Mongolia.

The level of uranium is $\geq 1$ μg/l in 58.7% of the all water samples. The uranium concentration in 4.19% of all water samples was determined higher than drinking water guidelines (30 μg/l) in World Health Organization (WHO) and United States Environmental Protection Agency (USEPA). The correlation analysis showed that uranium is correlating with electrical conductivity (EC) and arsenic content. Abnormally high concentrations of uranium in water were determined in some sampling points in the city area. Uranium can create complexes with carbonate ($CO_3^{2-}$) and bicarbonate ions ($HCO_3^-$ is 53-73% of all ions) in water. In the ground and drinking water, micro-elements concentration did not exceed the guidelines of WHO and USEPA except for as in the water sample from the Janchiwlan health resort, Bagakhangai district. Some physicochemical characterizations are found specific results in the Bagakhangai district (BKhD) due to uranium vein in this area. Geological structure and ground water flow direction is main factor of relatively high content of uranium in groundwater and it might influence the drinking water quality.

**References**

[1] S.L. Benjamin, C. B. Philip, P. Tamir and G. Ochir Environ Earth Sci, 62 (2011) 171-183.
[2] V.P. Isupov, A.G. Vladimirov, N.Z. Lyakhov, and S.L. Shvartsev, Doklady Earth Sciences, 437(1) (2011) 352-356.
[3] S. Kansal, R. Mehra and N.P. Singh, Journal of Public Health and Epidemiology, 3(8) (2011)352-357.

---

* Corresponding author, *E-mail: bolormuis@gmail.com*

O-51

# Novel Magnetic Dispersive μ-SPE Method using $Fe_3O_4/Ni/Ni_xB$ Nanocomposite Adsorbent for the Analysis of Pesticides

**İlknur Bağatır Erbaş, Tülin Deniz Çiftçi and Füsun Okçu Pelit***

Ege University, Faculty of Science, Department of Chemistry, 35100, İzmir, Turkey

*E-mail: ilknurbgtr@ gmail.com*

In the last years, to overcome the drawbacks of solid phase extraction (SPE), a new procedure based on the use of magnetically modified adsorbents called magnetic SPE (MSPE) has been developed. This technique has gained much attention due to easy separation under an applied external magnetic field, minimum solvent consumption and the extraction efficiency. Because of unique physical and chemical properties, a series of magnetic particles have been used for the extraction of organic pollutants by MSPE method. These particles include, nano $Fe_3O_4$, $Fe_3O_4$-grafted graphene [1], carbon nanotubes [2], graphene [3], $Fe_3O_4$-CNT [4] and so on.

In this study, a novel magnetic adsorbent $Fe_3O_4/Ni/Ni_xB$ nanocomposite was synthesized and used for the determination of pesticides by magnetic dispersive μ-SPE method. Characterization of the adsorbents was performed using scanning electron microscopy combined with energy dispersive X-ray spectroscopy (SEM-EDX). The performance of extraction of Bromopropylate (BRP) and Lambda-Cyhalothrine (LMD) were compared by using GC-ECD system. For this purpose 7 mL of sample (pH:7.0) was placed in a centrifuge tube containing 5.0 mg of $Fe_3O_4/Ni/Ni_xB$ nanocomposite material. Adsorption process was made by using a shaker for 30 min. After this process, centrifugation was made and nano particles were isolated from the sample by placing a strong magnet at the bottom of the tube. The preconcentrated target analytes were desorbed with 75 μl ethyl acetate by ultrasonication for 15 min. After centrifugation process for 1 min, 50 μl of the extract was placed in an insert containing 1 mg of $Na_2SO_4$ for the removal of excess amount of water. Inserts were centrifugated in a micro centrifuge and at the end, 20 μl of the sample was placed in a vial and 1 μl was injected to the GC system. This method was applied for pesticide determination in tap water samples. The regression coefficients relating to linearity were at least 0.99. Under optimized conditions the linear range was found between 0.1 – 5 ng $mL^{-1}$, and the detection limits for BRP and LMD were calculated as 0.02 and 0.03 ng $mL^{-1}$, respectively. This micro extraction method shares the advantages of the classical extraction methods such as excellent enrichment performance, easy operation and ability to employ a wide range of "green" extraction way.

**References**

[1] X. Cao, J. Chen, X. Ye, F. Zhang, L. Shen and W. Mo, J. Sep. Sci., 36 (2013) 3579-3585.
[2] Z. Du, M. Liu and G. Li, J. Sep. Sci., 36 (2013) 3387-3394.
[3] Q. Wu, G. Zhao, C. Feng, C. Wang and Z. Wang, J. Chromatogr. A, 1218 (2011) 7936-7942.
[4] B. Maddah and M. Hasanzadeh, Int. J. Nanosci. Nanotechnol., 13(2) (2017) 139-149.

---

* Corresponding author, *E-mail: fusun.okcu@ ege.edu.tr*

O-52

# Antibacterial and Mechanical Properties of PU/ZIF-8 Nanocomposite Coated Polyester Fabric

**Sevilay Nigar and Sennur Deniz***

Yıldız Technical University, Chemical Engineering Department, Davutpasa cd.,
34210, Esenler, İstanbul, Turkey

*E-mail: sevilay.nigar@gmail.com*

Polymer nanocomposites can offer significant improvements compared to neat polymers such as enhancement of elasticity and tensile strength, as well as antibacterial, thermal, electrical and gas barrier properties; due to their properties derived from several components. Metal-organic frameworks (MOFs) represent a new class of porous crystalline materials for which it is possible to design organic linkers and inorganic joints. MOFs have received huge attention in the past decade due to their unique properties, i.e. huge surface area, high porosity, low density, controllable structure and tunable pore size [1]. Zeolitic imidazolate frameworks (ZIFs) are a subclass of MOFs that are porous hybrid materials with structures analogous to zeolites that are built upon 4-connected nets of tetrahedral units, wherein metal ions, such as $Zn^{2+}$ or $Co^{2+}$, are linked through N atoms in ditopic imidazolate anions [2]. ZIF-8, one of the most widely studied ZIFs made by zinc ions coordinated by four imidazolate rings. As a result of their many benefits, MOFs appear to be excellent candidates for biomedical applications due to their antimicrobial activities [3]. The aim of this study was to prepare and investigate the polyurethane/ZIF-8 (PU/ZIF-8) coated fabric with unique properties, including antibacterial activity, mechanical properties and water vapor permeability. In this study, ZIF-8 was successfully synthesized under room temperature by using solvothermal synthesis route and characterized in terms of structure, adsorption isotherms and surface area by SEM, FT-IR and BET analysis. PU was used a polymer layer of coated polyester fabric. The mixture of PU/ZIF-8 nacomposite with 1 wt.% ZIF-8 content was prepared in dimethyl formamid as a solvent and coated on polyester fabric using indirect transfer coating method. After preparing PU/ZIF-8 coated fabric, different mechanical tests such as tensile strength, tear strength, accelerated life, water penetration and water vapor permeability tests were performed. Also, antibacterial activities of PU/ZIF-8 nanocomposite coated polyester fabrics were tested against Gram-positive *Staphylococcus aureus* (*S. aureus*, ATCC 25923) according to ISO 22196:2011 test method. It was found that PU/ZIF-8 nanocomposite coated polyester fabrics have antibacterial and good mechanical stability.

## References

[1] F.S. Ke, Y.S. Wu and H. Deng, Journal of Solid State Chemistry, Volume 223 (2015) 109-121.
[2] Y.R. Lee, M.S. Jng, H.Y. Cho, H.J. Kwon, S. Kim and W.S. Ahn, Chemical Engineering Journal, 271 (2015) 276-280.
[3] G. Wyszogrodzka, B.Marszalek, B. Gil and P. Dorozynski, Drug Discovery Today 21, 6, 2016.

## Acknowledgments

This work was supported by the Yıldız Technical University (No: 2014-07-01-DOP05).

---

* Corresponding author, *E-mail*: *sennurdeniz@gmail.com*

O-53

# Preparation of High-surface Area Activated Carbons from Sunflower Seed Extracted Meal Seed by $ZnCl_2$ Activation using Taguchi Robust Product Design

**Uğur Moralı***, **Hakan Demiral and Sevgi Şensöz**

Eskisehir Osmangazi University, Faculty of Engineering and Architecture,
Department of Chemical Engineering, Eskisehir, Turkey

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

In this study, sunflower seed extracted meal (SSEM) obtained from oil plant have been explored for its potential use in the preparation of activated carbon by the method of chemical activation with zinc chloride. The optimization of the preparation of activated carbon with high surface area has been achieved by using a combination of statistical tools including Taguchi matrix, signal to noise ratio, and analysis of variance (ANOVA). The following two controllable design factors were used in the Taguchi method: activation temperature and impregnation ratio (IR) [1]. The Taguchi orthogonal array L9 was applied with three level of consideration for each factor. The optimum parameters for the preparation of activated carbon have been identified as: activation temperature of 600 °C and an impregnation ratio of $ZnCl_2$: SSEM of 3. As a result, the activation temperature used was found to be the most influential parameter. The porous texture of the obtained activated carbons (ACs) was characterized by physical adsorptions of $N_2$ at 77K. The resulting activated carbon obtained under optimum conditions was characterized for its functional groups and surface morphology. The BET surface area and total pore volume of the optimized activated carbon were obtained as 1535 $m^2/g$ and 0.94 $cm^3/g$, respectively, at 600 °C and with an IR of 3:1. The main conclusion of this study was that through Taguchi optimization of activated carbon preparation a desired response is possible. Together with the optimization method adopted, the results allow for a more detailed and accurate assessment of the activated carbon production. This study also demonstrated the potential of using SSEM biomass as cheap and efficient raw materials to produce activated carbon for wastewater treatment.

## References

[1] H. Demiral and G. Gündüzoğlu, Bioresource Technology, 101 (2010) 1675-1680.

---

* Corresponding author, *E-mail: umorali@ogu.edu.tr*

O-54

# Investigation of Properties of Canola Oil and Its Exploitation in Mineral Oil Industry

**Zehra Gülten Altın**[1]*, **Mustafa Dağ**[1] **and Ruken Esra Demirdöğen**[2]

[1]Çankırı Karatekin University, Faculty of Engineering, Department of Chemical Engineering, 18100, Çankırı, Turkey
[2]Çankırı Karatekin University, Faculty of Science, Department of Chemistry, 18100, Çankırı, Turkey

*E-mail: zaltin@karatekin.edu.tr*

Vegetable oils have been preference of choice as lubricants since they have high viscosity index, low volatility, high ignition point. Moreover, their resources are edible and low cost coming from agri-source. However, they also suffer from some disadvantages such as having low hydrolytic resistance and oxidative stability, not being compatible with some additives, high viscosity and high yield point [1,2]. Among the vegetable oils canola appears as a good alternative because it is eco-friendly. Since its saturated fatty acid content is between %5,4-9,5 and total fatty acid content is between %90,5-94,2 it is of preference of choice. This high level of unsaturated fatty acids of canola enable it to react with a variety of molecules [3]. This study, targets at improving physical and chemical properties of canola and thus investigating its place in lubricant industry. Therefore, crude canola oil was modified with a polymeric product commercially known as Elvaloy Ret in super polyphosphoric acid media at 80-100°C in N2 atmosphere. The mixture was stirred at various stirring rates. It is known that Canola oil consists of 15–30% linoleic acid and 51–71% oleic acid. The oleic acid of canola oil (OA) and the glycid metacrylate epoxy groups (GMA) of the reactive elastomeric terpolymer (etylene acrylate copolymer) form epoxy groups in glycide metacrylate were observed at 910 $cm^{-1}$ in the FT-IR spectrum. The acid indexes, dynamic and kinematic visocities of the samples obtained in the experiments were evaluated. The acid index, dynamic and kinematic viscosities of the modified canola oil and oxidative stability and rheological analysis were determined. It was observed that the acid indexes and viscosity values of canola oil have increases upon modification. This may be due to decomposition of oil at such high temperature and thus the free fatty acid amount increased. The increase in the kinematic viscosities of the modified oil is indicates that this oil can be a new derivative for those named oils named Light Oil. The liquidity properties of the modified Canola oil at different temperatures (rheological analysis) showed that the samples were in the viscoelastic liquid form.

## References

[1] Ö. Salman and D. Durak, Sigma 29 (2011) 412-421.
[2] L.R. Rudnick, Syntetic Mineral Oils and Bio-based Lubricants, Chemistry and Technology, 2006.
[3] S.Z. Erhan, Industrial Crops and Products, 11 (2000) 277-282.

## Acknowlegement

This research was funded by Çankırı Karatekin University BAP Coordination Unit. Project No: F060515B21 (2015-2017).

---

* *Corresponding author, E-mail: zaltin@karatekin.edu.tr*

O-55

# Indoor Air Quality of Selected Places in Ulaanbaatar City, Mongolia

**Dorjkhand Jigjid**[1,2], **Altangerel Baterdene**[2] **and Amgalan Natsagdorj**[1]*

[1]School of Arts and Science, Department of Chemistry, National University of Mongolia, Ulaanbaatar, Mongolia
[2]Greencrown LLC, Environmental Laboratory, Ulaanbaatar, Mongolia

*Email: doogii.j@gmail.com*

The aim of the present study was to characterize Indoor Air Quality (IAQ) and conducted to assess [1] levels of volatile organic compounds (VOCs) and particulate matter (PM) in various rooms of public places such as the gas station, welding factory, auto repair center, new apartment building, heavy machinery repair center and printing facility of Ulaanbaatar city, Mongolia.

An automatic, continuous sampling system and a multi-gas monitor were employed to quantify the air pollutants, along with environmental comfort factors, including temperature, $CO_2$, and relative humidity at six sampling sites over eight days.

A screening study of VOC and the determination of benzene, toluene, ethylbenzene, xylenes (BTEX), sampled with Radiello® diffusive samplers suitable for thermal desorption, were carried out in the sampling sites. The Gas Chromatography-Flame Ionization Detector and Electron Capture Detector technique was used for the analysis. The analysis results showed a prevalent indoor contribution for all VOC expect for BTEX presented similar concentrations in indoor air. Several locations were higher than the recommendation of 0.2 mg/m$^3$ proposed by the European Commission.

The concentrations of VOC pollutants were within the limits defined by WHO guideline values that exceeded 8–12-fold higher than the European Commission. Benzene, styrene, xylene were detected in all the samples, with the highest mass fraction in the samples of the heavy machinery repair and maintenance. Trichloroethylene, 1.2-dichlorobenzene and 1.4- dichlorobenzene were commonly detected with compositions of 70.8-6652.93, 19.39-398.29 and 13.3-355.35 µg/m$^3$ respectively, in the welding victory, heavy machinery repair and maintenance and printing facility.

**References**

[1] L.K. Sahu, D. Pal, R. Yadav and J. Munkhtur, Physicial Research Laboratory (PRL), Navrangpura, Ahmedabad, India. Aromatic VOCs at Major Road Junctions of Metropolis in India: Measurements Using TD-GC-FID and PTR-TOF-MS Instruments (2015) 1.

---

* Corresponding author, *E-mail: n_amgalan@num.edu.mn*

O-56

# Essential Elements and the Ratio in Children's Scalp Hair in Autism Spectrum Disorder

**Khulan Uranchimeg**[1], **Bayasgalan Tserensodnom**[2], **Nyamgerel Ihagvadogmid**[3] **and Bolormaa Oyutstseg**[1]*

[1]Department of Chemistry, School of Arts and Sciences, National University of Mongolia, Ulaanbaatar, Mongolia
[2]Senior Lecturer, Department of Neurology, School of Medicine, Mongolian National University of Medical Sciences, Ulaanbaatar, Mongolia
[3]Mongolian Autism Association, Ulaanbaatar 14201, Mongolia

*E-mail: halanu@gmail.com*

Autism is a behaviorally defined disorder, which involves social withdrawal, communication deficits and repetitive behavior [1]. The autism symptoms both genetic and environmental factors (their interactions) have been implicated in all over the world [1,2]. International discussion has focused high content of lead with autism disorder for children [1-3]. In recent years, autism spectrum disorder is a problem and importantly concerned in Mongolia. This study's purpose is source of exposure lead and other elements children scalp hair with autism spectrum disorder.

Twenty seven children's scalp hair samples were collected between the age of 2 to 10 years old. They were either diagnosed previously with autism spectrum disorder. The scalp hair samples were pre-treated and wet digested using nitric acid and hydrogen peroxide. [4]. The measurements of scalp hair samples were carried out by using Ta-lab (Tomi-Analyte) and spectrophotometry (UV-M51) for nutritional or essential elements (Ca, K, Cu, Zn, Fe, Se) and toxic elements (As, Cd, Pb ). All the data were compared with ranges of worldwide [5]. The mean lead's content (0.42 µg/g) was lower than range of worldwide (1-5 years children's average lead content is 1.0 µg/g) in all participants. It means that the lead content not related with autism disorder directly. The mean concentration of selenium was lower than the worldwide range for 60 % of the total number of samples. Selenium is an important component of an antioxidant enzyme, takes part in defending against free radical damage and inflammation, gutathione peroxidase which acts to prevent the decay of cellular function and plays a key role in maintaining a normal metabolism [2]. The cluster analysis using Centroid Linkage was processed by nutritional or essential elements. From the cluster analysis, were observed six clusters. Nutritional elements are calculated by ratio Zn/Cu, Fe/Cu and Ca/K from 6 clusters. It is estimated that the ratio of Fe/Cu was higher than the ranges of worldwide for all analyzed samples. The ratio of Fe/Cu high causing lipid peroxide damage within neurological tissues. Currently, the results of this study are basic material and it should be investigated further more.

## References

[1] E.B. Busch, O.R. Amin and T. Rabah, Medica-Journal of Medicine 6 (2011) 247-254.
[2] E.B. Busch, O.R. Amin, H.H. Dessoki and T. Rabah, Medica-Journal of Medicine 7 (2012) 38-48.
[3] M. Damodaran, L. Priya and A. Geetha, Humana press (2010) doi: 10.1007/s2011-010-8766-2.
[4] O. Bolormaa, M. Tsuji, K. Kawasaki, S. Narantsetseg and T.Hattori, Pixe 16 (2006) 29-38.
[5] International Federation of Clinical Chemistry (IFCC), Reference values (RV's) and Reference intervals (ranges), (RI's), (Poulsen et al., 1997).

---

* Corresponding author, *E-mail: bolormuis@gmail.com*

O-57

# Air Particulate Matter in Ulaanbaatar Urban Environments Mongolia: Trace Elements, Patterns and Transports

**Barkhasragchaa Baldorj**[1], **Amgalan Natsagdorj**[2]*, **Dashnyam Baasanjav**[3], **Shagjjamba Davga**[4] and **Bolormaa Oyuntsetseg**[2]

[1]Central Laboratory of Environmental and Metrology Governmental Implementing Agency for Meteorology and Environmental Monitoring of Mongolia
[2]School of Arts and Science, Department of Chemistry, National University of Mongolia, 24100, Ulaanbaatar, Mongolia
[3]Department of Applied Chemistry, School of Engineering and Applied Science, Ulaanbaatar 14201, Mongolia
[4]Nuclear Research Center, Ulaanbaatar, Mongolia

*E-mail: bnbarkhas@gmail.com*

The impacts of atmospheric aerosols on public health, climate and atmospheric composition are currently among the most widely studied topics in environmental science research. Many epidemiological studies have shown the association between health effects and particulate matter (PM) in ambient air. Health effects of PM are likely to depend on several factors, however, ambient concentrations, size and composition of the particles belong to the most important ones [1].
In this study, PM sources at two different sites (Zuun ail and Nuclear Research Center) in Ulaanbaatar analyzed for elemental content and black carbon (BC). Black carbon concentrations were determined using light reflection and $PM_{10}$ concentrations were recorded using co-located continuous PM monitors. Multi-elemental analysis was determined by Roentgen Fluorescence Analysis (RFA) using SPESTRO XEPOS spectrometer. Additionally, time and size-resolved PM samples are being collected for a Raman spectral mapping analysis, which will allow an unprecedented window into the chemical composition and morphology of Ulaanbaatar PM on a particle-by-particle basis.

Positive matrix factorization (PMF) was used to determine the PM sources and their contributions on an hourly time-scale at each site using the hourly elemental, BC and $PM_{10}$ data. The significant factors (sources) were determined to be: high temperature combustion, household waste furnace, soil, motor vehicle. The high concentrations of PM pollution observed in Ub severe in the Gers area, demonstrating that domestic stoves were the main emission sources.

## References

[1] Z. Li, Q. Wen and R. Zhang, Science of the Total Environment, 586 (2016) 610-622.

---

* Corresponding author, *E-mail: n_amgalan@num.edu.mn*

O-58

# Benotriazoles–Impreganted Activated Carbon for Enhanced Adsorptive Removal of Radionuclides from Aqueous Solution

**Muna AbuDalo[1]*, Svetlana Nevostrueva[2] and Mark Hernadez[3]**

[1]Jordan University of Science and Technology, Faculty of Science, Department of Chemistry, Irbid, Jordan
[2]Intel Corporation, 5000 W. Chandler Blvd. CH7-336, Chandler, AZ 85226, USA
[3]University of Colorado at Boulder , Civil and Environmental Engineering, Campus Box 428, mBoulder, CO 80309-0428, USA

*E-mail: maabudalo@just.edu.jo*

Benzotriazole derivatives form very strong bonds with transition metals. The amphipathic behavior and metal-binding capacity of these compounds was leveraged to remove model radionuclides, Eu(III), Ce(III), Sr(II), and U(VI) from aqueous solution by sorbing carboxybenzotriazole (CBT) and methylbenzotriazole (MeBT) to different activated carbons and subsequently exposing them to acidic solutions carrying model radionuclides. Batch and small scale breakthrough experiments were used to evaluate the effectiveness of the developed method for removing model radionuclides under pH range between 1.0 and 4.5. The sorption potential of model radionuclides significantly improved with carbon oxidation (depression of $pH_{PZC}$) and its impregnation with carboxybenzotriazole (CBT). The amount of metal ions sequestered from solution was found to be sensitive to pH changes and the effectiveness of the metal removal capacity of granular activated carbons (GACs) remained unchanged despite the initial high concentrations of MeBT and CBT in the washout solution. No significant sorption was observed with these model radionuclides, where methylbenzotriazole (MeBT) was pre-adsorbed either to oxidized or non-oxidized GACs. The effectiveness of the metal removal capacity of columns packed with oxidized CBT-impregnated activated carbons demonstrated significant improvement over the carbon alone with the best affinity and elimination capacity for U(VI) ions. The results demonstrate the potential implication of the developed method for the cost-effective remediation for removing uranium ions from acidic environments [1].

## References

[1] M. Hernandez, M. Abu-Dalo, G. Khannan and Al. Quick, Metal removal system and method**,** US20130001169 A1.

---

* Corresponding author, *E-mail: maabudalo@just.edu.jo*

O-59

# Coupling Activated Carbon with Surface Active Materials for Olive Mill Wastewater Treatment

**Heba Kanaan**[1], **Abeer Al Bawab**[2], **Nathir Al-Rawashdeh**[1] **and Muna AbuDalo**[1]*

[1]Jordan University of Science and Technology, Faculty of Science, Department of Chemistry, Irbid, Jordan
[2]The University of Jordan, Faculty of Science, Chemistry Department, Amman, Jordan

*E-mail: kanaanhm14@yahoo.com*

The Mediterranean region is known as the main olive oil producing region worldwide. However, olive mill wastewater (OMW), a liquid by-product of the olive oil industry, creates a major environmental problem. The high polluting power of OMW is associated to its acidic pH, high amount of low biodegradable organic matter such as polyphenols. Only 2% of the total phenolic content of the olive fruit passes in the oil phase, while the remaining amount is lost in the OMW [1]. A reliable olive mill wastewater treatment method that meets communal needs in the most cost-effective way is a vital need, especially for Jordan, in which it faces serious problem pertaining water resources and environmental quality. In this work, different media were modified by oxidation or reduction and impregnating with different surfactant types. The modified media was tested in a batch approach using real OMW samples and under different experimental conditions (surfactant types, surfactant concentration, time, pH). Media was characterized by EuroEA Elemental Analyzer, and Scanning Electronic Microscope (SEM) (Figure 1). The specific surface area of GAC was determined by Brunauer–Emmett–Teller (BET) analysis technique (Table 1). Phenolic contents were estimated via Folin Ciocalteu's method (UV-Vis test), high performance liquid chromatography (HPLC), and chemical oxygen demand (COD). The results of this study showed that the highest removal efficiencies were for OMW samples treated with reduced GAC at pH 9 and in the absence of surfactant(s) with the maximum removal of 88%.

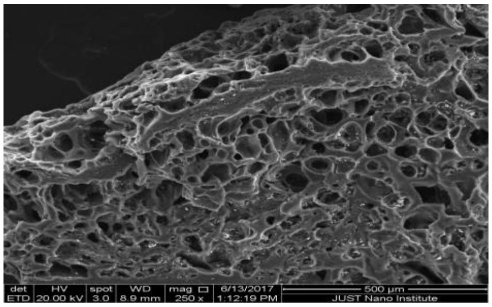


**Figure 1.** SEM micrograph of reduced GAC

**Table 1.** Reduced GAC properties

| | |
|---|---|
| Surface area (m$^2$/g) | 924.3 |
| Total pore volume (cc/g) | 0.48269 |
| Average pore diameter (A°) | 20.889 |

**Reference**

[1] P.S. Rodis, V.T. Karathanos, and A. Mantzavinou, Journal of Agricultural and Food Chemistry, 50 (2002) 596-601.

---

* Corresponding author, *E-mail: maabudalo@just.edu.jo*

O-60

# Effectiveness of Plants Fiber Impregnated with Green Nanoparticles for Water Disinfection

**Azza Jaradat[1], Borhan Albiss[2], Nathir Al-Rawashdeh[1] and Muna AbuDalo[1]***

[1]Jordan University of Science and Technology, Faculty of Science, Department of Chemistry, Irbid, Jordan
[2]Jordan University of Science and Technology, Faculty of Science, Department of Physics, Irbid, Jordan

*Email: jaazzah14@sci.just.edu.jo*

It is well known that safe water is essential to human health and the development of the country. More than one billion in the word do not have access to safe drinking water. In order to improve the quality of water that meet communal needs, a reliable and adequate safe water supply in a cost-effective way is a vital need [1]. In this research plants fiber impregnated with green manufactured ($TiO_2$) nanoparticles has been investigated for their potential in removing 99% of bacteria and algae for water disinfection. Throughout the research, green chemistry was applied to minimize the use or generation of potentially harmful compounds during the manufacture, application and disposal. The media was prepared by mixing nanoparticles with plant extract (pomegranate peel extract) and biological activity was evaluated at different concentration and with different type of bacteria (*Staphylococcus aureus*, *Pseudomonas aeruiginosa*, *Escherichia coli*). Our result showed that the prepared natural media has reproducible, effective antibacterial activity against tested bacteria assessed by well diffusion method, Microbial Inhibition Concentration (MIC), Minimum Bactericidal Concentration (MBC) and live/dead cell, and has a potential to be used for water disinfection (Figure 1 and Figure 2).

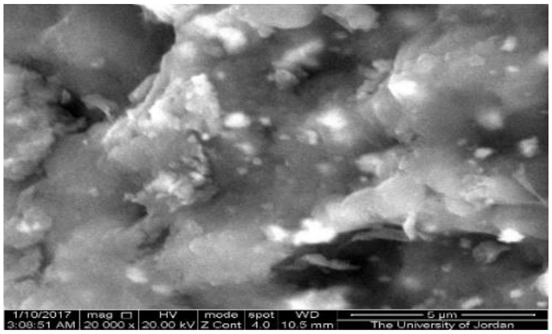


**Figure 1.** SEM micrograph of the natural media

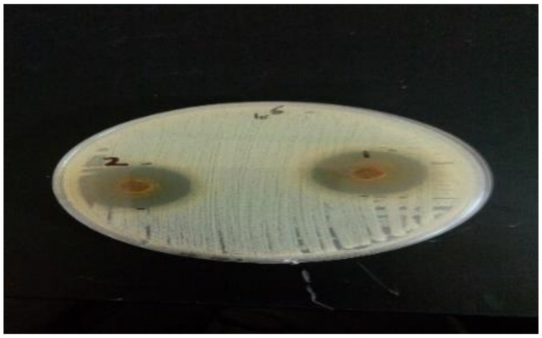


**Figure 2.** Inhibition effect of the natural media against *Staphylococcus aureus*

**References**

[1] World Health Organization. Guidelines for drinking-water quality. Vol. 1. World Health Organization, 2004.

---

* Corresponding author, *E-mail: maabudalo@just.edu.jo*

O-61

# Environmental Competence of Future Engineers – a Structural Component of Life Competence

**Tetiana Lukashenko**, Nina Kushchevskaya, Viktor Malyshev* and Ivan Kucheriavyi

University “Ukraine”, 23 Lvivska St., Kyiv 03115, Ukraine

*E-mail: taniainst@gmail.com*

The actual task of nowadays education is to prepare competitive personality, able to accept globalized, European integration processes, to the functioning in the new socio-economic and socio-cultural transformations including modern views according to the common man and nature evolution (co-evolution). So, without refusing national characteristics and interests, in Ukraine we have to take the best experience from abroad according to the mentioned problems and its adaptation to the national ground. Particularly, it applies to the specialist training who should be competent in the field of ecology. Ecological competence is a structural component of vital competence and as the indicator of quality number of ecology education only recently became important. Ecological competence includes knowledge and skills that are essential for future chemical engineers in further practical work. The condition of the successful formation of ecological competence of students is new content, use of forms and methods of pedagogical influence that include an experiment and scientific research (especially on the master level), develop intellectual skills (analysis, synthesis, reasoning, etc.), the ability to reflect events, information and experience critically, to find and to give grounds of alternate solutions of ecological problems.

In the «Programme of Actions» on the subject of Bologna Declaration implementation in higher education and science of Ukraine is stressed about creating a system of determining of graduates competence level and developing methods of objective assessment of professional competence of specialists of different educational levels in Ukraine. A special role in the implementation of this task is played by the universities because the necessary conditions for free development, the formation of a sustainable ecological position and professional competence of students are created there. Ecological competence enables for future professionals to solve production and living situation, subjecting them to the principles of sustainable development. The coordination of economic and social development and environmental protection applies the particular attention to the ecological education. Ecological competence of future engineers consists of motivational, cognitive, active and reflective components and requires further development of criteria and indicators of components that are mentioned above. The use of new and high technologies in the modern conditions while increasing harmful emissions into the atmosphere and water bodies, poor development of technologies of recycling raw materials contribute new and higher requirements to the professional competence of engineers and especially to the chemical engineers. Training of chemical engineer that is capable to the realization of professional activity is definitely associated with the formation of his/her ecological competence. The last provides professional ability to participate actively in preventing and overcoming ecological crisis, reducing the harmful impact of industrial chemical wastes, prevention of emergency ecological situation and, if it is necessary, the ability to liquidate it. The ecological crisis, in turn, leads to the rethinking of relations in the triangle "nature - man - society" and to the searching ways of its harmonization [1].

## References

[1] V. Geissen, H. Mol, E. Klumpp, G. Umlauf, M. Nadal,M. van der Ploega, S.E.A.T.M. van de Zee and C.J. Ritsema, International Soil and Water Conservation Research, 3 (2015) 57-65.

---

* Corresponding author, *E-mail: victor_malyshev@mail.ru*

O-62

# Algorithm of Formation of Ecological Competence of Chemical Engineers

**Tetiana Lukashenko, Nina Kushchevskaya, Viktor Malyshev* and**
**Ivan Kucheriavyi**

University “Ukraine”, 23 Lvivska St., Kyiv 03115, Ukraine

*E-mail: Kucheriavyi@email.ua*

Analysis of psychological and pedagogical sources of the ecological competence formation of future engineers allowed to confirm three main areas of consideration of this problem: features of engineering profile training; grounding of the need of ecological education and ecological training and thinking; theoretical and methodological principles of ecological competence formation of the individual. The analysis results and the facts of the threat growing of environmental conditions show that the question of ecological competence formation requires further study and development [1]. At the same time in the pedagogical science and in the practice of ecological competence formation of future chemical engineers requires clarification of certain aspects, in particular, increased the need to resolve the contradictions that objectively have the occur in the theory and practice of teaching. The main of them is a discrepancy: a) requirements applicable to the chemical engineers, as a subject of ecological safe activity, that is proposed with educational program content, on the one hand, and the level of students' training of the given profession - on the other; b) experimentally detected experience of ecological training of future specialists-chemists and the lack of focused ecological training; c) the need of develop and introduction of modern effective forms and methods of the teaching with the aim of forming ecological competence on the one hand, and on the other - an excess of old approaches to the training of specialists-chemists in the engineer education system. Relating to the purpose of research, the following tasks were determined: 1. To analyze the state of studied problem in the pedagogical theory and practice. 2. To develop a model of ecological competence formation that would include didactive basics of training, development of forms and methods of students' teaching of chemical specialties, personality-oriented teaching technologies for students with disabilities, organizational and pedagogical conditions of course functioning "Ecochemistry". 3. To make experimental verification of the effectiveness of the developed model of students' teaching activity in the ecology sphere and its impact on the ecological competence formation of graduates. 4. To develop the system of recommendations for practical implementation of ecological competence formation model of future chemists-engineers. Experimental-researching work was carried out in the training groups in Kyiv and Zaporizhzhia in the sphere of different engineering specialties of three universities. The total number of students both in the experimental and control groups was about 400 people. The material basis of laboratories and specialized classrooms of all experimental and control groups was roughly the same. This allowed to have the same specifications and to impose the same requirements on conducting chemical experiments under the program of chemical disciplines.

**References**

[1] O. Perfilova and Y. Alizade, Procedia Social and Behavioral Sciences, 15 (2011) 2293-2298.

---

* Corresponding author, *E-mail: victor_malyshev@mail.ru*

# Pyrolysis of Almond Shells and Characterization of Pyrolysis Liquid

**Pınar Acar Bozkurt***, Büşra Doğanay and Meral Yaşar

Ankara University, Faculty of Science, Department of Chemistry, 06100, Ankara, Turkey

*E-mail: p3acar@hotmail.com*

Biomass use with energy aims is increasing in most countries as a clean and renewable substitute for fossil energy. Therefore, different thermochemical conversions such as combustion, gasification and pyrolysis are used to recover energy from biomass materials. Biomass pyrolysis has received special attention since it leads to useful products and moreover contributes to diminish the environmental pollution arising from waste accumulation. However, different applications for the three fractions obtained in the pyrolysis have been reported. Thus, the char is a carbon-rich nonvolatile solid residue that could be used as fuel, briquettes, or activated carbon. The liquid fraction has the potential to be used as a fuel-oil substitute or may contain chemicals in economically recoverable. The gases have a sufficiently higher heating value (HHV) to be used for the total energy requirements of a biomass waste pyrolysis plant, to feed gas turbines or gas-fired engines [1,2]. Recently, pyrolysis process is becoming a potential technology, which has proved its efficiency through the energy conversion of various types of feedstocks. Moreover, almond shells are a relatively abundant lignocellulosic agricultural by-product in Turkey. Turkey is one of the important almond producers and 44,366 tons of almonds and 23,205 tons of almond shells are produced annually. One of the wastes which can be considered to have a good potential as a biomass feedstock is fruit shells. Like most biomass wastes, almond shells are biodegradable material composed of cellulose, hemicellulose, and lignin, when they heated in an inert atmosphere, they decompose into various pyrolysis products depending on the operating conditions principally temperature. In this study, pyrolysis of almond shells is performed in nitrogen atmosphere in a fixed bed reactor. The influence of the temperature (400-600°C) on the composition and properties of the different fractions were analyzed. As the temperature was increased a decrease in the char yield and an increase in the liquid and gas yield was observed. The highest liquid yields were obtained from the samples at 600°C. Aliphatic and aromatic hydrocarbons and hydroxyl and carbonyl compounds were the major components of the liquid fraction, which suggests their use as a source of chemicals.

## References

[1] M. Asadullah, N. S. Rasid, S. A. S. Kadir and A. Azdarpour, Biomass and Bioenergy, 59 (2013) 316-324.
[2] A. Veses, M. Aznar, I. Martinez , J. D. Martinez , J. M. Lopez, M. V. Navarro, M. S. Callen, R. Murillo and T. Garcia, Bioresource Technology, 162 (2014) 250-258.

## Acknowlegment

This study is supported by a grant (Project Number: 15B0430003) from Scientific Research Projects Committee of Ankara University.

---

* Corresponding author, *E-mail: p3acar@hotmail.com*

O-64

# Water Chemistry for Irrigation

**Gülüzar Duygu Semiz***

Ankara University, Faculty of Agriculture, 06100, Ankara, Turkey

*E-mail: semiz@ankara.edu.tr*

All natural water contains more or less soluble ions which are called SALT. Integrated and sustainable use of water and soil resources is one of the most important issues in irrigation and agricultural practices. It is very well known that irrigation with low water quality causes such extensive damage that to reclaim the soil back would be either too expensive or impossible. Soil and water chemistry play an important role in sustainable agriculture. During the course of human history, thriving civilizations whose existence were based on irrigated agriculture have declined or disappeared, in part due to poor irrigation water management practices. For example, the Harappa civilization in the Indus Plain region of India and Pakistan, the inhabitants of the lower Viru Valley in Peru, and the Hohokam Indians in the Salt River region of Arizona have all succumbed to the degradative effects of soil salinization [1]. Salts, depending on the ionic composition and concentration, can also affect many soil processes, such as soil water dynamics, soil structural stability, solubility of essential nutrients, and pH and pE of soil water—all indirectly hindering plant growth. The direct effect of salinity includes the osmotic effect affecting water and nutrient uptake and the toxicity or deficiency due to high concentration of certain ions [2]. The aim of the study is to show the importance of recognition to water chemistry for world food security.

## References

[1] M.E. Essington, Soil and Water Chemistry, CRC PRESS, (2004) 534.
[2] R. Rengasamy, 2015. Soil Salinization. Oxford Research Encyclopedia of Environmental Science. DOI: 10.1093 /acrefore/9780199389414.013.65.

---

* Corresponding author, *E-mail: semiz@ankara.edu.tr*

O-65

# Production of α-Gypsum Based on Flue Gas Desulphurization Gypsum

**<u>Sead Hrustanović</u> and Azra Jaganjac***

University of Sarajevo, Faculty of Science, Department of Chemistry, 71000 Sarajevo,Bosnia and Herzegovina

*Email: s.hrustanovic@hotmail.com*

The power generation industry has made an effort to develop an innovative industrial scheme for utilizing FGD gypsum and put them into practical use [1]. Development of α-gypsum technology proved its value on an industrial scale. For instance, in the Knauf process shown in the Figure 1 [2]. FGD gypsum is dehydrated under controlled condition into α-gypsum hemihydrat. Additives in the suspension change the crystal habit of the α-plaster and yield a product of defined and consistent properties. By using FGD gypsum the α-gypsum manufacturing costs are significantly lower and it is now-a-days used en-masse for manufacturing special materials in construction as fluid floor screeds, coal mining for Spraying Coal Refuse Piles and Oil wells as injection cement [3].

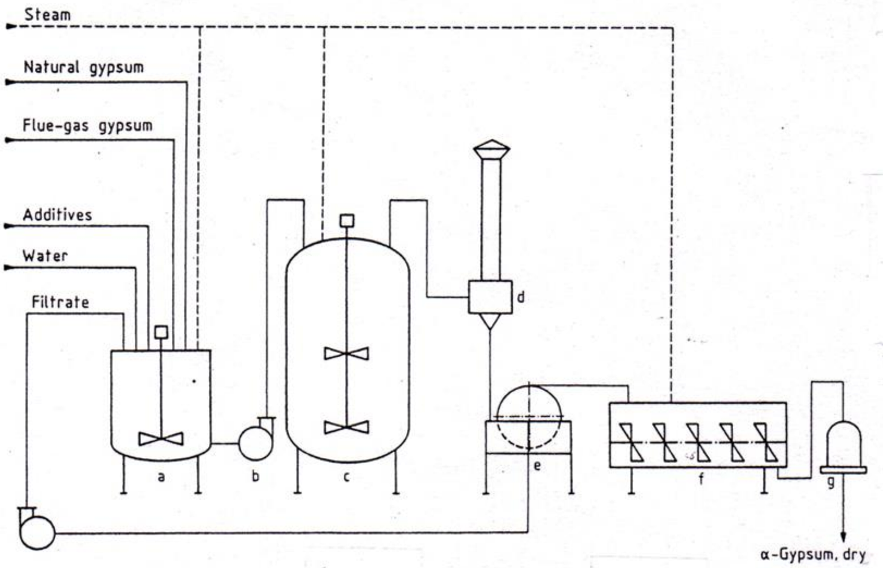


**Figure 1.** Production of α-gypsum from natural or FGD-gypsum

**References**

[1] F. Wirsching and R. Hüller, ZKG INTERNATIONAL 42(5) (1989) 223-228.

[2] S. Hrustanović, (2013): Chemical Characteristics of Natural Gypsum of some Mines in B&H as a Criteria for Use in Production α-Hemihydrates, Doctoral Thesis, University of Sarajevo, Faculty of Science.

[3] A. Jaganjac and S. Hrustanović, Gypsum Binder Production from FGD-Gypsum, European Conference on Raw Building Materials and Coal: New Perspectives, Sarajevo, May 20-21 (2004).

---

* Corresponding author, *E-mail: ElizabethB1943@hotmail.com*

# Food Chemistry

O-66

# Fatty Acid Profile of Mare’s Milk Produced in the Mountain and Highland of Kyrgyzstan during Milking Season.

**Aichurok Mazhitova*, Asylbek Kulmyrzaev and Zhyldyzay Ozbekova**

Engineering Faculty, Kyrgyz-Turkish Manas University, Bishkek 720038, Kyrgyzstan

*E-mail: mazhitova.aichurok@gmail.com*

In Kyrgyzstan, mare's milk is used for preparation of the fermented dairy beverage koumiss and fresh mare's milk has also uses to treat lung diseases as a traditional method of treatment, but mare milk production is seasonal [1-3]. Accordingly the effect of the milking season on fatty acid profile ($P<0.05$) of mares' milk of the Kyrgyz Novokirgizskaya horse breed grazing on the pastures at 1700 (mountain) and 2200 m (highland) above the sea level was investigated. The animals were kept under extensive pasture conditions and received no additional feed supplements. Milk samples were collected monthly from May to July and from May to August from mares grazing on mountain and highland, respectively. Fatty acid composition of the milk obtained from highland was richer in unsaturated fatty acids (linoleic acid, CLA) than that of produced in the mountain. Concentrations of linoleic acid and CLA from highland were at the highest level in the mid of the milking season in both pastures. The results of the study have shown that the fatty acid composition of the mare milk is influenced by milking season and geographical location of pastures.

## References

[1] J. Csapó, J. Stefler, T.G. Martin, S. Makray and Z. Csapó-Kiss, International Dairy Journal, 5(4) (1995) 393-402.
[2] J. Pikul and J. Wójtowski, Livestock Science, 113 (2008) 285-290.
[3] N. Minjigdorj, A. Haug and D. Austbo, Acta Agriculturae Scandinavica, Section A–Animal Science, 62(2) (2012) 73-80.

## Acknowledgment

This work was financially supported by Kyrgyz-Turkish Manas University.

---

* Corresponding author, *E-mail: mazhitova.aichurok@gmail.com*

# Investigation of Meat and Meat Products by Fluorescence Spectroscopy

**Zhyldyzai Ozbekova*** and **Asylbek Kulmyrzaev**

Department of Food Engineering, Kyrgyz-Turkish Manas University, Prospekt Mira, 56, 720042 Bishkek, Kyrgyz Republic

*E-mail: zhyldyzaiozbekova@gmail.com*

The objective of this study was to evaluate the potential of fluorescence spectroscopy [1-3] coupled with multivariate chemometric techniques to study meat, sausages and ground meat samples containing various ratios of soybean gel (5%, 10%, 20%, 40%, 60%, 80% and 100%). The emission fluorescence spectra of tryptophan (305-400 nm), riboflavin (410-700 nm) and vitamin A (340-540) were recorded at 290, 382 and 322 nm, respectively. The chemical compositions such as a moisture, fat and protein content of the samples were measured. Fluorescence spectral and chemical data were evaluated with chemometric methods such as Principal Component Analysis (PCA), Partial Least Squares (PLS) Regression and Partial Least Squares Discriminant Analysis (PLSDA). As a result, high correlations were observed between the chemical composition, fluorescence spectra of the samples and the content of soybean gels in meat samples. Chemical compositions of the investigated samples were predicted from fluorescence spectra with high correlation coefficients (moisture $R^2$=0.89, protein $R^2$=0.85 and fat $R^2$=0.89). It was concluded that fluorescence spectroscopy in combination with multivariate chemometric techniques has a high potential as a fast and accurate method for the study of meat and meat products.

## References

[1] A. Sahar, T. Boubellouta, J. Lepetit and É. Dufour, Meat Sci., 83 (2009) 672-677.
[2] R. Karoui., E. Dufour and J. De Baerdemaeker, Food Chem., 101 (2007) 1305-1314.
[3] A.A. Kulmyrzaev, R. Karoui, J. De Baerdemaeker and E. Dufour, Int. J. Food Prop., 10 (2007) 299-320.

## Acknowledgment

This work was financially supported by Kyrgyz-Turkish Manas University.

---

* Corresponding author, *E-mail: zhyldyzaiozbekova@gmail.com*

O-68

# Physicochemical and Rheological Behavior of Kyrgyzstan Honey Varieties

**Jamila Smanalieva**[1]*, **Kunduz Kadyrova**[1], **Carsten Eschenbaum**[2], **Uli Lemmer**[2] **and Coskan Ilicali**[1]

[1]Department of Food Engineering, Kyrgyz-Turkish Manas University, Prospekt Mira, 56, 720042 Bishkek, Kyrgyz Republic
[2]Light Technology Institute, Karlsruhe Institute of Technology (KIT) Engesserstrasse 13, D-76131 Karlsruhe, Germany

*E-mail: jamila.smanalieva@gmail.com*

The chemical, rheological and sensory properties of 25 Kyrgyz polyfloral honey were analyzed to demonstrate the relation between geographical origin and physicochemical properties [1-3]. Pure honeys of seven selected regions Suusamyr, Sary-Chelek, Toktogul, Issyk-Kul, Talas, Chon-Kemin and Uzgen (Kara-Shoro) were chosen as subjects of the study. The results showed that chemical parameters such as moisture content, reducing sugar content, total acidity and pH of the honey samples were within the limits established by normative documents. The maximum diastase number was found in honey varieties collected from mountain regions and this demonstrates the high quality and superiority of mountain honeys. The rheological properties of Kyrgyzstan mountain honey were determined by a wide range of temperature (10, 20, 30, 40, 50 °C). The validity of the rheological constitutive equations by Herschel-Bulkley, Ostwald-De Waele and Newton was investigated at different temperatures. Irrespective of geographical origin, all the honey varieties showed a Newtonian behavior at higher temperatures. The apparent viscosity of all honey varieties showed a strong dependence on temperature, and Arrhenius model was examined to describe this. Smell of honey samples was determined using a gas sensor array E-Nouse Kamina. Seven geographical origin honeys were classified based on physicochemical, rheological and E-Nouse data using statistical method Linear Discriminant Analysis (LDA). The result showed that the honey sample from different floral and geographical origins could be discriminated and identified by LDA clearly based on physicochemical and E-Nouse data.

## References

[1] J. Smanalieva and B. Senge, European Food Research and Technology 229 (2009) 107-113.
[2] E. Anklam, E., Food Chemistry 63 (1998) 549-562.
[3] M.L. Rodriguez-Mendez, Electronic Noses and Tongues in Food Science, Elsevier, Amsterdam, 2016.

**Acknowledgment**:

This work was financially supported by Kyrgyz-Turkish Manas University and Deutsche Forschungsgemeinschaft. The grant number is GZ LE 878/18-1.

---

* Corresponding author, *E-mail: jamila.smanalieva@gmail.com*

O-69

# Comparative Study of Fatty Acid Profile and Thermal Parameters of Yak (Bos Grunniens) and Cow (Bos Taurus) Fats

**Jamila Smanalieva[1]*, Zhyldyzai Ozbekova[1], Peggy Heunemann[2], Asylbek Kulmyrzaev[1] and Coskan Ilicali[1]**

[1]Department of Food Engineering, Kyrgyz-Turkish Manas University, Prospekt Mira, 56, 720042 Bishkek, Kyrgyz Republic
[2]Institute of Food, Nutrition and Health, ETH Zurich, CH-8092 Zurich, Switzerland

*E-mail: jamila.smanalieva@gmail.com*

Fat is an important source of essential fatty acids and facilitates the absorption of fat-soluble vitamins [1-3]. An increasing consumer demand on halal sausages, has encouraged research on alternative fat sources, such as yak fat.Yaks are an important animal on the high mountain regions in Kyrgyzstan, because they are critical to the livelihood security of the herders in a rather difficult environment. Besides milk, meat and wool, yak can give 1.2 kg to 10 kg fat. In this study the fatty acid profile and thermal parameters of yak fat were investigated to demonstrate nutritional value and to obtain functional parameters compared to cow fat. Result of fatty acid profile analysis revealed that the main fatty acids in investigated fats were palmitic (C16:0), stearic (C18:0) and oleic acids (C18:1). The content of oleic acid (18:1) in yak fat was significantly higher 32.06 % ($P < 0.05$); whereas in cow it was significantly lower 22.34% ($P < 0.05$). The unsaturated fatty acids (UFA) content in yak fat was higher compared to cow fat (about 27.1 %). Differential scanning calorimetry (DSC) was used to characterize the fat thermal behavior by monitoring associated changes in enthalpy upon heating. The melting temperatures were found to be 55.18±0.71, 54.98±3.01 °C for yak and cow fat, respectively. Data of fatty acid profile and thermal parameters were analyzed using PLSR (Partial Least Squares Regression) method. The regression analysis showed that there are a high positive correlation (R2 = 0.93 – 0.94) between melting temperature obtained from DSC-Analysis and saturated fatty acids (SFA), UFA contents of samples. These results can be used for future developments of new functional meat products that satisfy consumer appetite and well-being likewise.

## References

[1] Q. Wang, J.P. Wu, S.G. Zhang, Y.B. Zhang, H.X. Zhang and E. Fan, Chromatographia, 69(1-2) (2009) 139-143.
[2] C. Liu, G. Jin, Z. Luo, S. Li, S. Sun, Y. Li and M. Ma, Eur. J. Lipid. Sci. Tech., 117(6) (2015) 899-902.
[3] I.B. Tonial, A.C. Aguiar, C.C. Oliveira, E.G. Bonnafé, J.V. Visentainer and N.E. de Souza, S. Afr. J. Anim. Sci., 39 (2009) 328-332.

**Acknowledgments**:
This work was financially supported by Kyrgyz-Turkish Manas University and DAAD (German Academic Exchange Program).

---

* Corresponding author, *E-mail: jamila.smanalieva@gmail.com*

# Acrylamide Formation in Foods and Its Effects on Human Health

**Başak Gökçe Çöl***

İstanbul Gelişim University, School of Health Science, Department of Nutrition and Dietetics, 06100, Istanbul, Turkey

*E-mail: bgcol@gelisim.edu.tr*

Acrylamide is a contaminant naturally occurred during the heat treatment such as frying, baking, or broiling, of carbohydrate-rich foods. Several studies have shown that acrylamide is formed from the Maillard reaction between amino acids, mainly asparagine, and reducing sugars under cooking temperature is above 120 degrees Celsius [1,2]. Acrylamide has been known to be carcinogenic, neurotoxic and genotoxic effects in animal and is classified in Group 2A, probable carcinogens to humans by the International Agency for Research on Cancer [3]. Researchers in Swedish National Food Administration (SNFA) and Stockholm University showed that carbohydrate-rich foods; in particular; potato crisps, French fries, and crisp bread during the high temperature cooking methods, have been found to produce relatively high levels of acrylamide [4]. The SNFA findings therefore led to much public concern and international public health alarm by its report of high acrylamide levels of the most commonly consumed foods [5,6]. People are exposed to acrylamide by diet as a result of the consumption of acrylamide rich food products. Potato, coffee and cereal products are the major contributors. Cereal products including biscuits, baby biscuits, breads, crackers and breakfast cereals contain acrylamide at various levels. According to the eating habits of adolescents and children, their exposure to acrylamide higher than the rest of the population. It has been indicated that children would generally have intakes, two or three times higher than those of adults due to the body weight basis. Various factors such as food composition, the ratio of surface area to volume of the food, cooking methods, temperature and time, etc. can affect the acrylamide formation. [7]. For this reason reducing methods for acrylamide formation during food processing is very important. The food industry has devised many strategies to find appropriate and practical solutions to reduce the overall dietary exposure to acrylamide. These have been compiled in a 'Toolbox' produced by Food Drink Europe [8]. Recently, acrylamide analysis regarding in food for rapid extraction methods with quick, effective, cheap, rugged and safe protocols are highlighting trends [9]. The fact that acrylamide is found abundantly in a wide range of starch-containing foods and has negative impact on health, especially in children, so it needs to reduce the level of acrylamide in these products for protecting public health.

## References

[1] V.A. Yaylayan and R.H. Stadler, J. AOAC Int., 88(1) (2005) 262-267.
[2] D.V. Zyzak, R.A. Sanders, M. Stojanovic, D.H. Tallmadge, B.L. Eberhart, D.K. Ewald, D.C. Gruber and T.R. Morsch, J. Agric. Food Chem., 51 (2003) 4782-4787.
[3]G. Arusoğlu, Academic Food Journal, 13(1) (2015) 61-71.
[4] E. Tareke, P. Rydberg, P. Karlsson, S. Eriksson and M. Törnqvist, J. Agric. Food Chem., 50 (2002) 4998-5006.
[5] H. Mojska, I. Gielecińska, L. Szponar and M. Ołtarzewski, Food Chem. Toxicol., 48(8-9) (2010) 2090-2096.
[6] V. Sirot, F. Hommet, A. Tard and J.C. Leblanc, Food Chem. Toxicol., 50(3-4) (2012) 889-894.
[7] C.P.B. Gündüz, A.K. Bilgin , M.F. Cengiz, Academic Food Journal, 15(1) (2017) 1-7.
[8] M. Palermo, V. Gökmen, B. De Meulenaer, Z. Ciesarová, Y. Zhang, F. Pedreschi and V. Fogliano, Food Funct., 7(6) (2016) 2516-2525.
[9] N. Altunay, R. Gürkan and U. Orhan, Talanta, 161 (2016) 143-150.

---

* Corresponding author, *E-mail: bgcol@gelisim.edu.tr*

# Materials Science

O-71

# Polyamorphism in $TiO_2$

**Murat Durandurdu***

Abdullah Gül University, Department of Materials Science & Nanotechnology Engineering, Kayseri, Turkey

*E-mail: murat.durandurdu@agu.edu.tr*

Based on constant pressure *ab initio* simulations, we propose, for the first time, two successive amorphous-to-amorphous phase transformations for $TiO_2$. The first one is a gradual phase transformation from a low-density amorphous phase to a high-density amorphous phase, whereas the second one is a first order phase transformation from the high-density amorphous phase to a very high-density amorphous phase. The low-density amorphous to high-density amorphous phase change is irreversible, whereas the high-density amorphous to very high-density amorphous phase transformation is reversible. The high-density amorphous and very high-density amorphous phases consist of differently coordinated configurations. The sevenfold and ninefold coordinated arrangements formed in amorphous $TiO_2$ under pressure are similar to the main building motif of the baddeleyite and cotunnite polymorphs of $TiO_2$, respectively, while the eightfold-coordinated configuration is different from the local structure of the cubic $TiO_2$ phase. The electronic structure calculations suggest that both dense amorphous phases present a semiconducting character with a band gap energy less than that of the original low density amorphous phase [1].

**References**

[1] M. Durandurdu, J. Am. Ceram. Soc. in press (Doi: 10.1111/jace.14947).

---

* Corresponding author, *E-mail: murat.durandurdu@agu.edu.tr*

O-72

# Temperature-induced Structural Transition Accompanied by a Valency Transition in Alkali Sesquioxide $Cs_4O_6$

**Havva Esma Okur[1]*, Ross H. Colman[2], Winfried Kockelmann[3], Annette Sans[4] and K Kosmas Prassides[5]**

[1]Bursa Technical University, Faculty of Natural Sciences, Architecture and Engineering, Department of Chemistry, 16310, Bursa, Turkey
[2] Durham University, Department of Chemistry, Durham DH1 3LE, UK
[3]ISIS Pulsed Neutron and Muon Source, STFC Rutherford Appleton Laboratory, Didcot OX11 OQX, UK
[4]Max-Planck-Institute für Chemische Physik fester Stoffe, Dresden, Germany
[5]WPI –Advanced Institute for Materials Research, Tohoku University, Sendai, Miyagi 980-8577, Japan

*E-mail: esma.okur@btu.edu.tr*

Among the alkali oxides, the black-coloured molecular sesquioxides, $A_2O_3$ (A = alkali metal), fall into the *p*-electron mixed-valence systems with dioxygen in two different oxidation states, comprising three molecular anions: one closed-shell non-magnetic peroxide anion, $O_2^{2-}$ and two open-shell magnetic superoxide anions, $O_2^{-}$ with their molecular formula written as $(A^+)_4(O_2^-)_2(O_2^{2-})$[1]. Crystallographic and spectroscopic studies of this material have hitherto revealed differing results: while X-ray diffraction and elastic neutron scattering studies showed that alkali sesquioxides are single valent and no reduction of symmetry or ordering of the differently-sized indistinguishable dioxygen anions takes place down to 5 K[2-4], spectroscopy has provided unambiguous evidence for two localized valence states of dioxygen[4-5]. However, no experimental crystallographic evidence has been found so far for the presence of two localized valence states of dioxygen in sesquioxides. Due to these conflicting electronic and structural properties reported in the literature, we have re-investigated the structural properties of $Cs_4O_6$ and established the true crystallographic symmetry. Here we report a comprehensive study of the temperature response of the structure of $Cs_4O_6$ at both ambient and low temperatures using time-of-flight neutron powder diffraction by appliying a typical cooling protocol. We have found that the structure adoped depends on the cooling protocol applied. Ultra slow cooling (1.68 K/h) leads to a symmetry-lowering structural transition and this low-temperature phase crystallizes with a previously unreported tetragonal cell ($I\bar{4}2d$) where splitting of the oxygen atoms into two crystallographically-distinct sites is allowed (valence ordering). Controversially, rapidly cooling *via* deep quenching suppresses the emergence of the low-temperature phase with the high-temperature cubic structure ($I\bar{4}3d$) surviving down to liquid helium temperatures.

## References

[1] M. Jansen and N. Korber, *Z.* Anorg. Allg. Chem., 1991, 598, 163.
[2] A. Helms and W. Klemm, Zeitschrift für Anorg. und Allg. Chemie, 242 (1939) 201-214.
[3] M. Jansen and N. Korber, Zeitschrift für Anorg. und Allg. Chemie, 598 (1991) 163-173.
[4] M. Jansen, R. Hagenmayer, N. Korber and J. Rouxel, Comptes Rendus l'Académie des Sci.-Ser. IIC-Chem., 2 (1999) 591-594.
[5] J. Winterlik, G. Fecher, C. Jenkins, S. Medvedev, C. Felser, J. Kübler, C. Mühle, K. Doll, M. Jansen, T. Palasyuk, I. Trojan, M. Eremets and F. Emmerling, Phys. Rev. B, 79 (2009) 1-6.

---

* Corresponding author, *E-mail: esma.okur@btu.edu.t*

O-73

# Influence of $Mg_2Si$ Phase on Corrosion Properties of AS Series Magnesium Alloys

**Şennur Candan* and Ercan Candan**

Bilecik Şeyh Edebali University, Faculty of Engineering, Department of Mechanical Engineering, 11230, Bilecik, Turkey

*E-mail: sennur.candan@bilecik.edu.tr*

Mg-Al-Si based alloys (AS series Mg alloys) are particularly attractive for electronic, aerospace and automotive industries due to their low densities [1,2]. In the last few years, numerous studies have been conducted on AS series alloys to understand their creep mechanisms at elevated temperatures [3,4]. Given the nature of the application environment, corrosion resistance also is an important parameter as well as creep resistance of the Mg alloys. However, studies on corrosion behavior of AS series Mg alloys, published in the journals are scarce and carried out in a non-systematic manner [5,6]. It is well known that alloying elements [7-9] and cooling conditions [9] overwhelmingly affect the microstructure and therefore the corrosion resistance of the Mg alloys. Therefore, a comparative investigation on the corrosion behaviours of AS21 and AS91 alloys, cast under the same cooling conditions and controlled alloying composition, were carried out. Optical microscopy and scanning electron microscopy were used for microstructural examinations. The corrosion behaviour was evaluated by immersion tests and potentiodynamic polarization measurements in 3.5% NaCl solution. Results from both immersion tests and the potentiodynamic polarization measurements showed that the corrosion attack at the samples made of AS91 is tremendous which was attributed to the influence of the morphology of β phase and the interruption of continuity of oxide film on the surface of the alloys owing to coarsened β and $Mg_2Si$ phases.

## References

[1] A.A. Luo and A.K. Sachdev, 12-Applications of magnesium alloys in automotive engineering, in: C. Bettles, M. Barnett (Eds.) Advances in Wrought Magnesium Alloys. Woodhead Publishing (2012) 393-426.
[2] M. Pekguleryuz, 5-Alloying behavior of magnesium and alloy design, in: M.O. Pekguleryuz, K.U. Kainer, A.A. Kaya (Eds.) Fundamentals of Magnesium Alloy Metallurgy, Woodhead Publishing (2013) 152-196.
[3] W. Blum, P. Zhang, B. Watzinger, B.V. Grossmann and H.G. Haldenwanger, Materials Science and Engineering A, 319-321 (2001) 735-740.
[4] A. Rudajevová and P. Lukáč, Materials Science and Engineering, 397 (2005) 16-21.
[5] E.N. El Sawy, H.A. El-Sayed and H.A. El Shayeb, Journal of Alloys and Compounds, 492 (2010) 69-76.
[6] R.K. Gupta, N.L. Sukiman, K.M. Fleming, M.A. Gibson and N. Birbilis, ECS Electrochemistry Letters, 1 (2012) B1-B3.
[7] S. Candan, M.Unal, M.Turkmen, E. Koc, Y. Turen, and E. Candan, Materials Science and Engineering A, 501 (2009)115-118.
[8] K. Gusieva, C.H.J. Davies, J.R. Scully and N. Birbilis, International Materials Reviews, 60 (2015) 169-194.
[9] S. Candan, M. Celik M and E.Candan, Journal of Alloys and Compounds, 672 (2016) 197-203.

---

* Corresponding author, *E-mail: sennur.candan@bilecik.edu.tr*

# Electrical Resistivity of Polyurethane/Nonadecane Nanocapsules Reinforced Concrete Nanocomposites

**Semahat Doruk[1], Tayfun Uygunoğlu[2], Barış Şimşek[1]* and Osman Nuri Şara[3]**

[1]Çankırı Karatekin Univ., Faculty of Eng., Dept. of Chemical Eng., Çankırı
[2]Afyon Kocatepe Univ., Faculty of Eng., Dept. of Civil Eng., Afyonkarahisar
[3]Bursa Technical Univ., Faculty of Natural Science Architecture and Engineering, Dept. of Chemical Eng., Bursa, Turkey

*E-mail: chem.eng.bsimsek@hotmail.com*

Phase change materials can improve the building energy efficiency through the thermal regulation and storage [1]. Besides the ability to store thermal energy, these materials can provide extraordinary properties to concrete composites. With this purpose; the effect of polyurethane nanocapsules containing phase-change material synthesized by interfacial polycondensation polymerization method of electrical resistance of concrete was investigated via two-probe method. *N-nonadecane* was employed as a core material in polyurethane nanocapsules production. The properties of nanocapsules used for concrete nanocomposites production were characterized by DSC, FT-IR and SEM (Figure 1a). The average particle size of nanocapsules varying between 55-165 nm was found to be 100 nm. Melting points and the latent heat of fusion of polyurethane/Nanodecane nanocapsules was found as 31.90°C and 92.846 J/g, respectively. The results show that the electrical resistivity of concrete was decreased with the increasing amount of polyurethane nanocapsules containing phase-change material. It was concluded that polyurethane nanocapsules containing *N-nonadecane* can be used for conductive concrete nanocomposites manufacturing.

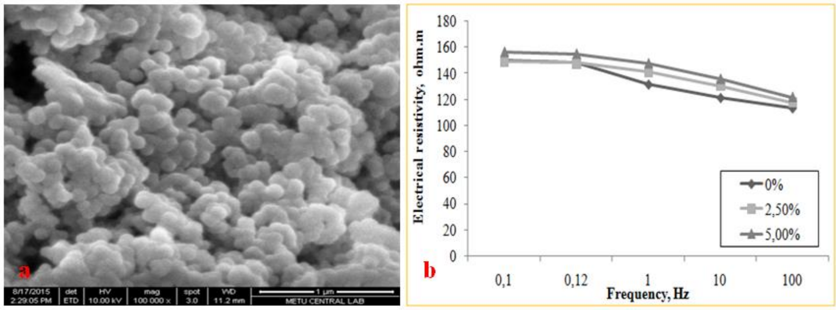


**Figure 1.** a) SEM image of PU/nonadecane nanocapsules, b) Electrical resistivity of polyurethane nanocapsules containing phase-change material reinforced concrete

## References

[1] F. Liu, J. Wang and X. Qian, Cement and Concrete Composites, 80 (2017) 317-325.

---

* Corresponding author, *E-mail: chem.eng.bsimsek@hotmail.com*

# Preparation and Characterization of BaMo$_4$:Eu@MCM-41 Composite

**Fatih Mehmet Emen**[1]*, **Ruken Esra Demirdöğen**[2], **Ali İhsan Karaçolak**[1], **Zeynep Yıldırım**[1], **Derya Kılıç**[1] **and Göktürk Avşar**[3]

[1]Mehmet Akif Ersoy University, Faculty of Arts and Sci., Dept. of Chemistry, Burdur, Turkey
[2]Çankırı Karatekin Univ. Faculty of Science, Dep. of Chemistry, Çankırı, Turkey
[3]Mersin University, Faculty of Arts and Science, Dept. of Chemistry, Mersin, Turkey

*E-mail: femen@mehmetakif.edu.tr*

Mesoporous materials which have photoluminescence property upon functionalization are of potential in the drug storage/release fields [1,2]. The design, preparation of non-toxic and stable luminescence systems have an important role in realizing this application. In this study, we aimed at preparing luminescent BaMO$_4$:Eu@MCM-41 composite via sol-gel process. The obtained composites were characterized by XRD, SEM-EDX, N$_2$ adsorption/desorption analysis and PL spectra. The excitation and emission spectrums of the composite are given in Figure 1.

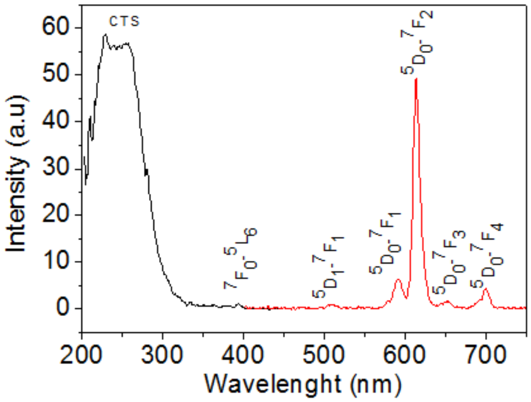


**Figure 1.** Photoluminescence spectra of BaMO$_4$:Eu@MCM-41 composite

**References**

[1] D.L. Shi, J. Lian, W. Wang, G.K. Liu, P. He, Z.Y. Dong., L.M. Wang and R.C. Ewing, Adv. Mater., 18 (2006) 189-193.
[2] J. Sauer, F. Marlow, B. Spliethoff and F. Schuth, Chem. Mater., 14 (2002) 217-224.

**Acknowledgement**

This study was supported by The Scientific and Technological Research Council of Turkey (TUBITAK) (Project Number: 116Z402).

---

* Corresponding author, *E-mail: femen@mehmetakif.edu.tr*

# Preparation of Modified MCM-48 with Thiourea Derivative Palladium Complex and Its Use as Catalyst

**Derya Kılıç[1], Fatih Mehmet Emen[1]*, Ruken Esra Demirdöğen[2], Göktürk Avşar[3], Zehra Gülten Altın[2], Tuncay Yeşilkaynak[4], Ali İhsan Karaçolak[1] and Zeynep Yıldırım[1]**

[1]Department of Material Technologies, Faculty of Engineering, Mehmet Akif Ersoy University, TR 15030, Burdur, Turkey
[2]Mehmet Akif Ersoy University, Faculty of Arts and Science, Department of Chemistry, 15100, Burdur, Turkey
[3]Çankırı Karatekin University, Faculty of Science, Department of Chemistry, 18100, Çankırı, Turkey
[4] Mersin University, Faculty of Arts and Science, Department of Chemistry, 33100, Mersin, Turkey

*E-mail: klc.derya13@gmail.com*

Mesoporous MCM-48 has high surface area (1600 $cm^2/g$) and pore volume (1.2 $cm^3/g$), regular pore size distribution, flexible synthesis conditions and cubic pore shape. These materials are used in various areas such as catalysis, gas adsorption, purification, pharmaceuticals and mecial applications, membrane production. However, the catalytic activity of pure MCM-48 is not sufficient for many reactions and applications. Metals, metal oxides and transition metal complexes are added into the structure to improve catalytic activity, selectivity and conversion rate in the reactions [1,2]. In this study, palladium complexes of the benzoylthiourea derivative ligands (Pd-carbamathionylbenzamid) activated mesoporous MCM-48 (MCM-48:$PdL_2$ (L=*N*-([1,1'-biphenyl]-2-ylcarbamothioyl)furan-2-carboxamide was prepared and characterized by FT-IR, H-NMR, XRD and SEM techniques. SEM image of MCM-48:$PdL_2$ is given in Figure 1. The prepared catalysts are used in the hydrogenation reaction of styrene and 1-octane.

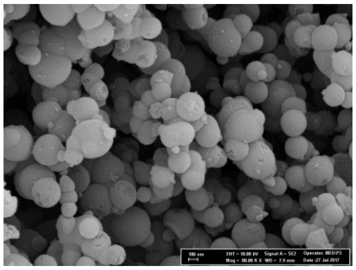


**Figure 1.** SEM image of MCM-48:$PdL_2$

**References**
[1] T.R. Pauly, V. Petkov, Y. Liu, S.J.L. Billinge and T. Pinnavaia, J. Am. Chem. Soc., 124 (2002) 97-103.
[2] W.G. Shim, D.Y. Choi, S.P. Choi, J.-W. Lee and H. Moon, Adsorption, 11 (2005) 503-507.

**Acknowledgement**
This work was supported by the Mehmet Akif Ersoy University Scientific Research Projects Coordination Unit. (Project Number: 0315-NAP-16).

---

* Corresponding author, *E-mail: femen@mehmetakif.edu.tr*

# Fabrication and Characterization of $Gd_2O_3$–$ZrO_2$ Binary System for IT-SOFCs via Pecchini Technique

**Emine Yalaz**[1]* **and Serdar Yılmaz**[2]

[1]Mersin University, Science Institute, Department of Nanotechnology and Advanced Materials, TR-33343, Mersin, Turkey
[2]Mersin University, Science and Letters Faculty, Department of Physics, TR-33343, Mersin, Turkey

*E-mail: yalazemine@gmail.com*

Solid oxide fuel cells have received much attention as a next generation alternative energy sources recently [1,2]. Particularly, current efforts are devoted to reducing SOFCs costs fuel cell systems and lowering the operational temperature. Zirconia ceramics have several advantages over other ceramic materials, due to their enormous applications in electrochemical devices. As the zirconia based solid electrolytes are used in SOFCs their electrolytic properties are very important and these properties can be suitably modified by doping with appropriate mixed valence cations [3,4]. In this study, a variety of powder solid mixtures prepared to synthesis in $(ZrO_2)_{1-x}(Gd_2O_3)_x$ binary system which is including the different stoichiometric ratio of pure ($ZrO_2$) and ($Gd_2O_3$) compound using of Pecchini technique. The most obvious advantage of this modified sol-gel Pecchini method is that reagents are mostly mixed in atomic level, which may increase the reaction rate and decrease the synthesis temperature. The produced Gd-stabilized $ZrO_2$ binary systems were characterized by X-ray diffraction method. According to the XRD analysis results, the lattice constants slightly increase with increasing $Gd_2O_3$ content. Also, the XRD data showed that the dominant single phase was the tetragonal type and lattice parameters varied from 3.6062 to 3.6211 Å, and from 5.1874 to 5.1672 Å, for a and c, respectively, in tetragonal forms [5].

**References**

[1] K. Haraldsson and P. Alvfors, Journal of Power Sources, 145 (2005) 289-306.
[2] S. Prince-Richard, M. Whale and N. Djilali, International Journal of Hydrogen Energy, 30 (2005) 1159-1179.
[3] V.G. Delgado, M.I. Cabrena and J. Gasga, Materials Characterization, 52 (2004) 179-186.
[4] W.D. Yang, Y.H. Changb and S.H. Huangb, Journal of the European Ceramic Society, 25 (2005) 3611-3618.
[5] E.N.S. Muccillo, R.A. Rocha and R. Muccillo, Materials Letters 62 (2002) 53-353.

---

* Corresponding author, *E-mail: yalazemine@gmail.com*

O-78

# Geometry and Surface Characteristic Dependent Biocompatibility Analysis of NiTi Alloys

**Sıdıka Mine Toker***

Eskisehir Osmangazi University, Metallurgical and Materials Engineering
Department, 26480 Eskişehir, Turkey

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

As in all biomaterials, biocompatibility of Nickel Titanium (NiTi) shape memory alloys (SMAs) is dependent on both the response of the surrounding tissue to the alloy, and the alloy's reaction to the tissue of contact. Moreover, the alloy's response to the physiological environment is influenced by various material properties, including its chemical content, microstructure and surface characteristics. Among these, surface characteristics constitute a critical parameter in determining biocompatibility, as the first biomaterial-tissue interaction takes place on the surface [1]. And for metallic materials, surface properties are strongly related to the processing history applied to obtain certain geometries and therefore the geometry of the sample. With this motivation, the current study aimed to analyze the biocompatibility of NiTi SMAs in relation to their surface characteristics, specifically surface roughness and groove properties. Specifically, two sets of cylindrical NiTi SMAs with different cross-sectional radii, therefore with different geometries and surface characteristics (Table 1) were tested via *in vitro* experiments. The results indicated that increased surface roughness does not necessarily provide a more favorable environment for cell attachment and proliferation; and surface characteristics such as grooves were observed to be more determining in terms of cellular response (Figure 1).

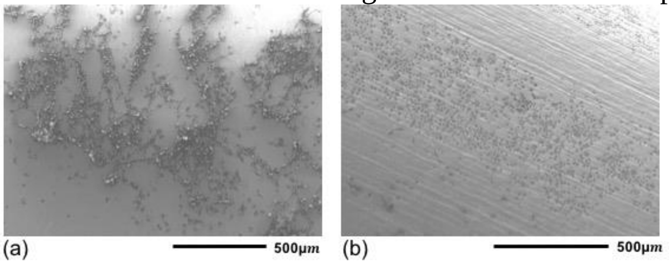


**Figure 1.** SEM images of thick wire (a) and thin wire (b) samples after 7 days of incubation with 3T3 fibroblast cells.

**Table 1.** Chemical content, geometry and surface roughness information of the NiTi samples

| Sample Name | Ni content (at. %) | Sample Height (cm) | Sample Radius (mm) | Surface Roughness ($R_a$ µm) |
|---|---|---|---|---|
| Thin wire | 50.4 | 2.75 | 1 | 0.70±0.11 |
| Thick wire | 60.7 | 1.5 | 1.75 | 0.45±0.06 |

## Reference

[1] B. Uzer, S.M. Toker, A. Cingoz, T. Bagci-Onder, G. Gerstein, H.J. Maier and D. Canadinc, Journal of the Mechanical Behavior of Biomedical Materials, 60 (2016) 177-186.

---

* Corresponding author, *E-mail: stoker@ogu.edu.tr*

# Silk Fibroin Microparticles Loaded with Extract of Olive Leaves

**Merve Deniz Köse** and **Oğuz Bayraktar***

Ege University, Faculty of Engineering, Department of Chemical Engineering, 35040, İzmir, Turkey

*E-mail: mervedenizkose@gmail.com*

The olive leaf extract has been reported to have high antioxidant and phenolic content. Oleuropein in the extract of olive leaf have attracted great interest due to its potential health benefits and antioxidant properties [1]. The main problem of using plant derived natural compound is their degradation in the gastrointestinal system before reaching the circulation system which limits their usage. Therefore, it is necessary to apply encapsulation systems. Spray-drying is a widely used method to prepare the micron sized polymeric material. Since synthetic polymers have many undesired properties, silk fibroin, is one of the most commonly used encapsulating biopolymers in biotechnological applications. The extract was prepared with dried leaves of *Olea europaea* in 70% aqueous ethanol solution. The liquid extracts were lyophilized after removal of ethanol under vacuum. A certain amount of olive leaf extract was added to the mixture of aqueous silk fibroin and maltodextrin solution, which was then spray-dried with a spray-dryer. The experimental conditions were the changing ratios of individual components in the sprayed dried solution, liquid flow rate, and inlet air temperature. Morphologies and sizes of microparticles alone and loaded with extract were investigated using Scanning Electron Microscopy (SEM). The antioxidant activity and antimicrobial activity of extract loaded microparticles were also determined. The aim of this study was to investigate the optimum spray-drying parameters to prepare the partially soluble silk fibroin microparticles loaded with olive leaf extract. In this study silk fibroin was successfully used along with maltodextrin to change the solubility and release properties of prepared microparticles having both antimicrobial and antioxidant properties.

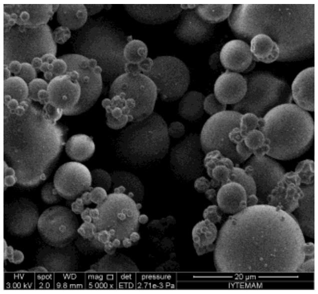


**Figure 1.** SEM images of extract loaded silk fibroin microparticles

**References**

[1] D. Baycin, E. Altiok, S. Ulku and O. Bayraktar, Journal of Agricultural and Food Chemistry 55(2007) 1227-1236.

---

* Corresponding author, *E-mail: oguz.bayraktar@ege.edu.tr*

O-80

# Enhanced Antimicrobial Activity of Lactoperoxidase Incorporated Hybrid Nanoflowers

**Süreyya Tavlaşoğlu[1], Cevahir Altınkaynak[1]*, Berrak Altınsoy[2], Nalan Özdemir[1], İsmail Öçsoy[3], Zeynep Köksal[4] and Hasan Özdemir[4]**

[1]Erciyes University, Faculty of Science, Dept. of Chemistry, Kayseri, Turkey
[2]Erciyes University, Faculty of Pharmacy, Dept. of Pharmaceutical Biotechnology, 38039 Kayseri, Turkey
[3]Erciyes University, Faculty of Pharmacy, Department of Analytical Chemistry, 38039 Kayseri, Turkey
[4]Atatürk University, Faculty of Science, Dept. of Chemistry, Erzurum, Turkey

*E-mail: s_tavlasoglu@hotmail.com*

The lactoperoxidase (LPO) is one of the prominent enzymes found in several sources, such as bovine milk, saliva and tears [1]. LPO damage bacterial cytoplasmic membranes by oxidizing the -SH groups of the enzymes in bacteria. Thus, bacteria growth and proliferation can be prevented. In this study, we synthesized LPO incorporated hybrid nanoflowers using a novel method protein-inorganic hybrid nanoflower for enhancing antimicrobial activity [2,3]. Then antimicrobial effect of LPO nanoflower and free form were investigated on gram negative and gram positive bacteria and *Candida albicans* (ATCC 90028). The study was performed with a microorganism concentration of 1x$10^8$ CFU/ml for bacteria in each milliliters of the NB, in which 24 hours incubated microorganisms were activated, and at 0.5 McFarland standard turbidity. Minimum inhibitory concentration [MIC] value of the samples was determined as the lowest concentration that inhibits microorganism growth after 24 h of incubation, was defined as ppm. Experiments were repeated as two parallels. As shown in Figure 1, the LPO nanoflowers exhibited higher antimicrobial activity on *Listeria monocytogenes* (ATCC 19115), *Salmonella typhimurium* (ATCC 14028), *Salmonella enteritidis* (ATCC 13076), *Escherichia coli* (ATCC 11230) and *Staphylococcus aureus* (ATCC 29213). Free form of LPO showed low antimicrobial activity on gram positive and gram negative bacteria. Besides both LPO nanoflowers and free LPO were observed no antimicrobial effect on *Candida albicans*.

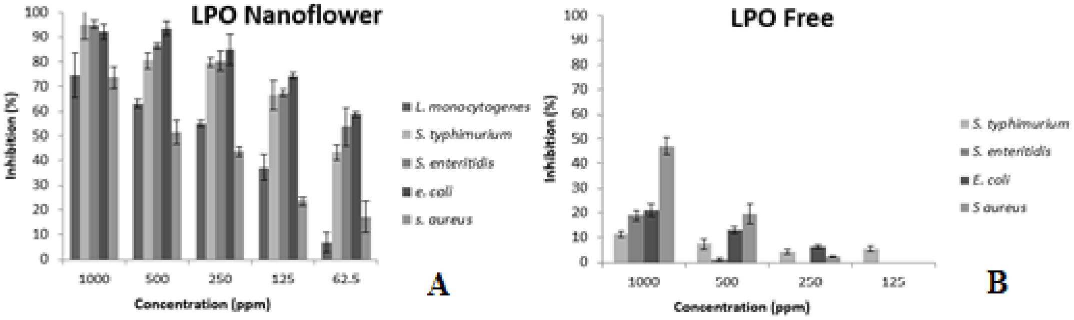


**Figure 1.** % inhibition values of (A) LPO nanoflower and (B) LPO free

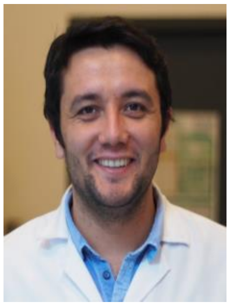
## References

[1] H. Ozdemir, I. Aygul and I. Küfrevioglu, Preparative Biochemistry and Biotechnology 31(2) (2001) 125-134.
[2] J. Ge, J. Lei and R.N. Zare, Nature Nanotechnology 7 (2012) 428-432.
[3] C. Altinkaynak, I. Yilmaz, Z. Köksal, H. Özdemir, I. Ocsoy and N. Özdemir, International Journal of Biological Macromolecules, 84 (2016) 402-409.

---

* Corresponding author, *E-mail: akcevahir@gmail.com*

O-81



# Novel Small Molecule Based Semiconductors for Solution-Processable and Ambient-Stable Ambipolar Organic Field-Effect Transistors

**Resul Özdemir[1], Mehmet Özdemir[1], Choongik Kim[2]* and Hakan Usta[1]***

[1]Abdullah Gül University, Department of Materials Science and Nanotechnology Engineering, Kayseri, Turkey
[2]Sogang University, Department of Chemical and Biomolecular Engineering, Mapo-gu, Seoul, Korea

*E-mail: resul.ozdemir@agu.edu.tr*

The design and development of novel ambipolar semiconductors is very crucial to advance the optoelectronic technologies such as organic complementary (CMOS) integrated circuits and light-emitting transistors (OLETs) technologies [1]. Although numerous high-performance ambipolar polymers have been realized to date, small molecules have been unable to provide high ambipolar performance in combination with ambient-stability and solution-processibility [2]. In this study, by implementing highly π-electron deficient, ladder-type **IFDK/IFDM** acceptor cores with bithiophene donor units in D-A-D π-architectures, two novel small molecules, **2OD-TTIFDK** and **2OD-TTIFDM**, have been synthesized and characterized in order to achieve low band-gap (1.21-1.65 eV) semiconductors with sufficiently balanced molecular energetics for ambipolarity. The HOMO/LUMO energies of the new semiconductors are estimated to be -5.5/-3.6 and -5.5/-4.2 eV, respectively. Bottom-gate/top-contact OFETs fabricated via solution-shearing of **2OD-TTIFDM** yield perfectly ambient stable ambipolar devices with reasonably balanced electron and hole mobilities of 0.13 $cm^2/V\cdot s$ and 0.009 $cm^2/V\cdot s$ with $I_{on/off}$ ratios of ~$10^3$-$10^4$, and **2OD-TTIFDK**-based OFETs exhibit ambipolarity under vacuum with highly balanced ($\mu_e/\mu_h \sim 2$) electron and hole mobilities of 0.02 $cm^2/V\cdot s$ and 0.01 $cm^2/V\cdot s$ with $I_{on/off}$ ratios of ~$10^5$-$10^6$. Our results clearly indicate that ambient-stability is a function of molecular orbital energetics stabilization via functional group (carbonyl *vs.* dicyanovinylene), and it's not a directly related to bulk π-backbone structure. **2OD-TTIFDM** stands out among the most ideal ambipolar small molecules in the OFET literature based on its solution-processibility and ambient-stability. Our results are expected to provide new directions in designing high-performance ambipolar small molecules with solution-processibility and ambient-stability.

## References

[1] K. Zhou, H. Dong, H.-L. Zhang and W. Hu, Phys. Chem. Chem. Phys., 16 (2014) 22448-22457.
[2] J. Zaumseil and H. Sirringhaus, Chem. Rev., 107 (2007) 1296-1323.

## Acknowledgement

This work has been supported by AGU-BAP (FYL-2016-65).

---

* Corresponding author, *E-mail: hakan.usta@agu.edu.tr & choongik@sogang.ac.kr*

# Influence of Samarium Doping on the Structural and Transport Properties of $La_{1.4}Ca_{1.6}Mn_20_7$ Manganites

**Nevin Soylu Koç***, **Sevgi Polat Altıntaş and Cabir Terzioğlu**

AIB University, Faculty of Arts and Science, Department of Physics, Bolu Turkey

*E-mail: nevinsoylu@ibu.edu.tr*

We have studied the influence of Sm substitution to La site on the structural and transport properties of $La_{1.4}Ca_{1.6}Mn_20_7$ manganites. Layered perovskite manganites were synthesized by the solid state reaction method with different fractional occupancy as $(La_{0.875}Sm_{0.125})_{1.4}Ca_{1.6}Mn_2O_7$, $(La_{0.75}Sm_{0.25})_{1.4}Ca_{1.6}Mn_2O_7$, $(La_{0.5}Sm_{0.5})_{1.4}Ca_{1.6}Mn_2O_7$. X-ray diffraction patterns were analyzed by using Rietveld profile fitting method and according to these results all samples crystallize in the tetragonal structure with the I4/mmm space group [1,2]. As the ratio of Sm increases in the compound, the A-site radius of manganite decreases and lattice parameters, grain size of the samples also decreases. The electrical resistivity measurements were carried out in the temperature range of 20-300K and all samples showed metal-insulator transition. The metal–insulator transition temperature ($T_p$) decreased with increasing doping rate. Magnetic susceptibility measurements reveal that the magnetic phase transition temperature ($T_c$) also decreased with Sm doping.

**References**

[1] A.K. Gupta, R. Kumar, V. Kumar, G.L. Bhalla and N.K. Khare, J. Phys. Chem. Solids, 70 (2009) 117–121.
[2] H. Asano, J. Hayakawa and M. Matsui, Appl. Phys. Lett., 68(25) (1996), 3638–3640.

---

* Corresponding author, *E-mail: nevinsoylu@ibu.edu.tr*

O-83

# Mixed-Ligand Boronic Acid UiO Type Metal-Organic Frameworks and Their Sugar Capture Properties

**Mustafa Erkartal***

Abdullah Gül University, Materials Science and Nanotechnology Engineering,
Kayseri, Turkey

*E-mail: merkartal@mail.com*

Metal-organic frameworks (MOFs) are crystalline/amorphous porous materials that are built by the organic linkers and inorganic metal/metal clusters nodes via coordination bonds. Unlike many other inorganic porous materials, MOFs have permanent high surface areas (porosity), adjustable pore sizes, and tailorable framework architectures. Benefitting from such potential, MOFs have attracted tremendous attention in gas storage/separation, catalysis, drug delivery, and electrochemical applications [1,2].

UiO-66 (Zr), consist of Zr6 clusters as the secondary building units and BDC (terephtalic acid) as the linkers, has recently attracted considerable interest due to its high thermal and chemical stability. In this study, we report the incorporation of active boronic acid moieties into UiO-66 by the mixed-linker (ML) approach. To this end, commercially available and inexpensive 4-carboxyphenylboronic acid (CPB) was utilized as fragment ligand to obtain the corresponding mixed linker MOF, UiO-66B. The resulting samples not only maintain their chemical and thermal stabilities but also show considerable sugar adsorption glucose, galactose, fructose- capacities, because of the good hydrogen bonding between the hydroxyl groups on saccarides and boronic acid moiety.

**References**
[1] M. Erkartal, U. Erkilic, B. Tam, H. Usta and J.T. Hupp., Chem. Commun., 23(53) (2017) 2028-2031.
[2] M. Erkartal, H. Usta, M. Çıtır and Ü. Şen, Journal of Membrane Science, 499 (2015) 156-163.

---

* Corresponding author, *E-mail: merkartal@mail.com*

O-84

# Investigation of Optimum Calcium Alumina Cement Dosage of Polymer Concrete Composites

**Barış Şimşek[1], Tayfun Uygunoğlu[2], Vedat Arda Küçük[1]*, Zehra Gülten Altın[1] and Mehmet Muhtar Kocakerim[1]**

[1]Çankırı Karatekin Univ., Faculty of Eng., Dept. of Chem. Eng., Çankırı, Turkey
[2]Afyon Kocatepe Univ., Faculty of Eng., Dept. of Civil Eng, Afyonkarahisar, Turkey

*E-mail: ardakucuk@karatekin.edu.tr*

Calcium aluminate cement is classified as a hydraulic binder provides various properties such as fast hardening at room temperature and appropriate rheological properties when compared the Portland cement [1]. In this study; the effect of using calcium alumina cement instead of the Portland cement-by adding 25%, 50% and 75%- on slump flow, the 3-days, 7-days and 28-days compressive strength, the percentage of water absorption, 28-days compressive strength of polymer concrete composites were investigated (Figure 1). Experimental results were compared with the polymer concrete containing 40% plastic aggregate and calcium aluminate cement between normal weight concrete containing 40% plastic aggregate and 100% Portland cement. The results showed that the 28-days splitting tensile strength was increased with increasing amount of calcium aluminate cement. When the splitting tensile strength test results are taken into consideration, the optimum calcium aluminate cement dosage was selected as 75% instead of the Portland cement. The results also showed that the slump flow was decreased with increasing amount of calcium aluminate cement. The percentage of water absorption of polymer concrete was negatively affected by calcium aluminate cement adding. However, since the air content change in small quantities, the effect of the amount of calcium alumina cement on air content can be neglected.

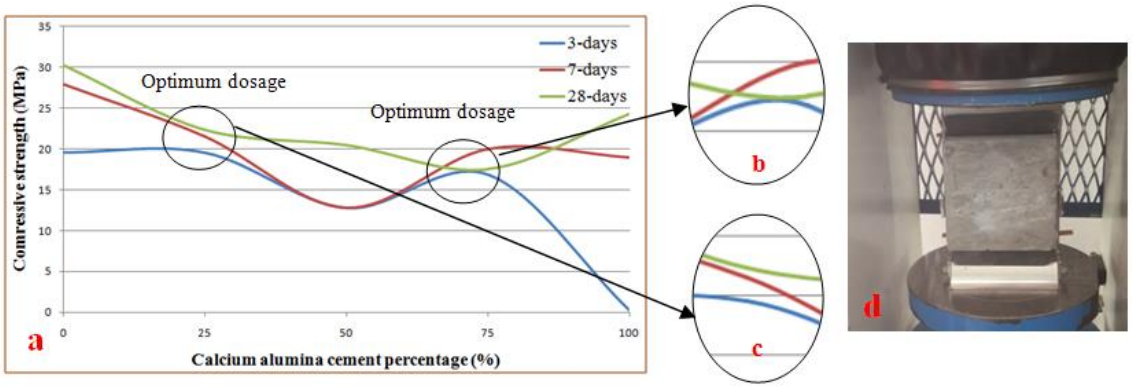


**Figure 1.** a) The effect of calcium aluminate cement on compressive strength of polymer concrete, b) and c) optimum dosage, d) experimental set-up for 28-days splitting tensile strength

**Reference**

[1] R.M. Parreira, T. L. Andrade, A. P. Luz, V. C. Pandolfelli and I. R. Oliveira, Ceramic International, 42 (10) (2016) 11732-11738.

---

* Corresponding author, *E-mail: ardakucuk@karatekin.edu.tr*

# Core-crosslinked Block Copolymer Micelles for Antibacterial Applications

**Melike Şeyma Kadayıfçı[1], Murat Topuzoğulları[1], Damla Gökkaya[1], Tuğba Atabey[2], Tülin Özbek Arasoğlu[2] and Mehmet Murat Özmen[1]***

[1]Yıldız Technical University, Department of Bioengineering, 34220, Istanbul, Turkey
[2]Yıldız Technical University, Department of Molecular Biology and Genetics, Istanbul, Turkey

*E-mail:mskadayifci.93@gmail.com*

Antibiotic resistance of bacteria is a global problem since it leads to increased mortality [1]. To overcome this resistance, highly efficient novel antimicrobial agents are required. Anti-bacterial polymers have been of great interest over the years as an alternative to the traditional anti-bacterial substances as they offer new anti-bacterial mechanisms and low costs. The positively charged polymers interact with the negatively charged surfaces of the bacteria causing their death. These polymers can be subjected to self-assembly to form micelles which can be used as antibacterial materials [2].

The aim of this study is to synthesize and characterize positively charged core crosslinked polymeric micelles for antibacterial applications. To achieve this aim, at first, Reversible Addition Fragmentation Chain Transfer Polymerization (RAFT) was used to prepare Poly(oligo ethylene glycol methyl ether methacrylate-b-4-vinylpyridine) P(OEGMA-b-4-VP) block copolymer. Then after, the copolymer was dissolved in water to self-assemble into core crosslinked micelles. The crosslinking was achieved via quarternization reaction using 1,6-dibromohexane as the quaternary crosslinker. To investigate the effect of quarternization ratios on the properties of the micelles, the amount of 1,6-dibromohexane was varied. Gel Permeation Chromatography (GPC), Fourier Transform Infrared Spectroscopy (FTIR), ZetaSizer, Scanning Electron Microscopy (SEM), Nuclear Magnetic Resonance Spectroscopy (NMR) and antibacterial assays were performed to characterize the obtained materials.

The results revealed that P(OEGMA-b-4-VP) block copolymer was successfully synthesized by the RAFT method in a controlled manner. The prepared core crosslinked micelles have an average particle size of 100 nm and zeta potential values within the range of (+25)-(+45) mV. Based on our findings, it can be concluded that the obtained positively charged core cross-linked micelles can be used for antibacterial applications.

**References**

[1] K.S. Kaye and J.M. Pogue, The Journal of Human Pharmacology and Drug Therapy, 35(10) (2015) 949-962.
[2] M. Talelli, M. Barz, C.J. Rijcken, F. Kiessling, W.E. Hennink, and T. Lammers, Nano today, 10(1) (2015) 93-117.

---

* Corresponding author, *E-mail: ozmenm@yildiz.edu.tr*

# Some Physicochemical Characteristics of Acid-activated Bentonite Samples

**Hale Bayram[1], Damla Erkakan[2], Müşerref Önal[2]* and Yüksel Sarıkaya[2]**

[1]Marmara University, Atatürk Faculty of Education, Science Teacher Education,
34722, Istanbul, Turkey
[2]Ankara University, Science Faculty, Chemistry Department, 06100, Ankara, Turkey

*E-mail: damlakumser@gmail.com*

To examine the effect of acid activation on the mineralogy, crystal structure and porosity, a white calcium bentonite (CaB) from Turkey was used as primary material. The natural CaB contains a calcium-rich smectite (CaS) and metahalloysite (MH) as major and minor clay minerals according to the X-ray diffraction (XRD) data [1]. In addition, the CaB includes opal-A, opal-CT, quartz, feldspar and calcite as impurities. The content of the CaS in the CaB is estimated from the particle size distribution curve as 80% by volume [2]. The mass loses by the dehydration and dehydroxylation of the natural sample was estimated from the thermogravimetry curve as 14.6 and 6.6%, respectively. The CaB samples were activated at 97°C with the different $H_2SO_4$% and the products were characterized by XRD and low temperature nitrogen adsorption/desorption. It was concluded from the XRD data that the crystallinity of the CaS decreases with increasing of the $H_2SO_4$% and disappears at 50% $H_2SO_4$ depending on the dissolution of the structural cations by the progress of the process [3,4]. This dissolution and corresponding altering of the smectite structure cause the increases approximately 5 and 2 times in the surface area and micro-mesopore volume of the CaS.

**References**

[1] D. M. Moore and Jr. R.C. Reynolds, X-Ray Diffraction and the Identification and Analysis of Clay Minerals, 2nd Ed., Oxford: Oxford University Press (1997).
[2] S. Kaufhold, R. Dohrmann, R. Ufer and F.M. Meyer, Applied Clay Science, 22 (2002) 145-151.
[3] P. Komadel, Clay Minerals, 38 (2003) 127-138.
[4] M. Önal and Y. Sarıkaya, Powder Technology, 172 (2007b) 14-18.

---

* Corresponding author, *E-mail: onal@science.ankara.edu.tr*

O-87

# A New Solution-Processable Molecules for Semiconducting Microfibers in Organic Thin-Film Transistors

**Mehmet Özdemir**, Resul Özdemir and Hakan Usta*

Abdullah Gül University, Department of Materials Science and Nanotechnology Engineering, Kayseri, Turkey

*E-mail: mehmet.ozdemir@agu.edu.tr*

The performances of organic field-effect transistors (OFETs) have been significantly improved in the last decade. Particularly, the *p*-channel OFET has now achieved many important milestones: high mobility, solution processability, air-stability, flexibility, low-voltage operation, and so on. For these achievements, the development of new superior materials, in particular, new organic semiconductors have contributed significantly [1]. Benzothieno[3,2-b][1]benzothiophene (BTBT) derivatives are promising organic semiconductors, because of their high mobility (5.0 $cm^2$ $V^{-1}$ $s^{-1}$ for the BTBT derivatives) and good air stability. On the other hand Electron-deficient π-conjugated small molecules can function as electron-transporting semiconductors in various optoelectronic applications [1]. Despite their unique structural, optical, and electronic properties, the development of BODIPY-based organic semiconductors has lagged behind that of other π-deficient units.

Here, we report the design and synthesis of two novel solution-proccessable BODIPY-based small molecules (BDY-3T-BDY and BDY-4T-BDY) for organic thin-film transistors (OTFTs). The new semiconductors were fully characterized by $^1H/^{13}C$ NMR, mass spectrometry, cyclic voltammetry, UV–vis spectroscopy, photoluminescence, differential scanning calorimetry, and thermogravimetric analysis. The single-crystal X-ray diffraction (XRD) characterization of a key intermediate reveals crucial structural properties. Solution-sheared top-contact/bottom-gate OTFTs exhibited electron mobilities up to 0.01 $cm^2$/V.s and current on/off ratios of $>10^8$. Film microstructural and morphological characterizations indicate the formation of relatively long (~0.1 mm) and micrometer-sized (1–2 μm) crystalline fibers for BDY-4T-BDY-based films along the shearing direction. Fiber-alignment-induced charge-transport anisotropy ($\mu_{\parallel}/\mu_{\perp} \approx 10$) was observed, and higher mobilities were achieved when the microfibers were aligned along the conduction channel, which allows for efficient long-range charge-transport between source and drain electrodes. These OTFT performances are the highest reported to date for a BODIPY-based molecular semiconductor, and demonstrate that BODIPY is a promising building block for enabling solution-processed, electron-transporting semiconductor films [2].

## References

[1] P.Bonaccorsi, M.C. Aversa, A. Barattucci, T. Papalia, F. Puntoriero and S. Campagna, Chem. Commun., 48 (2012) 10550-10552.
[2] M.E. El-Khouly , C.A. Wijesinghe, N. Nesterov, M.E. Zandler, S. Fukuzumi, D'Souza and F. Ultrafast, Chem.-Eur. J., 18 (2012) 13844-13853.

## Acknowledgement

This work has been supported by AGU-BAP (FDK-2017-97).

---

* Corresponding authors, *E-mail: hakan.usta@agu.edu.tr*

# Characterization of In-Situ Synthesized Hexagonal Boron Nitride and Silicon Carbide Composites with Conventional and Advanced Transmission Electron Microscopy Methods

**Umut Savacı[1]*, Zuhal Yılmaz[2], Nuran Ay[1] and Servet Turan[1]**

[1]Anadolu University, Faculty of Engineering, Materials Science and Engineering Department, 26555, Eskisehir, Turkey
[2]Bilecik Seyh Edebali University, SMYO, 11230, Bilecik, Turkey

*E-mail: umutsavaci@anadolu.edu.tr*

Structure-property relationship has great importance in materials science. The microstructural features e.g. present phases and their distributions and grain orientations have impact on the material properties. For characterization of aforementioned structural features, electron backscatter technique (EBSD) is widely used, however due to the resolution limits of this method transmission electron microscope (TEM) based advanced methods like precession electron diffraction (PED) method had been developed for phase and orientation mapping at high resolution [1]. In this method, nearly parallel nano sized probe is tilted with an angle from an optical axis and scanned over the sample with scan generator. While electron beam scanning, electron diffraction patterns are collected from every single point with an external CCD camera and then indexed via template matching algorithm to obtain phase and orientation maps [3].

Silicon carbide (SiC) has various applications but for applications that require complex geometries it is very limited because of low machinability. To overcome the machinability problem of SiC, addition of h-BN particles can be a solution. Since homogeneous mixing of SiC and h-BN particles cannot be achieved with conventional mixing methods, in-situ formation of h-BN particles during sintering is an alternative approach to overcome this problem. In this study, composite structure of SiC matrix with various amounts of in-situ synthesized hexagonal boron nitride (h-BN) particles during spark plasma sintering (SPS) process were characterized by conventional TEM/STEM imaging methods as well as advanced PED techniques to investigate the orientation relation between matrix and in-situ synthesized phases for the first time. For this purpose, TEM samples were prepared by mechanical thinning followed by Ar ion beam milling and prepared samples were characterized by using 200keV field emission TEM (JEOL-JEM2100F) equipped with STEM high angle annular dark field (HAADF) detector and energy dispersive X-ray (EDX) spectrometer. TEM phase and orientation maps were obtained at nano beam mode and the probe is scanned over an area up to 0.7° of precession angle. In this presentation, we focused on the characterization of composite structure with conventional TEM/STEM imaging methods to investigate the size and distribution of in-situ synthesized particles. PED method is used to obtain orientation maps to reveal the question of "Is there any orientation relation between different phases?" and results will be discussed. While these investigations it was also found that h-BN particles have also various types of defects within a grain and these defects were characterized with TEM and PED methods and obtained results will be discussed. Finally, effects of sample preparation method on the microstructure will be discussed.

## References

[1] J.G. Brons and G.B. Thompson, Jom, 66(1) (2013) 165-170.
[2] E.F. Rauch and A. Duft, Materials Science Forum, 495-497 (2005) 197-202.
[3] NanoMEGAS. Available from: http://www.nanomegas.com/.

## Acknowledgement

The authors would like to acknowledge the financial support from the Scientific Research Project Commission of Anadolu University (grant numbers:1504F168 and 1406F321) and The Scientific and Technological Research Council of Turkey (TUBITAK) 2211 scholarship programme.

---

* Corresponding author, *E-mail: umutsavaci@anadolu.edu.tr*

# Effects of Calcium and Magnesium Containing Additives on Crystallization of Sodium Carbonate from Trona Ore

**Zeynep Ören**[1]* and Derya Yeşim Hopa[2]

[1]Eti Soda A.Ş., 06730, Ankara, Turkey
[2]Afyon Kocatepe University, Faculty of Engineering, Department of Chemical Engineering, 03200, Afyonkarahisar, Turkey

*E-mail: zeynep-turkmen@hotmail.com.tr*

Trona is one of the forms of natural sources in which sodium carbonate occurs. The solution mining application is used for trona mining. In solution mining, crystallization step for sodium carbonate ($Na_2CO_3$) production has a great importance. Most important goals of crystallization stage are high efficiency and production of crystals with high quality. Among the parameters that effect crystallization process (like temperature, mixing, high saturation) additives have the biggest effect on crystallization. Even very small amounts of additives are enough to affect seed formation, crystal growth and shape [1]. In this study, the effects of three different calcium compounds [$CaCO_3$, $Ca(OH)_2$, CaO] and two different magnesium compounds [MgO and $Mg(OH)_2$] on physical and chemical properties of sodium carbonate crystals were investigated. The laboratory crystallization procedure was designed to mimic industrial crystallization conditions of Eti Soda Company, Turkey. Different amounts of calcium and magnesium compounds (0.1g; 0.2g; 0.5g; 1.0g) were added into the crystallization solution. After crystallization, the efficiency of crystallization, the purity of crystals and the grain size distribution of crystals were determined according to the ASTM E 359 2010 test methods. XRD and SEM analyses for selected samples were conducted. According to the results, among calcium containing additives 0.5 g of $Ca(OH)_2$ and among magnesium containing additives 0.5 g of MgO created the most positive effects on crystallization, crystal growth and shape of crystals. The physical and chemical properties of crystals that were produced with additives and the standard sample produced without additives are given in Table 1.

**Table 1.** Properties of crystals

| **Properties** | **Standard sample** | **Sample produced with 0.5 g $Ca(OH)_2$** | **Sample produced with 0.5 g MgO** |
|---|---|---|---|
| Purity (wt.% $Na_2CO_3$) | 98.73 | 96.19 | 99.24 |
| Crystallization efficiency (wt.%) | 15.12 | 19.29 | 17.94 |
| Particles above 150µm (wt.%) | 79.8 | 80.3 | 72.3 |

## References

[1] Ö. Doğan, Ö. "Effects of Homopolymers and Copolymers on Calcium Sulfate Dihydrate Crystallization", Yıldız Technical Unv., Institute of Science, Master Thesis (1997).

---

* Corresponding author, *E-mail: zeynep-turkmen@hotmail.com.tr*

# Exhaled Breath Analysis with Sn-doped ZnO sensors for the Identification and Characterization of Asthma Disease

**Irmak Karaduman[1]*, Tuğba Çorlu[1], Sezin Galioglu[2], Burcu Akata[2], Memet Ali Yıldırım[3], Aytunç Ateş[4], Hacı Hasan Örkçü[5] and Selim Acar[1]**

[1]Department of Physics, Science Faculty, Gazi University, Ankara, Turkey
[2]Department OF Micro and Nanotechnology, Middle East Technical University, Ankara, Turkey
[3]Department of Electric Electronics Engineering, Engineering Faculty, Erzincan University, Erzincan, Turkey
[4]Department of Material Engineering, Engineering and Natural Sciences Faculty, Yıldırım Beyazıt University, Ankara, Turkey
[5]Department of Statics, Science Faculty, Gazi University, Ankara, Turkey

*E-mail: karaduman.irmak@gmail.com*

In this study, Sn-doped ZnO ($Zn_{1-x}Sn_xO$ $0 < x < 0.5$) sensors are grown by Successive Ionic Layer Adsorption and Reaction (SILAR) method and zeolite A (LTA) film as a filter were coated on the thin films by using seeded hydrothermal synthesis. The ZIF modified Sn-doped ZnO sensors showed outstanding selectivity toward NO gas in comparison with other gases such as ethanol, aceton, ammonia, hydrogen, and carbon dioxide at 20 ppb. The ZIF modified sensors showed significant selectivity toward the analyte NO [1]. The operation temperature of the ZIF modified sensors shifted to room temperature with respect to unmodified sensors. These results represent potential feasibility for the detection of NO in exhaled breath for diagnosis of asthma. In addition, pattern recognition of all the five analyte species was performed by principal component analysis (PCA) method, which demonstrates the potential application of the selective breath analysis.

## References

[1] S. N. Talapaneni, J. Grand, S. Thomas, H.A. Ahmad and S. Mintova, Materials and Design, 99 (2016) 574-580.

---

* Corresponding author, *E-mail: karaduman.irmak@gmail.com*

# Bis(η5-cyclopentadienyl)iron Attached Nanoparticles; Application on Qualitative Analysis of Glucose

**Elvan Hasanoğlu Özkan***, **Nurşen Sarı and Ali Dişli**

Gazi University, Faculty of Science, Department of Chemistry, 06500, Ankara, Turkey

*E-mail: elvanelvan_06@hotmail.com*

Many novel nanomaterials have been investigated for immobilize of Glucose oxidase (GOx) enzyme. As is known, GOx is redox enzyme catalyzes the oxidation of glucose to gluconic acid [1]. GOx enzyme has been extensively used in the fabrication of determination for glucose. A number of immobilization supports including Fc for GOx have been investigated to improve its stabilities. Fc-Supports have been reported as useful catalysts. Gülce *et al.* reported that polymer poly(vinylferricinium) as an effective carrier support for glucose oxidase [2]. In the present work, by taking the advantages of ferrocene, to improve performance on the recycling stability for determination of glucose new a support has been prepared (PS-2G-D), as illustrated in Figure 1. And then (PS-2G-D) characterized by FT-IR, SEM and GPC analyses (Table 1). The experimental results showed that the prepared ferrocene attached nanosphere had high sensitivity and good operational stability for detection glucose.

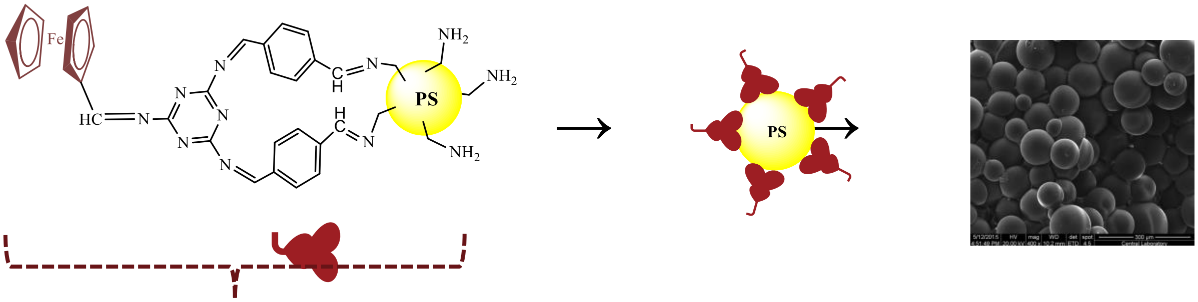


**Figure 1.** Rotation Synthesis of (PS-2G-D)

**Table 1.** Important FTIR spectrum of (PS-2G-D) and its Mw and Mn value

| Important IR vibration frequencies (cm$^{-1}$) | | | | $M_w$ / $M_{n\ (GPC)*}$ |
|---|---|---|---|---|
| ν(O–H) | 3433 | ν-CH=N (m) | 1611 | 1.86 / 2.01 |
| í-CH=N (Fc) | 1635 | í-CH=N(5-An) | 1605 | |
| í-Fe-Cp (ring) | 541 | | | |

*Gel permeation chromatography

**References**

[1] A. A. Sehat, A. A. Khodadadi, F. Shemirani, Y. Mortazavi, Int. J. Electrochem. Sci., 10 (2014) 272-286.
[2] H. Gülce, H. Özyörük, S. S. Çelebi, A. Yıldız, J. Electronal. Chem., 394 (1995) 63-70.

---

* Corresponding author, *E-mail: elvanelvan_06@hotmail.com*

O-92

# Response Surface Methodology Based D-optimal Design to Analyze the Silver Nanoparticles' Production Yield

**Özge Bildi Ceran[1], Öznur Karhan[1], Osman Nuri Şara[2] and Barış Şimşek[1]***

[1]Çankırı Karatekin Univ., Fac. of Eng., Department of Chemical Eng., Çankırı, Turkey
[2]Bursa Technical University, Fac. of Natural Sciences Arch. and Eng,, Department of Chemical Engineering, Bursa, Turkey

*E-mail: chem.eng.bsimsek@hotmail.com*

Production yield is a very important issue, especially for the nano materials industry, which has high cost production processes. In this study, silver nanoparticles (AgNPs) were synthesized using an environmentally friendly synthesis approach that is more advantageous than conventional methods with toxic properties. Processing parameters were statistically optimized in order to produce high yield AgNPs using Response Surface Methodology. Glucose/$AgNO_3$ mole ratios, reaction temperature and pH of mixture have been selected as a factors' effect on the production yield of silver nanoparticles. The produced AgNPs obtained by Response Surface Methodology were characterized via UV-visible analysis. The absorption peak is observed between 400 and 500 nm in the UV-visible spectrophotometric graphs which are confirmed in the presence of the silver nanoparticles for all experimental runs. The absorbance at 420 nm is shown in Figure 1a. The AG2 was determined as the optimum experiment in which the highest product efficiency is obtained. Transmission Electron Microscopy (TEM) image of the AG2 could be seen in Figure 1b.

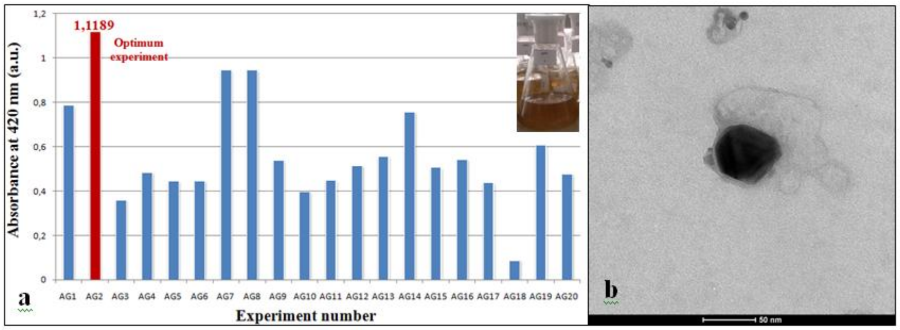


**Figure 1.** a. Absorbance values at 420 nm of AgNPs (optimum experiment has been shown in Red)
b. TEM image of AG2

**References**

[1] S. Chowdhury, F. Yusof, M. O. Faruck and N. Sulaiman, Procedia Engineering, 148 (2016) 992-999.
[2] Ö. Karhan, Ö.B. Ceran, O.N. Şara and B. Şimşek, Industrial & Engineering Chemistry Research (2017), In Press, DOI:10.1021/acs.iecr.7b01150.

---

* Corresponding author, *E-mail: chem.eng.bsimsek@hotmail.com*

# High Performance Supercapacitor based on rGO-$Fe_3O_4$/PANI Nanocomposite

**<u>Gülşah Kuruçam</u>*, Zafer Çıplak, Seray Türköz, Nuray Yıldız and Ceren Atila Dinçer**

Ankara University, Faculty of Engineering, Department of Chemical Engineering,
06100, Ankara, Turkey

*E-mail: gulsahcocu@hotmail.com*

As a result of the limited and decreasing energy sources in the world, renewable energy and energy storage systems have great importance. Main energy storage systems are fuel cells, batteries and supercapacitors [1]. Because of their high power density and great cycling stability supercapacitors are promising energy storage devices for wide spectra of application areas. Nanocomposites have drawn great attention as electrode materials for supercapacitors. Metal oxide nanoparticles such as ($Fe_3O_4$) and polyaniline (PANI) are redox active materials so they can exhibit higher capacitance [2]. In addition to high mechanical strength, electrical and thermal conductivity and good chemical stability of graphene prevent swelling-shrinking process of polyaniline during charge-discharge cycle [3].

In our study, rGO-$Fe_3O_4$/PANI nanocomposite was prepared with a facile two step method. First rGO nanosheets were decorated by $Fe_3O_4$ nanoparticles under $N_2$ atmosphere, then PANI coated rGO-$Fe_3O_4$ structure via in-situ polymerization approach. The effects of component amounts on the electrochemical performance were also investigated. The prepared nanocomposites were characterized by fourier transform infrared spectroscopy (FTIR), ultraviolet-visible spectroscopy (UV-vis), scanning electron microscopy (SEM), transmission electron microscopy (TEM) and x-ray diffraction spectroscopy (XRD), Electrochemical properties were characterized by cyclic voltammetry (CV), galvanostatic charge/discharge and electrochemical impedance spectroscopy (EIS) techniques.

In conclusion, rGO-$Fe_3O_4$/PANI nanocomposites were prepared successfully. The as-prepared ternary rGO-$Fe_3O_4$/PANI nanocomposite shows better electrochemical performance than rGO-$Fe_3O_4$ nanocomposite and $Fe_3O_4$ nanoparticles.

## References

[1] Q. Wang, L. Jiao, H. Du, Y. Wang and H. Yuan, Journal of Power Sources, 245 (2014) 101-106.
[2] S. Saha, M. Jana, P Samanta, N. C. Murmu, N. H. Kim, T. Kuila and J. H. Lee, Royal Society of Chemistry, 4 (2014) 44777-44785.
[3] P.K. Kalambate, R.A. Dar, S.P. Karna and A.K. Srivastava, Journal of Power Sources, 276 (2015) 262-270.

## Acknowledgement

This work was financially supported by the Scientific and Technical Research Council of Turkey (TÜBİTAK; Project No: 115M456).

---

* Corresponding author, *E-mail: gulsahcocu@hotmail.com*

# Investigation of $Fe_3O_4$/rGO Nanocomposite Performance for Supercapacitor Application

**Seray Türköz**, Nuray Yıldız*, Zafer Çıplak, Gülşah Kuruçam and Ceren Atila Dinçer

Ankara University, Faculty of Engineering, Department of Chemical Engineering, 06100, Ankara, Turkey

*E-mail: trkzseray@hotmail.com*

Due to the rapidly increasing world population and industrialization, the demand for energy is also increasing. In order to supply with energy need alternative energy sources have been developed. Supercapacitors (SC), which are electrochemical energy storage systems, draw attention because of their high power density, high rate capacity and long cycle life [1]. SCs are classified into three types of their energy storage mechanisms: high surface area and conductive carbon-based materials that store charge at the interface between electrode and electrolyte, named as electrical double layer capacitance, redox active materials such as transition metal oxides and conducting polymers, that undergo fast and reversible Faradic redox reactions, known as pseudocapacitance. Hybrid capacitors make use of both physical and chemical charge storage mechanism together in a single electrode. Therefore, hybrid capacitors have the advantage over the other two SCs [2]. Graphene-based nanocomposite materials have drawn serious attention. $Fe_3O_4$, which is a transition-metal oxide, utilize fast and reversible redox reactions to provide high power density as well as high energy density. It is distributed between the rGO sheets to prevent agglomeration and can also be integrated with rGO to improve the electrochemical performance of materials [3].

In our work, we prepared rGO/$Fe_3O_4$ nanocomposite via a one pot, green and facile method. The nanocomposites were characterized by transmission electron microscopy, scanning electron microscopy, Fourier Transform Infrared Spectroscopy, X-ray Diffraction, Thermogravimetric analysis, Ultraviolet-visible spectroscopy, cyclic voltammetry, electrochemical impedance spectroscopy and galvonastatic charge/discharge techniques. In summary, rGO nanosheets were decorated by $Fe_3O_4$ nanoparticles successfully. The prepared $Fe_3O_4$/rGO composite showed higher capacitance than pure $Fe_3O_4$ as a result of the synergetic effect between rGO and $Fe_3O_4$, the composite served as a supercapacitor electrode exhibits high specific capacitance, remarkable rate capability and excellent cycling stability.

## References

[1] Q. Wang, L. Jiao, H. Du, Y. Wang and H. Yuan, Journal of Power Sources, 254(2014) 101-106.
[2] P.K. Kalambete, R.A. Dar, S.P. Karna and A.K. Srivatava, Journal of Power Sources, 276 (2015) 262-270.
[3] J.P. Cheng, Q.L. Shou, J.S. Wu, F. Liu, V.P. Dravid and X.B. Zhang, Journal of Electroanalytical Chemistry, 698 (2013) 1-8.

## Acknowledgement

This work was financially supported by the Scientific and Technical Research Council of Turkey (TÜBİTAK; Project No: 115M456).

---

* Corresponding author, *E-mail: nyildiz@eng.ankara.edu.tr*

# Impact of A-site Cation Size Disorder on Electronic Properties of Perovskite Manganites

Sevgi Polat Altıntas[1]* and Nabil Mahamdioua[2]

[1]Abant Izzet Baysal University, Department of Physics, Bolu, Turkey
[2]Lend, Universite´ de Jijel, B. P 98 Jijel, Algeria

*E-mail: sevgialtintas@ibu.edu.tr*

We investigated the influence of the size mismatch effect of a series of $La_{2/3-x}RE_xCa_{1/3-y}Sr_yMnO_3$ with RE: Y, Gd and Ce. A-site cationic size mismatch, $\sigma^2$, is kept constant while the average cationic radius $<r_A>$ is varied. After characterizing the samples by X-ray diffraction, scanning electron microscope and energy dispersive X-ray spectrometer, a systematic investigation of electrical and magneto-transport properties were investigated. Also, electrical resistivity data were carried out using theoretical models to understand the conduction mechanism [1].

**Reference**

[1] G. Li, H.D. Zhou, S.J. Feng, X.J. Fan and X.G. Li, Journal of Applied Physics, 92 (2002) 1406-1410.

---

* Corresponding author, *E-mail: sevgialtintas@ibu.edu.tr*

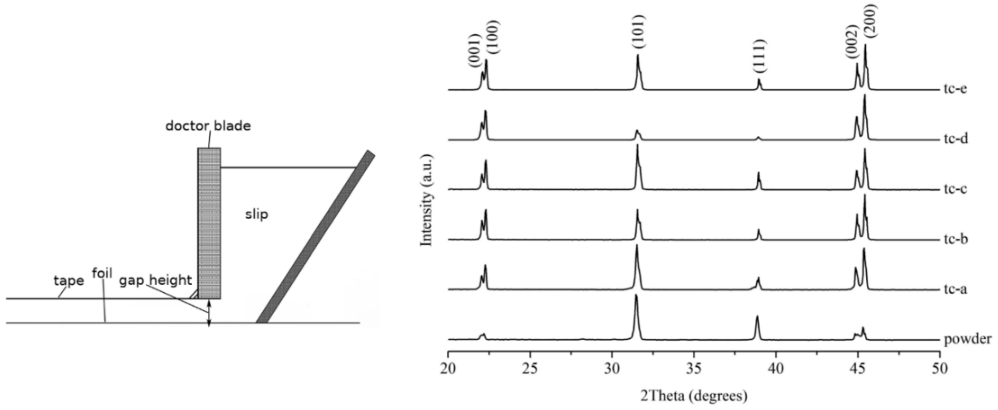
# Texturing Properties of Hydrothermally Synthesized Barium Titanate Powders by Aqueous Tape Casting

**Murat Özen**[1]*, Myrjam Mertens[2], Frans Snijkers[2] and Pegie Cool[1]

[1]University of Antwerp, Department of Chemistry, Laboratory of Adsorption and Catalysis (LADCA), Universiteitsplein 1, B-2610 Wilrijk, Belgium
[2]Flemish Institute for Technology Research (VITO nv), Boeretang 200, B-2400 Mol, Belgium

*E-mail: murat.ozen@outlook.com*

Aqueous slurries of hydrothermally prepared barium titanate ($BaTiO_3$) powders were tape casted in this work. About 64 vol% of $BaTiO_3$ was casted with a single doctor blade setup (Figure 1a). After drying of the green tapes, the tapes were sintered at 1400°C or 1500°C, and at different oven parameters (heating rates, holding times). The crystallographic texture of the sintered tapes was evaluated by the semi-quantitative XRD (Figure 1b) Lotgering method and the microstructure was studied by SEM. The Lotgering factor or the texturing degree (*f*) [1] of the sintered $BaTiO_3$ tapes was positively influenced by two main variables. Firstly, sintering in a one-step heating process resulted in a 22% to 30% increase of *f* (tc-b and tc-e). Secondly, the final sintering temperature had a positive effect on *f*. Sintering in the liquid-phase (Ti-excess) temperature region (> 1400°C) and at a high enough temperature (≥ 1500°C) drastically improved the relative intensity of the {001}-lines in XRD by 72% (tc-d), at the expense of the {101}- and {111}-lines. The average volume weighted grain-size of the sintered tapes was decreased up to 77%, relative to sample tc-a.



(a) (b)

**Figure 1.** (a) A single doctor blade setup and
(b) X-ray diffractograms (XRD) of $BaTiO_3$ tapes sintered at different heating conditions

**References**

[1] M. Özen, M. Mertens, F. Snijkers and P. Cool, Ceramics International, 42 (2016) 5382-5390.

---

* Corresponding author, *E-mail: murat.ozen@outlook.com*

# Selective Encapsulation of Volatile Compounds from Essential Oil of *Cistus Creticus*

**Emre Taylan Duman**[1] and Oğuz Bayraktar[2]*

[1]Ege University, Faculty of Engineering, Department of Bioengineering,
35040, İzmir, Turkey
[2]Ege University, Faculty of Engineering, Department of Chemical Engineering,
35040, İzmir, Turkey

*E-mail: emretaylanduman@yahoo.com*

*Cistus creticus* is one of the members of the Mediterranean flora which contains 45-50 different volatile molecules [1]. These phytochemicals have great potential of antimicrobial and cytotoxic activity [2]. But most of them volatile components. This causes difficulties in applying them to final products. Because of their volatility, they are mostly unstable and requires for a solvent. Encapsulation may be used for overcoming these problems. Cyclodextrins (CDs) are torous shaped molecules which are used for forming molecule-CD complexes which has increased solubility in water and also increased stability of the specific molecule [3]. This molecule-CD interaction named as inclusion complexes. In this specific work, development of new methods for encapsulation of volatile compounds by electrospraying CDs was developed, also characterization of the volatile components of *cistus creticus* was made (Figure). By this application encapsulating specific molecule or molecule groups selectively which has a potential for pharmaceutical and cosmetic applications. The potential of the application leads to reduce costs of separation and purification steps and make volatile compound water soluble. *Cistus creticus* leafs and twigs were collected on their natural season (May-June), and hydrodistillation was applied for seperation of volatile compounds and essential oil of the plant material. At the end of the process, essential oil was collected and analyzed for comparing molecular content with commercial essential oil. After active molecules were identified, a new method was applied to the volatile molecules.

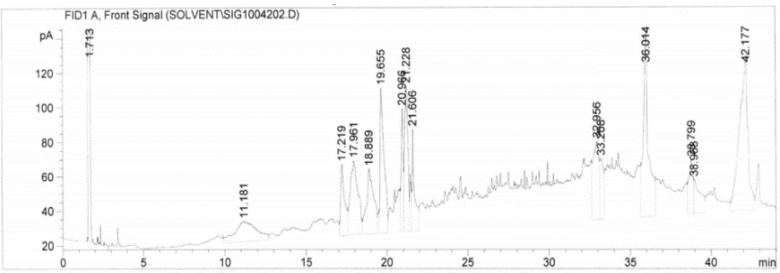


**Figure 1.** GC results of encapsulated molecules

## References

[1] C. Demetzos, H.E. Katerinopoulos, A. Kouvarakis, N. Stratigakis, A. Loukis, C. Ekonomakis and J. Tsaknis, Planta Medica, 63(5) (1997) 477-479.
[2] O. Bayraktar, E. Altıok, Ö. Yılmazer, D. Ruscuklu and M.Y. Buyukoz, Biointerface Research in Applied Chemistry, 6(4) (2016) 1417-1421.
[3] R.L. Abarca, F.J. Rodriguez, A. Guarda, M.J. Galotto and J.E. Bruna, Food Chemistry, 196 (2016) 968-975.

---

* Corresponding author, *E-mail: oguz.bayraktar@ege.edu.tr*

# Effect of Secondary Stabilizers Additives on The Polyene Formation of Plasticized Poly(Vinyl Chloride) Films during Heat Treatment

**A. Pınar Tüzüm Demir* and Çağıl Korkusuz**

Uşak University, Chemical Engineering Department, Uşak, 64200, Turkey

*E-mail: pinar.demir@usak.edu.tr*

Poly(vinyl chloride) (PVC), has many favorable characteristics such as easily modification and low cost [1]. However, PVC still has numerous problems, in particular, its low thermal stability during manufacture and use. Many applications consider PVC longevity as an important requirement, so investigation and improvement of its thermal stability and durability are necessary [2]. The material goes under degradation due to the thermal processes during its manufacturing process and service life [3]. When plasticized PVC (p-PVC) film is heated, plasticizer evaporates from the surface of the film and PVC degrades by the loss of hydrogen chloride (HCl) gas with the formation of conjugated double bonds during thermal decomposition [4]. The generation of HCl gas causes contamination of all product streams, creates corrosion problems and discoloration of the resin occurs along with important changes in physical and chemical properties [5]. The aim of the present work is to assess the effect of secondary stabilizer additives on the polyene formation of p-PVC films during heat treatment. In the first instance, p-PVC plastisols were produced from the formulations; di-izononil 1,2-siklohegzan dikarboksilik asit (DINCH) and di-2-etil hegzil ftalat (DEHP) as plasticizer, calcium-zinc stearate (CaSt2-ZnSt2) mixture as synergic thermal stabilizers, and epoxidized soy bean oil (ESBO), epoxidized linseed oil (ELO), tri phenyl fosfit (TFF), tri nonylphenyl fosfit (TNFF), diphenyl urea (DFÜ) as secondary heat stabilizer. 120µm thickness films on glass plates were cured for 15 minutes at 160°C. Then, the p-PVC films were produced. These films were subjected to heat treatments at 100 and 150$^{o}$C up to 420 minutes. Ultra Violet -visible (UV-vis) spectroscopy was utilized to follow polyene formation upon dehydrochlorination of PVC. Meanwhile, discoloration assessed in terms of Yellowness Index (YI) followed by the colorimeter.

## References

[1] C. Wan, Y. Zhang and Y. Zhang, Polymer Testing, 23 (2004) 299-306.
[2] B. Wu, S. Qi, X. Wang, Polymer Testing 29 (2010) 717–722.
[3] H. Zweifel, 2009. Plastics Additives Handbook, 5th Edition, Hanser Verlag, Munich, Germany, 1026-1107.
[4] T.O. Egbuchunam, D. Balköse and F.E. Okieimen, Polymer Degradation and Stability, 92 (2007) 1572-1582.
[5] Y.B. Liu, W.Q. Liu and M.H. Hou, Polymer Degradation and Stability, 92 (2007) 1565-1571.

## Acknowledgement

The financial support of Uşak University Research Fund (Project No: 2016/MF002) is gratefully acknowledged, as well.

---

* Corresponding author, *E-mail: pinar.demir@usak.edu.tr*

# Novel Techological Processes for Obtaining Modern Nanomaterials

Nina Kushchevska, Victor Malyshev* and Olena Paprotska

University “Ukraine”, 23 Lvivska St., Kyiv 03115, Ukraine

*E-mail: kushchevskaya@email.ua*

Among modern nanomaterials materials based on ferromagnetic powders occupy an important place. The problem is that existing, technological conditions of synthesis don't permit to obtain them in not pyrophorus chemically inert state with the necessary combination of physico-chemical and medico-biological properties, realized simultaneously in practice. We were the first to propose physico-chemical principle for metal-based powders synthesis by chemical precipitation of their salts with subsetuent reduction. Physico-chemical regularities for formation of initial nanodisperse systems with oxidation-resistant particle surface have been established. This permitted to work out technology of obtaining ferromagnetic powders with given structure and properties [1]. Complex of requirements to such powders is: a) the size of particles must correspond to the nanodispersed range; b) powders must be not pyrophoric, stable to corrosion, hydrophilic; must possess the high magnetic features; c)must not contain harmful admixtures and possess adsorption, catalytic and bactericidic characteristics (for biomedical purposes ). We solved scientific and technical problem of synthesis of nanosize ferromagnetic powders in stable chemically inert condition and made an attempt to create on their basis efficient materials of biomedical and technical use. Nanosized ferromagnetic powders have created for the first time, and on their basis with metals-additives Ag, Pt, Au, Cu, Zn, Co, and Ni with close to ellipsoidal and round form and with average size of particles 0,005-0,25 μm, specific surface area 25-50 $m^2$/g, heat moistening of particle surfaces by water 0,5-2,0 $Am^2$/kg, and with magnetic properties: coercitivity power Hc 24-60 kA/m, specific induction of saturation $\sigma_{S\ s}$ 85-200 $Am^2$/kg, specific residual induction or 20-80 $Am^2$/kg and area of their use has been determined. For oncology, neurooncology and surgery: 1) suspensions, magnetic liquids; 2) containers with ferromagnetic powders on basis of physiological solution, blood substitutes, medicinal preparations. For surgery and festering surgery: a) activated carbon material (ABBM Dnipro) MP; b) the unguent-emulsion “Magnolia”; c) films-adsorbents, membranes-adsorbents, application-dressing materials; d) sprinklings and others. For endocrinology, therapeutics and oncology: - capsules (magnetic containers for direct transport of medicines into key organ). Materials science: 1) glue-plumbers; glue compositions; 2) plumbers; strengthening materials; 3) magnetic fillers working in extreme conditions; 4) magnetic materials for fastening photographic magazines, sensors of acoustic emission and others. Results of work presented indicate prospects of technology of obtaining such ferromagnetic powders by thermochemical way and perspectives of creation on their basis of modern nanomaterials of different purposes.

**Reference**

[1] M.A. Garcia, J.M. Merino, E.F. Pinel, A. Quesada, J. de la Venta, M.L.R. González, G.R. Castro, P. Crespo, J. Llopis, J.M. G.-Calbet, and A. Hernando, Nano Letters, 7 (2007) 1489-1494.

---

[*] Corresponding author, *E-mail: victor_malyshev@mail.ru*

O-100

# Electrodeposition of Molybdenum and Tungsten Carbides Coatings: fron Initial Stages of Nucleation to the Continuous Layers Formation

**Viktor Malyshev[1]*, Angelina Gab[1], Marcelle Gaune-Escard[2] and Alla Sushchenko[1]**

[1]University “Ukraine”, 23 Lvivska St., Kyiv 03115, Ukraine
[2]Ecole Polytechnique, CNRS UMR 6595, Technopole de Chateau-Gombert, France

*E-mail: lina_gab@ukr.net*

Coatings of molybdenum carbide from the electrolyte of $Na_2WO_4$–$Li_2MoO_4$–$Li_2CO_3$ are deposited at similar (within 2.5 mol%) concentrations of lithium molybdate and carbonate. Solid coatings of molybdenum carbide were obtained at 1073-1223 K and current densities above 0.5 $A/cm^2$. The deposition rate of coatings in the studied current density range was 5-25 μm/h, the current efficiency of molybdenum carbide deposition in the form of a coating was up to 80%. The maximum coating thickness was up to 100 μm. The application of the reverse electrolysis mode allowed one to reduce the macrocrystalline structure and increase the coating thickness of 200 μm. The optimum parameters are as follows: the ratio of $\tau_k/\tau_a = 20\text{-}40$, the anodic period duration was 0.5-2.0 s, and its current density was 0.15-0.50 $A/cm^2$ [1]. Coatings of tungsten carbide $W_2C$ from the $Na_2WO_4$-$Li_2CO_3$ electrolytes are deposited at the $Li_2CO_3$ concentrations up to 15 mol. %. We showed that carbide electrodes in tungstate-molybdate-carbonate melts of certain compositions have equilibrium electrode potentials. The repeated switching-on of the current within a short period of time (5-10 s) does not give rise to peak formation. These facts indicate that the crystallization overvoltage is associated with the three-dimensional nucleation. Based on the experimental results, we evaluated the crystallization overvoltage due to a considerable energy loss for component nucleation at the first moments of synthesis. These energy losses at the Ag electrodes in the temperature range 973-1023 K attain values of 8-40 mV. An increase in the melt temperature may complicate the crystallization process because of the interaction between the deposited components and the material matrix. For metals forming alloys with the deposited components, crystallization overvoltage is observed for a surface oxide film. It is characteristic that the height of the overvoltage maximum for the above metals is proportional to the reciprocal time of their formation. This seems to be associated with the penetration of the part of the deposited components into the substrate bulk due to solid-phase diffusion, which allowed us to qualitatively characterize the degree of inertness of the substrate material. An increase in the melt temperature usually activates the cathode surface, increases the rate of mutual diffusion of the deposited components of the synthesized material and the substrate, and also intensifies the reactions of their chemical interaction. Studying the electrodeposition of carbides onto different single-crystal substrates, we observed a structural mismatch. The heteroepitaxial $Mo_2C$ and $W_2C$ layers on the single-crystal Mo and W substrates of various orientations were deposited from the $Na_2WO_4$-$MoO_3(WO_3)$-$CO_2$ melts at $T = 1123$ K and $i = (0.5\text{-}1.0)\times 10^3$ $A/m^2$.

**References**

[1] V. Malyshev, A. Gab, I. Astrelin, A.-M. Popescu and V. Constantin, Rev. Chim. (Bucureşti), 61 (2010) 387-389.

---

* Corresponding author, *E-mail: victor_malyshev@mail.ru*

O-101

# Electrochemical Synthesis of Dispersed Powders of Chromium, Molybdenum, and Tungsten Silicides in Halide-Oxide Melts

**Viktor Malyshev[1,2]*, Dmytro Shakhnin[1,2], Liliia Molotovska[2] and Alla Sushchenko[1]**

[1]University "Ukraine", 23 Lvivska St., Kyiv 03115, Ukraine
[2]V.I. Vernadsky Institute of General and Inorganic Chemistry of the NAS of Ukraine, 32/34 Palladina Ave., Kyiv 03142, Ukraine

*E-mail: liliiamolotovska@gmail.com*

For synthesis of Cr, Mo, and W silicides, their oxygen compounds were used to dissolved in KCl-KF and NaCl-$Na_3AlF_6$ mixtures. In current-voltage curves for chloride-cryolite melts, under joint presence of sodium molybdate and silicon oxide, two waves are observed. The first of them is caused by electroreduction of molybdenum oxyfluoride complex, and the second one – by an oxy-fluoride complex of silicon. Difference between half-wave potentials is 0.8-0.9 V. A Similar situation is observed in the presence of sodium tungstate, with the only difference that difference of half-waves potential is 100-150 mV lower. These data confirm that silicides synthesis could be carried out by electrolysis alone in kinetic regime [1]. It causes the following sequence of steps for electrosynthesis of silicides of molybdenum and tungsten: I – deposition of more electropositive metals (molybdenum or tungsten); II – deposition of the second component-silicon-on the surface of Mo or W deposited earlier; III – silicon reaction diffusion into the depth of metal-salt "pear" with formation of silicides phases of different compositions up to higher silicides. Essential role in electrochemical synthesis of silicides of Mo and W is played by temperature and current density values. Lowering the temperature below 850 ºC does not ensure completeness of interaction of Mo (W) and Si, and temperature rise above 950 ºC reduces the stability of metal-salt "pear" due to which silicides are not formed. With optimal melt composition, pure products were obtained with current density 0.5-1.2 A/cm$^2$ for $MoSi_2$ and 0.5-1.5 A/cm$^2$ for $WSi_2$. With $i_k < 0.5$ A/cm$^2$, obtained product is contaminated with Mo or W. Within the range of current density 0.5-1.5 A/cm$^2$, with current density increase, dispersity of Mo and W silicides increases. Similar dependence of phase composition on electrolysis duration is observed in the NaCl-$Na_3AlF_6$-$Na_2WO_4$-$SiO_2$ system. Initially, high-temperature electrochemical synthesis of chromium silicide is carried out from a mixture of molten NaCl-$Na_3AlF_6$-$K_2CrO_4$-$SiO_2$. Voltammetric curves show reduction waves of oxyfluoride complexes of Cr and Si at significantly different potentials, - (0.7-0.9) *V* and - (1.6-1.9) *V*, respectively. Depending on composition and electrolysis parameters, $Cr_2O_3$, higher silicide $CrSi_2$, and silicide $Cr_3Si$ phases were obtained as a mixture with aluminum compounds. To optimize synthesis conditions for chromium silicides containing no aluminum compounds, electrochemical synthesis was carried out in KCl-KF-$K_2SiF_6$- $K_2CrO_4$ system. The resulting current-voltage dependences show reduction waves for oxyfluoride complexes of Cr and Si at significantly different potentials. Depending on electrolyte composition and electrolysis parameters, both individual phases $Cr_2O_3$, $Cr_3Si$, and $CrSi_2$, and also mixtures of these phases with low silicon content were obtained.

**References**

[1] V.V. Malyshev, A.I. Hab, D.B. Shakhnin and D. Schuste, Materials Science, 52 (2017) 550-558.

---

* Corresponding author, *E-mail: victor_malyshev@mail.ru*

# Novel Ferromagnetic Nanocomposites for Biomedical Applications

**Nina Kushchevska[1], Victor Malyshev[1]*, Olena A. Paprotska[1],**
**Mustafa Oğuzhan Çağlayan[2]* and Zafer Üstündağ[3]**

[1]University of “Ukraine”, Institute of Engineering and Technology, Kyiv, Ukraine
[2]Cumhuriyet University, Faculty of Engineering, Department of Nanotechnology Engineering, Sivas, Turkey
[3]Dumlupınar University, Faculty of Arts and Science, Department of Chemistry, Kütahya, Turkey

*E-mail: paprotskaya@email.ua*

Today, there are problems of creating new biomaterials using scientific advances in the field of powder metallurgy, materials science, biochemistry, biotechnology and medicine. These problems can be resolved on the basis of studying physicochemical and biomedical properties of these powders. Theoretical and methodological recommendations for assessment of the influence of nanocomposites onto living organism’s cells through the study of their physicochemical and biomedical properties are also absent. Ferromagnetic nanocomposites with desired physical, chemical, medical, and biological properties were obtained by thermochemical method. Mechanism of formation of nanodisperse particles of metal compounds with desired physical, chemical, and medico-biological properties was studied. Physico-chemical conditions of synthesis of metal-based composite powders, and also physical and chemical changes occurring during the ferromagnetic nanoparticles formation by chemical methods with subsequent reduction in reducing environments were investigated. Investigation of physical properties of ferromagnetic nanocomposites was done by methods of X-ray phase, structural, and fluorescent analysis, of electron microscopy, NGR spectroscopy, of determination of specific surface of powders by thermal desorption of argon, and by magnetometric methods. Thus, phase composition, structure, specific surface, magnetic properties, particle size etc. were determined. Investigation of chemical properties of ferromagnetic nanocomposites was done by methods of elemental analysis, derivatography, corrosion studies, determination of surface hydrophilicity by the heats of wetting, adsorption properties studies, and by spectral methods. Chemical composition of ferromagnetic nanocomposites, the chemical state of metal atoms in their composition, the degree of hydrophilicity and adsorption properties of the surface were determined [1].

Experimental medico-biological estimation of the relative safety of ferromagnetic nanocomposites was made by determination of the degree of solubility of nanopowders of different dispersion degree, by study of the acute toxicity of powders during peroral, intravenous, and parenteral administration of them. Hazard class of ferromagnetic nanocomposites was determined, recommendations for their use in biology and medicine were developed.

**References**

[1] Y. Namiki, S. Matsunuma, T. Inoue, S. Koido, A. Tsubota, Y. Kuse and N. Tada, Nanotechnology and Nanomaterials "Nanocrystal", (Ed. Y. Masuda) 2011 (DOI: 10.5772/16424).

---

* Corresponding author, *E-mail: victor_malyshev@mail.ru* & *caglayanmoguzhan@gmail.com*

# Molybdenum (Tungsten)–Nickel (Cobalt) Alloys and Intermetallic Compounds: Electrochemical Properties of Melts and Electrodeposition of Coatings

**Viktor Malyshev[1,2]*, Nataliya Uskova[2], Nina Kushchevskaya[1] and Alla Sushchenko[1]**

[1]University "Ukraine", 23 Lvivska St., Kyiv 03115, Ukraine
[2]V.I. Vernadsky Institute of General and Inorganic Chemistry of the NAS of Ukraine, 32/34 Palladina Ave., Kyiv 03142, Ukraine

*E-mail: uskova@email.ua*

For the cathodic codeposition of metals, the correspondence of their crystalline lattices and the difference in their standard electrode potentials are of great importance.The directly proportional dependence of the ultimate current on the oxide concentration, the $i_p$/nFC ratio constant over a wide interval of polarization rates, and the $i_p$/nFC value indicate that the electrode process is limited by the diffusion of electroactive particles to the electrode surface. Therefore, under such polarization conditions, the rate of formation of electrochemically active particles imposes no restrictions on the electrode process. The analysis of the experimental data suggests that reversible equilibria and processes involving nickel and cobalt(II) can occur in the sodium tungstate melt [1].

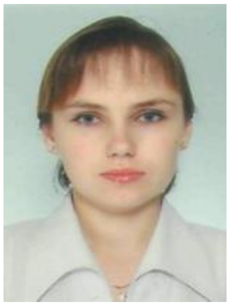
The addition of molybdenum(VI) oxide to the nickel-containing tungstate melt induces the dimolybdate-ion reduction wave. The concentration of $MoO_3$ was maintained at 1.0–2.5 mol %, and the NiO concentration was varied from 0.1 to 1.0 mol %. The molar ratio of the molybdenum and nickel ions changed from 250 to 1. An increase in the NiO concentration or the temperature and a decrease in the cathodic current density increase the nickel content in the deposit. Continuous layers of the intermetallics MoNi, $MoNi_3$, and $MoNi_4$ are sequentially deposited on the cathode at 1123–1173 K from the melts containing 0.1–1.0 mol % NiO. The introduction of tungsten(VI) oxide into a nickel-containing tungstate melt produces the ditungstate-ion reduction wave. The difference in the potentials of nickel and tungsten deposition is 0.13–0.16 V at 1173 K, and this potential is higher for nickel. The procedure of alloy deposition is similar to the procedure described above, but the starting melt was the $Na_2WO_4$–5.0 mol % $WO_3$ melt. The addition of tungsten(VI) oxide to a cobalt-containing tungstate melt results in the appearance of the ditungstate-ion reduction wave. The difference in the potentials of cobalt and tungsten deposition is 0.08–0.14 V at 1173 K. The $WO_3$ concentration was maintained at 0.1–1.5 mol %, and that of CoO was changed from 0.01 to 1.0 mol %. The molar ratio of the tungsten to cobalt ions was varied from 250 to 1. An increase in the CoO concentration, a rise in temperature, and a decrease in the cathodic current density increase the cobalt content in the deposit. Continuous layers of the CoW and $Co_3W$ intermetallics are sequentially deposited on the cathode at 1123–1173 K from the melts containing 0.1–1.0 mol % CoO. The addition of molybdenum(VI) oxide to the cobalt-containing tungstate melt of $MoO_3$ induces the dimolybdate-ion reduction wave. The difference in the potentials of cobalt and molybdenum deposition is 0.06–0.110 V at 1173 K. These dependences of electrodeposition of tungsten–cobalt alloys are also characteristic of the deposition of molybdenum–cobalt alloys. Depending on the ratio of the $MoO_3$ and CoO concentrations and the cathodic current density, continuous deposits of Mo, CoMo, $Co_3Mo$, and Co can be prepared from a $Na_2WO_4$–$MoO_3$–NiO melt.

## References

[1] V. Malyshev, A. Gab, I. Astrelin, A.-M. Popescu and V. Constantin, Rev. Chim. (Bucureşti), 61 (2010) 387-389.

---

* Corresponding author, *E-mail: victor_malyshev@mail.ru*



# VI-B Metal Electroreduction and Electroplating from Ionic Melts

**Victor Malyshev[1]*, Diana-Maria Bruskova[1], Dmytro Shakhnin[1] and Zafer Üstündağ[2]**

[1]University "Ukraine", Institute of Engineering and Technology, Kyiv, Ukraine
[2]Dumlupınar University, Faculty of Arts and Science, Department of Chemistry, Kütahya, Turkey

*E-mail: diana.bruskova@gmail.com*

The Cr(III) electroreduction in halide melts proceeds in two steps Cr(III) → Cr(II) → Cr(0). The structure of Cr(III) and Cr(II) complexes in chloride and bromide melts is more or less clear. Fluoride melts were studied less thoroughly. Chloride and bromide melts containing Cr(II) should be preferred in the metal deposition [1].

Quantity of stages in electrochemical reactions in molybdenum (tungsten) containing melts is determined by their composition. Considerable success was achieved in the electrodeposition of molybdenum (tungsten) coatings from halide systems. The use of halide–oxide melts extends the range of substrates for the molybdenum deposition to copper, nickel, and iron in addition to graphite and noble metals. The use of melts based on tungstates and molybdates of alkali and alkali-earth metals is very promising from the standpoint of conducting direct electrolysis and their use as the solvents in the synthesis of refractory, heavy, and nonferrous metals and their compounds. In the majority of studies, it was noted that electrochemically active species represent the cationized and dimeric complexes. Molten borates, phosphates, and silicates of alkali metals are also suitable solvents for the molybdates (tungstates) of alkali and alkali-earth metals, molybdenum (tungsten) oxide and their sulfides [1,2].

To date, the processes of electroplating of VI-B group metals from ionic melts are sufficiently well developed. Their preparation as cathodic deposits of a definite form is determined by the electrolyte composition and the choice conditions for the electrolysis. Many electrodeposition processes are still in the stage of their introduction into the industry and semi-industrial tests.

**References**

[1] A.I. Hab Materials Science, 43 (2007) 383-397.
[2] V.V. Malyshev, H.B. Kushkov and V.I. Shapovali, J. Appl. Electrochem., 32 (2002) 573-579.

---

* Corresponding author, *E-mail: viktor.malyshev.igic@gmail.com*

# Molybdenum Carbide Electrodeposition onto Semiconducting Materials Surface in Ionic Melts

**Victor Malyshev[1]*, Dmytro Shakhnin[1], Vladimir Danielik[2] and Marta Ambrova[2]**

[1]University "Ukraine", Institute of Engineering and Technology, Kyiv, Ukraine
[2]Technical University in Bratislava, Department of Inorganic Chemistry, Bratislava, Slovakia

*E-mail: vladimir.danielik@stuba.sk*

Deposition of metal-containing coatings onto particles of semiconducting abrasives provides an effective means of improving the performance of abrasive tools. Metallized abrasives are characterized by increased mechanical strength and adhesion to the substrate and are, therefore, consumed in smaller amounts. For coating electrodeposition to be possible, it is important that the corrosion potential of the substrate is higher than the deposition potential. To find out whether silicon carbide and boron carbide can be coated with molybdenum carbide, we measured their stationary potentials relative to the $Na_2WO_4$-$0.2WO_3$ | $O_2$, Pt half-cell. The deposition potential of molybdenum carbide is lower than the corrosion potentials of the materials examined, making possible the deposition of high-quality coatings [1,2].

Metallization of semiconductors is possible in melts that ensure the occurrence of redox reactions at the interface and the controllability of the electrode potential. For example, molybdenum carbide can be deposited from a tungstate-molybdate-carbonate melt at a temperature of 1073-1173 K and a current density of 10-100 $A/m^2$. In this melt, the particle surfaces serve as active substrates for electrodeposition. The cathodic current density in this process was set with regard for the particle surface area. The extent of metallization was determined as the difference between the weights of the metallized and initial samples. $Mo_2C$ was deposited at 1123 and 1173 K and a cathodic current density of 50, 100, and 200 $A/m^2$ for 15, 30, 45, 60, and 90 min. Both the deposition rate and the extent of metallization at a fixed treatment time grow with increasing electrolyte temperature and cathodic current density. The maximum attained thickness of carbide coating was 5 μm.

The principles of galvanic treatment formulated here have served as the theoretical basis in the deposition of refractory metals and their carbides onto dielectric and semiconducting powder particles of various sizes.

**References**

[1] V.V. Malyshev, A.I. Gab, A.D. Pisanenko, V.V. Soloviev and L.A. Chernenko, Materials Science and Engineering Technology, 45 (2014) 51-56.
[2] V.V. Malyshev, H.B. Kushkov and V.I. Shapovali, J. Appl. Electrochem., 32 (2002) 573-579.

---

* Corresponding author, *E-mail: viktor.malyshev.igic@gmail.com*

O-106

# Preparation of SiC from Ionic Melts

**Victor Malyshev[1]*, Aslı Erkal[2], Angelina Gab[1], Oksana Tereshchenko[1] and Arife Yurdakul[2]***

[1]University “Ukraine”, Institute of Engineering and Technology, Kyiv, Ukraine
[2]Alanya Alaaddin Keykubat University, Faculty of Engineering, Department of Metallurgical and Materials Engineering, Alanya, Antalya, Turkey

*E-mail: tereschenko230479@gmail.com*

A necessary condition for electrodeposition is the occurrence of a reaction involving electrons. Therefore, the cathode (or the surface layer of the pseudocathode) must possess electronic conductivity; that is, it must be a metal or a semiconductor. The satisfaction of this condition was checked by voltammetry. During the electroreduction of $CO_2$ at an elevated pressure, we observed an appreciable increase in the reduction current through the SiC ($B_4C$) electrode relative to that through the empty platinum container. At an elevated $CO_2$ pressure, the stationary potential of the SiC ($B_4C$) electrode is -0.40 to -0.45 V (vs. platinum-oxygen electrode). The $CO_2$ reduction current was determined by subtracting the current through the platinum net from the total current through the platinum-SiC ($B_4C$) electrode. Using literature data ($i(CO_2) = 4.5$ mA/cm$^2$ at $p(CO^2) = 1.52 \times 10^3$ kPa and V = 0.1 V/s), we calculated the electrochemically active surface of the SiC ($B_4C$) powder electrode to be 25 cm$^2$. This value is in good agreement with the specific surface area calculated for the SiC ($B_4C$) powder of the specified particle size from literature data [1].

Basing on our data on the electroreduction of the $MoO_4^{2-}$ ($WO_4^{2-}$) anions in the NaCl-KCl melt at the platinum net silicon carbide (boron carbide) electrodes in the presence of $Mg^{2+}$ cations, to determine the portion of the platinum net involved in the cathodic reaction, we studied the i(E) dependences with the empty and filled containers. The reduction of $MO_4^{2-}$ ions at the empty container electrode is similar to that at a platinum pin electrode. The stationary potential of the latter differs from that of the platinum reference electrode by no more than 5-10 mV. After the platinum container had been filled with SiC ($B_4C$), its stationary potential shifted from the platinum net potential to -0.35 to -0.40 V (vs. the platinum-oxygen electrode). A marked rise in the reduction current was also observed providing evidence of an increase in the surface area of the working electrode. From the observed difference between the currents through the Pt and SiC ($B_4C$) electrodes, one can determine the partial $MoO_4^{2-}$ reduction current at the surface of SiC ($B_4C$) particles. From our data ($i = 9.5$ mA/cm$^2$ at $C = 5 \times 10^{-5}$ mol/cm$^3$ $Na_2MoO_4$ and V = 0.1 V/s), we calculated the working SiC ($B_4C$) surface area to be 21 and 47 cm$^2$ at an SiC ($B_4C$) weight of 0.025 and 0.050 g, respectively. These values are in good agreement with the surface area calculated for the SiC powder with the specified particle size from literature data.

## References

[1] A.I. Hab, Materials Science, 43 (2007) 383-397.

---

* Corresponding author, *E-mail: viktor.malyshev.igic@gmail.com* & *arife.yurdakul@alanya.edu.tr*

O-107

# Electrochemical Synthesis of Zirconium Diboride Powders and Coatings from Ionic Melts

**Victor Malyshev[1], Nataliia Uskova[1], Ana-Maria Popescu[2], Virgil Constantin[2] and Arife Yurdakul[3]***

[1]University “Ukraine”, Institute of Engineering and Technology, Kyiv, Ukraine
[2]Ilie Murgulescu Institute of Physical Chemistry, Bucharest, Romania
[3]Alanya Alaaddin Keykubat University, Faculty of Engineering, Department of Metallurgical and Materials Engineering, Alanya, Antalya, Turkey

*E-mail: popescuamj@yahoo.com*

Zirconium diboride ($ZrB_2$) is a useful ceramics with a high melting point, high hardness and high electrical conductivity. It has excellent corrosion resistance against molten iron and slags and superb thermal shock resistance [1]. The purpose of the present work is to study the electrochemical behavior of zirconium in the KCl–NaCl–NaF–$K_2ZrF_6$ melt, its reduction jointly with the boron complexes, the way that zirconium diboride is synthesized, and to estimate the possibility of its high-temperature electrometallurgical production [2].

The following were found:

(1) In the KCl–NaCl–NaF–$K_2ZrF_6$ melt, the zirconium (IV) ions are present in the form of mixed chloride–fluoride or fluoride complexes, depending on the concentration of the fluoride ion.
(2) The electrometallurgical reduction of zirconium, depending on the concentration of the fluoride ion, proceeds according to the scheme of auto-inhibition or with the four-electron reversible one-stage transfer.
(3) The electrometallurgical synthesis of zirconium diboride is preceded by the reaction of the formation of the combined zirconium (IV) and boron (III) complexes limiting the electrode process.
(4) The stage of the charge transfer at the reduction of the combined complex in the wide interval of the polarization velocities proceeds reversibly with the one-stage transfer of 10 electrons.
(5) The compositions of electrolytes and the electrolysis regimes for the practical implementation of the high-temperature electrochemical synthesis of zirconium diboride powders and coatings are determined.

**References**

[1] F. Monteverde, A. Bellosi and S. Guicciardi, Journal of the European Ceramic Society, 22 (2002) 279-288.
[2] V.V. Malyshev and A.I. Gab, Russian Journal of Non-Ferrous Metals, 50 (2009) 485-491.

---

* Corresponding author, *E-mail: arife.yurdakul@alanya.edu.tr*

O-108

# Change of Electrochemical and Corrosion Titanium Behavior in the Result of Tungsten Carbide Electroplating

**Victor Malyshev*, Angelina Gab and Larisa Ursuliak**

University "Ukraine", Institute of Engineering and Technology, Kyiv, Ukraine

*E-mail: larieta@ukr.net*

The aim of the present work is to study the electrochemical and the corrosive behaviour of titan with tungsten coating produced by method of high-temperature electrochemical synthesis (HTES), in sulfuric acid solution. Tungsten was not widely used as construction material at normal temperatures in the industry due to deficiency and high cost. However, this material is essential as alloying component for coating deposition. Phase analysis of tungsten-coated with the HTES method titanium sample surface layer has shown the presence of intensive tungsten lines. Microhardness values of tungsten were within 4.0-4.2 GPa. Microhardness values of substrate layers next to coating increase showing interdiffusion of elements of the coating and substrate [1].

Corrosion potential of tungsten covered titan increases substantially from -0.59-0.61 up to 0.26-0.31 V transferring into a passive/active area of titan corrosion and failing to reach tungsten corrosion potential only by 0.02-0.04 V. The photocolorimetric analysis of solution was carried out after 5, 10, 15, and 30 h of the experiment. Average speed of titan dissolution for these time intervals was constant for sample with coating and equal to 0.005-0.01 g/($m^{2}$·h). The titan dissolution rate of potential of free corrosion was 19.1-19.3 g/($m^{2}$·h). As a result of coating deposition, titan dissolution speed diminishes 2000-4000 times. Average speed of corrosion of tungsten coating lowers with an increase of duration of corrosion experiment from 0.03-0.04 g/($m^{2}$·h) in the first 5 h down to 0.007-0.011 g/($m^{2}$·h) after 30 h. It was also found that similar dependence of the average corrosion speed on time takes place during the study of corrosive and electrochemical properties of tungsten in solutions of sulfuric and hydrochloric acids of different concentration. According to anode polarization curves, titan free corrosion potential is equal to -0.59 ÷ -0.61 V under the experimental conditions. It is characterized by area of active dissolution with relatively low critical passivation potential (-0.27 ÷ -0.29 V) and with high critical current. For tungsten sample, the active dissolution area is absent, and it is passive up to the potential of over passivation. Anode polarization curve of titan with tungsten coating is similar to tungsten sample one and practically coincides with latter with polarization more than 0.1 V. Potential of coated sample is close to potential of tungsten overpassivation. Anode current in passive and trans-passive areas are mainly determined by tungsten oxidation. According to cathode polarization curves, efficiency of cathode processes for tungsten sample and for coated titan one is considerably higher than for uncoated titan. The cathode curve of tungsten crosses its anode curve practically at the beginning of the active/passive area. Therefore, with comparable surface areas, tungsten cathode is not able to complete passivation of titan anode. Cathode curve of tungsten coating crosses anode curve of titan very close to passive area. Therefore, coating is more effective as cathode. Thus, it is possible to establish the following: galvanic tungsten coating passivates titanium and lowers the speed of its corrosion in $H_2SO_4$ (9.5 ppm) at 70-80°C by 2000-4000 times. Anode and cathode behaviour of titanium samples coated with tungsten is determined by electrochemical properties of tungsten. Efficiency of the cathode process at coating is higher than at tungsten by itself. Its value allows to passivate titan and to provide electrochemical protection.

## References

[1] A. Bodaghi and J. Hosseini, Int. J. Electrochem. Sci., 7 (2012) 2584-2595.

---

* Corresponding author, *E-mail: viktor.malyshev.igic@gmail.com*

# Surface Plasmon Resonance Enhanced Total Internal Reflection Ellipsometric Application for Detection of DNA Concentration

**Victor Malyshev**[1] and Mustafa Oğuzhan Çağlayan[2]*

[1]University "Ukraine", Institute of Engineering and Technology, Kyiv, Ukraine
[2]Cumhuriyet University, Faculty of Engineering, Department of Nanotechnology Engineering, Sivas, Turkey

*E-mail: viktor.malyshev.igic@gmail.com*

Surface plasmon resonance enhanced total internal reflection ellipsometry (SPRe-TIRE) is a golden tool for monitoring surface interactions especially in bioaffinity systems [1]. Oligonucleotide interactions can be monitored real time even at low concentrations (pM range). Nowadays cancer is a major problem both in terms of health and the global economy with its high death rate. In 2007, 13% of the world's deaths were due to cancer and it is estimated deaths due to cancer to be 12 million people per year in 2030 [2]. The presented study aims to suggest a SPRe-TIRE (Figure 1) based biosensor for the early detection of breast cancer, which is a common cancer type following lung cancer [3]. In this study, the major The BRCA1 (breast cancer 1) gene specific (5' SH-C$_6$-T$_{10}$-AAT GGA TTT ATC TGC TCT TCG-3') oligonucleotide probe was used for a breast cancer diagnosis purpose. The synthetic target gene sequence was used in order to determine biosensor performance. The limit of detection was 4.6 nM with an active detection range of 10-500 nM.

**Figure 1.** SPRe-TIRE setup

**References**

[1] A. Keske, A. Atar, I. Ustundag and M.O. Caglayan, Journal of Computational and Theoretical Nanoscience, 11 (2014) 981-986.
[2] H.G. Tompkins, W.A. McGahan, Spectroscopic Ellipsometry and Reflectometry: A User's Guide, John Wiley and Sons, New York (1999).
[3] J.T. Gohring, P.S. Dale and X. Fana, Sensors and Actuators B: Chemical, 146 (2010) 226-230.

---

* Corresponding author, *E-mail: caglayanmoguzhan@gmail.com*

# Nanomorphological Properties of Electrospun Vascular Grafts

**Stefan Talu**[1], **Mustafa Oğuzhan Çağlayan**[2]*, **Emel Berna Yılmaz**[2] **and Merve Küçükoflaz**[2]

[1]Universitatea Tehnica Cluj-Napoca, Faculty of Mechanical Engineering,
Cluj-Napoca, Romania
[2]Cumhuriyet University, Faculty of Engineering, Department of Nanotechnology
Engineering, Sivas, Turkey

*E-mail: stefan_ta@yahoo.com*

Nanomechanical elastic deformation properties of the non-woven vascular graft made of the electrospun copolymer of poly(L-lactate) and poly($\varepsilon$-caprolactone) was evaluated by AFM. Mechanical properties of vascular grafts, which are implemented in traumas with vascular damage in order to maintain blood flow to corresponding tissue, are extremely important due to mechanical stresses during and after the surgical operations. Force-replacement (nN-nm) curves were obtained over the 5 $\mu$m x 5 $\mu$m sample area by nanoindentation of a single sub-micron fiber of electrospun graft [1]. Approximately 200 of F-s curve data were acquired for a specimen to get histograms of elastic modulus for each specimen (Figure 1). Elastic moduli of 50% (by weight) PLLA-co-PCL was tenfold higher than other PLLA/PCL copolymers and PLLA/PCL blends.

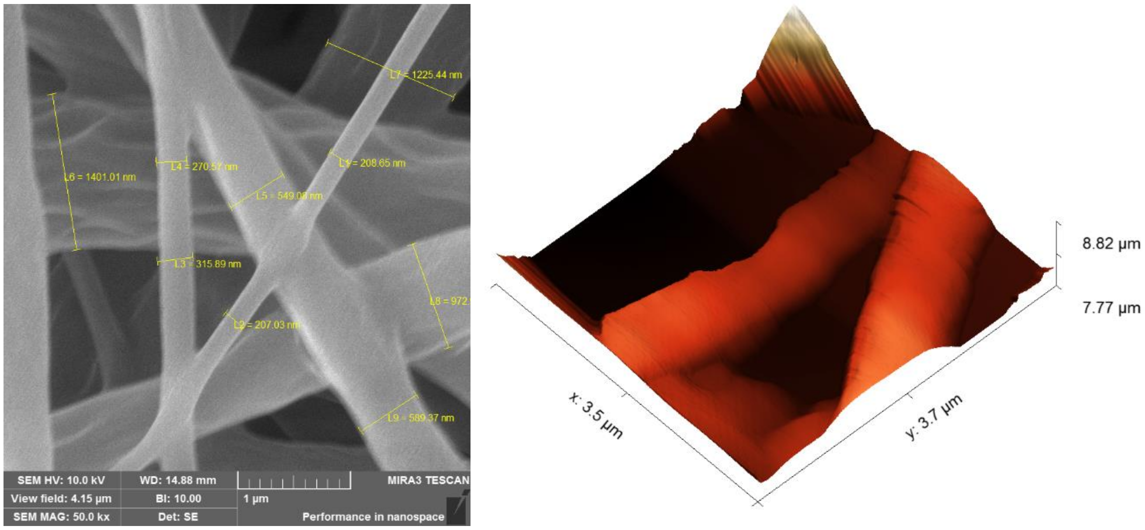


**Figure 1.** SEM and AFM images of electrospun fibers

**References**
[1] S. Talu, K. Stepien, M.O. Caglayan, MO, Microscopy Research and Technique, 78 (2015) 1026-1031.

---

* Corresponding author, *E-mail: caglayanmoguzhan@gmail.com*

O-111

# 2-Benzo*[c]*cinnoline Attached Graphene Oxide Modified Glassy Carbon Electrode for the Voltammetric Determination of Heavy Metals

**Munawar Saed Qureshi[1], Gamze Kuzu[2], Sirajuddin[3]*, Ali Osman Solak[4], Emine Kılıç[5] and Zafer Üstündağ[2]***

[1]Khwaja Fareed Engineering University and Information Technology, Department of Basic Sciences and Humanties, Rahimyar Khan 64200, Pakistan
[2]Dumlupınar University, Faculty of Arts and Science, Department of Chemistry, Kütahya, Turkey
[3]University of Sindh, National Center of Excellence in Anal. Chem. Jamshoro, Pakistan
[4]Kyrgyz-Turkish Manas University, Faculty of Engineering, Department of Chemical Engineering, Bishkek, Kyrgyzstan
[5]Ankara University, Faculty of Science, Department of Chemistry, Ankara, Turkey

E-mail: *drsiraj03@hotmail.com*

2-Aminobenzo[*c*]cinnoline (2-ABCC) modified graphene oxide (GO) electrode was prepared, and it was denoted as (BCC-GO). The material was characterized with Scanning electron microscopy (SEM), Raman spectroscopy, X-ray photoelectron spectroscopy (XPS), cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS). The nanomaterial was modified on glassy carbon electrode [1,2].

BCC-GO modified GC electrode (BCC-GO/GCE) was used for simultaneous determination of Pb, Cd and Zn in aqueous media by differential pulse anodic stripping voltammetry (DPASV). Optimum parameters such as incubation time, constant potential, incubation temperature and pH were investigated. Under the optimum conditions, a linear response was observed for the metals in the range from 1.0 to 150 µg $L^{-1}$. The detection limits of $Pb^{2+}$, $Cd^{2+}$ and $Zn^{2+}$ were 0.67, 0.48 and 0.55 µg $L^{-1}$, respectively. Finally the method had been applied to the simultaneous determination of $Pb^{2+}$, $Cd^{2+}$ and $Zn^{2+}$ in seawater water samples and the results were quite corresponding to the value obtained by ICP-OES. Application of the sensors to the samples produced recovery values in the range 96,4 to 103.2 percents

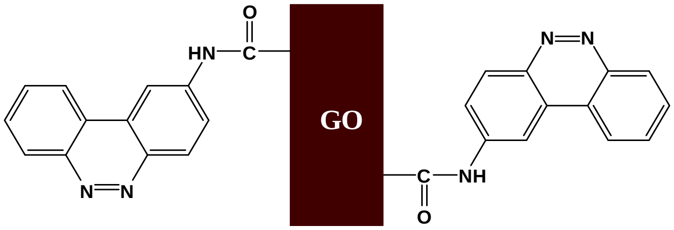


**Figure 1.** 2-BCC modified graphene oxide (BCC-GO)

## References

[1] G. K.-Çelik, A.F. Üzdürmez, A. Erkal, E. Kılıç, A.O. Solak and Z. Üstündağ, Electrocatalysis, 7 (2016) 207-214.
[2] A. Erkal, İ. Üstündağ, S. Yavuz and Z. Üstündağ, J. Electrochem. Soc., 162 (2015) H213-H219.

---

* Corresponding author, *E-mail: drsiraj03@hotmail.com & zustundag@gmail.com*

# Gold Nanoparticle Size and Shape Effects on Graphene Oxide Modified Carbonaceous Electrode for the Voltammetric Determination of Dopamine

**Munawar Saed Qureshi**[1], **Abdull Rahim Mohd Yusoff**[2] **and Zafer Üstündağ**[3]*

[1]Khwaja Fareed Engineering University and Information Technology, Department of Basic Sciences and Humanties, Rahimyar Khan 64200, Pakistan
[2]Universiti Teknologi Malaysia, Ibnu Sina Institute for Scientific and Industrial Research, Skudai, Johor, Malaysia.
[3]Dumlupınar University, Faculty of Arts and Science, Department of Chemistry, Kütahya, Turkey

*E-mail: arahimy@utm.my*

In this study, spherical- and rod-shaped gold nanoparticles (s-AuNPs and r-AuNPs) terminated graphene oxide (GO) were prepared via 4-aminothiol bridge. Firstly, 4-aminothiophenyl was added into a GO suspension containing 1-ethyl-3(3-(dimethlyamino)propyl)-carbodiimide (EDC) as an activating agent. And then gold nanoparticles were attached to the -SH included material as self assemble monolayer. The electrode materials were modified on glassy carbon electrode (GCE). The materials were characterized with IR, XPS, Raman, TEM [1]. Both electrodes were used for determination of dopamine in the presence of ascorbic acid [2] media by differential pulse voltammetry (DPV) under optimum parameters such as particle shape and size.

Under optimized experimental conditions in DPV technique, dopamine gave a linear response over the ranges 0.05–100.0 μM ($R^2 = 0.9935$) with r-AuNP modified electrode and 0.2–80.0 μM ($R^2 = 0.9783$) with s-AuNP modified electrode. The detection limits (S/N = 3) were found to be 0.03 μM and 0.12 μM for DA on r-AuNP and s-AuNP modified glassy carbon electrodes, respectively. The present methods were applied to the determination of DA in human serum samples, using standard adding method.

## References

[1] A. Erkal, İ. Aşık, S. Yavuz, A. Kariper and Z. Üstündağ, Journal of the Electrochemical Society, 163 (2016) H269-H277.
[2] İ. Üstündağ and A. Erkal, Sensors and Materials, 29 (2017) 85-94.

---

* Corresponding author, *E-mail: zustundag@gmail.com*

# Microstructural Control of High-Temperature Thermoelectric Perovskite Oxides for Efficient Energy Harvesting

**Uzma Hira** and **Falak Sher***

*Department of Chemistry, Syed Baber Ali School of Science and Engineering (SBASSE), LUMS, Lahore 54792, Pakistan*

*E-mail: 14130002@lums.edu.pk*

Thermoelectric materials have attracted much attention owing to their potential applications in waste heat recovery, power generation and solid state cooling [1]. Perovskite-type oxides are considered as interesting candidates for thermoelectric renewable power generation because of their complex crystal structure, unusual magnetic and electrical properties and high chemical and thermal stability [2]. We have synthesized $Sr_{2-x}Bi_xCoRuO_6$ ($0.0 \leq x \leq 1.2$) and $Ba_{2-x}Bi_xCoRuO_6$ ($0.0 \leq x \leq 0.8$) materials by conventional solid state reaction method and $La_{0.4}Bi_{0.4}Ca_{0.2}Mn_{1-x}Co_xO_3$ ($0.0 \leq x \leq 0.4$) manganites by sol-gel method. X-ray diffraction (XRD) analysis confirmed the phase purity of all the samples [3]. Lattice parameters and unit cell volumes calculated through Rietveld refinement of XRD patterns. TGA analysis indicated that perovskites are thermally stable and the total weight loss is about 6-7 wt. % from room temperature to 1200 °C in air. SEM micrographs showed that the morphology and size of the particles change significantly with increasing Bi doping. The magnetic data revealed that double perovskites have spin glass type behavior and Neel temperature ($T_N$) is 95K and 85K for $Sr_2CoRuO_6$ and $Ba_2CoRuO_6$ samples respectively. Thermoelectric properties measured from room temperature to a maximum of 700 K temperature. Seebeck coefficient ($S$) showed that $Sr_{2-x}Bi_xCoRuO_6$ with $x = 0.0$ and 0.2 samples are *n*-type and the rest of the compositions of this series have *p*-type behavior. All $Ba_{2-x}Bi_xCoRuO_6$ ($0.0 \leq x \leq 0.8$) samples exhibited *p*-type nature of the material. Electrical resistivity ($\rho$) decreased with increasing temperature for all the samples, indicating the semiconducting behavior of the oxide materials. The highest power factor (3.46 $\mu W/mK^2$) was achieved in $Sr_{1.6}Bi_{0.4}CoRuO_6$ sample at 700K, (12.94 $\mu W/mK^2$) in $Ba_2CoRuO_6$ sample at 700 K and ($8.68 \times 10^{-4}$ $\mu W/mK^2$) for $La_{0.4}Bi_{0.4}Ca_{0.2}Mn_{0.9}Co_{0.1}O_3$ sample nearly at room temperature.

## References

[1] L.E. Bell, Science, 321 (2008) 1457-1461.
[2] D.M. Rowe, Renewable Energy, 16 (1999) 1251-1256.
[3] C.M. Kim, J.W. Seo, J.S. Cha and K. Park, Int. J. Hydrogen Energy, 40 (2015) 15556–15558.

## Acknowledgement

We thank the Higher Education Commission (HEC) of Pakistan (Grant no.: 1981) and the British Council, UK for providing financial support for this research project.

---

* Corresponding author, *E-mail: fsher@lums.edu.pk*

O-114

# Antibacterial Activity of Cu Nanoparticles Synthesized by the Electrical Discharge in Liquid

**Emil Omurzak**[1]*, **Guzel Umetova**[1], **Ruslan Adil Akai Tegin**[2], **Abduraim Satyvaldiev**[3], **Zhanarbek Zhasnakunov**[3] **and Zhazgul Kelgenbaeva**[4]

[1]Kyrgyz-Turkish Manas University, Faculty of Engineering, Department of Chemical Engineering, Chyngyz Aitmatov Campus, Jal, 720038, Bishkek, Kyrgyzstan
[2]Kyrgyz-Turkish Manas University, Faculty of Engineering, Department of Food Engineering, Chyngyz Aitmatov Campus, Jal, 720038, Bishkek, Kyrgyzstan
[3]Arabaev Kyrgyz State University, Faculty of Biology and Chemistry, Bishkek, Kyrgyzstan
[4]Kyrgyz National Academy of Sciences, Institute of Chemistry, Bishkek, Kyrgyzstan

*E-mail: emil.omurzak@manas.edu.kg*

Copper nanoparticles are commonly applied and many researchers have stressed the emphasis of copper nanoparticles properties, applications and synthesis [1]. Because of their high reactivity due to the large surface to volume ratio, nanoparticles are expected to play a crucial role in water purification [2]. Copper in the form of nanoparticle has good bactericidal activity. The United States Environmental Protection Agency has approved the registration of copper as an antibacterial agent able to reduce specific harmful bacteria linked to potentially deadly microbial infections (European Copper Institute, 2008).

Cu nanoparticles of about 10 nm in size were synthesized by the pulsed plasma in aquatic solution of 0.2 % gelatine as surfactant material. By means of XRD and FESEM analysis, it is established that copper nanoparticles with sizes less than 10 nm are formed during the chemical reduction, which form aggregates mainly with a spherical shape. Presence of gelatin during the chemical reduction of copper induced formation of smaller size distribution nanoparticles than that of nanoparticles synthesized without gelatin and it can be related to formation of a protective layer.

Synthesized Cu nano-powders have sufficiently high activity against the Erwinia amylovora bacterium, and the bacterial growth inhibition depends on the Cu nanoparticles concentration. At a concentration of 5 mg/mL of Cu nanoparticles, the exciter growth inhibition zone reaches a maximum value within 72 hours and the lysis zone is 20 mm, and at a concentration of 1 mg/mL this value is 16 mm, which also indicates the significant antibacterial activity of this sample.

## References

[1] K. Ghandi and Y. Zeraatkish, Journal of NanoAnalysis, 1(2) (2014) 65-69.
[2] V. Knight, J.-J. Sanglier, D. Di Tullio, S. Braccili, P. Bonner, J. Waters, D. Hughes and L. Zhang, Appl. Microbiol. Biotechnol., 62 (2003) 446-458.

## Acknowledgment

This work was financially supported by the Ministry of Education and Science of the Kyrgyz Republic.

---

* Corresponding author, *E-mail: emil.omurzak@manas.edu.kg*

O-115

# Antibacterial Activity of Cu Nanoparticles Synthesized by the Electrical Discharge in Liquid

**Emil Omurzak**[1]*, **Asel Bekpolot kyzy**[1], **Ruslan Adil Akai Tegin**[2] **and Jyldyzai Ozbekova**[2]

[1]Kyrgyz-Turkish Manas University, Faculty of Engineering, Department of Chemical Engineering, Chyngyz Aitmatov Campus, Jal, 720038, Bishkek, Kyrgyzstan
[2]Kyrgyz-Turkish Manas University, Faculty of Engineering, Department of Food Engineering, Chyngyz Aitmatov Campus, Jal, 720038, Bishkek, Kyrgyzstan

*E-mail: emil.omurzak@manas.edu.kg*

Nano-sized silver particles are vastly studied because of growing demand in various fields such as chemical and biological sensing, electronics and optoelectronics applications owing to the highest electrical and thermal conductivity, energy harvesting, catalysis, imaging, and biomedicine [1,2]. One of the most important properties of silver nanoparticles (AgNPs) is their antimicrobial action against several bacteria, fungi, and viruses [3]. Surprisingly, AgNPs are safe and non-toxic to human and animal cells at low concentrations because the possible toxicity of AgNPs to the environment is considered extremely low as compared to other materials [4].

Silver nanoparticles (AgNPs) were prepared by solution-based chemical reduction routes and using pulsed plasma in a liquid. Silver nitrate was used as a precursor, tri-sodium citrate as reducing agents, while polyvinylpyrrolidone (PVP), cetrimoniumbromide (CTAB), Sodium n-Dodecyl Sulphate (SDS) were used as a stabilizing agent. Morphology, and structural properties of obtained nanoparticles were characterized by UV-visible spectroscopy (UV-VIS), and X-ray diffraction techniques. The characteristic surface plasmon resonance peaks of different spherical silver colloids occurring in the wavelength range of 397 to 504 nm, whereas triangular particles showed two peaks, first at 392 nm and second at 789 nm. The XRD spectra of the prepared samples indicated the face-centered cubic crystalline structure of metallic Ag nanoparticles. The in vitro antibacterial properties of all synthesized Ag nanoparticles against gram-negative bacteria Escherichia coli were examined by Kirby–Bauer disk diffusion susceptibility method. It was noticed that the stabilized with SDS AgNPs demonstrated a better antibacterial activity against bacterial strains as compared to the stabilized with PVP, CTAB AgNPs.

## References

[1] N.G. Bastus, F. Merkoci, J. Piella and V. Puntes, Chem. Mater., 26 (2014) 2836-2846.
[2] S. Iravani, H. Korbekandi, S.V. Mirmohammadi and B. Zolfaghari, Res. Pharm. Sci., 9 (2014) 385-406.
[3] S. Galdiero, A. Falanga, M. Vitiello, M. Cantisani, V. Marra and M. Galdiero, Molecules, 16 (2011) 8894-8918.
[4] N. Duran, P.D. Marcato, G.I.H. De Souza, O.L. Alves and E. Esposito, J. Biomed. Nanotechnol., 3 (2007) 203-208.

## Acknowledgment

This work was financially supported by the Ministry of Education and Science of the Kyrgyz Republic.

---

* Corresponding author, *E-mail: emil.omurzak@manas.edu.kg*

# Adsorption Kinetics of Malachite Green and Methylene Blue from Aqueous Solutions using Surfactant-modified Organoclays

**Haseeb Ullah[1], Muhammad Nafees[2], Farhat Iqbal[3],**
**Muhammad Saifullah Awan[4], Afzal Shah[1] and Amir Waseem[1]***

[1]Quaid-i-Azam University, Department of Chemistry, 45320, Islamabad, Pakistan
[2]Nanjing University, School of Chemistry and Chemical Engineering, State Key Laboratory of Coordination Chemistry, 210093, Nanjing, China
[3]University of Balochistan, Department of Statistics, Quetta, Pakistan
[4]Ibn-i-Sina Institute of Technology, H-11/4, Islamabad, Pakistan

*E-mail: chemist.ktk.06@gmail.com*

The main objective of this research is to study the adsorption behavior of malachite green and methylene blue dyes onto the surfactant modified natural clays [1]. The results of SEM, XRD, IR, and thermal analysis confirms the intercalation of organic moiety into the clay. The adsorption results show that pseudo-first order kinetics best fitted for both the dyes adsorbed on organo-clay. The data also reveal that both dyes are in a good agreement with Langmuir isotherm in both types of modified clays. The value of separation factor, $R_L$, from Langmuir equation and Freundlich constant, n, give an indication of favorable adsorption. The maximum adsorption capacity $q_m$ based on the Langmuir model was found to be 294-303 mg/g at 25 °C, is in good agreement with the experimental values.

**References**

[1] H. Ullah, M. Nafees, F. Iqbal, M.S. Awan, A. Shah and A. Waseem. Acta Chim. Slov., 64(2) (2017) 449-460.

---

* Corresponding author, *E-mail: waseem2000@hotmail.com*

# Synthesis & Characterization

O-117

# Anisotropy of Different Types of Alloys

**Fae'q A. A. Radwan***

Near East University, Faculty of Engineering, Lefkosa, KKTC

*E-mail: faeq.radwan@neu.edu.tr & frdwnk@gmail.com*

The norm of elastic constant tensor and the norms of the irreducible parts of the elastic constants of the alloys Iron-Silicon at different percentages of silicon, lead-indium at different percentages of indium, molybdenum-rhenium at different percentages of rhenium, niobium-hydrogen at different percentages of hydrogen, niobium-molybdenum at different percentages of molybdenum, niobium-oxygen at different percentages of oxygen, niobium-zirconium at different percentages of zirconium, palladium-rhodium at different percentages of rhodium, palladium-rhodium at different percentages of rhodium, and palladium-silver at different percentages of silver are calculated [1-3]. The relation of the scalar parts norm and the other parts norms and the anisotropy of the alloys are presented. The norm ratios are used as a criterion to present the anisotropy degree of the properties of the alloys [1,2].

## References

[1] F.A.A. Radwan, "Norm Ratio and Anisotropy Degree", Journal of Applied Sciences, Science Alert. 1, No. 3, 2001, PP, 301-304.
[2] F.A.A. Radwan, Science Alert, 1(3) (2001) 270-274.
[3] Landolt-Börnstein, Group III, "Crystal and Solid State Physics", Volume, 11, Springer-Verlag.

---

* Corresponding author, *E-mail: faeq.radwan@neu.edu.tr & frdwnk@gmail.com*

# Hybrid Systems Based on Perylene Diimide Derivatives or Ball-type Dinuclear Metallophthalocyanines for Photovoltaic Applications

**Abdurrahman Şengül***

Bülent Ecevit University, Faculty of Arts and Sciences, Department of Chemistry,
67100, Zonguldak, Turkey

*E-mail: sengul@beun.edu.tr*

Hybrid materials as triads and diads based on the symmetrically and unsymmetrically substituted perylene diimides (PDIs) appended at the imide positions with monodentate imidazole or pyridine ligands, and also bidentate chelating 1,10-phenanthroline ligand have been synthesized (Figure 1) [1]. Supramolecular self-assembly of these fluorescent bridging ligands with terpyridyl or bipyridine complex ions of platinum (II) and also palladium(II) have produced very soluble triads in organic and aqueous solution. These syntheses of these hybrids were inspired by the previous works based on the ball-type phthalocyanines showing better photovoltaic properties in comparison to those of mono-nuclear metallophthalocyanines. The isolated hybrid complexes were fully characterized by FT-IR, 1D-NMR ($^1$H NMR and $^{13}$C NMR), 2D-NMR ($^1$H-$^1$H COSY, $^1$H-$^{13}$C HSQC, $^1$H-$^{13}$C HMBC), MALDI TOF mass and UV-vis spectroscopy. The UV–vis spectra of the Pt(II) and Pd(II) complexes showed red-shifted and intense absorption bands derived from the conjugated structure of the new ligands. Here their electrochemical, spectroelectrochemical and photovoltaic properties are discussed.

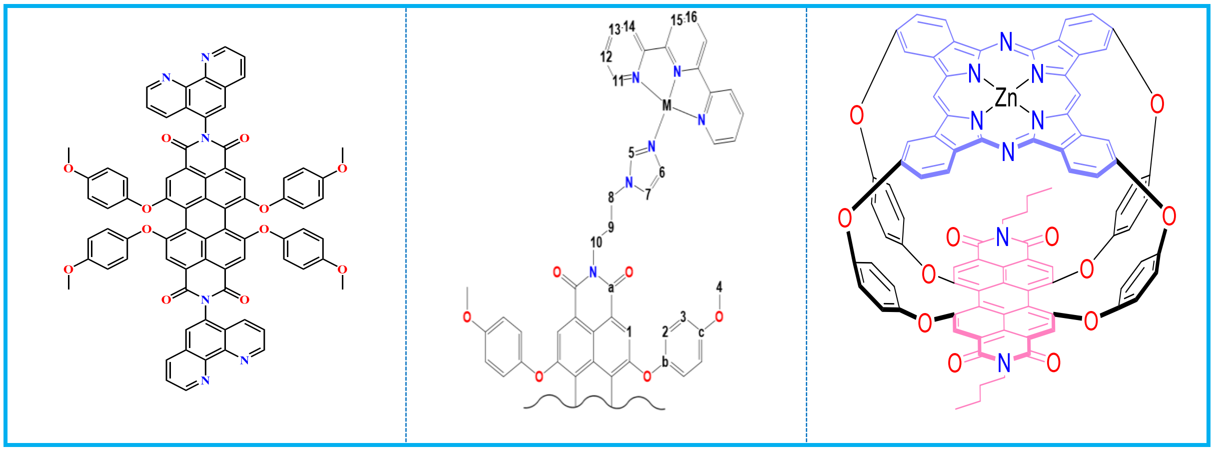


**Figure 1.** Hybrid materials for photovoltaic applications

**References**
[1] A. Sengul, S.I. Büyükekşi, E.B. Orman, A.R. Özkaya and A. Altındal, Dyes and Pigments, (2017), in press.

---

* Corresponding author, *E-mail: sengul@beun.edu.tr*

# Microwave-assisted Synthesis of 5-Hydroxymethylfurfural (5-HMF) over Metal Doped Alumina: Catalyst Screening Study

**Tuğçe Ayas[1], Halit L. Hoşgün[1]*, E. Zafer Hoşgün[2] and Ayşe Gül Türe[1]**

[1]Bursa Technical University, Department of Chemical Engineering, Bursa, Turkey
[2]Anadolu University, Department of Chemical Engineering, Eskişehir, Turkey

*E-mail: hlevent.hosgun@btu.edu.tr*

The fossil resources like oil, coal and natural gas are still primary energy and chemical sources. Lignocellulosic biomass has a potential as a renewable resource to fossil resources for energy and chemicals production. Lignocellulose, consist of cellulose, hemicellulose and lignin. Cellulose and hemicellulose are very important materials because they are transformed to C5 and C6 sugars. Bozell and Petersen identified many platform chemicals derived from C5 and C6 sugars in 2010. 5-hydroxymethylfurfural (5-HMF) and furfural were playing an important role as building block chemicals [1-3]. In this study, the effect of metal additives on the catalytic performances of alumina was investigated for the microwave-assisted synthesis of 5-Hydroxymethylfurfural from glucose. Zn, Ni, Cu, Fe and Cr doped alumina was synthesized by sol-gel method. All catalysts were characterized by nitrogen adsorption/desorption and X-Ray Diffraction method. Microwave-assisted experiments were carried out with a microwave oven (MILESTONE Ethos Easy) in Teflon vessels with 30 ml of water, 0.2 g of glucose and 0.2 g of catalyst. At the end of the treatment, the treated slurry was filtered to separate the solid and liquid fractions for further analysis. Compositions of liquid products were analyzed by high-performance liquid chromatography [4]. Catalyst screening experiments of metal doped catalysts for the transformation of glucose into 5-HMF were listed in Table 1. In the presence of 5% Cu doped alumina catalyst gave higher selectivity than other catalysts in the 5-HMF yields. On the other hand, 5%Ni has the highest glucose conversion.

**Table 1.** Conversion of glucose into 5-HMF by metal doped alumina catalysts

| **Catalysts** | **5% Ni** | **5% Cu** | **5% Cr** | **5% Fe** | **5% Zn** | **10% Ni** | **10% Cu** | **10% Cr** | **10% Fe** | **10% Zn** |
|---|---|---|---|---|---|---|---|---|---|---|
| **Glucose conversion (%)** | 84.07 | 79.69 | 17.74 | 83.38 | 71.38 | 70.40 | 28.48 | 43.71 | 57.77 | 46.46 |
| **5-HMF yields (%)** | 22.02 | 24.15 | 5.38 | 20.74 | 20.82 | 20.15 | 2.88 | 9.81 | 24.70 | 5.60 |

## References

[1] J. Liu, H. Li, Y.C. Liu, Y.M. Lu, J. He, X.F. Liu, Z.B. Wu and S. Yang, Catalysis Communications, 62 (2015) 19-23.
[2] A. Corma, S. Iborra and A. Velty, Chemical Reviews, 107 (2007) 2411-2502.
[3] J. J. Bozell and G. R. Petersen, Green Chemistry, 12 (2010) 539-554
[4] A. Sluiter, B. Hames, R. Ruiz, C. Scarlata, J. Sluiter and D. Templeton, (2006), National Renewable Energy Laboratory, Golden, CO.

---

* Corresponding author, *E-mail: hlevent.hosgun@btu.edu.tr*

O-120

# Synthetization and Characterization of Silver Nanoparticles from Black Morus Nigra and Its Applications in Microbial Activities

**Muhammad Arshad[1], Zainab Hussain[2] and Ghulam Hussain Bhatti[3]***

[1]Govt. Post Graduate Islamia College, Gujranwala, Pakistan
[2]Superior University, Department of Chemistry, Gujranwala, Pakistan [3]Presenting
[3]Cadet College Hasan Abdal Attock 43730, Pakistan

*E-mail: chemgcu@gmail.com*

Silver nanoparticles were synthesized by using green synthetic method in which various concentrations of silver nitrate $AgNO_3$ and Black Morus Nigra leaf extract have been used (Figure 1). The changing in color while performing the experiment indicates the formation of silver nanoparticles. Several techniques like (TGA, XRD, and SEM) were being used for the characterization of silver nanoparticles. Silver nanoparticles have several applications on microbial activities (bacterial action). Some of these applications were being discussed here. The Morus nigra is an excellent source of iron [1]. It is also a good source of minerals like potassium, magnesium and copper [2]. It contains some specific qualities which are successful for the cure of cancer [3].

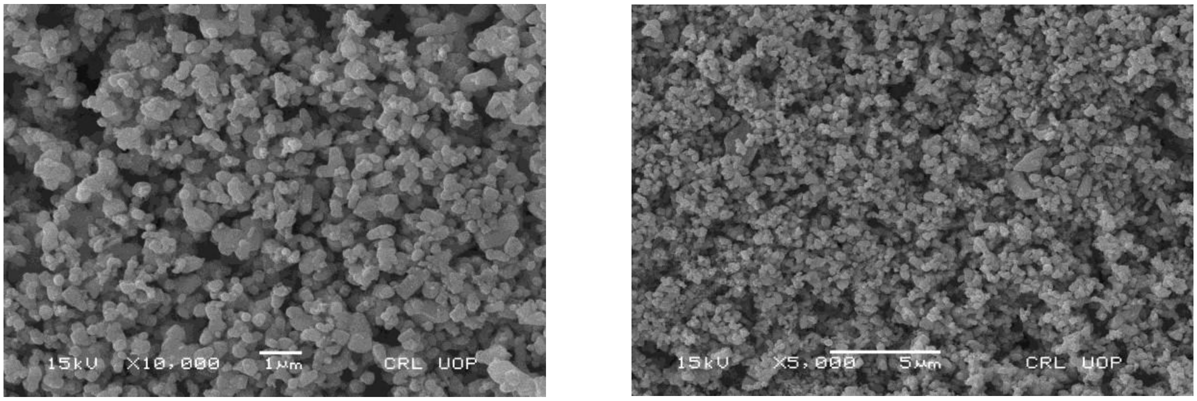


**Figure 1.** SEM pictures of the nano particles synthesized in 0.2 and 0.1 concentrations

## References

[1] J. Ahmad, A.H. Farooqui and T.O. Siddiqui, Morus Nigra Hamdard Med., 15 (1985) 76-78.
[2] D. Bown, 1995. Encyclopadia of Herbs and Their Uses, Dorling, London, U.K.
[3] R. Channabasava, M. Govindappa, Bangladesh J. Pharmacol., 9 (2014) 129-139.

---

* Corresponding author, *E-mail: chemgcu@gmail.com*

# Synthesis, Spectroscopic and Thermal Studies of Copper(I) Chlorido Complexes of Thioureas

**Muhammad Mufakkar[1], Ghulam Hussain Bhatti[2]*, Shakil Ahmad[3] and Maryem Rana[4]**

[1]Department of Chemistry, Govt. College Ravi Road Shahdara Lahore 54950, Pakistan
[2]Cadet College Hasan Abdal, Attock 43730, Pakistan
[3]Department of Chemistry, Govt. MAO College Lahore 54890, Pakistan [4]Department of Chemistry, Govt. College of Science, Wahdat Road Lahore 54890, Pakistan

*E-mail: chemgcu@gmail.com*

The study of the coordination behavior of thiones is of considerable interest due to the similarity of their binding sites to those in living systems [1]. The complexation of thiones towards Copper(I) has also received considerable attraction in view of their variable bonding modes, structural diversity and promising biological implications [2,3]. Copper (I) complexes of thioureas of the general formula: CuLCl, $CuL_2Cl$ and $CuL_3Cl$ [where L= Thiourea and its N-and N, N/- mono and di alkyl and phenyl derivatives] have been prepared using Cu(I)CN in the presence of HCl. The complexes have been characterized by thermal technique, IR (Figure 1 and Figure 2) and NMR ($^1$H and $^{13}$C) spectroscopy. An upfield shift in $^{13}$C NMR and downfield shifts in $^1$H NMR are consistent with the sulfur coordination to Copper(I) [4,5]. The disappearance of a band around 2200 cm$^{-1}$ in IR and a resonance around 146 ppm in $^{13}$C NMR indicates that during the course of the reaction the cyanide group of the Copper(I) salt has been replaced by chloride leading to the formation of chlorido complexes.

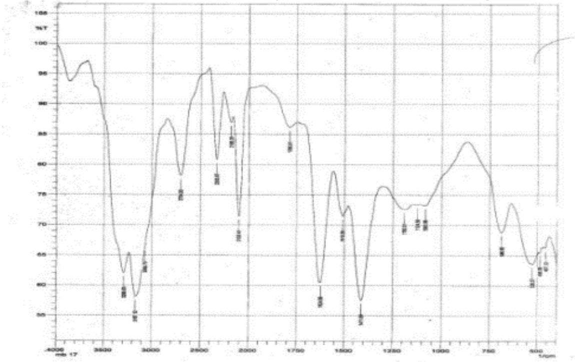


**Figure 1.** IR spectrum of Cu(Tu)Cl

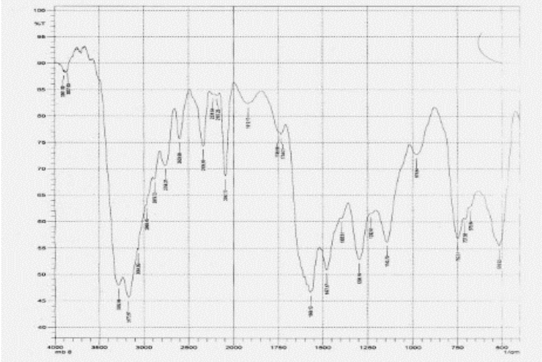


**Figure 2**. IR spectrum of $Cu(Metu)_4Cl$

## References

[1] P. Zoufala, T. Ruffer, H. Lang, S. Ahmad and M. Mufakkar, Anal. Sci., 23 (2007) 219.
[2] G. Marverti, M. Cusumano, A. Ligabue, M.L. Di Pietro, P.A. Vainiglia, A. Ferrari, M. Bergomi, M.S. Moruzzi and C. Frassineti, J. Inorg. Biochem., 102 (2008) 699.
[3] F.B. Stocker, M.A. Troester and D. Britton, Inorg. Chem., 35 (1996) 3145.
[4] M. Fettouhi, M.I.M. Wazeer and A.A. Isab, J. Coord. Chem., 60 (2007) 369-377.
[5] A.A. Isab and M.I.M. Wazeer, J. Coord. Chem., 58 (2005) 529-537.

---

* Corresponding author, *E-mail: chemgcu@gmail.com*

# The Effect of Leaving in the Electrophilic Amination of Diarylcadmium Reagents

**Tahir Daşkapan**[1] and **Adem Korkmaz**[2]*

[1]Ankara University, Science Faculty, Department of Chemistry, Ankara-Turkey
[2]Muş Alparslan University, Technical College Vocational School, Muş-Turkey

*E-mail: a.korkmaz@alparslan.edu.tr*

In this work, the synthesis of functionalized aryl amines, which are used in important chemical processes such as drug and dye synthesis [1-3], by electrophilic amination of diarylcadmium reagents with *o*-substituted ketoximes is given. The effect of leaving group of the oxime on the amination reaction and thus on the yield of aryl amine was investigated using acetone *O*-(4-fluorophenylsulfonyl)oxime and acetone *o*-(methylsulfonyl)oxime, as electrophilic amination reagents (Figure 1). The results showed that, the presence of an electron withdrawing on the leaving group increased the success of electrophilic amination reaction to give aryl amines in higher yields.

$$Ar_2Cd + (CH_3)_2C{=}NOSO_2LG \xrightarrow{CuCN} \left[(CH_3)_2C{=}NAr\right] \xrightarrow{Conc.\ HCl} ArNH_2$$

Ar : Phenyl, 4-methylthiophenyl, 4-methoxyphenyl, 3-methoxyphenyl, 4-chlorophenyl, 3-chlorophenyl, 3,5-dichlorophenyl, 3,5-dimethoxyphenyl, 4-methylphenyl, 2,5-Dimethylphenyl, 4-fluorophenyl, 4-chloro-2-methylphenyl, 1-naphtyl.
LG : 4-Fluorophenyl, Methyl

**Figure 1.** Aryl C-N bond formation by electrophilic amination of diarylcadmiums with acetone O-(4-fluorophenylsulfonyl)oxime and acetone O-(methylsulfonyl)oxime

All reactions involving organocadmium reagents were performed in flame-dried glassware with standard syringe / cannula techniques under an atmosphere of dry, oxygen-free argon. Arylamines as the final products were isolated as their *N*-benzoyl derivatives and these known compounds were identified from their melting points and $^1$H NMR spectrums.

**References**

[1] T. Daşkapan, Arkivoc, 230-262 (2011).
[2] A. Ricci; Amino Group Chemistry, From Synthesis to the Life Sciences; Wiley-VCH: Weinheim, (2007).
[3] E. Ciganek; Organic Reactions, (Editor: Denmark, S. E.) John Wiley & Sons, Inc., 72 (2009).

**Acknowledgement**

Financial supports from Ankara University Research Fund (grant no. 15L0430009) and Turkish Higher Education Council (ÖYP Program) are greatly acknowledged by the authors.

---

* Corresponding author, *E-mail: a.korkmaz@alparslan.edu.tr*

O-123

# Fluorescence of Indoles on Zeolite-Polymer Multilayers

**Dilek Ünal**[1]* and Tayfun Taş[2]

[1]Hacettepe University, Faculty of Medicine, 06100, Ankara, Turkey
[2]METU, Department of Micro and Nanotechnology, 06800, Ankara, Turkey

*E-mail: dlkunal@hotmail.com*

Indoles are significant molecules for biological activity. They exist as regulatory molecules, pharmaceutical agents or metabolites in biosystems. Sensitive determination of indoles in biofluids plays an important role in diagnosis of biosystem disorders or dysfunctions [1]. Fluorescence is a sensitive method for the evaluation of indolic molecules; concentrations as low as $10^{-8}$ $molL^{-1}$ can be detected for tryptophan [2]. Fluorescence intensity can be enhanced by changing a number of variables such as increasing the rigidity of the fluorescent molecule or changing the pH of the medium [3]. In this study, fluorescence of indolic molecules with various substituents on zeolite-polymer multilayers has been studied.

**References**

[1] N.K. Kaushik, N. Kaushik, P. Attri, N. Kumar, C.N. Kim, A.K. Verma and E.H. Choi, Molecules, 18 (2013) 6620-6662.
[2] D.M. Reynolds, Water Research, 37 (2003) 3055-3060.
[3] X. Meng, T. Harricharran and L.J. Juszczak, Photochemistry and Photobiology, 89(1) (2013) 40-50.

---

***** Corresponding author, *E-mail: dlkunal@hotmail.com*

O-124

# Preparation of Organically-linked Silica Membranes

**Tuğçe Kurt and Berna Topuz***

Ankara University, Faculty of Engineering, Department of Chemical Engineering,
06100, Ankara, Turkey

*E-mail: tugkurtt93*@gmail.com

In the field of separation research, the basic objective is to develop robust high-flux molecular sieving inorganic membranes with polymer-like flexibility by cheap and simple ways. Such membranes will greatly reduce the energy consumption used in separation and purification processes in chemical and petroleum industry. It is important to design hydrothermally stable membrane microstructures, with fine and well-controlled pore structure, to increase the efficiency of membrane processes used in separation technologies. The purpose of this work is to fabricate hydrophobic, ultra-thin (ca. 100 nm), and high-performance silica based microporous membranes by using low cost of sol-gel processing.

Up to now, surface hydroxyl ions have been found to limit their use in the amorphous silica membranes prepared by the sol-gel method, causing their structural stability to weaken in the water vapor environment and in high temperature applications. Organic-inorganic hybrid silica membranes prepared, using the precursor molecule modified with organic group, by sol-gel method have improved hydrothermal stability because they show more hydrophobic property due to Si-$(C)_n$-Si bonds formed in the microstructure [1,2]. The hydrothermal stability of the membranes produced by this approach is increasing proportionally to the size of the organic molecule added to the structure. Since the membrane pore size/affinity can be controlled by this method, water vapor-resistant hybrid organic-inorganic silica membranes are mostly used for pervaporation, but their use for separating gas molecules with small kinetic diameters is limited.

Hydrophobic silica membrane with a thickness of less than 80 nm was prepared on graded alumina supports which resulted in a helium permeance of $6.6\text{x}10^{-7}$ $\text{molm}^{-2}\text{s}^{-1}\text{Pa}^{-1}$ and a He/$N_2$ ideal selectivity of 6.5. This is the thinnest ceramic supported organosilica membrane reported.

## References

[1] M. Kanezashi, K. Yada, T. Yoshioka and T. Tsuru, J. Am. Chem. Soc. 131 (2009) 414-425.
[2] H.L. Castricum, A. Sah, R. Kreiter, D.H.A. Blank, J.F. Vente and J.E. ten Elshof, Chemical Communication, (2008) 1103-1105.

---

***** Corresponding author, *E-mail: topuzb@ankara.edu.tr*

O-125

# Synthesis, Characterization and Application of a Novel Multifunctional Stationary Phase for Hydrophilic Interaction/Reversed Phase Mixed-mode Chromatography

**Hayriye Aral***, K. Serdar Çelik, Ramazan Altındağ and Tarık Aral

University of Batman, Faculty of Science and Art, Department of Chemistry, Batman, Turkey

*Email: hayriye.aral@batman.edu.tr*

A novel multifunctional stationary phase was synthesized starting from L-isoleucine and 4-phenylbutylamine and evaluated as a hydrophilic interaction/reversed-phase mixed-mode stationary phase for high-performance liquid chromatography (HPLC). The prepared stationary phase was characterized by elemental analysis, infrared spectroscopy, scanning electron microscopy, Brunauer, Emmett and Teller and solid-state $^{13}$C NMR. Successful separation could be achieved among several aromatic compounds having different polarities under both hydrophilic interaction liquid chromatography (HILIC) and reversed phase (RP) condition. The effects of different separation conditions, such as pH value, mobile-phase content, column temperature, buffer concentration and flow rate, on the separation of nucleotides/nucleosides in HILIC mode were investigated. The six of them were separated within 10 minutes by isocratic elution under HILIC condition. To determine the influence of the new multifunctional stationary phase under the RP condition, a number of moderately and weakly polar and nonpolar compounds, such as 10 substituted anilines and eight substituted phenols were separated successfully under the RP condition. Additionally, nine mixtures of polar/nonpolar test compounds were simultaneously separated under HILIC/RP mixed-mode conditions. Compared to traditional C18 and commercial HILIC columns, the new stationary phase exhibited both HILIC and RPLC performance, and the scope of analyte separation was thus enlarged [1-2].

## References

[1] T. Aral, H. Aral, B. Ziyadanoğulları and R. Ziyadanoğulları, Talanta, 131 (2015) 64-73.
[2] H. Aral, K. Serdar Çelik, R. Altındağ and T. Aral, Talanta, 174 (2017) 703-714.

## Acknowledgement

University (BTÜBAP) (Project No: BTÜBAP-2012-FED-03).
The authors gratefully acknowledge the financial support provided by the Research Project Council of Batman.

---

* Corresponding author, *E-mail: hayriye.aral@batman.edu.tr*

O-126

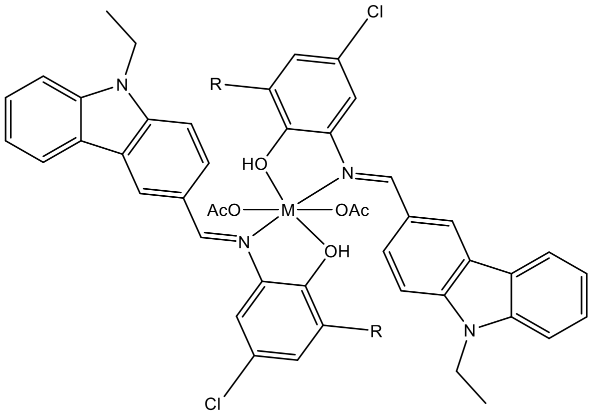
# Carbazole Derived Compounds, Synthesis, Elucidation, Catalytic and Thermal Features

**Selma Bal***

Kahramanmaraş Sütçü İmam University, Faculty of Science, Department of Chemistry, 46100, Kahramanmaraş, Turkey

*E-mail: selmadagli9@hotmail.com*

As a result of their synthetic adaptability, imines and their coordination compounds had been and are yet being examined comprehensively up until present day. They had caused great awareness among the many areas like biological functioning, catalytic power and exceptionally in olefin oxidations [1], ring breachings of epoxides [2]. Two Novel ligands and their Cobalt (II), Manganese (II) and Nickel (II) coordination compounds have been synthesized (Figure 1) and elucidated through many spectroscopic approaches. Catalytic activities of the synthesized and elucidated ligands have been searched in the oxidations of styrene and cyclohexene. Manganese (II) coordination compounds of the ligands proved the highest catalytic power in alkene oxidations. Synthesized complex compounds showed good stability thermally and proved that they could be practiced as catalysts in chemical experiments demanding extreme conditions. All the new compounds were further presented for their electronic characteristics.



M: Cobalt(II), Manganese(II), Nickel(II)

**Figure 1.** Chemical structure of compounds

**References**

[1] A. Mavrogiorgoua, M. Papastergioua, Y. Deligiannakis, M. Louloudi, J. Mol. Catal. A-Chem. *393* (2014), 8-17.

[2] V.I. Maleev, D.A. Chusov, L.V. Yashkina, N.S. Ikonnikov, M.M. II'in, Tetrahedron-Asymmetr. *25* (2014), 838-843.

---

* Corresponding author, *E-mail: selmadagli9@hotmail.com*

O-127

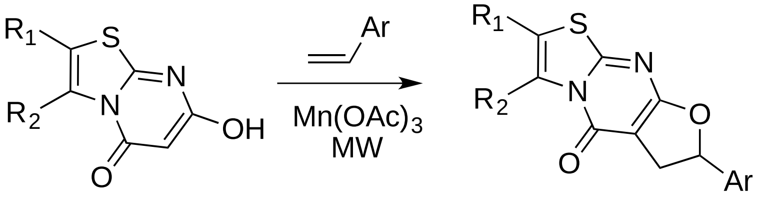
# Microwave Assisted Synthesis and Acetylcholine Esterase Inhibition of 6,7-Dihydro-5*H*-furo[2,3-*d*]thiazolo[3,2-*a*]pyrimidin-5-ones

**Aslı Ustalar** and **Mehmet Yılmaz***

Kocaeli University, Faculty of Art and Science, Department of Chemistry, 41380, Kocaeli, Turkey

*E-mail: asliustalar@hotmail.com*

Heterocyclic ring systems such as thiazole, thiazolopyrimidine and dihydrofuran form the skeletal structures of molecules displaying a wide-range of biological activities. Thiazole containing compounds have been reported to show antitumor, antimicrobial, anthelmintic, anti-leishmanial, anticonvulsant and anti-inflammatory effects [1]. Ritanserin [2] and setoperone [3] are thiazoloprymidine containing drugs used in the treatment of psychological diseases. Also, it has been reported the radical addition and cyclization of various active methylene compounds to unsaturated systems using manganese(III) acetate and cerium(IV) ammonium nitrate, resulting in the formation of functionalized dihydrofurans containing compounds [4]. A new class of compounds, 6,7-dihydro-5*H*-furo[2,3-*d*]thiazolo[3,2-*a*]pyrimidin-5-ones, were synthesized *via* the microwave assisted radical addition of compounds 7-hydroxy-5*H*-thiazolo[3,2-*a*]pyrimidin-5-one to various alkenes using manganese(III) acetate (Figure 1). Also, inhibition effects against acethylcholine esterease was investigated. AchE inhibition of compound **4e** showed excellent (92%) inhibitory potential, comparable with the standard drug Donapezil®



4 examples
60-98% yield

15 examples
80-90% yield

**Figure 1.** Synthesis steps of compounds 7-hydroxy-5*H*-thiazolo[3,2-*a*]pyrimidin-5-ones

## References

[1] A. Rana, N. Siddiqui and S. A. Khan, Indian J. of Pharm. Sci. 69 (2007) 10-17.
[2] S. Akhondzadeh, M. Malek-Hosseini, A. Ghoreishi, M. Raznahan and S.A. Rezazadeh, Prog. Neuro-Psychoph., 32 (2008) 1879-1883.
[3] R. Lewis, S. Kapur, C. Jones, J. DaSilva, G.M. Brown, A.A. Wilson, S. Houle and R.B. Zipursky, Am. J. Psychiat., 156 (1999) 72-78.
[4] B. Gregory, A.F. Parsons, C.B. Thomas, Tetrahedron, 57 (2001) 4719-4728.

---

* Corresponding author, *E-mail: mehmet.yilmaz@kocaeli.edu.tr*

# Novel Thiazolo[3,2-*c*]pyrimidine-based Anticancer Molecules

Muhammet Yıldırım[1]*, Arzu Yıldırım[2] and Derya Çelikel[1]

[1]Abant İzzet Baysal University, Faculty of Arts and Sciences, Department of Chemistry, 14030, Gölköy, Bolu
[2]Abant İzzet Baysal University, Faculty of Agricultural and Natural Sciences, Department of Field Crops, 14030, Gölköy, Bolu

*Email: muhammetyildirim@ibu.edu.tr*

For two decades, microwave energy has been frequently using in many types of organic reactions due to its various advantages [1]. Besides, heterocyclic enamines are important key building blocks for the preparation of natural products [2,3]. More specifically, studies utilizing the β-substituted enamines (**3**), and electrophiles (aldehydes, ketones, acyl chlorides, isocyanates) are very rare in recent literature [2,3]. Moreover, thiazolopyrimidine derivatives constitute the main body of important molecules exhibiting various biological activities. Especially, thiazolo[4,5-*d*]pyrimidines and thiazolo[3,2-*a*]pyrimidines, which are S-analogs of purine bases, attracts great attention by the researchers developing new drug molecules. Molecules having those two main structures are known to exhibit various biological activities such as antitumor, immunomodulator, antimicrobial, antiinflammatory, antipsychotics, antiparkinson and anticancer [5]. In the present work, as third derivative, novel thiazolo[3,2-*c*]pirimidines (**6a-b**), which are not present in recent literature, have been synthesized in short reaction times with excellent yields by multicomponent reactions of *β*-substituted enamines (**3a-b**) with formaldehyde and different amines under microwave or conventional heating conditions [4]. After that, novel thiazolo[3,2-*c*]pirimidines were fully characterized by means of physical and spectroscopic techniques (IR, NMR, MS).

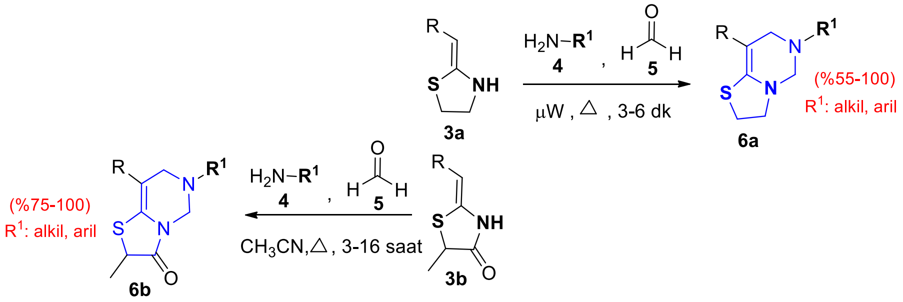


**Figure 1.** Route for preparation of anticancer thiazolo[3,2-*c*]pyrimidines

Finally, isolated **6a-b** derivatives in different concentrations were subjected to some cytotoxic activity studies on different cancer cell lines. It has been understood that at least six of **6a-b** derivatives exhibited strong cytotoxic effects on human breast (MCF-7) and liver (Hep/G2A) carcinoma cell lines when treated at very low doses.

## References

[1] C.R. Strauss, Microwaves in Organic Synthesis [Ed.: A. Loupy), Wiley-VCH, Weinheim (2002) 35-60.
[2] A. Zhang and J.L. Neumeyer, Organic Lett., 5 (2003) 201-203.
[3] S. Rajappa, Tetrahedron, 37 (1981) 1453-1480.
[4] M. Yıldırım, D. Çelikel, Y. Dürüst, D.W. Knight and B.M. Kariuki, Tetrahedron, 70 (2014) 2122-2128.
[5] A.E. Amr, M.M. Ashraf, F.M. Salwa, A.A. Nagla and A.G. Hammam, Bioorg. Med. Chem., 14 (2006) 5481-5488.

---

* Corresponding author, *Email: muhammetyildirim@ibu.edu.tr*

O-129

# Copper(II)-Catalysed Asymmetric Henry (Nitroaldol) Reactions: Recent Developments

**Leman Alkan*** and Stephen T. Astley

Ege University, Faculty of Science, Department of Chemistry, İzmir, Turkey

*E-mail: alkanleman@gmail.com*

The Henry or nitroaldol reaction is an important route for the construction of carbon-carbon bonds in synthetic chemistry (Figure 1). The chiral product of this asymmetric reaction is of particular interest. For example, the corresponding adducts can be easily transformed into valuable functionalized structural motifs, such as chiral β-amino alcohols and α-hydroxy carboxylic acids [1,2].

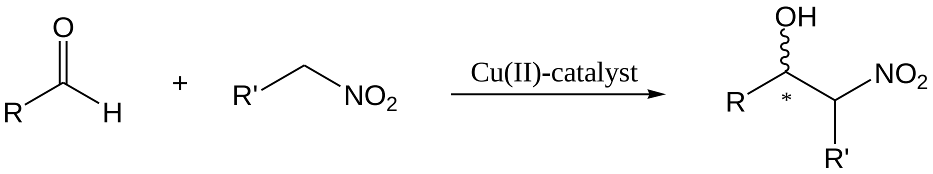


**Figure 1.** Henry (nitroaldol) reaction

Since the pioneering work of Shibasaki [3], where the heterobimetallic catalyst was used, various versions of metal-catalyzed asymmetric Henry reactions have been described. Copper has a special place among the metals used as catalysts because it is a cheap, low toxicity metal and has been widely used in organic synthesis. The excellent chelating properties of that metal allow coordination of it with bidentate as well as with polydentate ligands. Copper(II) complexes with various ligands, which include bisoxazolines [4], bisoxazolidines [5], $C_2$-symmetric diamines [6] and, in particular, chiral Schiff bases [7] catalyze an asymmetric Henry reaction.

## References

[1] B.M. Trost, V.S.C. Yeh, H. Ito and N. Bremeyer, Org. Lett., 42 (2002) 621-2623.
[2] T. Kudoh, T. Ishikawa, Y. Shimizu and S. Saito, Org. Lett., 5 (2003) 3875-3878.
[3] H. Sasai, T. Suzuki, S. Arai, T. Arai and M. Shibasaki, J. Am. Chem. Soc., 114 (1992) 4418-4420.
[4] D. Didier and E. Schulz, Tetrahedron: Asymmetry, 24 (2013) 769-775.
[5] Q. Liang, J. He and B. Ni, Tetrahedron: Asymmetry, 25 (2014) 1146-1149.
[6] J. Cho, G.H. Lee, S. Nayab and J.H. Jeong, Polyhedron, 99 (2015) 198-203.
[7] A. Akıncı, D.B. Celepci, L. Alkan, N. Korkmaz, M. Aygün and S.T. Astley, Appl. Organometal. Chem. article in press.

---

* Corresponding author, *E-mail: alkanleman@gmail.com*

# Synthesis, Spectroscopic Properties and Biological Activities of *spiro*-4-methoxybenzylaminophosphazenes

**Nur Güven Kuzey**[1], **Nuran Asmafiliz**[1]*, **Leyla Açık**[2] **and Tuncer Hökelek**[3]

[1]Ankara University, Faculty of Science, Department of Chemistry, Ankara, Turkey
[2]Gazi University, Faculty of Science, Biological Science, Ankara, Turkey
[3]Hacettepe University, Faculty of Science, Department of Physics, Ankara, Turkey

*E-mail: nurrguven@gmail.com*

The chemistry of cyclophosphazenes $[NPX_2]_n$ (n=3-40; X=halogens, different inorganic, organic and organometallic substituents) has attracted attention, especially in terms of Cl replacement reactions $[NPCl_2]_n$ (n = 3; trimer, n=4; tetramer) with the different nucleophilic reagents for the syntheses of a wide range of cyclotri- and tetraphosphazenes, polyorganophosphazenes and coordination compounds of the phosphazene ligands [1]. Hexachlorocyclotriphosphazene (cyclic trimer, $N_3P_3Cl_6$) is used largely for the preparation of many phosphazene frameworks with mono-, di- and multi-functional reagents [1,2]. In this study, the reactions of 4-methoxybenzaldehyde with the appropriate aliphatic diamines (N-methyl-ethylenediamine, N-ethyl-etylenediamine, N-methyl-1,3-diaminopropan) produced N/N donor-type bidentate ligands. The condensation reactions of $N_3P_3Cl_6$ with the synthesized ligands gave the new tetrachloro spiro-trimeric phosphazenes. The partly substituted phosphazenes reacted with pyrrolidine and piperidine to give tetrapyrrolidino- and tetrapiperidino compounds (Figure 1). The structures of all the phosphazenes were evaluated using FTIR, MS, $^1$H, $^{13}$C{$^1$H} and $^{31}$P{$^1$H} NMR spectral data. The crystal structure of one compound was determined using X-ray crystallography. Besides, DNA interactions and antimicrobial activity against some G(+) and G(-) bacteria and fungi of the partly and fully substituted phosphazenes were investigated.

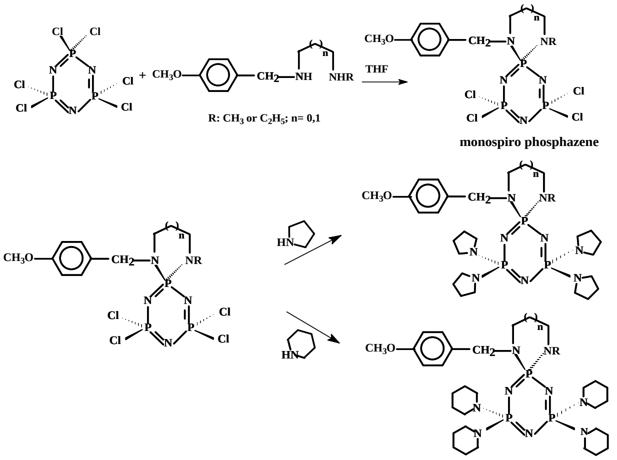


**Figure 1.** The reaction pathway of the N/N-substituted trimeric phosphazene derivatives

**References**
[1] M. Gleria and R. De Jaeger, Phosphazenes: A Worldwide Insight, Nova Publishers, 2004.
[2] N. Asmafiliz, Z. Kılıç, M. Civan, O. Avcı, L.Y. Gönder,L. Açık, B. Aydın, M. Türk and T. Hökelek. New. J. Chem., 40 (2016) 9609-9626.

---

* Corresponding author, *E-mail: gurun@science.ankara.edu.tr*

# Effective Synthesis of 3-Pyrrolin-2-one Derivatives using Aromatic Amine Compounds

**İbrahim Evren Kıbrız**[1]*, **Mustafa Saçmacı**[1] **and İsmail Yıldırım**[2]

[1]Bozok University, Faculty of Arts and Science, Department of Chemistry, 66100, Yozgat, Turkey
[2]Erciyes University, Faculty of Science, Department of Chemistry, 38039, Kayseri, Turkey

*E-mail:e.kibriz@hotmail.com*

Lactams such as 3-pyrrolin-2-one and its derivatives have shown anti-tumor activity. In the recent years, *N*-substituted maleimides and 3-pyrrolin-2-ones have received growing attention [1-4] due to their biological activity features and potencies for organic synthesis as key compounds for the synthesis of bio-active molecules, which are *Oteromycin, Talaroconvolutin A, Azaspirene, Fusarin and Clausenamide*..., etc. [5,6].

In this study, a new 3-pyrrolin-2-one compounds (**3a-d**) were synthesized from 2-aminooxazole (**1**) and aromatic amines (**2**) by refluxing in methanol (Figure 1). The product was characterized by molecular spectroscopic techniques (FT-IR, $^{1}$H-NMR and $^{13}$C-NMR) and HRMS analysis.

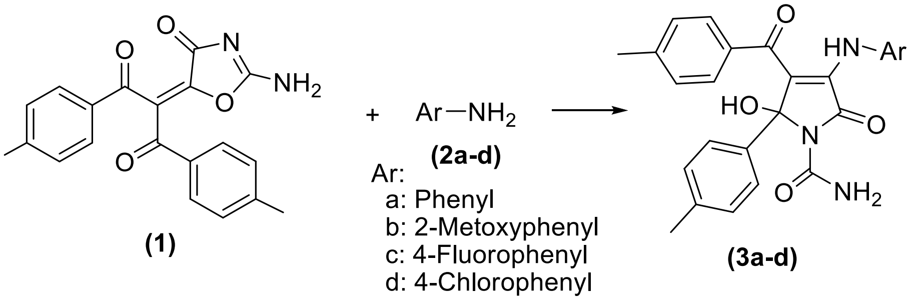


**Figure 1.** Synthesis of Compounds **3a-d**

**References**
[1] S. Kiren, X. Hong, C.A. Levertt and A. Padwa, Tetrahedron, 65 (2009) 6720-6729.
[2] M. Dubernet, V. Caubert, J. Guillard, M.C. Massuard, Tetrahedron 61 (2005) 4585-4593.
[3] J. Clayden, D.W. Watson, M. Helliwel and M. Chambers, Chem. Commun., 2582 (2003) 2582-2583.
[4] A. Alizadeh, A. Rezvanian and L.G. Zhu, Helv. Chim. Acta, 90 (2007) 2414-2420.
[5] B.B. Snider and S.B. Neubert, J. Org. Chem., 69 (2004) 8952-8955.
[6] Z. Feng, X. Li, G. Zheng and L. Huang, Bioorg. Med. Chem. Lett., 19 (2009) 2112-2115.

**Acknowledgement**
This study was supported financially by Bozok University Project Coordination Application and Research Center (Project No.: 6602c-FEF/17-72).

---

* Corresponding author, *E-mail: e.kibriz@hotmail.com*

# Mn(Oac)$_3$ Mediated Synthesis of Novel Piperazine Bearing Dihydrofurans and Investigation of Their Enzyme Inhibiton Capabilities. Part 1

**Sait Sarı and Mehmet Yılmaz***

Kocaeli University, Faculty of Arts and Sciences, Department of Chemistry, 41380, Umuttepe, Kocaeli, Turkey

*E-mail: sait.sari@kocaeli.edu.tr*

Dihydrofurans are a significant class of compounds since they show a wide range of biological activities and form the basic structure of many natural compounds [1]. It is known that dihydrofurans can be synthesized from transition metal salts capable of transferring single electrons that form α-carbon radicals with enolizable functional groups and the addition of this radical to unsaturated system can be used to generate new C-C bonds. Among these metal salts, manganese(III) acetate and cerium(IV) ammonium nitrate are widely used [2]. Piperazine is an organic compound that consists of a six membered ring containing two nitrogen atoms at opposite positions in the ring. Piperazine derivatives are one of the most important heterocyclic class of compounds which have diverse biological and farmacological activities [3,4]. In this study, dihydrofurans connected to piperazines were synthesized by oxidative radical cyclization between α,β-unsaturated diacyl piperazines and 1,3-dicarbonyl compounds, mediated by Mn(OAc)$_3$ (Figure 1). These molecules were characterized by NMR spectroscopy, and their enzyme inhibition capabilities were studied.

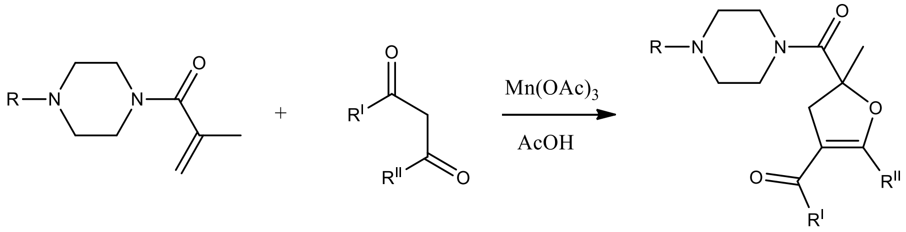


**Figure 1.** Synthesis of Mn(OAc)$_3$ mediated dihydrofuran compounds

## References

[1] F.M. Dean and A.R. Katritzky (Ed.), Advances in Heterocyclic Chemistry, 30 (1982) 167-238.
[2] A. Ustalar and M. Yılmaz, Tetrahedron Lett., 58 (2017) 516-519.
[3] M. Rudrapal and B. De, Int. Res. J. Pur. Appl. Chem., 3 (2013) 232-249.
[4] A.C. Tripathi, S.J. Gupta, G.N. Fatima, P.K. Sonar, A. Verma and S.K. Saraf, Eur. J. Med. Chem., 72 (2014) 52-77.

## Acknowledgement

This study was financially supported by the Scientific and Technical Research Council of Turkey (TBAG-116Z455). S. SARI thanks to TUBITAK for doctoral fellowship.

---

* Corresponding author, *E-mail: mehmet.yilmaz@kocaeli.edu.tr*

# Regioselective Synthesis of Some Novel Isoxazolidines and Isoxazoles Carrying Caprolactam Moiety

**Akın Sağırlı*** and Yaşar Dürüst

Abant İzzet Baysal University, Department of Chemistry, 14030, Bolu, Turkey

*E-mail: sagirli_a@ibu.edu.tr*

Isoxazole and isoxazolidine cores have significant importance of being a part of many biologically active compounds. They are known to exhibit analgesic [1], antibacterial [2], anticancer [3] and antifungal [4] properties. On the other hand, ε-caprolactams have drawn great attention in the construction of many heterocycles [5]. Taking into account of the above considerations, we have focused, in this study, on the synthesis of various isoxazoles and isoxazolidines bearing ε-caprolactam ring (Figure 1). 16 New aryl substituted 2-methyl-3-phenylisoxazolidin-5-yl)azepan-2-ones and (3-phenyl-4,5-dihydroisoxazol-5-yl)azepan-2-ones were obtained regioselectively by the means of the cycloaddition reaction of nitrones and nitrile oxides with *N*-vinyl caprolactam, respectively. The structures and absolute configurations of the cycloadducts were fully characterized by spectral/physical methods including X-ray diffraction data.

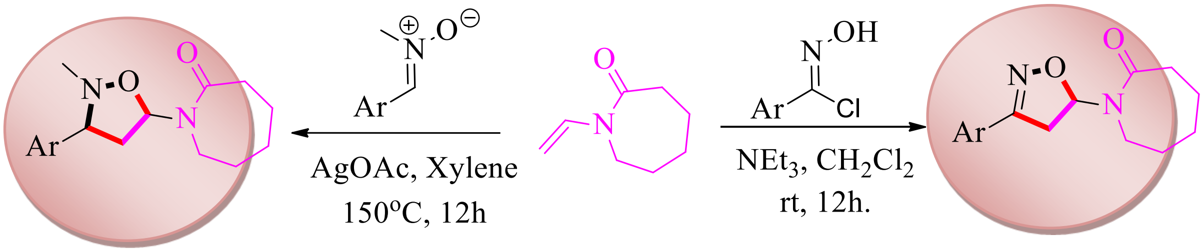


**Figure 1.** Synthesis of isoxazolidinesand isoxazoles bearing ε -caprolactam ring

**References**

[1] S. Kankala, R. K. Kankala, P. Gundepaka, N. Thota, S. Nerella, M. R. Gangula, H. Guguloth, M. Kagga, R. Vadde and C. S. Vasam, Bioorg Med Chem Lett., 23 (2013) 1306-1309.

[2] M. Ma, Y. Cheng, Z. Xu, P. Xu, H. Qu, Y. Fang, T. Xu and L. Wen, Eur. J. Med. Chem., 42 (2007) 93-98.

[3] W.T. Li, D.R. Hwang, C.P. Chen, C.W. Shen, C.L. Huang, T.W. Chen, C.H. Lin, Y.L. Chang, Y.Y. Chang, Y.K. Lo, H.Y. Tseng, C.C. Lin, J.S. Song, H.C. Chen, S.J. Chen, S.H. Wu and C.T. Chen, J. Med. Chem., 46 (2003) 1706-1715.

[4] S.B. Jadhav, R.A. Shastri, K.V. Gaikwad and S.V. Gaikwad, Eur. J. Chem., 6 (2009) 183-188.

[5] S.G. Durón, T. Polat and C.H. Wong, Org. Lett., 6 (2004) 839-841.

---

* Corresponding author, *E-mail: sagirli_a@ibu.edu.tr*

O-134

# Coumarin-based Fluorescent Chemosensor for Selective Detection of Phosgene

Sandip V. Mulay[1,3], Amgalan Natsagdorj[2]* and David G. Churchill[3]

[1]Center for Catalytic Hydrocarbon Functionalizations, Institute for Basic Science (IBS), Daejeon, 305–701, Republic of Korea
[2]Department of Chemistry, School of Arts and Science, National University of Mongolia, Ulaanbaatar, 24601, Mongolia
[3]Department of Chemistry, Korea Advanced Institute of Science and Technology (KAIST), Daejeon, 305–701, Republic of Korea

*Email: sandipm@kaist.ac.kr*

Phosgene ($COCl_2$), is highly toxic chemical but widely used in industrial processes, which have been regarded as a serious threat to our health and public security. Thus, it is imperative to develop a convenient and reliable detection method for this noxious agent. For this reason, it is an urgent need to develop facile and selective detection method of phosgene. In this work, we present a reaction-based fluorescent probe **CoumNMe$_2$** containing a coumarin-4-dimethyaminoaryl scaffold (Figure 1) for the selective detection of phosgene. The **CoumNMe$_2$** showed fluorescence enhancement (~45-fold) selectively with phosgene. More importantly, the sensor exhibits good selectivity to phosgene over close competitors diethyl chlorophosphate (DCP), diethyl cyanophosphonate (DECP), and diethyl methylphosphonate (DEMP) with very little interference from metal ions. The probe undergoes sequential phosgene-mediated nucleophilic substitution and intramolecular cyclization reaction to give a highly rigid system which shows an increase in fluorescence intensity by an intramolecular charge transfer (ICT) process.

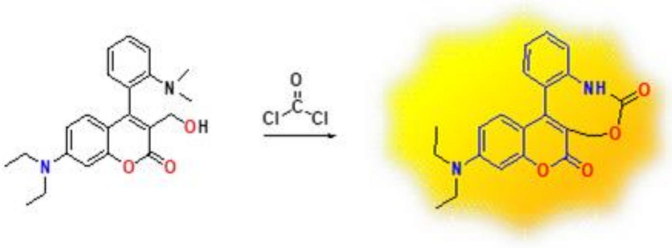


**Figure 1.** Chemical Structure of the Probe **CoumNMe$_2$**

**References**

[1] H.-C. Xia, X.-H. Xu and Q.-H. Song, Anal. Chem., 89 (2017) 4192–4197.
[2] Y.J. Jang, S.V. Mulay, Y. Kim, P. Jorayev, D.G. Chirchill, New J. Chem., 41 (2017) 1653-1658.

---

* Corresponding author, *E-mail: n_amgalan@num.edu.mn*

O-135

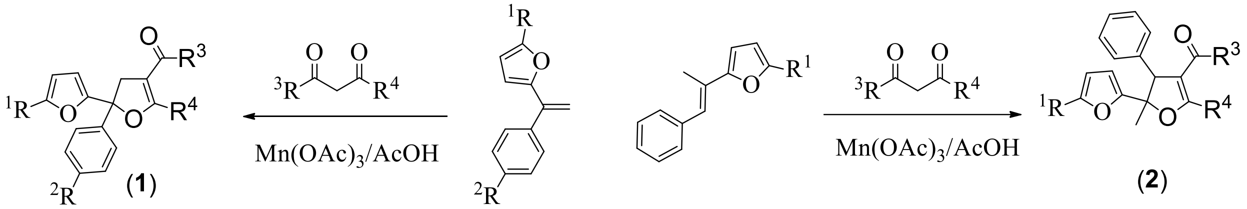
# Synthesis of New Furyl-substituted Dihydrofuran Compounds

**Mehtap Özgür**[1]*, Oğuzhan Alagöz[2] and Mehmet Yılmaz[3]

[1]Ankara University, Faculty of Science, Department of Chemistry, 06100, Ankara, Turkey
[2]Afyon Kocatepe University, Faculty of Engineering, Department of Chemistry, 03200, Afyon, Turkey
[3]Kocaeli University, Faculty of Arts and Sciences, Department of Chemistry, 41380, Kocaeli, Turkey

*E-mail: mehtapyakut@gmail.com*

Dihydrofurans are one of the most abundant molecules of biologically active compounds and they are commonly used as versatile intermediates in natural products synthesis [1]. Due to their structural features they are building blocks for synthetic chemistry areas. The radicalic addition-cyclization reaction of active methylene compounds with alkenes or alkynes promoted manganese(III) acetate [$Mn(OAc)_3$] represents one of the most common method [2]. Our research group was interested in preparing of heteroaryl substituted dihydrofurans by manganese(III) acetate, which have shown antifungal and antibacterial activity [3].



$^1$R= H, $^2$R= F (**2a**)
$^1$R= Me, $^2$R= H (**2b**)
$^1$R:=Me, $^2$R= F (**2c**)

$^1$R= H (**2d**)
$^1$R= Me (**2e**)

**Figure 1.** New furyl-substituted dihydrofurans

For this purpose, we studied the oxidative cyclizations of dimedone (**1a**), 1,3-cyclohexanedion (**1b**), acetylacetone (**1c**) and ethyl acetoacetate (**1d**) with 2-[1-(4-fluorophenyl)vinyl]furan **(2a)**, 2-methyl-5-(1-phenylvinyl)furan **(2b)**, 2-[1-(4-fluorophenyl)vinyl]-5-methylfuran **(2c)**, **(**E**)**-2-(1-phenyl-prop-1-en-2-yl)furan (**2d**) and **(**E**)**-2-methyl-5-(1-phenyl-prop-1-en-2-yl)furan (**2e**) using manganese(III) acetate at elevated temperature in acetic acid under an argon atmosphere (Figure 1). As a result of these cyclization reactions, we obtained various new furyl-substituted dihydrofurans in good yields.

## References

[1] M. Mondaland, U. Bora, RSC Adv., 3 (2013) 18716-18754.
[2] H. Aslan, D. E. Akpınar, A. Öktemer, M. Yakut, O. Alagöz, Helv. Chim. Acta, 97 (2014) 652-663.
[3] M. Yılmaz, N. Uzunalioğlu, M. Yakut, A.T. Pekel, Turk. J. Chem., 32 (2008) 1-12.

---

* Corresponding author, *E-mail: mehtapyakut@gmail.com*

# Synthesis and Spectroscopic Investigation on Ferrocenyldithiophosphonato Cd(II) and Hg(II) Complexes

**Ertuğrul Gazi Sağlam**[1]*, **Özgür Tutsak**[1] **and Hakan Dal**[2]

[1]Bozok University, Science and Art Faculty, Department of Chemistry, 66000, Yozgat, Turkey
[2]Anadolu University, Science Faculty, Department of Chemistry, 26470, Eskişehir, Turkey

*E-mail: saglameg@gmail.com*

Perthiophosphonic acid anhydrides, namely, 1,3,2,4-dithiadiphosphetane 2,4-disulfides, are important starting materials for the synthesis of organodithiophosphorus compounds [1,2]. The first example of ferrocenyl perthiophoshonic acid anhydrides, FcLR, was first explored by Woollins and coworkers [3].

In this work, we performed that ammonium ferrocenyl dithiophosphonates (FcLn, n=1, 3-methyl-1-butyl-; n=2, 3-pentyl-) were treated with the $CdCl_2$ and $HgCl_2$ to prepare their Cd(II) and Hg(II) complexes ($[M_2(\mu\text{-}FcLn)_2(FcLn)_2]$) (Figure 1).

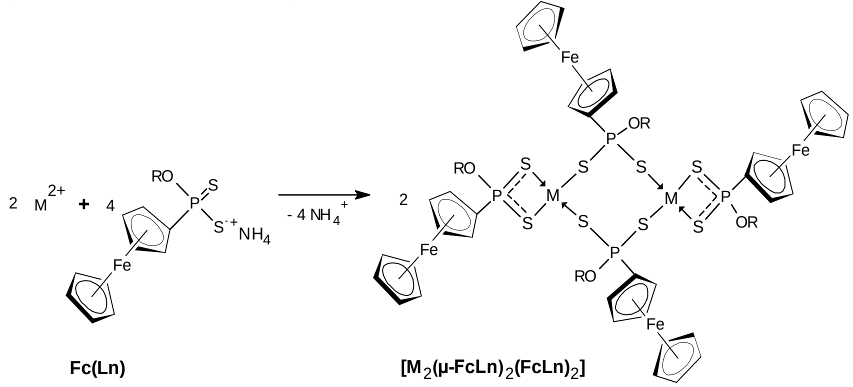


**Figure 1.** Syntheses reactions of the new Cd(II) and Hg(II) complexes

Structures of the new complexes were elucidated with the help of elemental analysis, mass spectroscopy, FTIR, Raman, $^{1}$H-, $^{13}$C- and $^{31}$P-NMR spectroscopy.

## References

[1] I. S. Nizamov, G.G. Sergeenko, A.E. Popovich, I.D. Nizamov, E.S. Batyeva and V.A. Al'fonsov, Russ. J. G. Chem., 72(9) (2002) 1356-1366.
[2] H. Beckmann, G. Grofimann, G. Ohms and J. Sieler, Heteroatom Chem., 5(1) (1994) 73-83.
[3] M. St. J. Foreman, A.M.Z. Slawin and J.D. Woollins, J. Chem. Soc., Dalton Trans., (1996) 3653-3657.

## Acknowledgement

This study is supported by a grant (Project Number: TBAG 114Z091, TUBITAK) from The Science and Technological Research Council of Turkey.

---

* Corresponding author, *E-mail: saglameg@gmail.com*

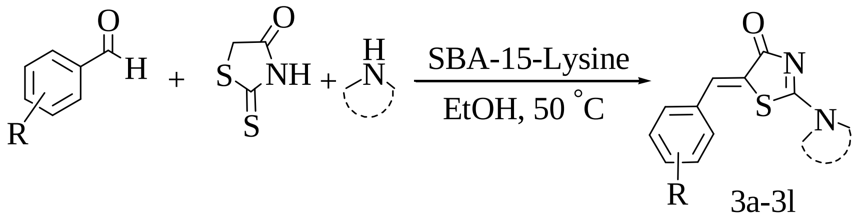
# Modified Mesoporous SBA-15/L-Lysine as Heterogeneous Catalyst for Synthesis of 2-amino-5-alkylidene-thiazol-4-ones

**Zakieh Yousofvand and Maryam Hajjami***

Department of Chemistry, Faculty of Science, Ilam University, P.O. Box, 69315516, Ilam, Iran

*E-mail: mhajjami@yahoo.com & m.hejami@ilam.ac.ir*

In recent years, nanostructure mesoporous materials have interested much attention for development of catalytic systems. Among them, SBA-15 is a highly ordered material possessing the largest pore size, thick walls, adjustable pore size from 3 to 30 nm, and high thermal and hydrothermal stabilities [1]. Thiazolidinone derivatives in particular, 2-amino-5-alkylidene-thiazol-4-ones have been extensively used in drug discovery and show a variety of biological activities such as anti-inflammatory effects, antimicrobial, antiviral, cardiotonic and etc [2,3]. In this work, new heterogeneous SBA-15/L-Lysine catalyst was developed for the synthesis of 2-amino-5-alkylidene-thiazol-4-ones from aldehydes, amines and rhodamine (Figure 1). This new catalyst has several advantages such as supply products in good yields, short reaction times and simple work-up procedure. The structure of catalyst was characterized by SEM, XRD, TGA, FT-IR, and BET analysis.



Amines= Piperidine, Morpholine, Pyrrolidine, Cyclohexylamine

**Figure 1.** Preparation of 2-amino-5-arylidenethiazol-4-ones

## References

[1] B. Yan and L.L. Kong, Nanoscale Res Lett., 5 (2010) 1195-1203.
[2] Z. Smelcerovic, A. Veljkovic, G. Kocic, D. Yancheva, Z. Petronijevic, M. Anderluhe and A. Smelcerovic, Chem. Biol. Interact.,229 (2015) 73-81.
[3] C. Mukhopadhyay, and S. Ray, Tetrahedron, 67 (2011) 7936-7945.

## Acknowledgement

Authors thank the research facilities of Ilam University, Ilam, Iran, for financial support of a research project.

---

***** Corresponding author, *E-mail: mhajjami@yahoo.com & m.hejami@ilam.ac.ir*

O-138

# One-Pot Synthesis of Quinazoline Tetracyclic Derivatives by Novel Ionic Liquid Supported on Magnetic Nanoparticles

**Zahra Taherinia and Arash Ghorbani-Choghamarani***

Department of Chemistry, Faculty of Science, Ilam University, P.O. Box, 69315516,
Ilam, Iran

*E-mail: a.ghorbani@ilam.ac.ir & arashghch58@yahoo.com*

Magnetic nanoparticles (MNPs) as catalyst supports have been attracting more and more attention because they are readily dispersed and exhibit an intrinsically high surface area to the active catalytic sites, low toxicity, and simple separation by an external magnetic field [1]. One of the twelve principles of green chemistry is the design of *chemical processes that reduce or eliminate* chemical waste, the cost of production. This can be achieved by developing alternative and sustainable technologies that are non-toxic to living things and the environment. This is the case of ionic liquids (ILs), due to their unique combination of thermal and chemical stability, low vapor pressure, low melting point, chemical stability, high conductivity, ability to dissolve organic and inorganic solutes and catalytic properties [2]. Among fused heterocyclic compounds, quinazoline tetracyclic has recently attracted much attention due to the exhibit a wide range of biological and pharmacological activities [3]. In this work nano-$Fe_3O_4$-supported, ionic liquid have been successfully synthesized and used for a series of quinazoline tetracyclic compounds by a three component reaction of a mixture of isatoic anhydride and amine with ninhydrin in PEG (Figure 1).

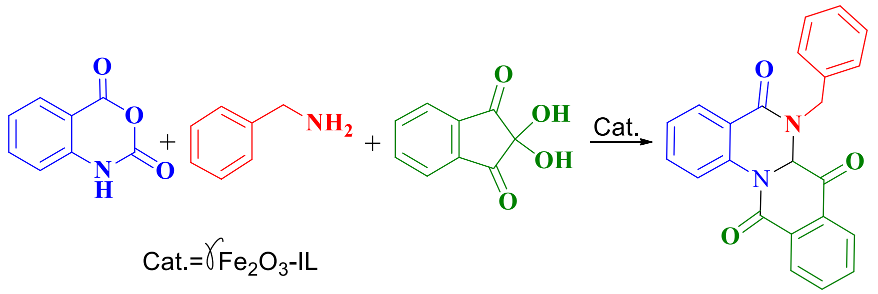


**Figure 1.** Synthesis of quinazoline tetracyclic

**References**
[1] C.R. Martin, Chem. Mater., 8 (1996) 1739.
[2] A. Aghayee, M.A. Zolfigol, H. Keypour, M. Yarie, and L. Mohammadi, Appl. Org. Chem., 8 (2016) 612.
[3] G.M. Whitesides, and B. Grzybowski, Science, 295 (2002) 2418.

**Acknowledgement**
Authors thank the research facilities of Ilam University, Ilam, Iran, for financial support of a research project.

---

* Corresponding author, *E-mail: a.ghorbani@mail.ilam.ac.ir & arashghch58@yahoo.com*

O-139

# High-Temperature Electrochemical Synthesis of Tungsten Carbide in Ionic Melts: Technologies of Obtaining and Regeneration

**Viktor Malyshev[1]*, Angelina Gab[1], Marcelle Gaune-Escard[2] and Alla Sushchenko[1]**

[1]University "Ukraine", 23 Lvivska St., Kyiv 03115, Ukraine
[2]Ecole Polytechnique, CNRS UMR 6595, Technopole de Chateau-Gombert, France

*E-mail: alla.suschenko@gmail.com*

An analysis of the literature shows that high-temperature electrochemical synthesis in ionic melts is a very promising method for obtaining tungsten carbides. An analysis of the state of the art in the high temperature electrochemical synthesis of tungsten carbide demonstrates that further advancement of this technology is possible only through working out its theory; elucidating the mechanism of electrodeposition; and learning to conduct and control the tungsten and carbon electrodeposition reactions, which are multielectron electrode processes. Since a necessary condition for electrodeposition of a compound is the similarity of the deposition potentials of its components, it is necessary to find ways of ensuring this similarity and the conditions under which the desired electrode reactions will occur simultaneously. Thermodynamic foundations of the electrosynthesis of tungsten carbides include the following: 1) calculating the equilibrium potentials of tungsten and carbon deposition from various electrolytes; 2) choosing the conditions and components for the electrochemical synthesis of tungsten carbides; 3) studying the effect of the acid-base properties of the melt on the discharge potential of oxygen-containing anions [1].

Theoretical foundations of the high-temperature electrochemical synthesis of tungsten carbides include the following: 1) investigating the simultaneous electroreduction of carbon dioxide and various molybdenum and tungsten ionic species in the KCl-NaCl melt; 2) investigating the simultaneous reduction of carbon dioxide and fluorotungstate complexes in the NaCl-KCl-NaF melt; 3) simultaneous electroreduction of carbon dioxide and dimeric tungsten species in tungstate melts; 4) simultaneous electroreduction of the carbonate and tungstate ions in chloride-fluoride and oxide melts. Realization of the high-temperature electrochemical synthesis of tungsten carbides includes the following: 1) electrosynthesis of tungsten carbide powders at a positive carbon dioxide pressure; 2) electrochemical synthesis of fine tungsten carbide powders from oxide melts; 3) electrodeposition of tungsten carbide coatings from tungstate-halide melts. The technology for high-temperature electrochemical synthesis of highly dispersed tungsten monocarbide powders is developed. Variation of a composition of electrolyte used in synthesis of tungsten carbide in a course of isothermal heating is investigated. The influence of the electrolysis period duration on the electrolyte composition and the cathode deposit structure and composition is studied. Development of the processing method for tungsten carbide and cobalt hard alloys wastes includes the determination of the potentials range where tungsten and cobalt alloys phases dissolve selectively in the phosphoric acid solutions forming soluble compounds of these metals and tungsten carbide phase remains in deposit. It is also shown that tungsten ores and concentrates decompose at 1323-1373 K in NaCl-$Na_2SiO_3$ melt with the formation of two immiscible phases: halide-tungstate one containing 96-99% of tungsten, and silicate one containing more than 90% of other ore components.

## Reference

[1] V.I. Shapoval, Kh.B. Kushkhov and I.A. Novoselova, Journal of Applied Chemistry of the USSR, 58 (1985) 1027-1030.

---

* Corresponding author, *E-mail: victor_malyshev@mail.ru*

# Syntheses and Structural Characterizations of 2-Pyridyl-*spiro*-Cyclotriphosphazenes

**Gamze Elmas*, Aytuğ Okumuş and Zeynel Kılıç**

Ankara University, Faculty of Science, Department of Chemistry, 06100, Ankara, Turkey

*E-mail: gegemen@ankara.edu.tr*

The hexachlorocyclotriphosphazene (trimer, $N_3P_3Cl_6$) is an important starting material used in the preparation of phosphazene derivatives in the field of phosphazene chemistry. There are a lot of reports on the nucleophilic substitution reactions of hexachlorocyclotriphosphazenes with mono, di and multidentate ligands in the literature [1,2]. A wide range of cyclotriphosphazene derivatives with different side groups and with diverse application potential have been obtained with these reactions [3]. In this study, the Cl replacement reaction of $N_3P_3Cl_6$ (**1**) with one equimolar amount of sodium salt of 3-*N*-(2-pyridyl)-methylamino-1-propanol containing N/O donor atom and *N*-methyl-*N′*-(2-pyridyl)-methyl-1,3-propanediamine containing N/N donor atom gave seperately two kinds of 2-pyridyl-spiro-cyclotriphosphazenes (**2** and **3**). The spiro products (**2** and **3**) reacted with excess morpholine afforded the fully substituted 2-pyridyl-spiro-cyclotriphosphazenes (**4** and **5**) (Figure 1). The structures of these compounds (**2-5**) were verified by elemental analyses, MS, FTIR, $^1$H, $^{13}$C{$^1$H} and $^{31}$P NMR techniques.

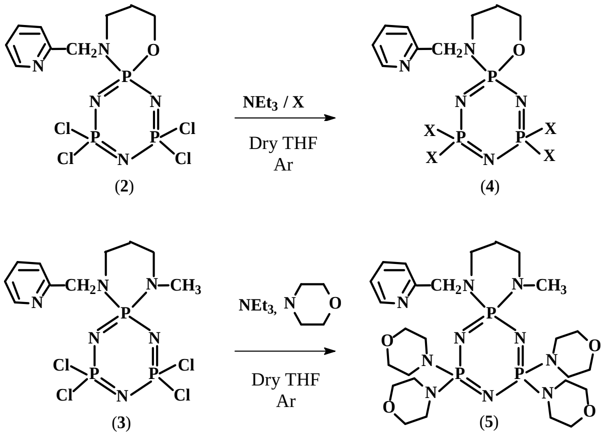


**Figure 1.** 2-Pyridyl-spiro-cyclotriphosphazene derivatives (**2-5**)

## References

[1] F.F. Stewart, Organophosphorus Chem. Royal Society of Chemistry, 44 (2015) 397-430.
[2] A. Okumuş, G. Elmas, Z. Kılıç, N. Ramazanoğlu, L. Açık, M. Türk, G. Akça, Turk. J. Chem., (2017) DOI: 10.3906/kim-1612-80.
[3] V. Chandrasekhar, R.S. Narayanan, Organophosphorus Chem. Royal Sciety of Chemistry, 45 (2016) 375-437.

## Acknowlegment

This study is supported by a grant "Scientific and Technical Research Council of Turkey" (Grant No. 216Z105).

---

* Corresponding author, *E-mail: gegemen@ankara.edu.tr*

# YAKUT HALL FOYER

# POSTER PRESENTATIONS

# Analysis

P-1

# Solid Phase Microextraction of Phthalate Esters by Using Graphene Oxide Sorbent Modified with Ionic Liquids

**Paniz Tashakkori**[1], **Pelin Erdem**[2], **Serap Seyhan Bozkurt**[2]* **and Melek Merdivan**[2]

[1]Dokuz Eylul University, The Graduate School of Natural and Applied Sciences, 35160, İzmir, Turkey
[2]Dokuz Eylul University, Faculty of Science, Chemistry Department, 35160, İzmir, Turkey

*E-mail: paniztashakkori@yahoo.com*

Solid phase micro-extraction (SPME) is an extraction and preconcentration technique that's used for trace level of compounds in various sample matrixes before analysis. This non-exhaustive extraction approach utilizes a fiber made of fused silica or metal core that coated with a small amount of sorbent material with thicknesses between 7 and 100 mm. SPME offers many advantages over conventional extraction techniques such as simplicity, ease of automation, high enrichment factors, low sample volume requirements, and it is clearly an environmentally friendly technique [1,2]. Furthermore, SPME can be used in the analysis of gas, liquid and solid samples and for the determination of volatile, semi-volatile, and non-volatile analytes. So, it is demonstrating great versatility [3]. Otherwise, phthalate esters crept into widespread use over the last several decades because of their many beneficial chemical properties. Now they are ubiquitous, not just in the products in which they are used, but also as contaminants in just about anything. Much of the literature focuses on phthalates toxicological properties on human health such as cancer, asthma, endocrine disorders and obesity. So, the determination of phthalates has become important [4]. In this study 1-(3-aminopropyl)-3-vinylimidazolium bromide/tetrafluoroborate and 1-(3-aminopropyl)-3-benzylimidazolium bromide/tetrafluoroborate ionic liquids (ILs) were synthesized and then, these ionic liquids were chemically bonded to graphene oxide (GO). The structures of GO-IL sorbents was characterized by FTIR and XRD. Thermal stabilities of them were investigated by TGA curves. Later, GO-IL based SPME fibers were prepared. Phthalate esters (dimethyl phthalate, dibutyl phthalate, dipentyl phthalate, dibutylhexyl phthalate and di-n-octyl phthalate, diethylhexyl phthalate) were separated from the matrix and preconcentrated with headspace and the immersion SPME method by means of prepared fibers and analyzed by gas chromatography-mass spectrometer (GC-MS).

## References

[1] P. Rocío-Bautısta, I. Pacheco-Fernández, J. Pasán and V. Pino, Analytica Chimica Acta, 939 (2016) 26-41.
[2] E.A. Souza-Silva, R. Jiang, A. Rodríguez-Lafuente, E. Gionfriddo and J. Pawliszyn, Trends Anal. Chem., 71 (2015) 224-235.
[3] A. Spietelun, L. Marcinkowski, M. De la Guardia and J. Namieśnik, J. Chromatogr. A, 1321 (2013) 1-13.
[4] E. Olkowska, J. Ratajczyk and L. Wolska, Trends Anal. Chem., 91 (2017) 77-90.

## Acknowledgements

The authors would also like to thank Scientific and Technological Research Council of Turkey (TUBITAK) financially supported by project 215Z212.

---

* Corresponding author, *E-mail*: *serap.seyhan@deu.edu.tr*

P-2

# Determination of Optimum Conditions to Prepare an Acid Activated Bentonite Sample with Maximum Bleaching Power

**Hale Bayram[1], Müşerref Önal[2]*, Damla Erkakan[2], Yüksel Sarıkaya[2]**

[1]Marmara University, Atatürk Faculty of Education, Science Teacher Education, 34722, Istanbul, Turkey
[2]Ankara University, Faculty of Science, Department of Chemistry, 06100, Ankara, Turkey

*E-mail: onal@science.ankara.edu.tr*

To investigate the effect of $H_2SO_4$ activation on the surface area ($S/m^2g^{-1}$), micro, mesopore volume ($V/cm^3g^{-1}$), and bleaching power (BP), a white calcium bentonite (CaB) from Ankara (Turkey) was used. The CaB samples were activated by changing $H_2SO_4$ dosage, temperature and time when two of these staying constant, respectively [1]. The representative ones of the obtained samples were examined by the X-ray diffraction (XRD), chemical analysis (CA), low temperature nitrogen adsorption/desorption ($N_2$-AD), and bleaching power (BP) measurement techniques. The CaB contains a calcium reach smectite (CaS) as major clay mineral, also illite (I), metahalloysite (MH), opal-A (OA), opal-CT (OCT), quartz (Q) and feldspar (F) in different amounts as impurities according to the XRD data [2]. The S and V values were calculated from the nitrogen adsorption and desorption data, respectively [3]. Although, the BP increases with increasing S and V values it depends more on the pore size of the acid activated samples. The optimum acid percent, temperature and time of the activation are determined as 35% $H_2SO_4$, 100°C, and 8h, respectively.

**References**

[1] H. Noyan, M. Önal and Y. Sarıkaya, Food Chemistry, 105 (2007) 156-163.
[2] H. Bayram, M. Önal, H. Yılmaz and Y. Sarıkaya, Journal of Thermal Analysis and Calorimetry, 101 (2010) 873-879.
[3] S. Brunauer, P. H. Emmett and E. Teller, Journal of American Chemical Society, 60 (1938) 308-319.

---

* Corresponding author, *E-mail: onal@science.ankara.edu.tr*

P-3

# Simple and Quick Determination of Trace Thiabendazole Residues in Fruits and Vegetables Utilizing IL-UA-DLLME Combined with Spectrophotometry

**Nail Altunay*, Ramazan Gürkan and Adil Elik**

Cumhuriyet University, Faculty of Sciences, Department of Chemistry, TR-58140,
Sivas

*E-mail: naltunay@cumhuriyet.edu.tr*

In agricultural practice, although the use of insecticides, herbicides, and fungicides provides unquestionable benefits in providing a plentiful, low-cost supply of high-quality fruits and vegetables, their incorrect application may present a main source of pollutions, which involve possible risks to human health [1]. Nowadays, food safety has reached alarming dimensions globally because of the increasing amount of pesticide residues in fruits and vegetables. The development of new, simple and inexpensive analytical methods is of great importance, especially for the analysis of pesticide residues in the real samples. Therefore, an eco-friendly ionic liquid-based ultrasound-assisted dispersive liquid–liquid microextraction (IL-UA-DLLME)-spectrophotometric method has been proposed for simple and rapid determination of trace Thiabendazole (TBZ) in fruits and vegetables in this study. The ionic liquid, 1,3-dibutylimidazolium hexafluorophosphate [BBim][PF6] was used for extraction of TBZ from the selected samples in the presence of 5 mg $L^{-1}$ $Cu^{2+}$ ions at pH 5.5. After optimizing the variables that influence the microextraction process, the analytical properties of the proposed method were determined by calibration curves prepared from both model solutions and matrix-matched solutions. The optimized method allows wide linear working range (0.3 to 280 µg $L^{-1}$), low LOD (0.1 µg $L^{-1}$), relative standard deviation (≥2.8% RSD), good recovery (≥94%), and high sensitivity enhancement factor (150) for model solutions while it allows a detection limit of 0.3 µg $L^{-1}$ in the range of 0.8-250 µg $L^{-1}$ for the matrix matched solutions. After the accuracy and precision of the method were performed, it was successfully applied to the determination of TBZ residues in fruits and vegetables at two different spiked concentrations, and satisfactory recoveries were obtained.

## References

[1] V. Boeris, J.A. Arancibia, A.C. Olivieri, Analytica Chimica Acta, 814 (2014) 23-30.

---

* Corresponding author, *E-mail: naltunay@.cumhuriyet.edu.tr*

P-4

# Ultrasonic Assisted Microextraction of As and Sb from Water and Plant Samples as Determined by HG-AAS

**Nail Altunay***, **Adil Elik and Ramazan Gürkan**

Cumhuriyet University, Faculty of Sciences, Department of Chemistry, TR-58140, Sivas

*E-mail: naltunay@cumhuriyet.edu.tr*

Especially, determination of toxic metal ions at ultra-trace levels is an important issue in the context of food chemistry [1]. A new and simple ultrasonic assisted microextraction (UAME) procedure was developed for the determination of arsenic and antimony in water and plant samples by hydride generation atomic absorption spectrometry (HG-AAS). Some factors such as ionic liquid amount, ligand concentration, pH, extraction time, sample volume, and HG-AAS conditions were investigated and optimized in details. Chemical hydride generation with 1.5% $NaBH_4$ after the pre-reduction of As(V) and Sb(V) with 1.0% l-cysteine in 0.02 mol $L^{-1}$ HCl (20 min contact time at 80±5 °C) was used. Under the optimal hydride generation conditions and analytical system operation the detection limits (ng $kg^{-1}$) were 15 (As) and 50 (Sb), whereas the precision was 1.1–6.0% for 30-150 ng $kg^{-1}$ As and 1.4–5.2% for 75–200 mg $kg^{-1}$ Sb. The sensitivity enhancement factor for As and Sb was 80 and 115, respectively. Trueness test for the entire analytical procedure was performed by means of the Standard Reference Material (SRM) NIST 1643e (Trace elements in water) and results were in good agreement with the certified values. The system was evaluated for quantitative determinations of total As and Sb in different kind of waters and plant samples. The method is simple and relatively cheap in comparison with other methodologies.

**References**

[1] LA. Brunborg, K. Julshamn, R. Nortvedt and L. Frøyland, Food Chemistry, 96(4) (2006) 524-531.

---

* Corresponding author, *E-mail: naltunay@cumhuriyet.edu.tr*

P-5

# Highly Sensitive Determination of Certain Antihypertensive Drugs in Their Pure and Combined Forms

**Nevin Erk**[1]*, **Gizem Tırıs**[2] **and Ali Kemal Ateş**[1]

[1]Ankara University, Faculty of Pharmacy, Department of Analytical Chemistry, 06100, Ankara, Turkey
[2]Bezmialem Vakıf University, Faculty of Pharmacy, Department of Analytical Chemistry, İstanbul, Turkey

*E-mail: erk@pharmacy.ankara.edu.tr*

The objective of this study was to develop and validate for the simultaneous determination of Nebivolol (NB) and Hydrochlorothiazide (HY) in pure drugs and their binary mixtures, without prior separation. In the first method, first derivative spectra ratio spectrophotometry is used solutions of standard and samples in methanol first derivative spectra ratio spectra absorbance signals were measured at 291.5 and 283.7 nm's for NB and 247.7 and 225.5 nm's for hydrochlorothiazide, respectively. The first derivative spectra ratio spectrophotometric calculations of regression equations were estimated for determination NB and HY nm by the least - squares method as follows: $y = 0.0104[NB]$ (µg/mL) - 0.0059 ($r^2 = 0.9991$) and $y = 0.0919[HY]$ (µg/mL) - 0.2373 ($r^2 = 0.9965$) , respectively. The second method was the ratio difference spectrophotometric method where the difference amplitude at 280.0-290.0 nm for NB and 239.5-256.5 nm for HY were selected to simultaneously determine this drugs in binary mixtures [1-3]. Also, the ratio difference spectrophotometric calculations of regression equations were estimated for determination NB and HY nm by the least - squares method as follows: $y = 0.0657$ [NB] (µg/mL) - 0.0259 ($r^2 = 0.9966$) and $y = 0.09817$ [HY] (µg/mL) - 0.0206 ($r^2 = 0.9971$) , respectively. The calibration curves were linear through the concentration range of 5.0-35.0 µg/mL for NB and HY, respectively. The correlation coefficients of calibration curves calculated from these two methods indicate good linearity for both methods. The results of the analysis were validated statistically, and recovery studies confirmed the accuracy of the described methods which were carried out by following the ICH guidelines.

## References

[1] H.M. Mohamed, H.M. Lotfy, M.A. Hegazy and S.Mowaka, Chemistry Central Journal, 11 (2017) 1-15.
[2] H.M. Lotfy, M.A.M. Hegazy, M.R. Rezk and Y.R.Omran, Spectrochimica Acta A, 126 (2014) 197-207.
[3] E.A. Abdel-Aleem, M.A. Hegazy, N.W.Sayed, M. Abdelkawy and R.M.Abdelfatah, Spectrochimica Acta Part A, 136 (2015) 707-713.

---

* Corresponding author, *E-mail: erk@pharmacy.ankara.edu.tr*

P-6

# Different Spectrophotometric Methods for Simultaneous Determination of Certain Antihyperlipidemic Drugs in Their Bulk and Mixtures

**Nevin Erk[1]* and Gizem Tırıs[2]**

[1]Ankara University, Faculty of Pharmacy, Department of Analytical Chemistry, 06100, Ankara, Turkey
[2]Bezmialem Vakıf University, Faculty of Pharmacy, Department of Analytical Chemistry, İstanbul, Turkey

*E-mail: gizem.tiris@gmail.com*

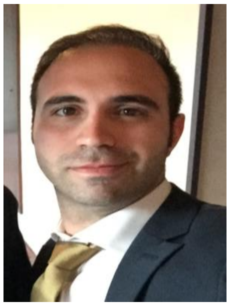
Ezetimibe (EZ), (3*R*,4*S*)-1-(4-fluorophenyl)-3-[(3*S*)-3-(4-fluorophenyl)-3-hydroxypropyl]-4-(4-hydroxyphenyl)azetidin-2-one, and atorvastatin (AT), [*R*-(*R*, *R*)]-2-(4-fluorophenyl)-β,δ-dihydroxy-5-(1-methylethyl)-3-phenyl-4-[(phenylamino)carbonyl]-1H-pyrrole-1-heptanoic acid were oral antihyperlipidemic drugs [1]. In this work is concerned with the simultaneous determination of AT and EZ in a binary mixture by using different methods. The first one was an extended ratio subtraction spectrophotometry procedure and the second one was ratio difference spectrophotometry [2]. This first one method was extended ratio subtraction spectrophotometry where the $\lambda_{max}$ signals at 241.2 nm for AT, or 230. 4 nm for EZ were selected for simultaneous determination AT or EZ in their binary mixtures. The method was applied in the concentration ranges of 2.0-40.0 μgml$^{-1}$ AT, or 6.0-42.0 μgml$^{-1}$ EZ, allowing a rapid, accurate and precise simultaneous determination of the concentration of both analytes. The rectilinear equation for calibration curves were found to be: $y = 0.0156x – 0.0314$ ($R^2$: 0.9934) (where y is analytical signals in the ratio $\lambda_{max}$ absorbances spectra in ratio spectra, and C is the concentration) at 241.2 nm and $y = 0.0192\ x - 0.0411$ ($R^2$: 0.99456) at 230.4 nm for AT and EZ, respectively. For the ratio difference spectrophotometry was involved measurement of the absorbance difference of the ratio spectra in binary mixture [3]. The difference amplitudes in the ratio spectra at 241.6 – 229.7 nm and at 230.3 – 243.0 nm were selected to determine AT and EZ in the binary mixture. The described methods can be easily applied by the quality control laboratories in routine analyses of these drugs it pharmaceutical preparations.

## References

[1] P. Beringer, Remington: The Science and Practice of Pharmacy, 2006 New York, NY Lippincott Williams & Wilkins.
[2] H.M. Lotfy, M.A.M. Hegazy, M.R. Rezk and Y.R.Omran, Spectrochimica Acta A, 126 (2014) 197-207.
[3] H.M. Mohamed, H.M. Lotfy, M.A. Hegazy and S.Mowaka, Chemistry Central Journal, 11 (2017) 1-15.

---

* Corresponding author, *E-mail: erk@pharmacy.ankara.edu.tr*



# Development Method for Rapid Estimation of Atenolol and Lercanidipine in Bulk and Pharmaceutical Dosage Forms

**Nevin Erk* and Berk Toker**

Ankara University, Faculty of Pharmacy, Department of Analytical Chemistry, 06100, Ankara, Turkey

*E-mail: berktoker*@me.com

Atenolol (ATE), 1-3, (*RS*)-2-{4-[2-hydroxy-3-(propan-2-ylamino)propoxy] acetamide, is a selective $\beta_1$ receptor antagonist. Lercanidipine (LER), 1,4-dihidro-2,6-dimethyl-4-(3-nitrophenyl)-3,5-pyridinedicarboxylic acid, is a calcium channel blocker of the dihydropyridine class. Recently, ATE was marketed in combination with LER in tablets. Simple, accurate and precise spectrophotometric techniques were developed for simultaneous determination of atenelol (ATE) and Lercanidipine (LER) by employing ratio difference and first derivative UV spectrophotometric techniques without prior separation. In the ratio difference technique [1-3], solutions of standard and samples in methanol were used, ATE and LER were determined by measuring the difference signals in the ratio spectra between at 275.01 – 281.6 nm and between at 249.29 – 258.88 nm in the bulk drugs and binary mixture, respectively. On the other hand, ATE and LER were determined using first derivative UV spectrophotometric technique by measuring the first derivative signals at 236.60 nm (zero-crossing point of LER) and 226.04 nm (zero-crossing point of ATE), respectively. Both spectrophotometric techniques were characterized by high sensitivity and accuracy for ATE and LER were in the concentration ranges 5.0 – 75.0 ug/mL and 5.0 - 40.0 ug/mL, with well accepted mean correlation coefficients for each drug, respectively. The intra-day and inter-day precision values for ATE and LER were less than 2.5 % (CV). The proposed methods were applied to the determination of both analytes in synthetic mixtures and pharmaceutical preparations, with satisfactory results in both cases.

**References**

[1] H.M. Lotfy, Int. J. of Pharm. and Pharm. Sci., 4 (2012) 107-114.
[2] H.M. Lotfy, M.A.M. Hegazy, M.R. Rezk and Y.R. Omran, Spectrochim. Acta A, 148 (2015) 328-337.
[3] C.V. Patel, A.P. Khandhar, A.A. Captain and K.P. Patel, Eurasian J.Anal.Chem., 2(3) (2007) 159-171.

---

* Corresponding author, *E-mail: erk@pharmacy.ankara.edu.tr*

P-8

# Simultaneous Analysis of Amphetamine, Methamphetamine and MDMA (ecstasy) in Pharmaceutical Dosage Forms by Gas Chromatography (GC)

**Nevin Erk* and Arzu Menteşe**

Ankara University, Faculty of Pharmacy, Department of Analytical Chemistry, 06100, Ankara, Turkey

*E-mail: arzumentese@hotmail.com*

Amphetamine belongs to the phenethylamine class. It is also the parent compound of the substituted amphetamines, which includes substances such as bupropion, cathinone, MDMA(ecstasy), and methamphetamine. Amphetamines were a group of synthetic psychoactive drugs called central nervous system stimulants [1]. Amphetamine (AMP) and methamphetamine (MAMP) were used in the treatment of attention deficit/ hyperactivity disorder, narcolepsy, obesity and depression. However, at large doses, these drugs were more likely to increase rapid muscle deterioration and impair coordination. Even higher doses may result in hallucinations, paranoia, and psychosis. In this study, we developed a qualitative method for gas chromatography/mass-spectrometry (GC/MS) and a quantitative method for gas chromatography (GC) for AMP. The oven temperature was carried out at $250^0$C. The internal standard method using tetracosane as the internal standard is used. The method was applied in the concentration ranges with a correlation coefficients of 10.6 - 332.0 $\mu g.ml^{-1}$ ($r^2$: 0.9992) for AMP, 10.7 - 334.0 $\mu g.ml^{-1}$ ($r^2$: 0.9990) for MAMP and 12.6 - 393.0 $\mu g.ml^{-1}$ ($r^2$: 0.9998) for MDMA, respectively. The analytical signals were observed at 2.612, 3.013 and 9.278 min for AMP, MAMP and MDMA, respectively. The aim of this research is to develop and validate the GC methods for the determination of the amphetamine derivatives.

## References

[1] A. Phonchai, B. Janchawee , S. Prutipanlai, S. Thanchaiwattana, T. Ruhland and M. Jorgensen, Journal Analytical Chemistry 65(9) (2010) 951-959.

---

* Corresponding author, *E-mail: erk@pharmacy.ankara.edu.tr*

P-9

# Acidity Constants of Ceftizoxime, Cefotaxime, Ceftiofur

**Sertaç Budak[1], Kader Poturcu[1], Sibel A. Özkan[2] and Güleren Alsancak[1]***

[1]Süleyman Demirel University, Arts and Science Faculty, Department of Chemistry, Isparta, 32200, Turkey
[2]Ankara University, Faculty of Pharmacy, Department of Analytical Chemistry, Ankara, 06100, Turkey

*E-mail: kaderpoturcu@sdu.edu.tr*

The cephalosporins are the most widely used groups of antibiotics. Based on the basis of bacterial susceptibility patterns and resistance to β-lactamases, cephalosporins have been classified as first, second, third and fourth generation. All the cephalosporins consist of a β-lactam ring fused with dihydrothiazine ring and side chains linked to C7 position and to C3 position. There are only few reports dealing with the acidity constant ($pK_a$) values of the third generation cephalosporins. Having this mind, this study deals with the $pK_a$ of some selected cephalosporins, cefotaxime, ceftizoxime and ceftiofur. Those three compounds are chosen due to its same basic (cephem 2) structure and the same substituent at C2 and C7 position, but differentiating in substituent R at C3 position. All three compounds have carboxylic group, as ionization center at C2 position, and the same C7 substituent bearing two ionization groups, amide and aminothiazole [1,2].

In the present study, the acidity constants of these three compounds were determined by using RP-LC method. Recently, some researchers successfully applied RP-LC method for determination of the $pK_a$ value of drug active compounds. Determination of $pK_a$ using RPLC was based on measurement of the retention time of studied substances as a function of eluent pH. This relationship was then fitted by a sigmoidal curve, where $pK_a$ is the value of pH in the sigmoid inflection point.

## References

[1] M. Aleksic, V. Savic, G. Popovic, N. Buric and V. Kapetanovic, Journal of Pharmaceutical and Biomedical Analysis 39 (2005) 752–756
[2] C. Horvath, W. Melander and I. Molnar, Analytical. Chemistry, 49 (1977) 142-154.

---

* Corresponding author, *E-mail: gulerenalsancak@sdu.edu.tr*

P-10

# Quantitative Structure-Property Relationship Method to Assess the Lipophilicity of Amphotheric Drugs

**Ebru Çubuk Demiralay[1], Kader Poturcu[1], Dilara Başat Dereli[2] and Güleren Alsancak[1]***

[1]Süleyman Demirel University, Arts and Science Faculty, Department of Chemistry, Isparta, 32200, Turkey
[2]Bitlis Eren University, Tatvan Vocational School of Higher Education, 13200, Bitlis, Turkey

*E-mail: kaderpoturcu@sdu.edu.tr*

Drug lipophilicity is a very important parameter governing pharmacokinetics and pharmacodynamics phenomena. The determination of the lipophilicity of pharmaceuticals is of great importance in quantitative structure-activity relationship studies. The determination of lipophilicity parameters of drug candidates is necessary from the early stages of the drug development process.

The lipophilicity of solutes is most commonly characterized by the logarithm of their partition coefficients (log P) in n-octanol/water systems. The reversed phase liquid chromatography (RP-LC) technique has grown in the lipophilicity estimation of solutes. The use of RP-LC to determine the lipophilicity for a wide range of compounds of diverse chemical structures has applied either isocratic or gradient elution techniques [1]. For a quantitative comparison of the relative lipophilicity of a series of drug analytes, best suitable option is their intercepts (log $k_w$) of the linear relationships between the logarithm of their retention times (log $t_r$) and the volume fraction organic modifier in hydro-organic eluents. The 1-octanol/water partition coefficient is also determined by applying a quantitative structure–property relationship (QSPR) model [1]:

$$\log P_{o/w} = 1.22p_{reference} + 1.89(HDCA\text{-}2) - 0.17(HOMO\text{–}LUMO) + 1.98(pol/d^2) - 1.27\cdot10^{-3}(DPSA\text{-}1) - 0.99$$

The determination of log $P_{o/w}$ of amphoteric compounds is more difficult due to the existence of at least two $pK_a$ values. In this work, log $P_{o/w}$ values of four amphoteric compounds (atorvastatin, rosuvastatin, rosiglitazone and mebendazole) were determined. Retention data were obtained with mobile phases containing acetonitrile and water at different pH for all compounds. To measure the log $P_{o/w}$ of the neutral form of the solute, the working pH values were carefully selected.

## References

[1] J.M. Pallicer, C. Calvet, A. Port, M. Rosés, C. Ràfols and E. Bosch, Journal of Chromatography A, 1240 (2012) 113- 122.

---

* Corresponding author, *E-mail: gulerenalsancak@sdu.edu.tr*

P-11

# Optimization of Hydrogen Yield by Design of Experiments Using Co-Culture of *Clostridium butyricum* and *Enterobacter aerogenes*

**Zeynep Yılmazer Hitit**[1,2] **and Patrick C Hallenbeck**[2,3]*

[1]Ankara University, Faculty of Engineering, Department of Chemical Engineering, 06100, Ankara, Turkey
[2]Département de Microbiologie, Infectiologie et Immunologie, Université de Montréal, CP6128 Succursale Centre-ville, Montréal, Québec, Canada H3C 3J7
[3]Life Sciences Research Center, Department of Biology, United States Air Force Academy 2355 Faculty Drive, USAF Academy, Colorado 80840

*E-mail:* zyilmazer@*ankara.edu.tr*

The effects of various factors on fermentative hydrogen production by co-cultures of *Clostridium butyricum* and *Enterobacter aerogenes* was investigated using the experimental design methods of Plackett Burman and Central Composite Design to better understand the process, achieve higher yields, and to improve performance through optimization [1]. Fermentative hydrogen production can be conducted using either pure cultures or co-cultures. Previous studies have evaluated hydrogen production by pure cultures of *C. butyricum* or *E. aerogenes* [2-4]. Evaluating hydrogen production by co-culture of these microorganisms is an interesting approach since *E. aerogenes* is a facultative microorganism with resistance to oxygen in contrast to the strict anaerobe *C. butyricum*, and therefore has the ability to maintain anaerobic conditions. The goal of the present study was to apply a Design of Experiments (DOE) approach to the field of microbiology in order to achieve optimal results for complex systems that require variation of different parameters. For this purpose, Plackett Burman design was used first to find effective parameters influencing biohydrogen production by varying the substrate concentration (g/L), inoculum ratio, and added reagent concentrations (g/L). After finding most effective parameters, Central composite design (CCD) was carried out. From Response Surface Methodology (RSM), the maximum hydrogen yield of 2.15 mole $H_2$/mole glucose and total hydrogen production of 936 μmole were achieved with the values of inoculum ratio, substrate concentration and $FeSO_4$ concentration of 8 mL, 1.3 g/L and 0.56 g/L, respectively [1].

**References**

[1] Z. Yılmazer Hitit, Karışım Kültür Kullanılarak Karanlık Fermantasyon Yöntemiyle Biyohidrojen Üretimi, Doktora Tezi, (2016), Ankara.
[2] İ. Karapınar Kapdan and F. Kargı, Enyzme and Microbial Technology, 38 (2006) 569-582.
[3] D. Leung, M. Leung, K. Sumathy and D. Ni, Fuel Processing Technology 87 (2006) 451–472.
[4] A.T. Jackson, Process Engineering in Biotechnology, (1990).

---

* Corresponding author, *E-mail: patrick.hallenbeck@umontreal.ca*

P-12

# Preconcentration of Cadmium(II) Ions Using Graphene Oxide Modified Expanded Perlite As a Sorbent

**Rukiye Saygılı Canlıdinç***, **Orhan Murat Kalfa, Zafer Üstündağ and Yunus Erdoğan**

Dumlupınar University, Faculty of Arts and Science, Department of Chemistry,
43100, Kütahya, Turkey

*E-mail: rukiye.saygili@dpu.edu.tr*

Heavy metals such as cadmium, copper, lead and zinc are serious hazards and non-biodegradable in the environment. FAAS is one of the most widely technique for the determination of these metals. However, the direct determination of extremely low concentrations of these metals can be difficult because of matrix interferences or insufficient sensitivity of most analytical techniques. For this reason, preliminary separation/preconcentration techniques are usually required. The most commonly employed technique for sample treatment is solid-phase extraction (SPE) [1-3]. In recent years we have seen intense interest grow in graphene (G) and graphene oxide (GO) as a sorbent material for SPE. Although G and GO have several advantages as adsorbents in SPE, very small particles of G and GO can cause high pressure in the SPE column and can escape from the SPE column [4]. To overcome these problems, we developed a new adsorbent by covalently binding GO sheets to expand perlite. The carboxy groups of GO were linked to the amino groups of an aminoterminated silica based expanded perlite sorbent. In this way, a new adsorbent (GO@Ex. Perlite) can be used in normal-phase SPE for preconcentration of cadmium ions. Perlite is an inert glassy volcanic ryholitic rock and can be expanded up to 10–20 times its original volume when heated rapidly at 700–1200 ˚C (expanded perlite). Most of perlite contains greater than 70% silica, and it is inexpensive and abundantly available in Turkish markets so this could make it available candidate as an economical sorbent for removing heavy metals such as lead, copper, cadmium and chromium [5]. In this study, preconcentration conditions of cadmium ions, prior to determination with AAS, using graphene oxide modified expanded perlite were investigated. Graphene oxide modified expanded perlite (GO@EP) was synthesized by covalently binding GO sheets to the expanded perlite. To determine optimum conditions, several parameters' effects such as pH, eluent type and concentration, flow rate was studied. The modification, size and morphology of sorbent were characterized by FT-IR, SEM, XRD and TGA/DTA.

## References

[1] C. Duran, D. Ozdes, D. Sahin, V.N. Bulut, A. Gundogdu and M. Soylak, Microchemical Journal 98 (2011) 317-322
[2] N. Pourreza, S. Rastegarzadeh and A. Larki, Journal of Industrial and Engineering Chemistry 20 (2014) 2680-2686.
[3] A.R. Türker, Separation and Purification Reviews, 41 (2012) 169-206.
[4] R. Sitko, B. Zawisza and E. Malicka, Trends in Analytical Chemistry, 51 (2013) 33-43.
[5] M. Alkan and M. Doğan, Journal of Colloid and Interface Science, 243 (2001) 280-291.

---

* Corresponding author, *E-mail: rukiye.saygili@dpu.edu.tr*

P-13

# Spectrophotometric Determination of Tungsten in Micel Media

**İlknur Bağatır Erbaş, Füsun Okçu Pelit, F. Nil Ertaş and Levent Pelit***

Ege University, Faculty of Science, Department of Chemistry, 35100, İzmir, Turkey

*E-mail: ilknurbgtr@ gmail.com*

Tungsten has many applications in military and environment and nowadays, its use as an alternative to lead is becoming widespread. Pollutant effects are observed in water and soil samples. The potential impact to human health has made the Centers for Disease Control to investigate the link of tungsten to human health in impacted areas [1]. The analytical methods used in the literature to identify and illuminate the behavior of tungsten metal in environmental samples are few and generally, graphite furnace atomic absorption spectrophotometer (GFAAS), X-ray fluorescence spectrophotometer (XRF), induced plasma atomic emission spectroscopy (ICP-OES) [2] and ICP-mass spectroscopy (ICP-MS) [3] methods are used for determination. These methods are quite expensive and require complicated devices. As preprocessing, spectrophotometric applications by liquid-liquid extraction have also been performed. In these studies, benzoinoximete, tributyl-phosphate, thiocyanate, dithiol and Amberlite XAD-1180 were used to separate tungsten from industrial waters and aqueous media [4]. Most of these methods have not been validated, and these methods involve preliminary steps that require long pretreatment steps. Nowadays, cheap methods that are easy to use are being sought and for this purpose, application areas of spectroscopic methods are increasing. It is known that tungsten complexes with pyrogallol red (PGR) reactant and is used for spectroscopic purposes. In addition, metal complexes showed bathochromic and hyperchromic effects in micellar environments and this reaction have been used for more sensitive analyzes. In this study, it was aimed to improve the spectroscopic signal of the complex formed by tungsten metal with PGR using micellar 1-methyl-3-octadecyl-imidazolium bromide (C18mimBr). Optimum conditions were obtained by operating in a pH 4.0 Acetic Acid / Acetate buffer, with 40 mL of $5.0 \times 10^{-3}$ M ionic liquid (C18mimBr) solution with $1.0 \times 10^{-3}$ M PGR (40 mL) with a 10 min waiting time. The limit of detection (LOD) and the limit of quantification (LOQ) were calculated as $2.3\text{x}10^{-7}$ M and $7.7\text{x } 10^{-7}$ M, respectively. Repeatability is 5.1%. The ionic liquid used to exhibited bathochromic and hyperchromic activity and could thus be reduced to lower specification limits.

## References

[1] A.J. Bednar, J.E. Mirecki, L.S. Inouye, L.E. Winfield, S.L. Larson and D.B. Ringelberg, Talanta, 72 (2007) 1828-1832.

[2] A.J. Bednar, W.T. Jones, M.A. Chappell, D.R. Johnson and D.B. Ringelberg, Talanta, 80 (2010) 1257-1263.

[3] S.S. Morrison, C.L. Beck, J. M. Bowen, T.A. Eggemeyer, C.C. Hines, M. Leizers, L.A. Metz, S.M. Morley, K.R. Restis, M.S. Snow, D.E. Wall, S.B. Clark and B.N. Seiner, Journal of Radioanalytical and Nuclear Chemistry, 311 (2017) 749–754

[2] M. Soylak, L. Elçi and M. Doğan, Talanta 42 (1995) 1513-1517.

---

* Corresponding author, *E-mail: levent.pelit@ege.edu.tr*

P-14

# Photoelectrocatalytic Degradation of Diquat by Using Nanotube Structured $TiO_2$ Photoanodes

Turan Mutlu[1], Levent Özcan[2]* and Sedat Yurdakal[1]

[1]Afyon Kocatepe University, Faculty of Science and Literature, Department of Chemistry, 03200, Afyonkarahisar, Turkey
[2]Afyon Kocatepe University, Faculty of Engineering, Department of Biomedical Engineering, 03200, Afyonkarahisar, Turkey

*E-mail: turanmutluu@gmail.com*

Diquat, a herbicide, is used mostly as non-selective contact herbicide meaning that causing injury only to the parts of the plant to which it is applied, crop desiccant and aquatic herbicides [1]. It is a highly toxic compound and in the case of contact or ingestion, great health problems could occur, such as corrosive effect on skin, kidney failure and central nervous system toxicity [1]. For this reason, it is important to investigate effective methods for degradation of diquat in water. Photoelectrocatalytic method, i.e. combination of the heterogeneous photocatalysis with the electrocatalytic one, has shown to be an effective tool to improve the performances of degradation reactions [2]. In this work, nano-tube structured $TiO_2$ photoanodes on Ti foil were prepared by using anodic oxidation methods in both aqueous and non-aqueous electrolytes. Photoanodes were characterized by XRD, SEM and electrochemical methods (Figure 1). The prepared photoanodes were used for photoelectrocatalytic degradation of diquat under UV irradiation. Non-nanostructured $TiO_2$ anodes were also prepared by the thermal oxidation method for comparison aim at different calcination temperatures, however, they showed worst activity due to their low active surface areas with respect to nano-structured ones. Photocatalytic and electrocatalytic experiments were also performed and it was obtained that photoelectrocatalytic degradation is more effective method than that of photocatalytic and electrocatalytic. In addition, the most effective degradation was obtained by nanotube structured $TiO_2$ photoanodes prepared in non-aqueous electrolyte. The obtained activity results were supported by characterization results. In order to improve the obtained results, we are also preparing noble metal (such as Pt and Au) loaded photoanodes for the same degradation experiments.

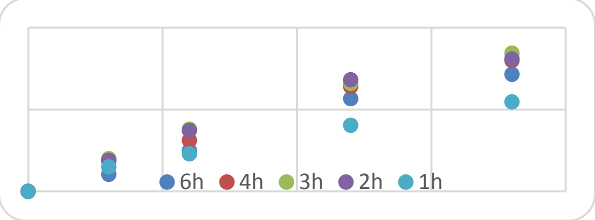


**Figure 1.** Comparison of photoelectrocatalytic performance of different photo anodes produced in different anodization time labelled as TiNTEG500-xh (x: Anodization time)

## References

[1] G.Z. Fortenberry, J. Beckman, A. Schwartz, J.B. Prado, L.S. Graham, S. Higgins, M. Lackovic, P. Mulay, H. Bojes, J. Waltz, Y. Mitchell, K. Leinenkugel, M.S. Oriel, E. Evans and G.M. Calvert, Environmental Research 146 (2016) 191-199.
[2] L. Özcan, S. Yurdakal, V. Augugliaro, V. Loddo, S. Palmas, G. Palmisano and L. Palmisano, Applied Catalysis B: Environmental, 132–133 (2013) 535-542.

---

* Corresponding author, *E-mail: leventozcan@aku.edu.tr*

P-15

# Sensitive and Rapid Determination of Protease Inhibitors in Pure Drugs and Their Mixtures using High Performance Liquid Chromatography

**Gizem Tırıs[1] and Nevin Erk[2]***

[1]Bezmialem Vakıf University, Faculty of Pharmacy, Department of Analytical Chemistry, İstanbul, Turkey
[2]Ankara University, Faculty of Pharmacy, Department of Analytical Chemistry, Ankara, Turkey

*E-mail: erk@pharmacy.ankara.edu.tr*

A simple, economic, sensitive and rapid high performance liquid method (HPLC) for the simultaneous determination of Abacavir (AB), Lamivudine (LM) and Zidovudine (ZD) in pure drugs and their mixtures was developed and validated in the present study. Better separation of the all drugs was achieved on Zorbax CN, (100 x 4.6 mm, 3.5 μm) column with the mobile phase consisted of a mixture of 0.05 M potassium dihydrogen phosphate buffer, methanol in the ratio of (55:45, v/v) with an isocratic elution. A diode-array detection was used in the 200- 300 nm range and the detection wavelength was set at 275 nm with a flow rate of 0.8 $\text{mL}\cdot\text{min}^{-1}$, loop of 20 μL and column at $25^0$C temperature. The internal standard method using acetaminophen as the internal standard is used. Calibration plots showed correlation coefficients $r > 0.9970$ which were calculated by the least square method. As for linearity the HPLC was applicable in the concentration ranges of 1.0 - 50.0 $\mu\text{g.ml}^{-1}$ for AB, LM and ZD. The proposed method was employed with a high degree of precision and accuracy in the determination of all active ingredients. The retention time was observed at 5.28, 3.59 and 3.30 min for AB, LM and ZD, respectively. The method was suitable for the simultaneous determination and it can be applied in the quality control department in industries, bio-pharmaceutics and bio-equivalence studies.

## References

[1] P. Djurdjevic, A. Laban, S. Markovic and M. Jelikic-Stankov, Anal. Lett., 37(13) (2004) 2649-2667.
[2] W. Kromdijk, S.A. Pereira, H. Rosing, J.W. Mulder, J.H. Beijnen and A.D.R. Huitema, Journal of Chromatogr. B: Anal. Technol. Biomed. Life Sci., 43 (2013) 919-920.

---

* Corresponding author, *E-mail: erk@pharmacy.ankara.edu.tr*

P-16

# Interactions with Metal Ions of the Functionalized-halloysite Nanotubes with Hydroxyl Groups

**Davut Laçin[1], Elif Avcu[2] and Tülay Bal Demirci[2]***

[1]İstanbul University, Faculty of Engineering, Deparment of Geological Engineering, 34320, Avcılar, İstanbul, Turkey
[2]İstanbul University, Faculty of Engineering, Department of Chemistry, 34320 Avcılar, İstanbul, Turkey

*E-mail: tulaybal@istanbul.edu.tr*

Halloysites (Hal) are naturally two-layered aluminosilicate clay with nanotubular morphology with external diameter of about 50–80 nm, an internal diameter (lumen) of 10–15 nm and a length of about 1000 nm in the nanoscale, are readily obtainable, and are 50 times less toxic than the usual table salt [1-2]. The crystal structure of each layer consists of scrolled layers composed of a sheet of corner-sharing $SiO_4$ tetrahedral bonded to a sheet of edge-sharing $AlO_6$ octahedral to form a 1:1 layer silicate terminated with hydroxyl groups [3]. A purified halloysite tube wall is composed of 10–15 bilayers of aluminum and silicon oxide. Halloysites have been used as an adsorbent for transition-metal ions and organic species, especially as supporting substrates for nanoparticles in various water purification systems [4].

In this work, we prepared *functionalized*-halloysite nanotubes with different hydroxyl groups (Hal-OH) and acid-leached halloysites (AHal). The products were treated with transition metal salts in water at different pH values and at different temperatures and were investigated adsorption on halloysite. The structures were characterized with AAS, ATR-FTIR, Powder XRD, EDX and SEM.

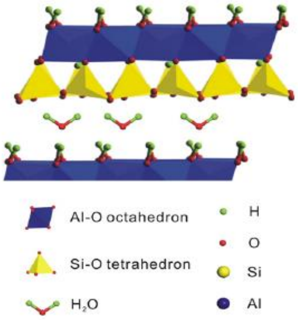


**Figure 1.** The crystalline structure of hydrated halloysite form

## References

[1] V. Bertolino, G. Cavallaro, G. Lazzara, S. Miliot and F. Parisi, Langmuir, 33 (2017) 3317-3323.
[2] B. Gradzik, A. Stenzel, A.R. Boccaccini and M. El Fray, Des. Monomers Polym., 18(6) (2015) 501-511.
[3] C.S. Yelleswarapu, G. Gu, E. Abdullayev, Y. Lvov and D.V.G.L.N. Rao, Opt. Commun., 283 (2010) 438-441.
[4] D. Presti, A. Pedone, G. Mancini, C. Duce, M. R. Tine´ and V. Barone, Phys.Chem.Chem.Phys., 18 (2016) 2164-2174.

---

* Corresponding author, *E-mail: tulaybal@istanbul.edu.tr*

# Archaeological Chemistry

# Investigation of Comparison Total Porosity of Some Glazed/Unglazed Hasankeyf Ceramics

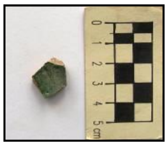
**Nurşen Özkul Fındık**[1]*, **Yılmaz Güler**[2], **Ali Akın Akyol**[3] **and Nurşen Sarı**[4]

[1]Gazi University, Faculty of Arts, Department of History of Art, 06500, Ankara, Turkey
[2]Van Yüzüncü Yıl University, Faculty of Arts, Department of History of Art, 65090, Van, Turkey
[3]Gazi University, Faculty of Fine Arts, Department of Conservation and Restoration of Cultural Properties, 06830, Ankara, Turkey
[4]Gazi University, Faculty of Science, Department of Chemistry, 06500, Ankara, Turkey

*E-mail: nursenozkul@gmail.com*

Halloysites (Hal) are naturally two-layered aluminosilicate clay with nanotubular morphology with Most of the ceramic objects found in archaeological excavations in Anatolia are made of glazed/ unglazed ceramics. The excavations which revealed a great number of glazed or unglazed ceramic pieces in addition to architectural ruins have necessitated both archaeological and archaeometric analyses. Ceramic pieces obtained from different areas of the Hasankeyf archaeological site and were investigated archaeometrically [1]. There are important to obtain information deal with the composition of archaeological ceramics in order to understand the structure of the ceramics of the past century. For this purpose, a variety of techniques have been used [2]. One of the techniques is thin section optical microscopy analysis. It is being used the DMLP Model Microscope to identify the composition of ceramics. Here, some glazed/unglazed Hasankeyf Ceramics were made a comparison of total porosity by means of thin section optical microscopy analysis (Table 1). It was determined that there were differences in the pores of glazed and unglazed.

**Table 1.** Glazed and unglazed comparison for pores (%P)

| Ceramic samples | Total Porosity (%P) | T (ºC) |
|---|---|---|
| <br>Unglazed | 4 | 850-900 |
| <br>Glazed | 7 | 900 |

**References**
[1] N. Özkul Fındık, A.A. Akyol and N**.** Sarı, Journal of Mediterranean Archaeology and Archaeometry, 14 (2014) 261-271.
[2] M. Tite, O. Watson, T. Pradell, M. Matin, G. Molina, K. Domoney and A. Bouquillon, Journal of Archaeological Science, 57 (2015) 80-91.

---

***** Corresponding author, *E-mail: nursenf@gazi.edu.tr*

P-18

# Comparison of TGA with SEM-EDX Analysis of Some Hasankeyf Ceramics

**Nurşen Özkul Fındık**[1]*, Ali Akın Akyol[2] and Nurşen Sarı[3]

[1]Gazi University, Faculty of Arts, Department of History of Art, 06500, Ankara, Turkey
[2]Gazi University, Faculty of Fine Arts, Department of Conservation and Restoration of Cultural Properties, 06830, Ankara, Turkey
[3]Gazi University, Faculty of Science, Department of Chemistry, 06500, Ankara, Turkey

*E-mail: nursenozkul@gmail.com*

Archaeology is the study of historic or prehistoric people and their culture through the study of their artifacts. Turkey is a treasure harboring ancient cultures. Hasankeyf is an important medieval town located in the southeast of Turkey. Its existence is currently threatened by the Ilısu Dam, whose construction is continuing in the region. Excavations for the documentation, conservation and protection of the natural and historical assets in Hasankeyf has been going on systematically since 1998 [1]. So the assessment of the residues is important of archaeological artifacts. As known, the common aim of the study on archaeological artifacts (especially ceramics) is to obtain representative information about the composition. For this purpose, a variety of techniques have been used [2]. One of the techniques is Scanning Electron Microscopy coupled with Energy Dispersive X-ray (SEM/EDX) Spectroscopy. SEM/EDX is the best known and most widely-used of the surface analytical techniques (Figure 1). For Hasankeyf ceramics used these technics also.

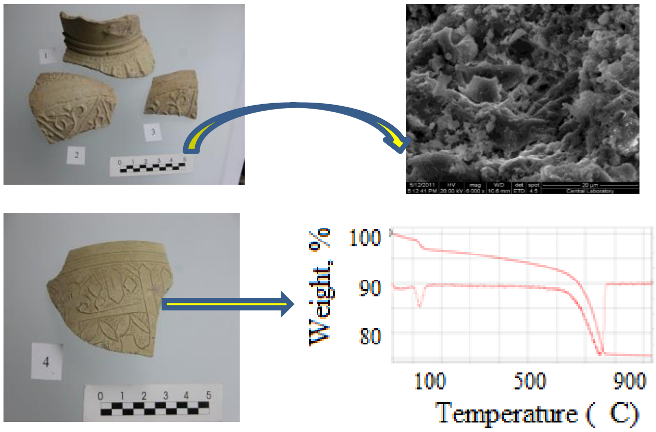


**Figure 1.** TGA analysis and SEM morphology for some Hasankeyf ceramıcs

**References**

[1] N. Özkul Fındık, A.A. Akyol and N. Sarı, Journal of Mediterranean Archaeology and Archaeometry, 14 (2014) 261-271.

[2] M. Tite, O. Watson, T. Pradell, M. Matin, G. Molina, K. Domoney and A. Bouquillon, Journal of Archaeological Science, 57 (2015) 80-91

---

* Corresponding author, *E-mail: nursenozkul@gmail.com*

# Bioscience & Biotechnology

P-19

# Determination of Chemical Content of *Sphagnum Molle* Plant and Investigation on Antiproliferative Activity with Real-Time Cell Analysis System

**Muhammed Altun**[1]* and **Gökhan Abay**[2]

[1]Çankırı Karatekin University, Faculty of Science, Department of Chemistry, 18100, Çankırı, Turkey
[2]Recep Tayip Erdogan University, Faculty of Architecture Design and Fine Arts, Department of Landscape Architecture, 53100, Rize, Turkey

*E-mail: muhammedaltun@karatekin.edu.tr*

Cancer is one of the major diseases in today's world. According to the World Health Organization, if no precautions are taken against cancer, 26 million people worldwide will have cancer until 2030. Plants synthesize many primary and secondary metabolites called organic compounds. Primary metabolites take part in important events such as photosynthesis, respiration, growth and development. Secondary metabolites are chemotaxonomically important natural products studied widely in the last decades. Bryophytes are potential therapeutic sources of cancer treatment due to the components they produce. *Sphagnum molle* was first recorded in our country in Rize, Fındıklı [1]. In this study, chemical component analysis of MeOH:$CHCl_3$ extract of the *Sphagnum molle* plant were carried out with HPLC/TOF-MS and investigated the antiproliferative effects of these components against PC3 (human prostate cancer) cell lines (Figure 1).

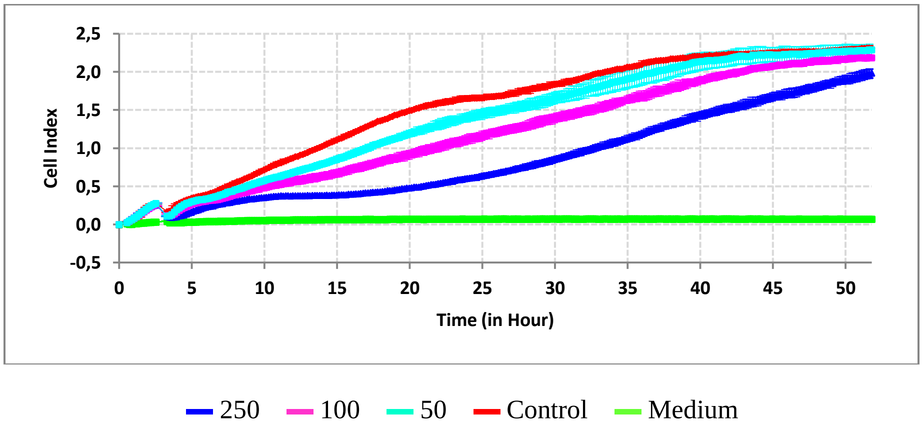


**Figure 1.** Antiproliferative effect of MeOH:$CHCl_3$ extract of *Sphagnum molle* against to PC3 cell lines

**References**
[1] G. Abay and T. Keçeli, Cryptogamie Bryologie, 35 (2014) 105-112.

**Acknowledgement**
The authors express their thanks to Çankırı Karatekin University for its financial support (BAP-FF090316B16).

---

* Corresponding author, *E-mail: muhammedaltun@karatekin.edu.tr*

# Optimizing the Physical Properties of Injectable Polymer/Calcium Phosphate Composite Bone Substitutes

**Öznur Demir Oğuz and Duygu Ege***

Boğaziçi University, Institute of Biomedical Engineering, 34684, Istanbul, Turkey

*E-mail: duygu.ege@boun.edu.tr*

The development of an injectable bone substitute (IBS) while mimicking the highly mineralized collagen-based matrix of native bone is crucial to obtain mechanically compatible and osteoconductive formulations. Calcium phosphate cements (CPCs) are widely exploited and promising bone substitutes but their injection into the body is limited due to their relatively poor cohesion [1]. To this end, an injectable and thermoresponsive polymer, methylcellulose (MC), was combined with CPCs in order to overcome limitations of CPCs and to improve the mechanical strength, viscosity, bio-absorbability, and injectability. Also, gelatin was incorporated to lower the phase transition temperature and to enhance cellular adhesion through presented RGD sequence within gelatin structure. IBS was prepared by mixing powder phase (tetra calcium phosphate (TTCP), and dicalcium phosphate dehydrates (DCPD) and calcium sulfate dehydrates (CSD) with the liquid phase (MC and gelatin). The amount of MC in the produced IBS varied from 0 to 12 wt% while the gelatin amount was 2.5 wt%. To prepare the powder phase first, TTCP and DCPD was mixed with 1 to 1 (wt to wt) ratio and TTCP-DCPD mixture was mixed with CSD with 1 to 4 (wt to wt) ratio [2]. The injectability was determined by measuring the mass % of liquid and powder phase mixture that could be extruded by hand from a 10 ml syringe with 18 gauge needle. The setting time and temperature were measured using the test tube inversion technique. Liquid phase prepared by 5 and 6 wt% MC solution was found to be more suitable for preparation of the injectable gel because the the gelation takes place at around 37°C within 15 min. For easy injection from the syringe, powder to liquid ratio should be between 1 to 1.8 wt%. After, the characterization of the samples was performed by using X-Ray Diffraction (XRD), Fourier Transform Infrared Analysis (FTIR), and rheometer. FTIR proved the hydrophilic interaction between MC and gelatin through both amides I at 1633 $cm^{-1}$ and β-glycosides bonds among saccharide units at 900-1230 $cm^{-1}$. XRD analysis of IBS showed the peaks for the crystalline phases of the samples which were for TTCP, DCPD, and CSD. The gelation behavior of liquid phase and the mixture of liquid and powder phase were examined using G' and G" measured by rheometer. Rheometer results showed that all the prepared formulations exhibited Newtonian flow [3]. When the concentration of MC increased, the gelation time decreased. Accordingly, IBS prepared by using liquid phase containing 6 wt% MC was found to be suitable for the preparation of an injectable gel due to its suitable viscosity, gelation time and gelation temperature. Overall, the synthesized thermo-responsive IBS represents promising platforms for future studies in bone tissue engineering and bone-defect repair.

**References**

[1] Z. Chen, X. Zhang, L.Kang, F. Xu, F.Z. Cui, Front Mater Sci, 9 (2015) 332-345
[2] V.V. Thai, B.T. Lee, J Mater Sci: Mater Med, 21(2010) 1867-1874.
[3] H. Park, M.H. Kim, Y.I. Yoon, W.H. Park, Carbohydrate Polymers, 157 (2017) 775-783.

---

* Corresponding author, *E-mail: duygu.ege@boun.edu.tr*

P-21

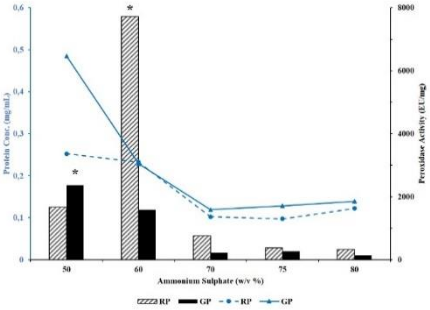
# Synthesis of Enzyme-inorganic Hybrid Nanoflowers Using the Purified Peroxidase from Ripe and Unripe Bitter Gourd and Its Use in Dye Decolorization

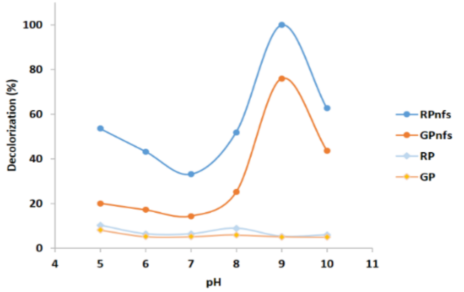
**Cevahir Altınkaynak[1]*, Ayşe Baldemir[2], Nalan Özdemir[1], Vedat Yılmaz[3] and İsmail Öçsoy[3]**

[1]Erciyes University, Faculty of Science, Department of Chemistry, Kayseri, Turkey
[2]Erciyes University, Faculty of Pharmacy, Department of Pharmaceutical Botany, Kayseri, Turkey.
[3]Erciyes University, Faculty of Pharmacy, Department of Analytical Chemistry, 38039, Kayseri, Turkey.

*E-mail: akcevahir@gmail.com*

Bitter gourd peroxidase enzyme can be purified from ripe and unripe (green) fruits and that procedure can be affect the amount and activity of the enzyme obtained. Bitter gourd peroxidases can catalyze dye decolorization reactions. In order to increase the use of enzymes, their activities, stability and recovery need to be increased [1,2]. Recently, protein-inorganic hybrid nanoflower synthesis method is described, an exciting and inspiring strategy known to increase enzyme activity, stability and reusability [1-3]. This procedure requires a metal ion, phosphate groups and proteins. Herein, we partially purified peroxidase from ripe and unripe fruits of Momordica caharantia Descourt, and identified the optimum conditions and yield of the synthesis procedure (Figure 1). Then we synthesized enzyme-inorganic hybrid nanoflowers using bitter gourd peroxidases purified from ripe and unripe fruit. Some characteristics of them were confirmed by SEM, EDX, XRD and FTIR. The hybrid nanoflowers exhibited enhanced enzymatic activity than free forms. The decolorization of direct blue 1 with hybrid nanoflowers and free forms were evaluated in the various pHs (5-10) (Figure 2) and temperatures (25°C, 40°C, and 60°C).





([GP] Bitter Gourd Unripe (Green) Peroxidase, [RP] Bitter Gourd Ripe Peroxidase, [nfs] Nanoflowers)

**Figure 1.** Effect of ripe and unripe (Green) fruits of *M. charantia* on ammonium sulphate fractionation of bitter gourd proteins. Marked (*) columns are the optimum conditions

**Figure 2.** Effect of pH on the enzymatic decolorization of Direct Blue 1

## References

[1] J. Ge, J. Lei and R.N. Zare, Nature Nanotechnology, 7 (2012) 428-432.
[2] C. Altinkaynak, S. Tavlasoglu, N. Özdemir and I. Ocsoy, Enzyme Microb Technol, 93-94 (2016) 105-112.
[3] C. Altinkaynak, I. Yilmaz, Z. Koksal, H. Özdemir, I. Ocsoy and N. Özdemir, Int. J. Biol. Macromolec., 84 (2016) 402-409.

---

* Corresponding author, *E-mail: akcevahir@gmail.com*

# Characterization of Electrospun Polyvinyl Alcohol/Chitosan Nanofiber: Using for Conversion of Glucose to Fructose

**Gökmen Arabacı[1], Yasemin İspirli Doğaç[2], Ceyhun Işık[1]*, İlyas Deveci[3] and Mustafa Teke[1]**

[1]Muğla Sıtkı Koçman University, Faculty of Science, Chemistry Department, Muğla, Turkey
[2]Muğla Sıtkı Koçman University, Muğla Vocational School, Chemistry and Chemical Processing Technology Department, Muğla, Turkey
[3]Selçuk University, Technical Sciences Vocational School, Chemistry and Chemical Processing Technology Department, Konya, Turkey

*E-mail: cyhn87@yahoo.com*

In this work, polyvinyl alcohol (PVA)/chitosan(Ch) nanofibers were synthesized by electrospinning technique. The operational parameters of nanofibers were PVA concentration (%), Ch concentration (%), voltage (kV), needle tip-collector distance (cm) and injection speed (ml/h). The criteria used in deciding the best PVA/Ch nanofiber structure was the taylor cone formation during electrospinning, fiber formation, no formation of polymer droplets at the needle tip or on the collector, stable system, easy removal of fiber from the collector, mechanically stable fiber. According to these criteria, the most appropriate operational parameters as electric voltage, distance between tip and collector, concentration of PVA and Ch, injection speed were found as 13 kV, 20 cm, 6% PVA, 1% Ch and 0.2 ml/h, respectively. The morphology and structure of the nanofibers were characterized by scanning electron microscopy (SEM), Fourier transform infrared spectroscopy (FTIR) and thermal gravimetric analysis (TGA) (Figure 1). As seen in the figure, the obtained nanofibers were randomly-organized, smooth and round-shaped. SEM results showed that the resulting nanofibers had the narrow diameter distribution. To use the nanofibers in glucose-fructose conversion process, glucose isomerase (GI) enzyme was immobilized onto the nanofibers by adsorption and crosslinking methods [1]. Optimum conditions and enzymatic characteristics of immobilized GI were investigated. The significance of this study is improving of stability properties of GI for the industrial usage.

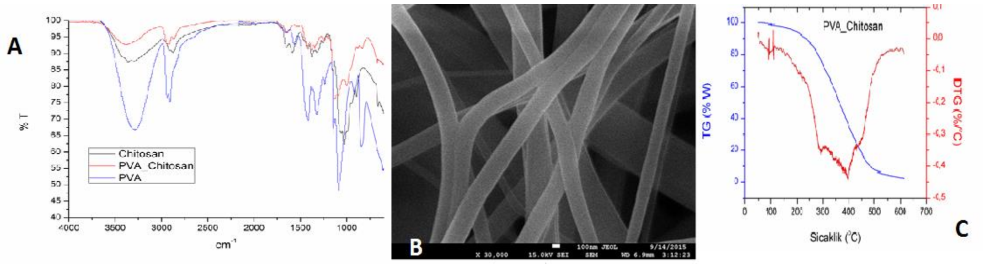


**Figure 1.** The electrospun PVA/Ch nanofiber characterization: A. FTIR spectrums; B. SEM image; C. TG and DTG curves

## References

[1] H. Zhao, Q. Cui, V. Shah, J. Xu, T. Wang, Journal of Molecular Catalysis B: Enzymatic, 126 (2016) 18-23.

## Acknowlengement

This work was supported by a grant from the Muğla Sıtkı Koçman University Scientific Research Projects (No:13/182 and 17/024).

---

* Corresponding author, *E-mail: cyhn87@yahoo.com*

P-23

# Structural Characterization of Different Magnetic Core-shells Nanogels Based on $NiFe_2O_4$

Yasemin İspirli Doğaç[1]*, Mustafa Kemal Sezgintürk[2], Funda Öztürk[3] and Mustafa Teke[4]

[1]Muğla Sıtkı Koçman University, Muğla Vocational School, Chem. and Chem. Processing, Muğla, Turkey
[2]Çanakkale Onsekiz Mart University, Faculty of Engineering, Department of Bioengineering, Çanakkale, Turkey
[3]Namık Kemal University, Faculty of Arts and Sciences, Department of Chemistry, Tekirdağ, Turkey
[4]Muğla Sıtkı Koçman University, Faculty of Science, Department of Chemistry, Muğla, Turkey

*E-mail: y-ispirli@hotmail.com*

Due to the advantages of magnetic nanoparticles and magnetic polymers such as observable nature and high surface area, they have been investigated for many applications [1]. Magnetic nanogels, a class of these structures, are a popular topic for research in recent years. In the submitted study, $NiFe_2O_4$ magnetic nanoparticles were covered by acrylamide/sodium acrylate copolymers and pHEMA. The $NiFe_2O_4$-acrylamide/sodium acrylate nanogels (NF-AM/AA) were synthesized by solution polymerization. The $NiFe_2O_4$- pHEMA nanogels (NF-pHEMA) were synthesized by photopolymerization. The operational parameters of nanogels were amount of $NiFe_2O_4$ nanoparticles (5-400 mg) and the rate of AM:AA-Na (25:75, 50:50, 75:25) or % HEMA concentration (0.5; 1; 2%). The effect of operational parameters was investigated for optimizing the morphology and structure of the magnetic nanogels by scanning electron microscopy (SEM), fourier transform infrared spectroscopy (FTIR), thermal gravimetric analysis (TGA) and atomic force microscopy (AFM) (Figure 1). According to our results, the magnetic nanogels were successfully formed as a core-shell structure and the most appropriate operational parameters were found as 100 mg $NiFe_2O_4$ and 50:50 (AM:AA-Na rate) for NF-AM/AA; 15 mg $NiFe_2O_4$ and % 1 HEMA for NF-pHEMA. Cross-linked with AM /AA copolymers $NiFe_2O_4$ nanogel (NF-AM/AA) and pHEMA-coated $NiFe_2O_4$ nanogel (NF-pHEMA) have not been reported in the previous works. For this reason, the synthesis and characterization of these structures will be the first record in the literature.

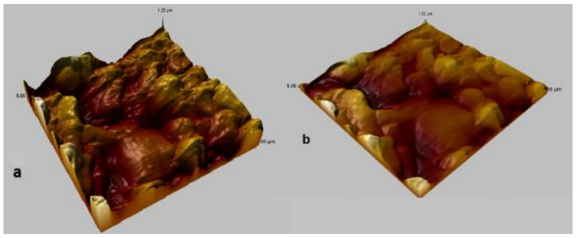


**Figure 1.** The AFM images of (a) NF-AM/AA, and (b) NF-pHEMA magnetic nanogels

## References

[1] A.M. Atta, O.E. El-Azabawy, H.S. Ismail and M.A. Hegazy, Corrosion Science, 53(5) (2011) 1680-1689.

## Acknowlengement

This work was supported by a grant from the Scientific and Technological Research Council of Turkey (TÜBİTAK)-National Postdoctoral Research Scholarship Programme (2218).

---

* Corresponding author, *E-mail: y-ispirli@hotmail.com*

# Optimization and Characterization of Urease Immobilization on Electrospun Polyvinyl Alcohol/Chitosan Nanofiber

**Nur Kutlu[1], Yasemin İspirli Doğaç[2*], İlyas Deveci[3] and Mustafa Teke[1]**

[1]Muğla Sıtkı Koçman University, Faculty of Science, Chemistry Department, Muğla, Turkey
[2]Muğla Sıtkı Koçman University, Muğla Vocational School, Chem. and Chem. Processing, Muğla, Turkey
[3]Selçuk University, Technical Sciences Vocational School, Chem. and Chem. Processing Konya, Turkey

*E-mail: y-ispirli@hotmail.com*

In this work, polyvinyl alcohol (PVA)/chitosan(Ch) nanofibers were used for urease immobilization. The nanofibers were prepared by electrospinning technique [1] with the most appropriate operational parameters as electric voltage, distance between tip and collector, concentration of PVA and Ch, injection speed were found as 13 kV, 20 cm, 6% PVA, 1% Ch and 0.2 ml/h, respectively. Urease immobilization was carried out in which the most suitable nanofiber formation was observed. The enzyme was immobilized onto the nanofibers by adsorption and then cross-linking methods. For the optimization of urease immobilization, the amount of nanofibers, the adsorption time, the amount of urease and the amount of glutaraldehyde were investigated as basic parameters. The optimum temperature, optimum pH, thermal stability, pH stability, kinetic parameters and reusability parameters were investigated in the characterization of urease immobilized nanofibers prepared under optimum conditions. Then, the urea removal performance of the artificial serum sample was investigated by the recycled column system of urease immobilized PVA/chitosan nanofibers, which is suitable for the activity and stability (Figure 1). Urease immobilization systems performed about 85% when compared with free enzyme activity. The $K_m$ and $V_m$ values of free urease were calculated as 0.177 mM and 0.369 U /mg protein, respectively, and the $K_m$ and $V_m$ values of urease immobilization system were calculated as 0.181 mM and 0.306 U/mg protein, respectively. Urease immobilization systems have improved pH stability from 3-10. It developed thermal stability at 58.0% at 50 ° C and 34.6% at 60 °C.

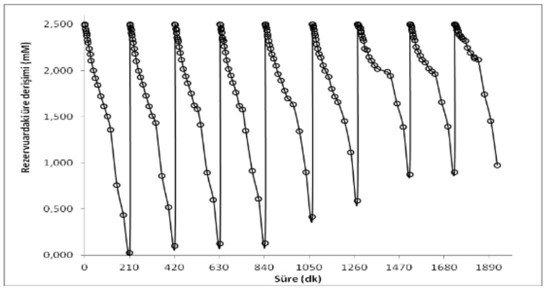


**Figure 1.** Urea removal performance from serum sample of urease immobilized nanofibers

**References**

[1] K. Paipitak, T. Pompra, P. Mongkontalang, W. Tchitdheer and W. Pecharapa, Procedia Engineering, 8 (2011) 101-105.

---

* Corresponding author, *E-mail: y-ispirli@hotmail.com*

P-25

# The Effect of Electronegative Substituents on "IC50 Value"

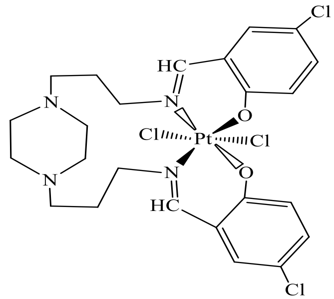
**Meryem Çat**, **Elvan Hasanoğlu Özkan, Nurşen Sarı, Özlem Çolak and Fatma Arslan***

Gazi University, Faculty of Science, Department of Chemistry, 06500, Ankara, Turkey

*E-mail: mrymcat@gmail.com*

Acetylcholinesterase enzyme (AChE), inhibitors have side effects, including hepatotoxicity, gastrointestinal tract excitement and hallucination. Therefore, the identification of new and better AChE inhibitors remains an important goal. Donepezil is a new class of ChE inhibitor having an N-benzylpiperidine and indanone moiety [1]. In the present study, the Schiff base and it's Pt(IV) complex were prepared by reacting of piperazine derivative (1.0 mmol, 15 mL methanol) with 5-chloro-salicylaldehyde **(**2.0 mmol, 10 mL methanol). The inhibitory effects of the synthesized compounds on AChE were evaluated using the Ellman method [2] with Donepezil.HCl as the positive control. We examined the inhibition effect of the synthesized compounds against the AChE enzyme, purified from *Electrophorus electricus* (electric eel) Type V-S, activity of 100 unit/mL. The $IC_{50}$ values for AChE inhibition and the selectivity for AChE are summarized in Table 1.

**Table 1.** $IC_{50}$ values of studied compounds and Donepezil.HCl



| **Compounds** | **$IC_{50}$ [ M ]** |
|---|---|
| Ligand | $1.27 \times 10^{-6}$ |
| Complex | $5.29 \times 10^{-7}$ |
| Donepezil.HCl | $1.29 \times 10^{-8}$ |

**References**

[1] H. Sugimoto, H. Ogura, Y. Arai, Y. Iimura and Y. Yamanishi, Jap. J. Pharmacol., 89 (2002) 7-20.

[2] A.T.Tunç, E. Aynacı Koyuncu and F. Arslan, Artif. Cells Nanomed. Biotech., 44 (2016) 1659-1664.

---

* Corresponding author, *E-mail: fatma@gazi.edu.tr*

P-26

# Enzyme Inhibition Study by means of Ellman Method for Pt(IV) Complex with Piperazine Derivatives

**Meryem Çat**, Elvan Hasanoğlu Özkan, Özlem Çolak, Nurşen Sarı and Fatma Arslan*

Gazi University, Faculty of Science, Department of Chemistry, 06500, Ankara, Turkey

*E-mail: mrymcat@gmail.com*

Alzheimer 's disease (AD) is characterized by memory loss, difficulty in speaking, problems with communication and reasoning [1]. There are many causes about the emergence of this disease, like genetic factors, autoimmune reactions, protein plaques and tangles [2]. One of these reasons is the cholinergic hypothesis that AD is caused by reduced synthesis of the neurotransmitter acetylcholine (ACh). AChE inhibitors inhibit the hydrolysis reaction of ACh, so low ACh level at AD patients is raised [3]. Many inhibitors such as tacrine, donepezil, physostigmine are used as drugs for AD treatment. In this study, a new series of 2,2'- ((1E,1'E)-((piperazine-1,4-diylbis(propane-3,1-diyl)) bis(azanylylidene))bis(methanylylidene)) bis(4-**X**phenol) [X:-F,-Cl,-Br]-$Pt^{+4}$ complexes were designed, synthesized, and evaluated as multi-potent anti-Alzheimer drug candidates. The synthesized compounds were characterized and then we tested the inhibitory effects of the synthesized complexes on the acetylcholinesterase enzyme. A fluoro substituent displayed higher activity compared to the chloro and bromo substituents. For the studied complexes all $IC_{50}$ against AChE were in the micromolar range.

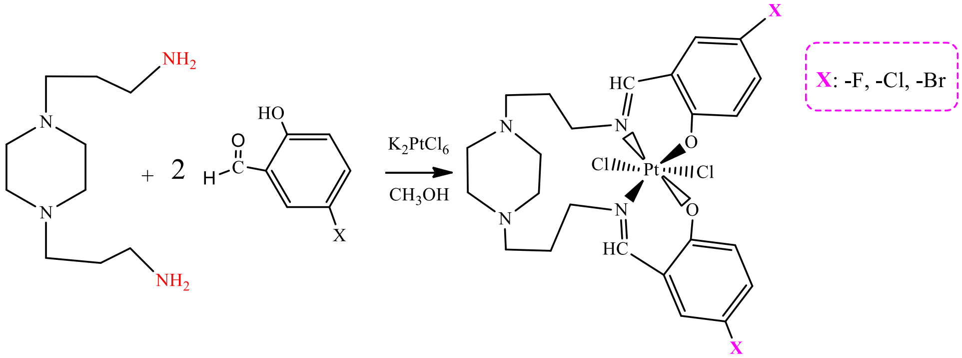


**Figure 1.** Synthesis rotation of complexes

**References**

[1] S. Akhondzadeh, M. Noroozian, M. Mohammadi, S. Ohadinia, A.H. Jamshidi and M. Khani, J. Clin. Pharm. Ther., 28 (2003) 53-59.

[2] A. Nordberg and A.L. Svensson, Drug Safety, 19 (1998) 465-480.

[3] P.T. Francis, A.M. Palmer, M. Snape and G.K. Wilcock, J. Neurol. Neurosur. Ps., 66 (1999) 137-147.

---

* Corresponding author, *E-mail: fatma@gazi.edu.tr*

# Computational & Theoretical Chemistry

P-27

# Investigation via Principal component analysis, DFT and Molecular Dynamics Simulations Approaches on the Anticorrosive Effects of Some Thiophene Derivatives against the Corrosion of Iron

**Burak Tüzün*** and **Şavaş Kaya**

Cumhuriyet University, Faculty of Science, Department of Chemistry, 58140, Sivas, Turkey

*E-mail: btuzun@cumhuriyet.edu.tr*

Some thiophene derivatives have been investigated by the DFT (Density Functional Theory) Method. All calculations were made using the Gaussian 09 program. The initial molecular models of all molecules were optimized by three different methods [1]. The molecular dynamic simulation approach is very important in terms of the explanation of the nature of the interactions between inhibitor molecules and metal surface. The most stable low energy adsorption configurations for A, B and C molecules on Fe (110) surface are given in Figure 1 [2]. In order to have a wider knowledge about the local reactivity of the thiophene derivatives, the Fukui indices for each one of the atoms in the molecules have been calculated at the B3LYP/6-31++G level of theory in gas phase [3].

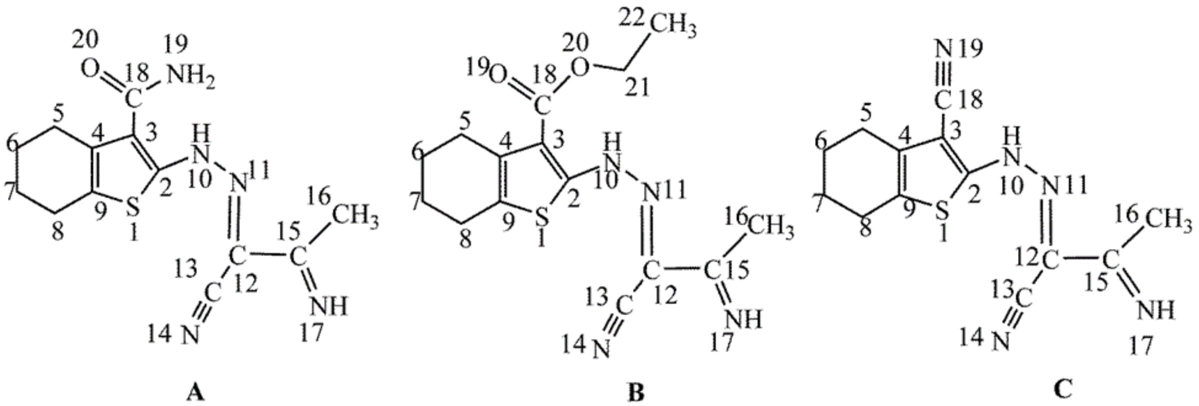


**Figure 1.** Chemical molecular structures of studied thiophene derivatives

**References**

[1] A.S. Fouda, A.A. Attia and A.A. Negm, Journal of Metallurgy 2014 (2014) 1-15.

[2] C. Zuriaga-Monroy, R. Oviedo-Roa, L.E. Montiel-Sánchez, A. Vega-Paz, J. Marín-Cruz and J.M. Martínez-Magadán, Ind. Eng. Chem. Res., 55 (2016) 3506-3516.

[3] S. Erdoğan, Z.S. Safi, S. Kaya, D. Özbakır Işın, L. Guo and C.A. Kaya, J. Mol. Struct. 1134 (2017) 751-761.

---

* Corresponding author, *E-mail: btuzun@cumhuriyet.edu.tr*

P-28

# Investigations on Small Molecular DFT and Molecular Dynamic Simulation Approaches

**Burak Tüzün**[1]* and Gamze Tüzün[2]

[1]Cumhuriyet University, Faculty of Science, Department of Chemistry, 58140, Sivas, Turkey
[2]Cumhuriyet University, Faculty of Pharmacy Department of Biochemistry, 58140, Sivas, Turkey

*E-mail: btuzun@cumhuriyet.edu.tr*

9 Small molecules were investigated by the DFT (Density Functional Theory) Method. All calculations were done using Gauss 09 program. The first molecular models of all molecules were optimized in three different ways [1-5]. The aim of the present work is to evaluate the corrosion inhibition efficiencies of $S^{2-}$, $HS^-$, $Se^{2-}$, $HSe^-$, $Te^{2-}$, $HTe^-$, $TeS_3^{2-}$, $NH^{2-}$, $OH^-$ from information provided by DFT.

Through such calculations, the corrosion inhibition efficiencies of molecules are associated with quantum chemical parameters such as the energies of the highest occupied molecular orbital ($E_{HOMO}$) and the lowest unoccupied molecular orbital ($E_{LUMO}$), HOMO–LUMO energy gap ($\Delta E$), chemical hardness ($\eta$), softness ($\sigma$), electronegativity ($\chi$), proton, affinity (PA), electrophilicity ($\omega$) and nucleophilicity ($\varepsilon$). A recent comprehensive review by us on the use of DFT as a tool in the design of corrosion inhibitors is available in the literature and the references therein.

Molecular Dynamics Simulation studies of these molecules have been studied [6].

## References

[1] K.F. Khaled, Electrochim. Acta, 53 (2008) 3484-3492.
[2] M.K. Awad, M.R. Mustafa and M.M. Abo Elnga, J. Mol. Struct. (THEOCHEM), 959 (2010) 66-74.
[3] I.B. Obot, D.D. Macdonald and Z.M. Gasem, Corros. Sci., 99 (2015) 1-30.
[4] R.D. Dennington, T.A. Keith and C.M. Millam, GaussView 5.0 (Gaussian Inc, Wallingford, 2009)
[5] M.J. Frisch et al., Gaussian 09, Revision C.01 (Gaussian Inc, Wallingford, 2009)
[6] M.A. Chidiebere, C.E. Ogukwe, K.L. Oguzie, C.N. Eneh and E.E. Oguzie, Ind. Eng. Chem. Res., 51 (2012) 668-677.

---

* Corresponding author, *E-mail: btuzun@cumhuriyet.edu.tr*

P-29

# Docking and Molecular Dynamic Simulations of the Complexes of Some Moracine Compounds with PTP1B

Şafak Ozhan Kocakaya* and Necmettin Pirinççioğlu

Dicle University, Faculty of Science, Department of Chemistry, 21280, Diyarbakır, Turkey

*E-mail: safakozhan@dicle.edu.tr*

PTP1B (protein-tyrosine phosphatase 1B) is a non-transmembrane enzyme found in the endoplasmic reticulum (ER) and is a widely expressed phosphatise. It plays a relevant modulator role in signalling pathways initiated by the activation of the tyrosine kinase receptor superfamily [1].

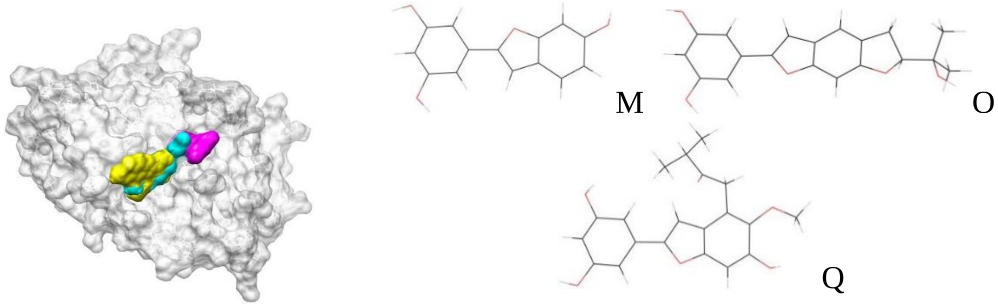


**Figure 1.** Docking results of ligands in the PTP1B catalytic pocket

The current study represents a computer assisted model to investigate the importance of specific residues in the binding site of protein tyrosine phosphatase 1B (PTP1B) with various Moracine derivatives isolated from nature. Molecular dynamics (MD) simulations were also performed to estimate the dynamic behaviours of the complexes. Absolute binding free energies were calculated with different components and accomplished by using the Molecular Mechanics-Poisson-Boltzmann Surface Area (MM-PB/SA) and Generalized Born Surface Area (MM-GB/SA) approaches. The results show that the predicted free energies of the complexes are generally consistent with the available experimental data. MM/GBSA free energy decomposition analysis indicates that the residues Arg24, Arg254, Met258, and Asp29 in the second active site in PTP1B are essential for the high selectivity of the inhibitors [2] (Figure 1 and Table 1).

**Table 1.** Dock results for the complexes of PTP1B with Moracine compounds

| Ligand | Electrostatic Energy, kcal/mol | van der Waals Energy, kcal/mol | Dock Score Energy, kcal/mol |
|---|---|---|---|
| **Moracine M** | -8.27 | -2.10 | -31.37 |
| **Moracine O** | -4.18 | -33.28 | -37.46 |
| **Moracine Q** | -4.77 | -32.45 | -37.22 |

## References

[1] A. Cheng, N. Dube, F. Gu and M.L. Tremblay, Eur. J. Biochem., 269 (2002) 1050-1059.
[2] D.A. Evans and D. Seidel, J. Am. Chem. Soc., 127 (2005) 9958-9959.

---

* Corresponding author, *E-mail: safakozhan@dicle.edu.tr*

# Synthesis and Crystal Structure of a Chiral Lactam and Three Amino Alcohols as Potent Protein Tyrosine Phosphates 1B Inhibitors

**Şafak Ozhan Kocakaya**[1]*, **Mehmet Karakaplan**[1] **and Rosario Scopelliti**[2]

[1]Dicle University, Faculty of Science, Department of Chemistry, 21280, Diyarbakır, Turkey
[2]Ecole Polytecnıcque Federale de Lausanne (EPFL), CH-1015, Lausanne, Switzerland

*E-mail: safakozhan@dicle.edu.tr*

Protein tyrosine phosphatase 1B (PTP1B) is an intracellular protein expressed in insulin responsive tissues including the classical insulin targeted tissues such as liver, muscle and fat. PTP1B plays an important role in insulin receptor signalling. PTP1B dephosphorylates the insulin receptor during its biosynthesis in endoplasmic reticulum as well as after it has been stimulated by the insulin, and thus play a central role in negative regulation of insulin signalling pathway [1,2].

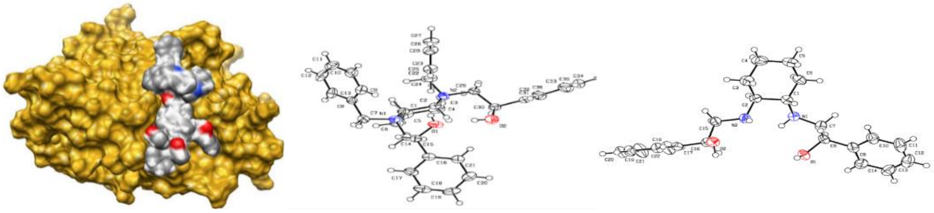


**Figure 1.** Docking results of ligand**s** in the PTP1B catalytic pocket and ORTEP plot of the compounds

Two chiral *β*-amino alcohols have been synthesized and characterized by spectroscopic techniques. Regioselective ring opening reaction of chiral styrene oxide by amine nücleophile was confirmed by X-ray diffraction data. Ligands crystallizes in the tetragonal, orthorhombic and tetragonal crystal lattice system respectively. Ligands have been used as potential inhibitors for Protein Tyrosine Phosphatase 1B enzyme (PTP1B). Potential inhibitor effect of these molecules to the target protein was investigated by Dock and molecular dynamics (MD) calculations. Dock score analysis was demonstrated that ligands have powerful enzyme inhibitor capacity towards PTP1B (Figure 1 and Table 1).

**Table 1.** Calculated thermodynamic parameters for complexation of ligands by docking method

| Ligand | Elektrostatic Energy kcal/mol | van der Waals Energy kcal/mol | Dock Score Energykcal/mol | İnternal_Energy kcal/mol |
|---|---|---|---|---|
| 1 | -0.435 | -24.911 | -25.346 | 1.876 |
| 2 | -3.909 | -37.297 | -41.206 | 7.734 |

**References**
[1] A.R. Saltiel and C.R. Kahn, Nature, 414 (2001) 799-806.
[2] J.L. Evans and B. Jallal, Expert Opin. Investig. Drugs, 8 (1999) 139-160.

---

* Corresponding author, *E-mail: safakozhan@dicle.edu.tr*

# Prediction of the Difference between Biorelevant p$K_a$ Values and Its p$K_a$ at 25˚C for Some NSAIDs by Using Abraham's Five LSER Solvation Descriptors

**Hale Seçilmiş Canbay[1], Kader Poturcu[2], Ebru Çubuk Demiralay[2] and Güleren Alsancak[2]***

[1]Mehmet Akif Ersoy University, Faculty of Engineering and Architecture, Department of Bioengineering, 15030, Burdur, Turkey
[2]Süleyman Demirel University, Arts and Science Faculty, Department of Chemistry, 32200, Isparta, Turkey

*E-mail: gulerenalsancak@sdu.edu.tr*

Non-steroidal anti-inflammatory drugs (NSAIDs) are analgesics, antipyretics and anti-inflammatory activities and are widely used in the treatment of acute and chronic pain, osteoarthritis, rheumatoid arthritis (1). Because of their effectiveness in suppressing and preventing inflammation, NSAIDs are becoming the most commonly used drugs around the world. The acidity constant (p$K_a$) is a very important property of drug candidates, because it is of main importance for their absorption, distribution, metabolism, and excretion (ADME) properties. In addition to these, the chemical state of a drug candidates determines other physicochemical properties such as solubility and lipophilicity.

The acidity constant as a thermodynamic parameter is temperature-dependent. For the precise determination of p$K_a$, experiments must be conducted under controlled constant temperature. In practice, the common reference value is 25˚C and reported p$K_a$ values are mainly clustered around room temperatures (78%). Only few data are available at biorelevant temperature (37˚C). The effect of temperature on p$K_a$ depends on the nature of the functional group. There is no significant difference between the biorelevant p$K_a$ and its p$K_a$ at 25˚C on simple carboxylic acid-containing drugs. In the present study, the temperature difference between its p$K_a$ at 25˚C and 37˚C for some NSAIDs were predicted by using a special equation. The A, B, S, E, V values were considered as molecular descriptors (2). The results show that, there is a good correlation between the predicted and experimentally determined acidity constants of NSAIDs studied.

## References

[1] B. Barfi, A. Asghari, M. Rajabi, A.G. Moghadam, N. Mirkhani and F. Ahmadi, Journal of Pharmaceutical and Biomedical Analysis, 111 (2015) 297-305.
[2] N. Sun and A. Avdeef, Journal of Pharmaceutical and Biomedical Analysis, 56 (2011) 173-182.

---

* Corresponding author, *E-mail: gulerenalsancak@sdu.edu.tr*

P-32

# Investigation of Retention Behavior of Naphthalene, Phenanthrene, Acenaphthene and Fluorene by Using Abraham's Five Terms LSER Equation

**Ali Nasıh Alı Alı, Kader Poturcu, Ebru Çubuk Demiralay and Güleren Alsancak***

Süleyman Demirel University, Arts and Science Faculty, Department of Chemistry, 32200, Isparta, Turkey

*E-mail:gulerenalsancak@sdu.edu.tr*

Retention in LC is a result of interactions between the solute and the mobile phase, the solute and the stationary phase and the mobile phase and the stationary phase. Retention mechanisms in reversed-phase liquid chromatography (RP-HPLC) are often described by the difference in various solutes hydrophobic and electronic interactions with both the stationary and mobile phase. The applicability of a LSER model for prediction of the retention behavior of non-polar solutes in RP-HPLC has been studied. The classical five term LSER equation has been applied to retention data evaluation.

$$logt_r = c + eE + sS + aA + bB + vV$$

Solute descriptors are represented by capital letters while the complementary effect on these interactions by the log tr is explained by the lower case letters, namely the system constants. These descriptors are excess molar refraction, combined dipolarity/polarizability, overall solute hydrogen bond acidity, overall solute hydrogen bond basicity and McGowan volume.

The classical five terms LSER equation was applied to retention data evaluation for naphthalene, phenanthrene, acenaphthene and fluorene. The predicted retention times were compared with experimental data and a good correlation has been found. It has been shown that LSER is a reliable model for description of retention, characterization of the stationary phase and prediction of solute retention on the basis of system characteristics. Acetonitrile–water systems fit better to the LSER model. The relative contributions of each descriptor to the measured retention times showed that the principal factor governing the retention on these reversed phase C18 columns is the volume (V), while the contribution of molar refractivity is of minor importance. In addition, the results presented in this work demonstrate that C4 stationary phase interacts with these nonpolar solutes simultaneously through both reversed phase and electrostatic interactions.

**References**

[1] J.M. Pallicer, C. Calvet, A. Port, M. Rosés, C. Ràfols, E. Bosch, Journal of Chromatography A, 1240 (2012) 113-122.

---

* Corresponding author, *E-mail: gulerenalsancak@sdu.edu.tr*

P-33

# Investigation of Anticancer Properties of Some Organo-Boron Complexes with Norfloxacin

**Koray Sayın*** and Duran Karakaş

Cumhuriyet University, Faculty of Science, Department of Chemistry, 58140, Sivas, Turkey

*E-mail: krysayin@gmail.com*

Quantum chemical calculations are performed over some boron complexes with norfloxacin. Complex **(1)** has been synthesized by Wang et al. Spectral investigations of mentioned complex have been done and structural properties and geometric parameters have not been reported in their paper [1]. There are no any data about the rest complexes. The mentioned boron complex with norfloxacin are represented in Figure 1 and optimized at M062X/6-31+G(d) level in gas phase. Structural properties, IR and NMR spectrum are examined in detail. Additionally, biological activities of mentioned complexes are investigated by molecular docking analyses. Interaction energies between vascular endothelial growth factor receptor 2 (VEGFRTK) (PDB code: 3WZE) taken from RCSB protein data bank and mentioned complexes are calculated. As a result, it is found that boron complex with fluorine atoms coordinated to boron atom is the best candidate for anticancer drug. This work is supported by the Scientific Research Project Fund of Cumhuriyet University under the project number F-492.

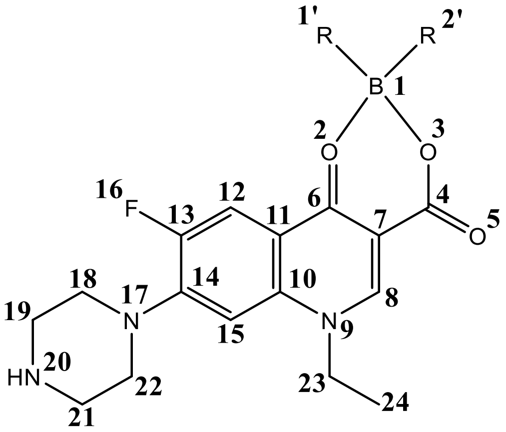


**Figure 1**. Schematic diagram of boron complexes with atomic labelling. R: -F$^-$ (**1**), -NO$^-$ (**2**), -CN$^-$ (**3**) and -CH$_3^-$ (**4**)

**References**
[1] L. Lin, Y. Zhai, D. Wang, G. Yin, L. Fan, Y. Hu, Journal of Fluorine Chemistry, 182 (2016) 7-11.

---

* Corresponding author, *E-mail: krysayin@gmail.com*

# A Theoretical Study on the Interaction Between Undoped or Doped (Si and Al) C60 Fullerenes and Piperazine-2,3,5,6-Tetraone

**Özgür Alver[1], Cemal Parlak[2] and Mustafa Şenyel[1]***

[1]Anadolu University, Science Faculty, Department of Physics, Eskisehir, Turkey
[2]Ege University, , Science Faculty, Department of Physics, Izmir, 35100, Turkey

*E-mail: msenyel@anadolu.edu.tr*

Piperazine and tetraone related compounds have been widely used for various kinds of proposing particularly in the drug industry. Further, heteroatom doped fullerenes have been extensively included in the search of new types of sensor devices and medical applications as drug delivery vehicles [1,2]. In this work, as seen from Figure 1, the interaction of pristine and Si or Al doped C60 fullerenes with piperazine-2,3,5,6-tetraone (ppto) and some important structural or electronic properties were examined based on the density functional theory. The obtained results propose that doped C60 fullerenes might be used to diagnose the presence of ppto and they might be used as delivery vehicles because of their high adsorption energies with ppto.

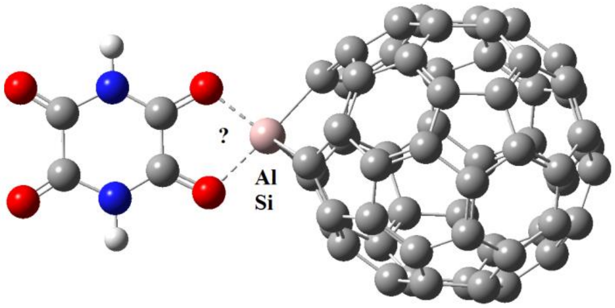


**Figure 1.** Schematic diagram of the compounds

**References**
[1] C. Parlak, Ö. Alver and P. Ramasami, Main Group Met. Chem., 39 (2016) 145-150.
[2] C. Parlak, Ö. Alver and M. Şenyel, J. Theor. Comput. Chem., 16 (2017) 1750011.

**Acknowlengement**
The Authors acknowledge the Fencluster system in Ege University, Science Faculty for the computing resources.

---

* Corresponding author, *E-mail: msenyel@anadolu.edu.tr*

P-35

# Theoretical and Experimental Vibrational Spectroscopic Study of 3X-thiophene-2-carbaldehyde [X=F, Cl or Br]

**Mustafa Şenyel**[1]*, **Esma Güneş**[1] **and Cemal Parlak**[2]

[1]Anadolu University, Faculty of Science, Department of Physics, Eskişehir, Turkey
[2]Ege University, Faculty of Science, Department of Physics, İzmir, Turkey

*E-mail: msenyel@anadolu.edu.tr*

The effects of halogen on the conformer, vibrational properties of thiophene-2-carbaldehyde ($C_5H_4OS$) and 3X-thiophene-2-carbaldehyde [$C_5H_3XOS$; X = F, Cl or Br] were investigated employing the DFT method. For theoretical calculations, the B3LYP functional was used with the 6-31++G(d,p) basis set. Computations were focused on the two different conformational isomers of the compounds in the gas phase. FT-IR and Raman spectra of 3X-thiophene-2-carbaldehyde have been experimentally reported in the region of 4000-400 $cm^{-1}$ and 4000-50 $cm^{-1}$, respectively. Thiophene-2-carbaldehyde and its halogen derivatives were calculated and the effect of halogen on vibrational spectra was investigated.

## References

[1] C. Parlak, Ö. Alver and P. Ramasami, Main Group Met. Chem., 39 (2016) 145-150.
[2] C. Parlak, Ö. Alver and M. Şenyel, J. Theor. Comput. Chem., 16 (2017) 1750011.

## Acknowledgement

This study was supported financially by Anadolu University BAP Commission (Project No: 1503F103).

---

* Corresponding author, *E-mail: msenyel@anadolu.edu.tr*

# A Nonlinear Least Squares Workbench with Variable Projection

**Mehmet Çetin Koçak***

Ankara University, Faculty of Engineering, Department of Chemical Engineering,
06100, Ankara, Turkey

*E-mail: mckocak@ankara.edu.tr*

Let T and x respectively denote the nonlinear and linear parameters to tune and t be the independent variable of a function $y(T, x, t)$. The problem of fitting y to N pairs of $(t, y_{dat})$ data often arises in many fields including science and engineering. It becomes overdetermined if N exceeds the combined lengths of T and x, in which case there may be a residue at one or more points so that $y(T, x, t) \approx y_{dat}$. The least squares (LS) approach to fitting a curve to given data is to minimize the norm of the residues z. The fitting problem is linear LS (shortly, LLS) if T is empty. It is nonlinear LS (shortly, NLLS) if T has at least one element. In separable NLLS (shortly, SNNLS), $y(T, x, t) = F(T, t)x \approx y_{dat}$ where each column in the design matrix F is associated with a basis function $f(T, t)$. Thus, y predictions are a linear combination of $f(T, t)$, the expansion coefficients being x. Variable projection (varpro) is a highly popular approach to SNLLS cases. A varpro published as a nested Matlab function [1] has been equipped with additional solver links in this research and tailored to serve the ultimate product which is a versatile and robust 2-wing workbench for nonlinear least squares. One wing calls solvers directly, the other via varpro. The workbench docks applications as a nested Matlab function, say Nest, housing two user blocks. The first block is the main function Nest which defines the experimental points, weights, bounds, and tolerances, initializes the parameters, calls the selected solver, and processes the results. The second block is the objective or model function that is called by the solver. The user supplies the models and utilities as child functions of Nest. The solvers nlinfit, lsqcurvefit, and lsqnonlin can operate in either wing; fminsearch, fminunc, and fmincon link only directly. Together, these solvers offer over ten algorithms. The triggered solver tries to minimize the residue norm until it encounters a convergence or failure condition. The points may be assigned unequal weights if some of them are more important or more accurate than others. In addition, there may be constraints.

The first case is a weighted SNLLS example [1]: $y = x_1 e^{-T_2 t} \cos T_3 t + x_2 e^{-T_1 t} \cos T_2 t$. nlinfit, lsqcurvefit, and lsqnonlin reproduce the original fit in either wing. Confined to the direct call wing, fminsearch and fminunc are also successful. The second case is a non-separable, dynamic NLLS case with constraints [2]:

$$\frac{dG(t)}{dt} = k_1(G_b - G(t)) - X(t)G(t), \quad G(t_0) = G_0$$
$$\frac{dX(t)}{dt} = k_3(S_I(I(t) - I_b) - X(t)), \quad X(t_0) = X_0$$

The choices are limited here. Run in the direct call wing, fmincon, lsqcurvefit, and lsqnonlin render results in good agreement with the original [2].

## References

[1] D.P. O'Leary, B.W. Rust, Variable projection for nonlinear least squares problems. Computational Optimization and Applications 54 (2013) 579-593.
[2] N. van Riel, Minimal models for glucose and insulin kinetics. http://bmi.bmt.tue.nl/sysbio/. (accessed 15.02.2017).

---

* Corresponding author, *E-mail: mckocak@ankara.edu.tr*

P-37

# Theoretical Studies on Corrosion Inhibitive Effects of Schiff Bases Containing Oxygen, Nitrogen and Sulphur Donors

**Celal Tuğrul Zeyrek**[1]*, **Hüseyin Ünver**[2] **and Ayhan Elmalı**[3]

[1]Ankara Nuclear Research and Training Center, Turkish Atomic Energy Authority, 06100, Beşevler, Ankara, Turkey
[2]Ankara University, Science Faculty, Department of Physics, 06100 Beşevler, Ankara, Turkey
[3]Ankara University, Faculty of Engineering, Department of Physics Engineering, 061000, Beşevler, Ankara, Turkey

*E-mail: ctzeyrek@gmail.com*

Corrosion is the destructive attack on metals or alloys by chemical or electrochemical reaction with their environment, leading to enormous economic losses. The organic inhibitors which containing heteroatoms like nitrogen, phosphorus, oxygen, sulfur generally have become widely accepted as applicable corrosion inhibitors in various media [1,2]. The corrosion inhibitive effects of 2-(2-Hydroxybenzylideneamino)-2-methylpropane-1,3-diol (BAMP), 2-((2-hydroxynaphthalen-1-yl)methyleneamino)-2-methyl-propane-1,3-diol (NAMP), 2-((pyridin-2-ylimino)methyl)phenol (PMP) and N-(thiophen-2-ylmethylene)pyridin-2-amine (TMP) were investigated by means of density functional theory (DFT) at B3LYP, CAM-B3LYP and B3PW91 level with 6-31G(d,p) base set (Figure 1). The quantum chemical parameters, such as the highest occupied molecular orbital, the lowest unoccupied molecular orbital, gap energy and other parameters, including electronegativity, global hardness, the total charges on the whole molecules and the total energies have been calculated and discussed to obtain information about the relationships between the molecular and electronic structures of the studied inhibitors and their experimental corrosion inhibition efficiencies.

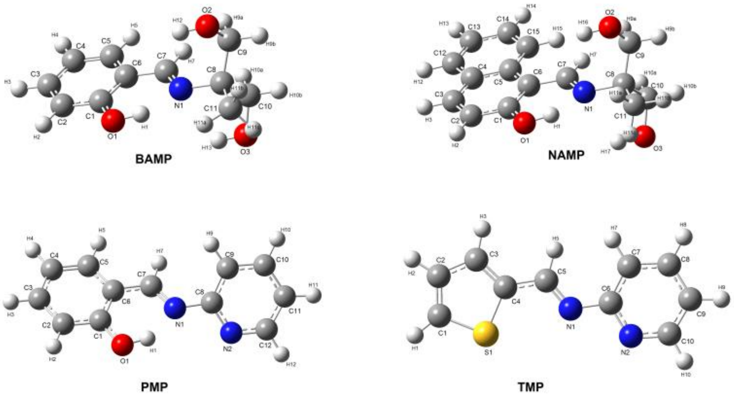


**Figure 1.** The optimized structures of the investigated compounds

**References**
[1] H. Jum Z.-P. Kai and Y. Li, Corros. Sci., 50 (2008) 865-871.
[2] M. Ajmal, A.S. Mideen and M.A. Quaraishi, Corros. Sci., 36 (1994) 79-84.

---

* Corresponding author, *E-mail: ctzeyrek@gmail.com*

P-38

# Computational Modelling the Effective Dichromate Selectivity of an Amin-Functionalized Calix-[4]-Arene Receptor

**Serkan Demir**[1]*, M. Soner Engin[2], Serkan Sayın[3] and Seydahmet Çay[3]

[1]Giresun University, Department of Industrial Engineering, 28200, Giresun, Turkey
[2]Giresun University, Department of Food Engineering, 28200, Giresun, Turkey
[3]Giresun University, Department of Environmental Engineering, 28200, Giresun, Turkey

*E-mail: serkan.demir@giresun.edu.tr*

The chemistry of anion recognition has recently emerged field of both supramolecular and analytical chemistry within the last decade. Quantum chemical computational modeling of receptor-anion interaction on the other hand is much more recent subject of interest for a more elaborate design and quantitative evaluation of receptor-anion interaction phenomenon. Among the most employed artificial receptors for anion recognition, calixarenes have been reported to be effective host platforms for the involvement of anionic guests by displaying dual binding function through electrostatic and hydrogen bonding sites [1-3].

In this study, selective behavior of an upper-rim tetraamine functionalized calix[4]arene derivative (CX4) towards dichromate anion among coexisting (Figure 1). Sulfate, nitrate and chloride anions was probed by DFT-thermodynamical computations and quantified by concenptual-DFT reactivity descriptors. In all computations, CX4-anion adducts were accessed randomly by using GUI programs. Once protonated form of CX4 at one amine sides was used in computations since within the working pH range of 3-5 CX4 is once protonated. Hence a dual binding function of CX4 towards anions through both hydrogen bonding and electrostatic interactions was provided.

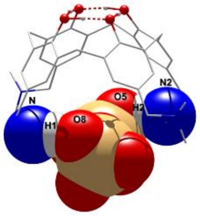


**Figure 1.** Optimized structure of CX4- $HCr_2O_7^-$ with space-filled represented anion and interacting atomic sites

**References**
[1] J.L. Sessler, P.A. Gale and W.S. Cho, Monogr. Supramol. Chem., (2006) 1-413.
[2] S.K. Kim, V.M. Lynch and J.L. Sessler, Org. Lett., 16 (2014) 6128-6131.
[3] N.Y. Edwards and A.L. Possanza, Supramol. Chem., 25 (2013) 446-463.

---

* Corresponding author, *E-mail: serkan.demir@giresun.edu.tr*

# A DFT Investigation on the Electronic Structure, Chemical Reactivity Behaviour, MEP Diagrams of the Harman Derivatives

**Goncagül Serdaroğlu*** and Mustafa Elik

Cumhuriyet University, Department of Mathematics and Science Education, Sivas, Turkey

*E-mail: Goncagul.serdaroglu@gmail.com*

Harman (1-methyl-9H-pyrido[3,4-b]indole) is a kind of the indole alkaloids having the biological and pharmacological interest and it is used as the traditional in anticancer treatment [1]. Harman and its derivatives have been commonly studied because of their pharmaceutical importance [2]. Figure 1 presents that the most stable conformer structure with respect to the conformational minima for each Harman derivative. The conformational analysis has been conducted to determine the stable conformer in PES (Potential Energy Surface) at B3LYP/631G** level of the theory [3,4] in the gas phase by using the Gaussian 09W[5] software. the most stable structures have been used as the starting structure in the further calculations. Also, the geometry optimization and frequency calculations have been repeated at 6311++G** basis set in the water phase to get the solvent effect on chemical reactivity behavior of studied structures. The stable structures have been verified with no imaginary frequency. MEP (molecular electrostatic potential) diagram is a very useful tool to evaluate the electronic interactions in any molecular system, and it is getting used in predicting the chemical reactivity behavior of any system.

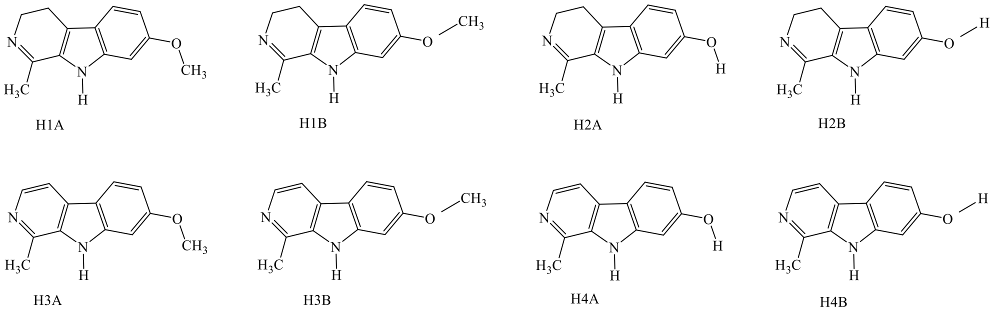

H1A H1B H2A H2B
H3A H3B H4A H4B

**Figure 1.** The most stable conformers of Harmaline (H1), Harmalol (H2), Harmine (H3), Harmol (H4)

**References**

[1] M.A. Munoz, O. Sama, M. Galan, P. Guardado, C. Carmona and M. Balon, J. Phys. Chem. B, 103 (1999) 8794-8798.

[2] S. Nafisi, M. Bonsaii, P. Maali, M. A. Khalilzadeh, and F. Manouchehri, Journal of Photochemistry and Photobiology B: Biology, 100 (2010) 84-91.

[3] A.D Becke, J. Chem. Phys., 98 (1993) 1372-1377.

[4] C. Lee, W. Yang, R.G. Parr, Phys. Rev., B37 (1988) 785-789.

[5] M. J. Frisch, et al. (2013) Gaussian 09 D.01. Gaussian, Inc, Wallingford CT.

**Acknowledgments**

The author thanks to Scientific Research Projects of Cumhuriyet University (Project No: EĞT-053). The all calculations have been conducted at TUBITAK ULAKBIM, High Performance and Grid Computing Center.

---

* Corresponding author, *E-mail: Goncagul.serdaroglu@gmail.com*

# Electrochemistry

# Electrochemical Reduction of Sulfasalazine in the Absence and Presence of Tryptophan

**Emine Coşkun* and Bahri Dağdeviren**

Ondokuz Mayıs University, Faculty of Arts and Sciences, Department of Chemistry, Samsun, Turkey

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

Rheumatoid arthritis (RA) is an autoimmune disease which provokes and systemic inflammation of the synovial joints, affecting many other tissues and organs, especially the lungs, pericardium and sclera. Sulfasalazine, 5-[4-(2-pyridylsulfamoyl) phenylazo], (SSZ) (Figure 1), is a pharmaceutical product that belongs to the anti-inflammatory class of azo-salicyclic acid derivatives used for the treatment of RA [1]. SSZ is also recommended for the other types of inflammatory arthritis, such as psoriatic arthritis, and is used for treatment of Crohn's disease and ulcerative colitis. Tryptophan (l-2-amino-3-(indol-3-yl)propionic acid, (TRP) is a vital constituent of proteins and it is an essential amino acid for humans, helping in the normal growth of infants establishing and maintaining a positive nitrogen balance in adults. TRP cannot be synthesized by the mammal body, being frequently added to dietary and feed products as a fortifier and to pharmaceutical formulations to supplement the typical diet, sometimes deficient in vegetables[2]. In this study, the interactions of SSZ with TRP in aqueous solutions at different pHs (4, 7 and 9) were monitored with square-wave voltammetry (SWV). With the addition of TRP to SSZ solution, the peak current of SSZ decreased and its peak potential shifted to more positive values and no new reductive peaks appeared.

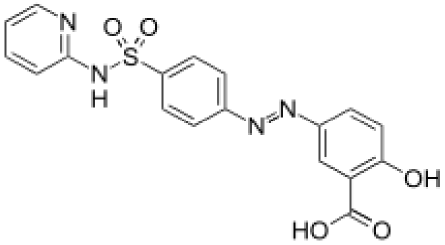


**Figure 1.** Chemical structure of sulfasalazine

**References**

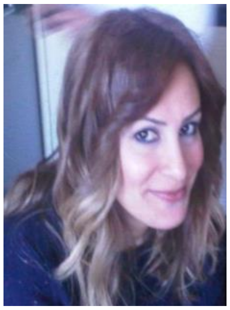
[1] R.M. Buoro, V.C. Diculescu, H.C. Lopes, S.H.P. Serrano and A.M.Oliveira-Brett, Electroanalysis, 26 (2014) 1-7.

[2] A.R. Fiorucci, P. Cervini, O.F. Filho and E.T.G. Cavalheiro, Journal of the Brazilian Chemical Society, 24(8) (2013) 1228-1236.

---

* Corresponding author, *E-mail: ecoskun@ogu.edu.tr*

P-41



# Multistate Proteinous Biomemory Device Based on Redox Controllable Hapten Cross-Linker

**Remziye Güzel**[1]*, Arzu Ersöz[2], İbrahim Dolak[3] and Rıdvan Say[2]

[1]Dicle University, Department of Chemistry, Diyarbakır, Turkey
[2]Anadolu University, Department of Chemistry, Eskişehir, Turkey
[3]Dicle University, Vocational School of Technical Science, Diyarbakır, Turkey

*E-mail: guzel.remziye@gmail.com*

A new concept for a biomemory device by the mimicking biomechanics is currently emerging to transfer the biomaterial function into a conventional electronic format even though silicon based memories have experienced a tremendous growth over the past decade in developing high speed, low cost and nonvolatile devices [1,2]. In particular, the electrical or electrochemical memory concepts using organic and biological molecules have been studied in combination with the current electronic system [3-5]. In this study, a multistate biomemory device consisting of cytochrome c (Cyt-c) photosensitively cross-linked by MACys-Ru(bipyr)$_2$-MACys hapten molecules, which have a memory effect through a charge transfer mechanism, was developed. In this study, it has suggested a highly resolute surface-confined switch composed a signal-enhanced electro-active protein (Cyt-c) co-polymerized on the gold substrates that can be controlled by the redox property through ruthenium based cysteine monomer hapten, MACys-Ru(bipyr)$_2$-MACys as an ANADOLUCA photosensitive cross-linker. The photosensitive cross-linking of the Cyt-c protein on the gold surface topography was determined by the scanning electron microscopy (SEM) (Figure 1). Two state memory functions, writing and erasing of the developed biomemory device, were investigated by the chronoamperometry (CA) and open-circuit potential amperometry (OCPA). The polymeric proteinous memory device, p(MACys-Ru(bipyr)$_2$-MACys-co-Cyt-c) layer, on the gold electrode is stable and repeatable up to with $10^4$ times continuous cycle.

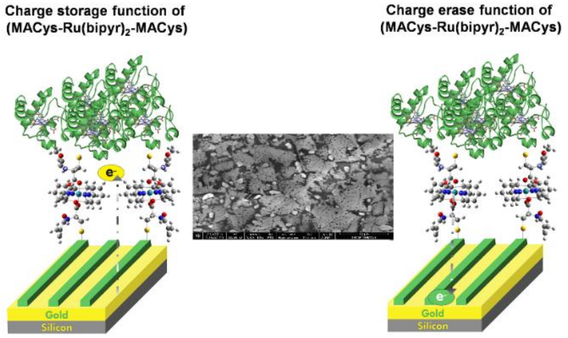


**Figure 1.** The charge transfer process for Cyt- c/MACys-Ru(bipyr)$_2$-MACys) along the memory device operation hapten/cyt-c co-polymerized gold substrate

## References

[1] R.J. Tseng,, C. Tsai, L. Ma, J. Ouyang, C.S. Ozkan and Y. Yang, Nature Nanotechology, 1(1) (2006) 72-77.
[2] D.Y. Zhang, A.J. Turbelfield, B. Yurke and E. Winfree, Science, 318(5853) (2007) 1121-1125.
[3] C.P. Collier, J.O. Jepesen, Y. Luo, J. Perkins and E.W. Wong, Journal of American Chemical Society, 123 (2001) 12632-12641.
[4] W.P. Lin, S.J. Liu, T. Gong, Q. Zhao and W. Huang, Advanced Materials, 26 (2014) 570-606.
[5] S.T. Han, Y. Zhou and V.A.L. Roy, Advanced Materials, 25 (2013) 5425-5449.

---

* Corresponding author, *E-mail: guzel.remziye@gmail.com*

# Development of Graphene and Molecularly Imprinted Polymer Based Sensor for Trinitrotoluene Detection

**Ömer Kılıç[1], Behice Yavuz Erdoğan[2] and A. Nur Onar[1]***

[1]Ondokuz Mayıs University, Faculty of Art and Sciences, Department of Chemistry, 55139, Samsun, Turkey
[2]Ondokuz Mayıs University, Technical Vocational School of Higher Education, Department of Food Technology Programmes, 55600, Terme, Samsun, Turkey

*E-mail: nonar@omu.edu.tr*

Sensors for the detection of explosives are important for various disciplines including humanitarian demining [1], remediation of explosives waste sites, homeland security, and forensic applications [2]. Nanotechnology has played a pivotal role in the production of nanosensors with low cost, portability, specificity, and ability in rapid identification [3]. Polymer-modified electrodes have many advantages when used in electrochemical methods of analysis and electropolymerization is a successful method for the immobilization of polymers. Polyaniline (PANI) is one of the most studied conducting-polymer owing to its high conductivity, unique redox properties, easy preparation, and potential applications in many areas. Graphene (GN) has attracted great interest in sensor technology because of its high elasticity, very large surface area, and high conductivity, which arises from its strictly 2D structure [4]. In this work, it is aimed to detect and determine trinitrotoluene (TNT) using an electrochemical sensor based on graphene and molecular imprinted polymer (MIP). Picric acid served as a model molecule. Waste carbon electrodes extracted from used batteries were used as the electrode instead of the commercial glassy carbon electrode. The reduction of the synthesized graphene oxide and polymer formation were carried out electrochemically using cyclic voltammetry by scanning in the potential range of -1.0 to + 1.2V (vs Ag / AgCl) as a one step process. Square wave voltammetry (SWV) was used for measurements between -1.2 and 1.0 V. The methanol-acetic acid mixture was used to remove the repressed picric acid from the sensor and the experimental conditions were optimized. After the sensor was developed, voltammetry and SEM were used for characterization. Then the sensitivity of the electrode to picric acid was tested (Figure 1).

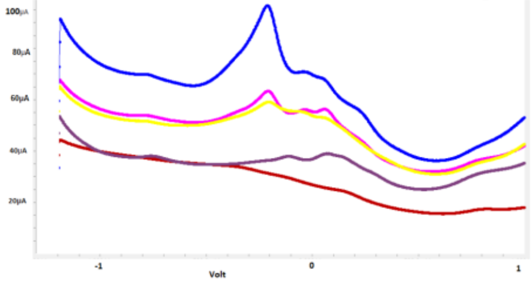


**Figure 1.** SWV measurements in 0.1 M phosphate buffer (pH 6.5) (a) MIP before template extraction, (b) MIP after template extraction, (c) After incubation for one min in a $2x10^{-4}$M picric acid solution, (d) After incubation for one min in a $2x10^{-3}$M picric acid solution, and (e) After incubation for one min in a $2x10^{-2}$M picric acid solution

## References

[1] A. Maureen Rouhi, Chemical Engineering News, 75 (1997) 14-22.
[2] K.D. Smith, B. McCord, W. MacCrehan, K. Mount and W. Rowe, Journal of Forensic Sciences, 44 (1999) 789-794.
[3] F. Akhgari and H. Fattahi, Sensors and Actuators B, 221 (2015) 867-878.
[4] L. Shi, A.G. Hou, L.Y. Chen and Z.F. Wang, Polymer Composites, 36 (2015) 1280-1285.

---

* Corresponding author, *E-mail: nonar@omu.edu.tr*

P-43

# Chemometric Optimization Approach for a New Voltammetric Quantitation of Cefdinir in Pharmaceutical Formulations

**Saadet Dermiş, Erdal Dinç*, Seda Akçasoy and Z. Ceren Ertekin**

Ankara University, Faculty of Farmacy, Department of Analytical Chemistry, 06100, Ankara, Turkey

*E-mail: dinc@pharmacy.ankara.edu.tr*

Cefdinir, third generation cephalosporin, is chemically known as [6R-[6a, 7β(Z)]]-7[[2-amino-4-thiazolyl) hydroxyimino) acetyl] amino]-3- ethyl-8-oxo-5-Thia-1-azabicyclo-(4.2.0.)-oct-2-one-2 carboxylic acid. Cefdinir is an extended-spectrum, semisynthetic, β-lactam antibiotic of the cephalosporin class for oral administration in the treatment of mild to moderate bacterial infections. In electrochemical researches, chemometric experimental design and optimization is a very powerful tool for finding the best experimental conditions with a small number of experiments [1,2]. In this study, a new voltammetric approach was applied to the quantitation of cefdinir in three different pharmaceutical preparations, tablets, efervesen tablets and suspension formulation using chemometric optimization technique. A $3^3$ full factorial design model was applied to the Osteryoung Square Wave Voltammetric method development procedure. From the results obtained by applying experimental design and optimization methodology, the optimal voltammetric experimental condition and settings were found to be pH 5.7 for supporting electrolyte (BR buffer), 61 mV for square wave amplitude and 36 Hz in frequency. Under optimized voltammetric conditions, square-wave voltammograms of calibration, validation and unknown samples were recorded between 0.0-1400 mV. The linear regression equation for the analysis of cefdinir in the working linear range of 0.5-20 μg/mL was computed by using the relationship between the concentration and peak current at 600 mV. The optimized voltammetric method was validated in according to ICH regulations. We concluded that the optimized and developed voltammetric approach was very suitable for the quantitative determination and routine analysis of commercial pharmaceutical preparations containing cefdinir.

## References

[1] R. Güzel, H. Eksi, E. Dinç and A.O. Solak, Journal of the Electrochemical Society, 160 (2013) B119-B124.
[2] S. Erden, D. Eskiköy Bayraktepe, Z. Yazan and E. Dinç, Ionics, 22 (2016) 1231-1240.

---

* Corresponding author, *E-mail: dinc@pharmacy.ankara.edu.tr*

P-44

# The Inhibiting Effect of Sodium Molybdate on the Corrosion of the Mild Steel in New Type of Cleaning Ink from a Printing Press

Aylin Aytaç*

Gazi University, Faculty of Science, Department of Chemistry, 06500 Teknikokullar, Ankara, Turkey

*E-mail:aylin.aytac@gmail.com*

Washing and cleaning solutions for use in offset printing are mixtures of different, chemical compounds such as hydrocarbons, solvent naphthas, oils, tensides, corrosion inhibitors and others [1]. The different compositions of the washing solutions are adjusted to the specific intended use. The inhibiting effect of sodium molybdate on the corrosion of the mild steel in a new type of cleaning ink from a printing press has been studied by means of the potentiodynamic polarization and electrochemical impedance spectroscopy. The inhibition efficiencies of sodium molybdate obtained from all methods employed are in good agreement. Results show sodium molybdate was the best concentration with a mean efficiency of 99% at 0.5 M. The potentiodynamic polarization curves showed both the cathodic and the anodic processes of steel corrosion were suppressed, and the Nyquist plots of impedance gave mainly a capacitive loop (Figure 1).

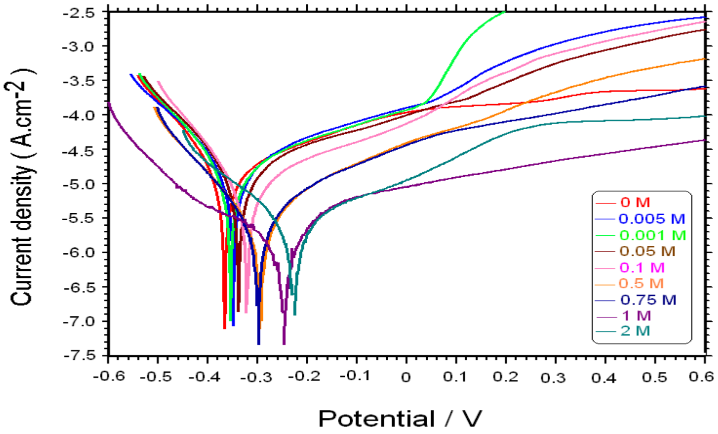


**Figure 1.** The anodic and cathodic polarization curves in the cleaning solution in the absence and presence of various concentrations of sodium molybdate

**References**

[1] I.W Bartlett, A.J.P. Dalton, A. Mc. Guinness and H. Palmer, The Annals of Occupational Hygiene, 43(2) (1999), 83-90.

**Acknowledgement**

This study was supported by Gazi University BAP.

---

* Corresponding author, *E-mail: aytaca@gazi.edu.tr & aylin.aytac@gmail.com*

# Voltammetric Mitoxantrone Determination in Biological and Pharmaceutical Samples Using a Carbon Paste Sensor Modified with Sepiolite Clay

**Dilek Eskiköy Bayraktepe***, **Ceren Yıldız and Zehra Yazan**

Ankara University, Faculty of Science, Department of Chemistry, 06560, Ankara, Turkey

*E-mail: dilekeskikoy@gmail.com*

Mitoxantrone (MTX) is a synthetic anthracycline with the chemical structure given in Figure 1. It has a planar anthraquinone ring which can intercalate between the base pairs of DNA helix and two nitrogen-containing side chains can bind to the negatively charged phosphate backbone of DNA electrostatically. These interactions have been demonstrated to inhibit the nucleic acid synthesis [1]. So, MTX is used as an antitumor drug against breast and prostate cancers, acute leukemia and non-Hodgkins lymphoma [2,3].

An anodic adsorptive stripping voltammetric method was developed to determine the Mitoxantrone (MTX) in biological and pharmaceutical samples. The method is based on a carbon paste electrode (CPE) modified by the addition of sepiolite clay. Square wave anodic adsorptive stripping voltammetry (AdsSWV) technique was employed. The anodic AdsSWV peak current of MTX is linearly proportional to the concentration within the range 0.137–100 n mol $L^{-1}$. Detection and quantification limits (LOD and LOQ) were calculated as 0.0411 nmol $L^{-1}$ and 0.137 nmol $L^{-1}$, respectively. The voltammetric technique was applied to the MTX analysis in human serum and also in flakon samples. The results were compared with those reported in the literature.

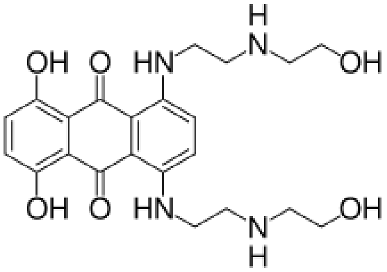


**Figure 1.** Chemical structure of MTX

**References**

[1] N. Li, Y. Ma, C. Yang, L. Guo and X. Yang, Biophys. Chem., 116 (2005) 199-205.
[2] R. Tietze, E. Schreiber, S. Lyer and C. Alexiou, BioMed. Res. Int., 2010 (2010) 597304.
[3] G. An and M. E. Morris, J. Pharm. Biomed. Anal., 51 (2010) 750-753.

---

* Corresponding author, *E-mail: dilekeskikoy@gmail.com*

# Voltammetric Determination of Hydroquinon in Some Cosmetic Products by Using Carbon Paste Electrodes

**Sevda Aydar[1] and Zehra Yazan[2]***

[1]Istanbul University, Faculty of Engineering, Department of Chemistry, 34320, İstanbul, Turkey
[2]Ankara University, Faculty of Science, Department of Chemistry, 06100, Ankara, Turkey

*E-mail: sevda.aydar@gmail.com*

Hydroquinone (1,4-dihydroxybenze, HQ) is isomer of dihydroxybenzenes. It is widely used as important industry raw and synthetic intermediates in many fields such as tanning, dye, chemical, pesticide and some other fields closely relate to our life [1]. Due to the high toxicity and low degradability in the ecological environment, the determination of dihydroxybenzene isomer has been one of the most important research topics in the field of environmental pollutant analysis [2]. Compared with the chromatographic and optical methods, electrochemical methods are preferable, and attractive for detection of such phenolic compounds due to the advantages of fast response, cheap instrument, low cost, simple operation, time saving, high sensitivity, and excellent selectivity [3]. A voltammetric method was developed to determine the Hydroquinone (HQ) content in cosmetic products. The method is based on a carbon paste electrode (CPE). Square wave voltammetry (SWV) technique was employed with the electrode as the anode. Furthermore, electrochemical redox properties of HQ were investigated by using cyclic voltammetry (CV) on the same electrode. The CV studies show that HQ has one oxidation signal at about +0.561 V in acidic media. The anodic peak current of HQ in SWV varies linearly with the concentration range of 0.1–100 $\mu$mol $L^{-1}$. Detection limits (LOD) and quantification (LOQ) limits were calculated as 0.027 $\mu$mol $L^{-1}$ and 0.092 $\mu$mol $L^{-1}$, respectively.

## References

[1] S. Zhu, W. Gao, L. Zhang, J. Zhao and G. Xu, Sensors And Actuators B, 198 (2014) 388-394.
[2] X. Ma, Z. Liu, C.T. Chen and H. Ma, Microchim. Acta, 180 (2013) 461-468.
[3] X. Yuan, X. Yuan, D. Yuan, F. Zeng, W. Zou, F. Tzorbatzoglou, P. Tsiakaras and Y. Wang, Applied Catalysis B: Environmental, 129 (2013) 367-374.

---

* Corresponding author, *E-mail: zdurmus@science.ankara.edu.tr*

P-47

# Voltammetric Determination of Hydroquinon in Cosmetic Products by Using Clay Modified Carbon Paste Electrodes

**Sevda Aydar[1] and Zehra Yazan[2]***

[1]Istanbul University, Faculty of Engineering, Department of Chemistry, 34320, İstanbul, Turkey
[2]Ankara University, Faculty of Science, Department of Chemistry, 06100, Ankara, Turkey

*E-mail: sevda.aydar@gmail.com*

Hydroquinone (1,4-dihydroxybenze, HQ) is isomer of dihydroxybenzenes which is widely used in cosmetics, dyes, pesticides, medicines, and pharmaceutical industries [1]. HQ is used as a topical application for skin whitening for reducing the color of the skin. However, numerous studies revealed that if a HQ taken orally may cause exogenous ochronosis, a disfiguring disease in which blue-black pigments are deposited onto the skin [2]. Dihydroxybenze isomers are widely distributed due to their variety sources. They are important environmental pollutants. Even at very low concentration, they are toxic to humans and difficult to degrade in the ecological environment [3]. New analytical procedures for the determination of HQ are expected to be welcome. For this purpose, an anodic adsorptive stripping voltammetric method was developed to determine the Hydroquinone (HQ) content in cosmetic products. The method is based on a carbon paste electrode (CPE) modified by the addition of sepiolite clay. Differential puls adsorptive stripping voltammetry (AdsDPV) technique was employed with the electrode as the anode. Electrochemical redox properties of HQ were investigated by using cyclic voltammetry (CV) on the same electrode. The CV studies show that HQ has one oxidation signal at about +0.422 V in acidic media. The anodic peak current of HQ in AdsDPV varies linearly with the concentration range of 0.01–700 μmol $L^{-1}$. Detection (LOD) and quantification (LOQ) limits were calculated as 0.01 μmol $L^{-1}$ and 0.033 μmol $L^{-1}$, respectively. This voltammetric technique has been applied to HQ analysis in cosmetic products and acceptable results were obtained.

## References

[1] X. Ma, Z. Liu, C. Qiu, T. Chen and H. Ma, Microchim Acta, 180 (2013) 461-468.
[2] H. Soltani, A. Pardakhty and S. Ahmadzadeh, Journal of Molecular Liquids, 219 (2016) 63-67.
[3] Y.I. Zhanga, S. Xiaoa, J. Xiea, Z. Yanga, P. Panga and Y. Gaoa, Sensors and Actuators B, 204 (2014) 102-108.

---

* Corresponding author, *E-mail: zdurmus@science.ankara.edu.tr*

P-48

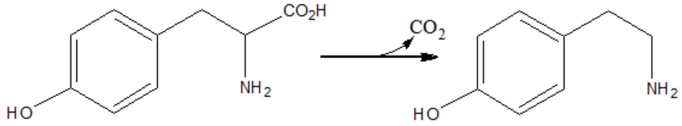
# Voltammetric Determination of Tyramine at a Glassy Carbon Electrode Modified with $TiO_2$-Ag-PPy Nanocomposites

**Zehra Özden Erdoğan**[1], **İlker Akın**[2] **and Semahat Küçükkolbaşı**[1]*

[1]Selçuk University, Faculty of Science, Department of Chemistry, Konya, Turkey
[2]Necmettin Erbakan University, Faculty of Science, Department of Biotechnology, 42075, Konya, Turkey

*E-mail: duruzera@gmail.com*

Biogenic amines are usually used as quality markers of foods due to their influence on human health. When they are consumed at high concentrations, biogenic amines can cause various diseases such as migraine, hypotension, and diarrhea [1]. Tyramine (p-hydroxyphenylethylamine), decarboxylation product of tyrosine (Figure 1), can be found in many food products (e.g., chocolate, wine, beer, cheese, beans, banana peel, ketchup, fish) and can be used as their quality indicator, due to the concentration of tyramine increases in perishable products [2].



**Tyrosine** **Tyramine**

**Figure 1.** The formation of tyramine

In this study, electrochemical sensor based on $TiO_2$-Ag-PPy nanocomposites was prepared for tyramine. An electrochemical and morphological property of the $TiO_2$-Ag-PPy/GC electrode surface was characterized by cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS) and scanning electron microscope (SEM). The results show that $TiO_2$-Ag-PPy modified GC electrode provides good electron transmission pathway than other electrodes.Optimum working conditions such as pH, working potential and the amount of $TiO_2$-Ag-PPy were investigated and performance factors of tyramine sensor were studied. The working range of the sensor biosensor was 0.041-3.065 μM with sensitivity of 8.027 $nA\mu M^{-1}$ and limit of detection of 0.02 μM. The sensor shows good repeatability, reproducibility and anti-interference property.

**References**

[1] I.M. Apetrei and C.Apetrei, Sens. and Actuators B, 178 (2013) 40-46.
[2] J.Kochana, K. Wapiennik, P. Knihnicki, A.Pollap, P. Janus, M. Oszajca and P. Kustrowski, Anal. Bional. Chem., 8 (2016) 5199-5210.

---

* Corresponding author, *E-mail: ksemahat@gmail.com*

P-49

# A Novel Modified Glassy Carbon Electrode as a Voltammetric Sensor for the Sensitive Determination of Ondansetron in Pharmaceuticals

**Mustafa Barış Koçer[1]*, Zehra Özden Erdoğan[1], Semahat Küçükkolbaşı[1], Serkan Sayın[2] and Mustafa Yılmaz[1]**

[1]Selcuk University, Faculty of Science, Department of Chemistry, Konya, Turkey
[2]Giresun University, Faculty of Engineering, Department of Environmental Engineering, Giresun, Turkey

*E-mail: mbariskocer@gmail.com*

Ondansetron (OND), (RS)-9-methyl-3-[(2-methyl-1H-imidazol-1-yl)methyl]-1,2,3,9-Tetrahydro-4H-carbazol-4-one monohydrochloride, is a selective serotonin 5-HT3 receptor antagonist widely used in the treatment of emetogenic side effects accompanying cancer chemotherapy or radiotherapy. The studies on the use of OND in new indications continue and, therefore, the development of a sensitive analytical method to evaluate the quality of its pharmaceutical product or to determine drug concentrations in biological fluids is highly required [1,2]. Electrochemical detection of OND is a very elegant method in pharmaceutical analysis due to its high sensitivity, rapid response, simple operations and low cost [3]. In this study, we prepared an electrochemical sensor based on carbon nanotube (CNT) and calix[4]arene (Calix) modified glassy carbon electrode for the determination of ondansetron (Figure 1). Before use, the CNT material was submitted to various chemical-physical procedures and new 5,11,17,23-tetra-ter-butyl-25,26,27,28-tetrahydroxycalix[4]arene/CNTs were performed by the reaction Calix and derivazited CNT. The electrochemical behavior of CNT-Calix was investigated by using cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS). The results indicate that CNT-Calix modified GC electrode provides good electron transmission pathway than bare GC electrode. The amount of ondansetron was determined by differential pulse anodic stripping voltammetric analysis as a sensitive detection technique. The experimental parameters such as pH, deposition time, deposition potential and the amount of Calix were optimized. Under optimal conditions, linear range and limit of detection for ondansetron were calculated. The developed sensor was applied successfully for quality control assay in tablets.

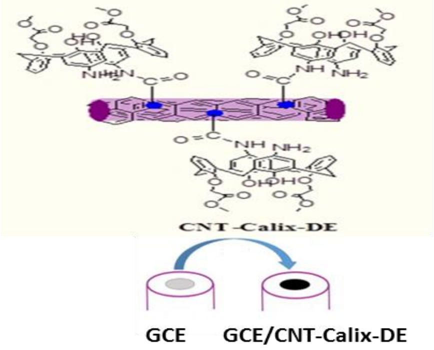


**Figure 1.** Schematic illustration of the electrode preparation

**References**
[1] A. Markham and E.M. Sorkin, Drugs, 45 (1993) 931-952.
[2] J.H. Ye, R. Ponnudurai and R. Schaefer, CNS Drug Rev., 7 (2001) 199-213.
[3] B. Nigović and S.B. Hocevar, Electrochim. Acta, 58 (2011) 523-527.

---

* Corresponding author, *E-mail: mbariskocer@gmail.com*

# Development of Voltammetric Method for Determination of Ethanol

**Halit Arslan***, **Demet Uzun and Fatma Arslan**

Gazi University, Faculty of Science, Department of Chemistry, 06500, Ankara, Turkey

*E-mail: halit@gazi.edu.tr*

Ethanol is an inflammable, colorless, a less toxic chemical substance that is mostly found in alcoholic beverages. Ethanol is used in the chemical and food industry, medicine and cosmetic industry. The accurate determination of ethanol in complex specimens is important in clinical and forensic medicine [1,2].

In this study for electrochemical determination of ethanol a new method has been developed. For this purpose various support electrolytes and working electrodes were studied. The most suitable supporting electrolyte was pH 5.0 BR buffer and a palladium electrode was determined as working electrode. In pH 5 Britton-Robinson (BR) support electrolyte using Palladium (Pd) electrode, received voltammograms with cyclic voltammetry (CV) and square wave voltammetry (SWV) showed that ethanol reduction peak is about -0,065 V. It is observed that in pH 5 BR buffer solution with addition ethanol, steady increase in the diffusion of the peak. With peak which the advantage of giving proper answers to additional ethanol on -0,065 V, calibration graph for ethanol is plotted. The linear working range of ethanol using pH 5 BR buffer and Pd electrode was determined to be $2.60\times10^{-6}$ M - $8.0\times10^{-4}$ M. For ethanol, the limit of detection was $7.78\times10^{-7}$ M and the limit of quantity was $2.60\times10^{-6}$ M.

The influences of some other commonly found inorganic and organic species on the determination of ethanol were also examined. The applicability of palladium electrode was tested by the determination of real samples.

## References

[1] S.H. Zhen, Y. Wang, C.G. Liu, G.M. Xie, C.S. Zou, J. Zheng and Y. Zhu, Forensic Science International., 207(1-3) (2011) 177-182.
[2] Z. Zhub, C.-T. Kaoa, R.-J. Wua, Applied Surface Science, 320(12) (2014) 348-355.

---

* Corresponding author, *E-mail: halit@gazi.edu.tr*

P-51

# Development of Voltammetric Method for Phenol Determination

**Halit Arslan*, Mustafa Balcı, Demet Uzun and Fatma Arslan**

Gazi University, Faculty of Science, Department of Chemistry, 06500, Ankara, Turkey

*E-mail: halit@gazi.edu.tr*

Phenolic compounds are toxic chemicals used by many industries, such as leather, paint, paper, pharmaceutical industry, and which cause pollution as a result of the release of these industries by their waste water. It is easily absorbed from the living skin in contact with the dirty environment and is toxic to organs and tissues such as the liver, lungs and kidneys. Therefore, the presence of some phenolic compounds in the water poses a danger to living things. Phenol-containing drinking water is converted to poisonous polychlorinated phenols when chlorinated. Therefore, it is important to determine the amounts of phenolic compounds in ground waters in wastewater, in terms of human and environmental health [1-3].

In this study, the electrochemical method for the determination of phenol was developed. Electrochemical behaviors for phenol, catechol and quinon were investigated with various electrodes and supporting electrolytes. As a result of this work, Au electrode was found to be the best electrode and pH 5 $CH_3COOH/NaCH_3COO$ buffer was observed as the best supporting electrode, for the determination of phenol. In this media, electrochemical behaviors of catechol, quinon and phenol were investigated with SWV, the reduction peaks were found +0.24 V from catechol and +0.16 V for quinon. In the buffer media (pH 5 $CH_3COOH/NaCH_3COO$) the peak was observed at -0.20 V regularly increases with additions of phenol. In the studies made by CV, the reversible peaks were of observed for katekol and kinon. Irreversible peak was observed for phenol. The interference effects of the some inorganic species which can be found in the waste water were investigated. The calibration graphic for phenol was drawn by using the peak at -0.20 V, increasing with phenol additions. Later known amount of phenol concentration was determined by the standard addition method. The method was performed to real sample.

## References

[1] J. Hervás Pérez, M. Sánchez-Paniagua López, E. López-Cabarcos, B. López-Ruiz, Biosensors and Bioelectronics, 22 (2006) 429-439.
[2] K.R. Rogers, J.Y. Becker, J. Wang and F. Lu, Field Analytical Chemistry and Technology, 3(3) (1999) 161-169.
[3] S.E. Stanca, I.C. Popescu and L. Oniciu, Talanta 61(4) (2003) 501-507.

---

* Corresponding author, *E-mail: halit@gazi.edu.tr*

P-52

# Independent and Simultaneously Determinations of Que, Kae, Lut and Chr using HNPC Modified Carbon Based Sensor Electrode

**Nagihan Durmuş, Bedrettin Mercimek, İbrahim Ender Mülazımoğlu* and Ayşen Demir Mülazımoğlu**

Necmettin Erbakan University, Ahmet Keleşoğlu Education Faculty, Chemistry Department, Konya, Turkey

*E-mail: iemulazimoglu@konya.edu.tr*

Polyphenols comprise different subgroups of phenolic acids and flavonoids and their derivatives, flavonoids and flavonoid derivatives, polyphenols, carotenoids, anthocyanins, etc., and they occur in plants, vegetables, and fruits or berries [1,2]. Polyphenols are ones of the most important phytochemical antioxidants used in the preservation of foodstuff nutritional quality. Phenolic compounds (originated from vegetables and fruits) also present antioxidant activity. In general, the antioxidant activity of the phenolic compounds is determined by its ideal chemical structure in terms of some properties such as free-radical scavengers or chain breakers agents. It also, the fact of the resulting antioxidant-derived radical, namely phenoxy radical is relatively stable due to the resonance delocalization and lack of suitable sites for attack by molecular oxygen. Various methods have been proposed for the evaluation of the total antioxidant capacity (TAC) in biological, chemical and food samples. These methodologies are based on UV-Vis spectrometry [3], chromatography [4] and electrochemical techniques [5]. Especially, different nanomaterials, nanofilms and nanoparticles can be used for the development of a selective method in nanotechnology [6]. Moreover, significant progress has been performed in the production of carbonaceous materials in the development of sensor electrodes (chemical, biochemical, electrochemical, etc.) [7]. In this study, electrochemical modification of a glassy carbon (GC) electrode with 4-hydroxyphenethyl-4-(4-nitrophenyl) piperazine-1-carbodithioate (HNPC) was carried out and the modified electrode was investigated independently and simultaneously for the availability in the determination of quercetin (Que), kaempferol (Kae), luteolin (lute) and Chrysin (Chr) (Figure 1). The surface modification of GC electrode was performed with HNPC using cyclic voltammetry (CV), whereas the characterization of this sensor electrode was performed using CV, electrochemical impedance spectroscopy (EIS) and scanning electron microscopy (SEM). The usability of the modified electrode was examined in the determination of some flavonoids using differential pulse voltammetry (DPV). Consequently, flavonoid derivatives can easily be determined as independently and simultaneously by using HNPC modified GC sensor electrode.

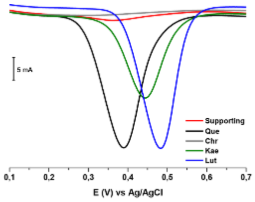


**Figure 1.** DPVs of Que, Kae, Lut, Chr and supporting electrolyte onto the HNPC/GC electrode surface

**References**

[1] H.F. Stich and M.P. Rosin, Adv. Exp. Med., 177 (1984) 1-29.
[2] R. Tsao and Z. Deng, J. Chromatogr. B, 812 (2004) 85-99.
[3] R. Apak, S. Gorinstein, V. Böhm, K.M. Schaich, M. Özyürek and K. Güçlü, Pure Appl. Chem., 85 (2013) 957-998.
[4] L. Jaitz, K. Siegl, R. Eder, G. Rak, L. Abranko, G. Koellensperger and S. Hann, Food Chem., 122 (2010) 366-372.
[5] İ.E. Mülazımoğlu and A. Demir Mülazımoğlu, Food Anal. Methods, 5 (2012) 1419-1426
[6] V.K. Gupta, M.L. Yola, N. Atar, Z. Üstündağ and A.O. Solak, J. Mol. Liq., 191 (2014) 172-176.
[7] V.K. Gupta, M.L. Yola, N. Atar, Z. Üstundağ and A.O. Solak, Electrochim. Acta, 112 (2013) 541-548.

---

* Corresponding author, *E-mail: iemulazimoglu@konya.edu.tr*

P-53

# Investigation of Spectroelectrochemical Behaviours of 3-HF, 6-HF and 3,6-DHF using Modified Carbonaceous Electrodes

**Nagihan Durmuş, Bedrettin Mercimek, Ayşen Demir Mülazımoğlu and İbrahim Ender Mülazımoğlu***

Necmettin Erbakan University, Ahmet Keleşoğlu Education Faculty, Chemistry Department, Konya, Turkey

*E-mail: admulazimoglu@konya.edu.tr*

Chemical modified electrode (CME), as a core part of electrochemical sensor, plays a vital role in trace analysis of different compounds and promotes the development of electrochemistry. Different from glassy carbon (GC) electrode, carbon paste electrode (CPE) has lower background current, multifaceted modifications and high sensitivity [1]. Antioxidants can be classified into two major groups: enzymatic and non-enzymatic. Some of them are endogenously produced, such as enzymes, low-molecular-weight molecules, and enzyme cofactors, while other, non-enzymatic antioxidants are obtained from dietary sources. Dietary antioxidants can be placed into various classes [2], of which polyphenols, i.e., phenolic acids and flavonoids, is the largest class. The other classes of dietary antioxidants include vitamins, carotenoids, organosulfural compounds, and minerals. Antioxidants are a class of compounds of great interest for the pharmaceutical industry and biochemists, known for their capacity to reduce damage caused by some reactive species: oxygen, nitrogen, or even chlorine. The discovery of the role of free radicals in several diseases is offering a new approach to health care. Great interest has been observed in research on the replacement, partial or total, of synthetic antioxidants with natural ingredients. Organisms are well protected against free radical damage due to the presence of oxidative enzymes or chemical compounds [3]. Herein, electrochemical modification of a GC electrode with 4-hydroxyphenethyl-4-(4-nitrophenyl) piperazine-1-carbodithioate (HNPC) was carried out and the modified electrode was investigated separately and simultaneously for the availability in the determination of 3-hydroxyflavone (3-HF), 6-hydroxyflavone (6-HF) and 3,6-dihydroxyflavone (3,6-DHF) (Figure 1). The surface modification of GC electrode was performed with HNPC using cyclic voltammetry (CV), whereas the characterization of this sensor electrode was performed using CV, electrochemical impedance spectroscopy (EIS) and scanning electron microscopy (SEM). The usability of the modified electrode has been examined in the determination of flavonoid derivatives using differential pulse voltammetry (DPV) and square wave voltammetry (SWV).

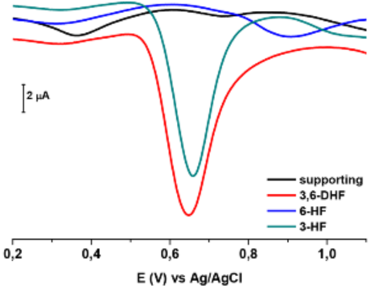


**Figure 1.** DPVs of 3-HF, 6-HF, 3,6-DHF and supporting electrolyte onto the HNPC/GC electrode surface

**References**
[1] A. Nezhadali and S. Sadeghzadeh, Sensors Actuat. B-Chem., 224 (2016) 134-142.
[2] E. Niki, H. Shimaski and M. Mino, Gakkai Syuppan Center: Tokyo, 1994.
[3] R.H. Liu, J. Nutr., 134 (2004) 3479-3485.

---

* Corresponding author, *E-mail: iemulazimoglu@konya.edu.tr*

P-54

# Mutated DNA Sensor on Carbonaceous Electrode by Impedimetry

**İhsan Aşık**[1] **and Zafer Üstündağ**[2]*

[1]Mehmet Akif Ersoy University, Gölhisar Vocational School of Health Services,
Department of Pharmacy Services, Gölhisar, Burdur, Turkey
[2]Dumlupınar University, Faculty of Arts and Science, Department of Chemistry,
43100 Kütahya, Turkey

*E-mail:ihsanasik@mehmetakif.edu.tr*

Carbonaceous materials, such as carbon nanotubes (CNT), graphene and its derivatives, graphene nanoribbons (GNR), polymers and their composites, coal tar pitch (CTP), and other carbonized materials are experiencing the golden age today. They have attracted thermal conductivity and low cost in recent decades, due to their special features such as refractory, mechanical properties, and electrical conductivity. The carbonized materials and their composites are widely used as carbon composites, carbon fiber manufacturing and electrode materials of sensor or battery studies [1,2]. Electrochemical DNA based sensors offer high sensitivity, high selectivity, and low cost for the detection of selected sequence or mutated genes associated with different disease and promise to provide an easy, accurate a low cost material [3].

In this study, a highly sensitive method for detection of DNA and mutated DNA hybridization was developed based on the carbonaceous electrode by impedimetry. The electrode material was synthesized from capture DNA array terminated gold nanoparticles included carbonaceous Viscum album (VA) modified pencil electrode. The VA on pencil electrode was carbonized with a tube furnace at 1000 °C under flowing inert $N_2$ at a heating ramp of 10 °C/min for a hold period of 1 h. The materials were characterized by SEM, TEM, XPS, XRD and IR. The performance of the developed nanosensor was optimized by determination of DNA and mutated DNA under suitable analytical parameters.

**References**

[1] A. Erkal, İ. Aşık, S. Yavuz, A. Kariper and Z. Üstündağ, J. Electrochem. Soc., 161 (2014) H696-H704.
[2] R. Narasimman and K. Prabhakaran, Carbon, 50 (2012) 1999-2009.
[3] A. Sassolas, B.D.L. Bouvier and L.J. Blum, Chem. Rev., 108 (2008) 109-139.

---

* Corresponding author, *E-mail: zustundag@gmail.com*

P-55

# Dihydroxybenzene Isomers Sensitive Polymerized Graphene Oxide based Electrochemical Sensor

**Mehmet Selçuk Erdoğan** and Zafer Üstündağ*

Dumlupınar University, Faculty of Arts and Science, Department of Chemistry,
Kütahya, Turkey

*E-mail: mse1977@gmail.com*

In this study, we investigated the selectivity, reliability of a novel, easily prepared and rapid detective electrochemical sensor composed of graphene oxide (GO) and 1,4 phenylenedimethanamine (PDMA) to form graphene oxide supported polyamide p[GO-PDMA] covered on a glassy carbon (GC) electrode for simultaneous determination of dihydroxybenzene isomers; resorcinol (RC),hydroquinone (HQ), catechol (CC) [1]. The surface topography and the structure of GC/p[GOPDMA] were characterized and analyzed in detail by scanning electron microscopy (SEM) (Figure 1). Cyclic voltammetry (CV), differential pulse voltammetry (DPV) and electrochemical impedance spectroscopy (EIS) were used for voltammetric determination of the isomers. Electrochemical analysis results indicate that the GC/p[GO-PDMA] sensor exhibited wide linear ranges with good correlation coefficients and detection limits. The limit of detection (S/N = 3) of the method was calculated as 0.06 μM for HQ, 0.12 μM for CC, and 0.10 nM for RC with the linear calibration curves ranged from 10 μM to 100 μM, 1 μM to 20 μM, and 5-80 μM, respectively. Also, as real sample electro analysis, the electrochemical determination of RC, HQ and CC in tap water was studied.

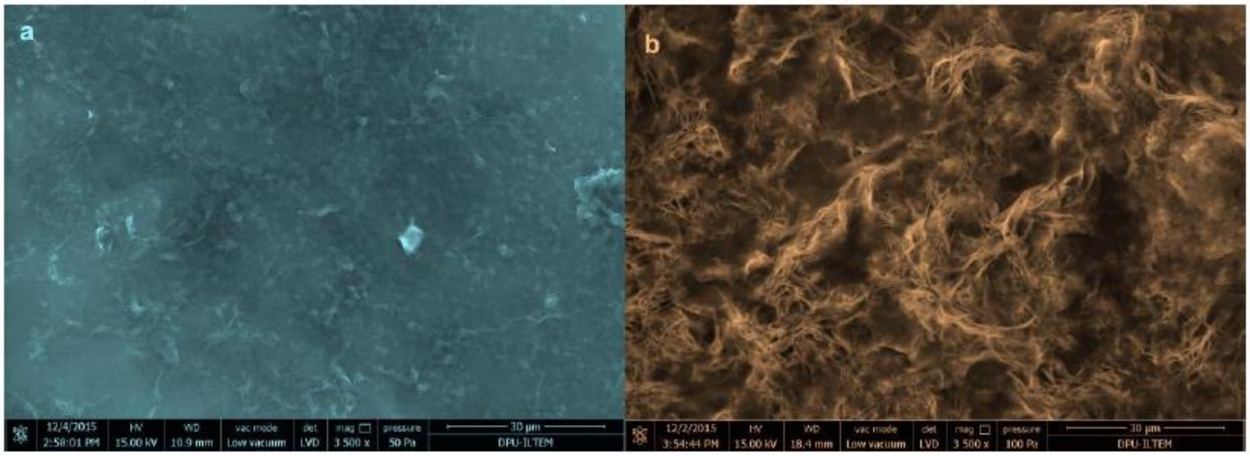


**Figure 1.** SEM images of GO and p[GO-PDMA]

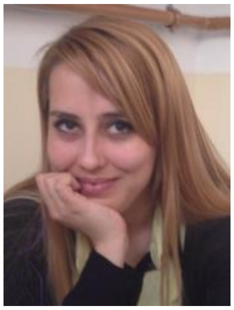
**References**

[1] H. Zhang, X. Bo, L. Guo, Sensors and Actuators B: Chemical, 220 (2015) 919-926.

---

* Corresponding author, *E-mail: zustundag@gmail.com*

P-56



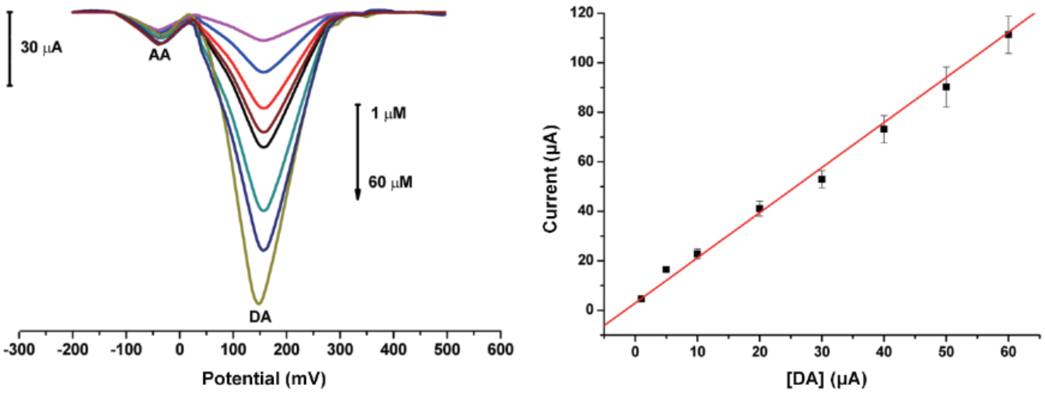
# Determination of Dopamine in the Presence of Ascorbic Acid on Glycoside-doped Carbonaceous Electrode

**İlknur Üstündağ[1]* and Aslı Erkal[2]**

[1]Dumlupınar University, Faculty of Arts and Science, Department of Physics, Kutahya, Turkey
[2]Alanya Alaaddin Keykubat University, Alanya, Antalya, Turkey

*E-mail: aaslierkal@gmail.com*

Recently, carbonaceous materials (CMs) and their hybrids have been actively pursued as electrocatalysts for electrochemical studies [1]. CMs such as glassy carbon (GC), vitreous carbon, pyrolyzed photoresist film (ppf)-coated substrates, carbon nanotubes, and graphene are very conductive surfaces as working electrodes [2]. Currently, CMs with natural carbon matrices including products such as plant and animal sources are used as next-generation electrodes. In addition, some chemicals such as polysaccharides/osazones, and polymers are preferred as raw materials [2]. A novel carbonaceous material was prepared from a digitonin (DG)-doped coal tar pitch (CTP) with a tube furnace under nitrogen atmosphere. It was used as an electrode after mixing the material with an organic binder. The new carbon electrode was denoted as CTP-DG. The CTPDG was characterized by cyclic voltammetry (CV), infrared spectroscopy (IR), X-ray photoelectron spectroscopy (XPS), scanning electron microscopy (SEM), and X-ray diffraction (XRD). The electrode was used for the determination of dopamine (DA) by differential pulse voltammetry (DPV). DPVs of 1–60 μM DA on CTP-DG in the presence of AA and their calibration curve are given in Figure 1. It exhibits a linear response to DA in the range of 1–60 μM. The detection limit (S/N = 3) for DA is 80 nM. Satisfactory results were achieved for the determination of DA in real samples [2].



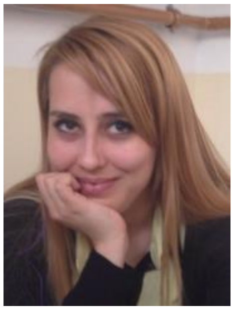
(a) (b)

**Figure 1.** (a) DPVs of 1–60 μM DA on CTP-DG in the presence of AA, and (b) their calibration curve

**References**
[1] J.C. García and C.R. Cabrera, Electrocatalysis, 5 (2014) 402-407.
[2] İ. Üstündağ and A. Erkal, Sensors and Materials, 29 (2017) 85-94.

---

* Corresponding author, *E-mail: iozkirim@gmail.com*



# Preparation and Application of Carbonaceous Graphene Nanocoil Electrodes

**Aslı Erkal**[1] and Zafer Üstündağ[2]*

[1]Dumlupınar University, Faculty of Arts and Science, Department of Physics, Kutahya, Turkey
[2]Alanya Alaaddin Keykubat University, Alanya, Antalya, Turkey

*E-mail: aaslierkal@gmail.com*

Graphene nanoribbons supported carbonaceous materials were synthesized as novel electrode material [1]. Graphene nanoribbons were synthesized with chemical oxidation methods from multi-walled carbon nanotubes. The nanoribbons, unzipped nanotubes, were added in coal tar pitch and then were carbonized on a glassy carbon substrate with high temperature tube furnace at 1000 ºC under $N_2$ atmosphere. The nanoribbons, carbonaceous materials were characterized with some techniques such as TEM, SEM, XRD, IR and electrochemical methods. Electrochemical properties of the nanoribbon supported carbonaceous nanocoil electrode (Figure 1) were investigated via cyclic voltammetry and electrochemical impedance spectroscopy. Electrochemical performance of the nanomaterials was tested as sensor applications. The modified electrode was used for determination of dopamine and uric acid via differential pulse voltammetry in the presence of ascorbic acid. The limit of detection (S/N = 3) of the method was calculated as 3.0 nM for dopamine and 6.0 nM for uric acid with the linear calibration curves ranged from 2 µM to 20 µM. The method shows good reproducibility and stability and was successfully applied to measure dopamine and uric acid in real samples.

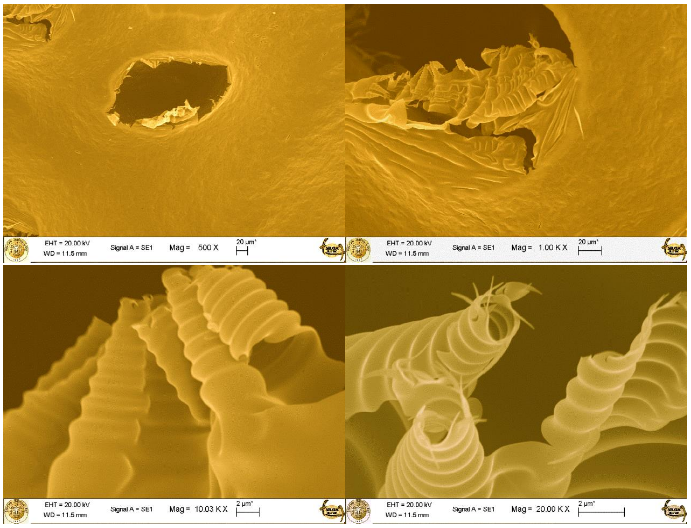


**Figure 1.** SEM images of nanocoil materials

## References

[1] A. Erkal, İ. Aşık, S. Yavuz, A. Kariper and Z. Üstündağ, Journal of the Electrochemical Society, 163 (2016) H269-H277.

---

* Corresponding author, *E-mail: zustundag@gmail.com*

# Energy

# Effect of Metal Loaded Zeolite Catalysts on Chemical Recycling by Pyrolysis of Polystyrene Wastes

**Havva Sarıkaya and Ali Karaduman***

Ankara University, Faculty of Engineering, Department of Chemical Engineering,
06100, Ankara, Turkey

*E-mail: hsarikaya@ankara.edu.tr*

Polystyrene (PS) is a thermoplastic widely used in packaging, telephone, computer and car interior parts. PS production has increased considerably in recent years and the amount of PS waste has increased accordingly. PS wastes must be disposed of by recycling processes for economical and environmental reasons [1-6]. Conventional methods of processing plastic wastes, including incineration of waste plastics, cause both the environment and the release of carcinogenic gases that adversely affect human health. Chemical recycling methods are necessary for the sustainable recovery of plastic wastes. In this study, pyrolysis of PS waste was investigated to utilize PS wastes and recover valuable chemicals such as styrene, methyl styrene and toluene. For this purpose, polystyrene waste was pyrolyzed using Ni and Co loaded MCM-41 and ZSM-5 zeolite catalysts. Metal loaded zeolite catalysts were prepared by the wet impregnation method. The experiments were carried out in a 250 ml stainless steel autoclave reactor at $N_2$ atmosphere and 350-425$^{o}$C temperature range. The obtained pyrolysis liquid products were subjected to vacuum distillation to separate from solid residue. The liquid was analyzed by GC-MS. The effect of temperature, zeolite type and metal loading on product yield and product distribution was determined.

## References

[1] V. Kříž and Z. Brožová, Acta Geodynamica et Geomaterialia, 4(2)(146) (2007) 39-42.
[2] M.F. Ali, S. Ahmed and M.S. Qureshi, Fuel Processing Technology, 92(5) (2011) 1109-1120.
[3] E.I. Andreikov, I.S. Amosova, Y.A. Dikovinkina, O.V. Krasnikova and M.G. Pervova, Russian Journal of Applied Chemistry, 85(1) (2012) 89-97.
[4] M.F. Ali and M.S. Qureshi, Petroleum Science and Technology, 31(16) (2013) 1665-1673.
[5] M.P. Aznar, M.A. Caballero, J.A. Sancho and E. Francés, Fuel Processing Technology, 87(5) (2006) 409-420.
[6] Z. Hussain, K.M. Khan, N. Basheer and K. Hussain, Journal of Analytical and Applied Pyrolysis, 90(1) (2011) 53-55.

---

* Corresponding author, *E-mail: ali.karaduman@ankara.edu.tr*

# The Effect of Tin oxide Addition to Carbon as Supports for Pt-based Electrocatalysts for High Temperature Fuel Cells

**Aylin Aytaç**[1,2]* and Werner Lehnert[2]

[1]Gazi University, Faculty of Science, Department of Chemistry, 06500 Teknikokullar, Ankara, Turkey
[2]Institute of Energy and Climate Research, IEK-3: Electrochemical Process Engineering, Forschungszentrum Jülich, 52425 Jülich, Germany

*E-mail:aylin.aytac@gmail.com*

In this study, we investigated the tin oxide as alternative support materials to activated-carbon for Pt electrocatalysts for high temperature polymer electrolyte fuel cell [1]. First tin oxide was synthesized with average particle sizes of 18.3 and mixed with heat treated VulcanXC-72. The electroless deposition method was used to deposit platinum on tin oxide-carbon mixtures and has been characterized using XRD, XPS and TEM. Electrochemical properties evaluated by cyclic voltammetry coupled with a rotating disk electrode in 0.5M $H_2SO_4$ showed improvements with tin oxide addition. The performance of the fuel cell using platinum supported tin oxide-carbon mixture and Vulcan carbon as a cathode catalyst was evaluated at 160 $^oC$ under $H_2$ and $O_2$ gases showed 0.62V at a current density of 200mAcm$^{-2}$,while 0.38 V was obtained in the case of Pt/C catalyst.

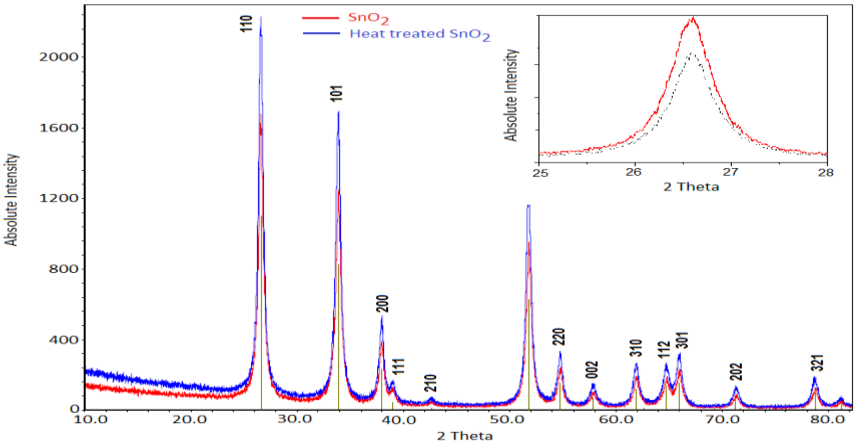


**Figure 1.** XRD characterization of $SnO_2$ and heat treated $SnO_2$ at 410 $^oC$ [inner: (1 1 0) peak of $SnO_2$]

## References

[1] Y. Shao-Horn, W.C. Sheng, S. Chen, P.J. Ferreira, E.F. Holby and D.Morgan, Topics in Catalysis, 46(3-4) (2007) 285-305.

## Acknowledgment

This study and Dr. Aylin Aytac was supported by TUBITAK-BIDEP 2219-International Postdoctoral Research Scholarship Program

---

* Corresponding author, *E-mail: aytaca@gazi.edu.tr & aylin.aytac@gmail.com*

# Occupational Health and Safety in Thermal Power Plants

**Hayrunnisa Mazlumoğlu***

Ataturk University, Faculty of Engineering, Department of Chemistry, 25000, Erzurum, Turkey

*E-mail: h.mazlumoglu@atauni.edu.tr*

As the comfort and level of welfare of humanity has increased over time, the need for energy has also increased. The most common method of energy production in the world, and in Turkey, is to use thermal power plants, which convert the thermal energy of solids, liquids and gaseous fossil fuels into electrical energy [1]. The increase in the number of thermal power plants caused by increased energy demands leads to environmental pollution, and thermal power plants are classified as "highly dangerous enterprises" because they pose various hazards in terms of occupational health and safety. For example, some workers in boiler rooms may suffer from diseases of the upper respiratory tract, such as bronchitis, and from conjunctivitis caused by vanadium compounds and $SO_2$ [2,3]. In this study, the occupational health and safety of thermal power plants is discussed.

**References**

[1] DPT, 2001.VIII Beş Yıllık Kalkınma Planı. Elektrik Enerjisi Özel İhtisas Komisyonu Raporu. DPT Yayın No: 2569 ÖİK: 585. Ankara.
[2] C. Davutoğlu, Termik Santral Baca Gazı Arıtma Tesisi Kaynaklı Koagülasyon Çamurunda Florür Giderimi. Y. Lisans Tezi, Çukurova Üniv., Adana (2008).
[3] K. Kavak, Dünyada ve Türkiye'de Enerji Verimliliği ve Türk Sanayiinde Enerji Verimliliğinin incelenmesi Devlet Planlama Teşkilatı Uzmanlık Tezi, Yayın No: DPT. 2689 (2005).

---

* Corresponding author, *E-mail: h.mazlumoglu@atauni.edu.tr*

P-61

# Synthesis of Novel Cobalt Complexes Redox Shuttle for Dye-Sensitized Solar Cells

**Melike Arslan Faideci**, **İbrahim Erden*** and **Fatma Aytan Kılıçarslan**

Yıldız Technical University, Faculty of Arts and Science, Department of Chemistry, 34210, Istanbul, Turkey

*E-mail: melikearslan92@gmail.com*

Solar energy systems, including photovoltaics, show a rapid increase in the development and industrialization and constitute to a very significant part in the field of renewable energy research. Dye-sensitized solar cells (DSC) achieve direct sunlight-to-electricity conversion by partially mimicking photosynthesis, rendering it a unique photovoltaic technology. Redox mediators play a major role determining the photocurrent and the photovoltage in DSCs. To maintain the photocurrent, the reduction of oxidized dye by the redox mediator should be significantly faster than the electron back transfer between $TiO_2$ and the oxidized dye. Since the discovery of DSCs, the iodide/tri-iodide redox couple has been conventionally used as the redox mediator. However, $I^-$/ $I_3^-$ redox system has a mismatch between its redox potential and dye redox potential In addition, it has been observed that there may be problems of corrosiveness and competitive visible light absorption. These disadvantages were overcome with one-electron-transfer cobalt complexes with more positive redox potentials, which resulted in an improved photovoltage and with overall higher efficiencies compared to those of the $I^-$/ $I_3^-$ systems [1-3]. Herein, we report new cobalt 4,5-Diazafluorene-9-on (dafo) complexes, $[Co(dafo)_3]^{2+}/^{3+}$. The structures of $Co^{2+}/Co^{3+}$ complexes were examined by FTIR, UV-Vis, H-NMR and MS. As alternative redox mediators, cobalt complexes ($Co^{2+}/Co^{3+}$) have been studied both as redox mediators (Figure 1). The photovoltaic tests of the samples are carried out by the current-voltage (I-V) measurements and it is observed that these materials exhibited significantly enhanced electrical properties such as increased photovoltaic cell efficiency.

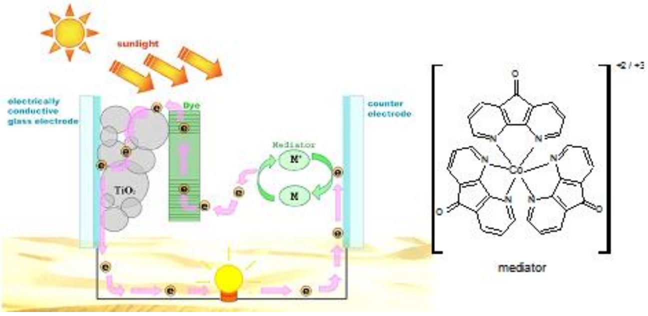


**Figure 1.** A systematic diagram of the energy flow in the dye sensitized solar cells (DSCs)

## References

[1] V.T. Annibale and D. Song, Dalton Transactions, 45 (2016) 32-49.
[2] J.H. Yum, E. Baranoff, F.Kessler, T. Moehl, S. Ahmad, T. Bessho, A. Marchioro, E. Ghadiri, J.E. Moser, C. Yi, M.K. Nazeeruddin and M. Gratzel, Nature Communication, 3(631) (2012) 1-8.
[3] Y. Saygili, M. Söderberg, N. Pellet, F. Giordano, Y. Cao, A.B. Munoz-Garcia, S.M. Zekeeruddin, N. Vlachopoulos, M. Pavone, G. Boschloo, L. Kavan, J. E. Moser, M. Gratzel, A. Hegfeldt and M. Freitag, J. Am. Chem. Soc., 138 (2016) 15087-15096.

---

* Corresponding author, *E-mail: ibrahimerden@hotmail.com*

P-62

# Pyrolysis Kinetics of Hornbeam Shell Residues (*Carpinus betulus* L.) by TGA

**Uğur Moralı* and Sevgi Şensöz**

Eskisehir Osmangazi University, Faculty of Engineering and Architecture,
Department of Chemical Engineering, Eskisehir, Turkey

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

The thermal degradation of hornbeam shell residue (*Carpinus betulus* L.) by using thermogravimetric analysis (TGA) technique was studied in an inert atmosphere at a heating rate of 10 °C $min^{-1}$ from ambient temperature to 1000 °C. The values of kinetic parameters were obtained via Coast-Redfern method have been determined by using termogravimetric data [1]. The activation energy and pre-exponential factor for the active pyrolysis zone were 34.88 kJ $mol^{-1}$ and 73.62 $min^{-1}$, respectively. The obtained kinetic parameters of the reaction were compared with those of the other biomass samples. The experimental results and calculated kinetic parameters provide useful data for the design and operation of the pyrolysis of the lignocellulosic biomass.

**References**

[1] S. Ren, H. Lei, L. Wang, Q. Bu, S. Chen and J. Wu, Biosysstems Engineering, 116 (2013) 420-426.

---

* Corresponding author, *E-mail: umorali@ogu.edu.tr*

P-63

# $Li_7La_3Zr_2O_{12}$ Fibers as an Electrolyte for All-Solid-State Li-ion Batteries

**Salim Erol***

Department of Chemical Engineering, Eskisehir Osmangazi University, Eskişehir 26040, Turkey

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

In all-solid-state Li-ion batteries, the components are all made up of solid phase. The nonflammability of the solid electrolyte overcomes the safety problem of the conventional Li-ion batteries. Since solid electrolytes neither leak nor vaporize easily, all of the cell components can be directly stacked in one container, instead of multiple containers as in the liquid- containing cells. Therefore, the battery size reduces, and thus the volumetric energy density significantly improves up to 3 times. Moreover, solid electrolytes physically separate the cathode from the anode, eliminating the need for separators. In addition, solid electrolytes have a wider range of operating potentials (over 5 V) and operating temperatures. They can be paired with certain high-voltage and high-capacity electrodes that are generally difficult to combine with liquid electrolytes. The best examples of these electrodes are lithium metal anodes and sulfur cathodes. Another feature of solid electrolytes is their single-ion conduction that suppresses side reactions and leads a long battery life. As a result of unity transference numbers indicating that $Li^+$ ions are the sole charge carriers, there is no concentration gradient inside the operating cells; thus, the cell over-potential is negligible. Furthermore, the capacity fade caused by the continuous decomposition of the electrode surface in contact with liquid is avoided [1-3].

The new methodology proposed in this work uses oxide filaments/fibers instead of a dense thin film electrolyte, allowing: (i) straightforward fabrication without the use of costly thin film production techniques, (ii) minor changes in the existing Li-ion battery production lines, and (iii) better mechanical stability and electrochemical performance. $Li_7La_3Zr_2O_{12}$ (LLZO) fibers as an electrolyte were prepared using the electrospinning technique. The crystallographic phase and morphology of the products was studied by X-ray diffraction (XRD) patterns and microscopic images. The results indicated that the produced electrolyte would be a good alternative of all-solid-state batteries for electric vehicles in terms of battery safety and performance.

**References**

[1] K. Takada, Acta Mater., 61 (2013) 759-770.
[2] M. Tatsumisago, M. Nagao and A. Hayashi, J. Asian Ceram. Soc., 1 (2013) 17-25.
[3] C. Cao, Z.B. Li, X.L. Wang, X.B. Zhao, and W.Q. Han, Front. Energy Res., 2(25) (2014) 1-10.

---

* Corresponding author, *E-mail: esalim@ogu.edu.tr*

# Investigation of the Effect of Deposition Time of ZnO Solution on Spray Pyrolysis Technique

**Mehmet Kurt[1]*, Ercan Karaköse[2], Ahmet Yartaşı[1] and Hakan Çolak[3]**

[1]Çankırı Karatekin University, Faculty of Engineering, Department of Chemical Engineering, Çankırı, Turkey
[2]Çankırı Karatekin University, Faculty of Science, Department of Physics, Çankırı, Turkey
[3]Çankırı Karatekin University, Faculty of Science, Departmen of Chemistry, Çankırı, Turkey

*E-mail*: *kurtmehmet1818@gmail.com*

Among various semiconducting materials, zinc oxide (ZnO) is a distinctive electronic and photonic wurtzite n-type semiconductor with a wide direct band gap of 3.37 eV and it has some significant advantages in its large free exciton binding energy that allows for efficient excitonic emission at room temperature. Many methods have been used to prepare ZnO films such as pulsed laser deposition [1], magnetron sputtering [2], metal–organic chemical vapor deposition [3], atomic layer deposition [4], and sol gel method [5]. Among these processes, spray pyrolysis offers several advantages like non-vacuum use of inexpensive equipment, ease of large-scale adoption and possibility of automation for industrial use. Moreover, it can offer control of the basic characteristics of the as-grown samples through the deposition conditions, such as substrate temperature, type and concentration of the precursor solution [6]. In this work, we investigate the influence of deposition time and on the morphological, structural, and optical characteristics of ZnO samples, which were deposited using the ultrasonic spray pyrolysis (USP) on glass substrates at 450 °C. X-ray diffractometer (XRD), field emission scanning electron microscopy (FE-SEM) and UV-Vıs measurements were used to characterize the deposited ZnO films. XRD results showed that the film's structure exhibited a polycrystalline with hexagonal wurtzite structure and (002) preferred orientation. SEM studies revealed the formation of ZnO films consisting of uniformly distributed over the entire surface of the substrates. The films are found to have a maximum transmittance 90% at 450°C of the optical measurements.

**References**

[1] A. Bikowski, K. Ellmer, J. Appl. Phys., 113 (2013) 053710.
[2] S.T. Tan, X.W. Sun, X.H. Zhang, S.T. Chua, B.J. Chen and C.C. Teo, J. Appl. Phys., 100 (2006) 033502.
[3] C.S. Ku, J.M. Huang, C.M. Lin, H.Y. Lee, Thin Solid Films 518 (2009) 1373-1376.
[4] Z. Yang, J.L. Liu, M. Biasini and W.P. Beyermann, Appl. Phys. Lett., 92 (2008) 042111.
[5] L. Xu, G. Zheng, J. Miao, F. Xian, Appl. Surf. Sci., 258 (2012) 7760-7765.

---

* Corresponding author, *E-mail*: *kurtmehmet1818@gmail.com*

# Enviromental & Green Chemistry

# Pipette Tipped µ-SPE for Green Extraction of Pesticides

**Füsun Okçu Pelit[1]*, İlknur Bağatır Erbaş[1], Tuğba Yavuz[1],
Kasım Ocakoğlu[2] and Levent Pelit[1]**

[1]Ege University, Faculty of Science, Department of Chemistry, 35100, İzmir, Turkey
[2] Mersin University, Advanced Technology, Education, Research and Application Center, 33343, Mersin Turkey

*E-mail: fusun.okcu@ege.edu.tr*

Pesticide residue analysis is generally carried out in a sequence of several steps, e.g. extraction with organic solvent(s) followed by liquid-liquid partitioning (LLE), clean up by column, concentration, and finally a separation and determination [1]. In these traditional sample preparation techniques, most steps are tedious, time consuming, labor-intensive, and rather complex, and they consume large amounts of solvents. Solid phase extraction (SPE) is an efficient method for improving the clean-up of the samples and high preconcentration factors can be reached by this means. Nevertheless, synchronous with modern trends in analytical chemistry towards simplification and miniaturization of sample preparation methods, some modifications must be considered for the SPE method. Miniaturization can be achieved by increasing the interfacial area between the solid adsorbent and sample solution and micro- or nanoscale sorbents are used for this purpose. The problems of SPE can be accomplished by using micro-SPE (µ-SPE) extraction technique developed in 2006 [2]. Microextraction also can be done by packed sorbent in a pipette tip. This is a new format for solid-phase extraction (SPE) that has been miniaturized to work with sample volumes as small as 10 µL. In this study, $TiO_2$, ZnO, $SiO_2$ nano adsorbents were filled in a pipette tip and used for the extraction of Chlorpyrifos (CP), Procymidone (PRC), Bromopropylate (BRP) and Lambda Chyalothrin (LMD) pesticides in tap water samples. The analysis was performed by gas chromatography with electron capture detection. The parameters related to the micropipette extraction procedure namely; pH, extraction solvent type and volume, washing and elution solvent type, sample volume, salt effect, sampling speed, drying type, elution time, drying time and sequential extraction effect on the extraction efficiency were screened by applying Plackett-Burmann design and then, selected parameters were optimized by using Box-Behnken Design. As a result, enrichment factors were calculated as 13.3, 1.60, 19.5 and 21.2 for CP, PRC, BRP and LMD, respectively. Especially BRP and LMD signals were improved by using $SiO_2$ nano material. The regression coefficients relating to linearity were at least 0.99. Recoveries from spiked well water sample range from 93 to 110% and relative standard deviations were no higher than 13% in the most unfavourable case. This new technique is very promising because it is fast, simple and green.

## References

[1] C. Basheer, A.A. Alnedhary, B.S.M. Rao,S. Valliyaveettil and H.K. Lee, Analytical Chemistry, 78 (2006) 2853-2858.
[2] C. Aftafa, F.O. Pelit, E.E. Yalçınkaya, H. Türkmen, İ. Kapdan and F.N. Ertaş, Journal of Chromatography A, 1361 (2014) 43-52.

---

* Corresponding author, *E-mail: fusun.okcu@ege.edu.tr*

P-66

# Magnetic Solid Phase Extraction Based on Carbon Coated $Fe_3O_4$ Nanoparticles Coupled with HPLC-UV for the Determination of Three Herbicides in Environmental Water Samples

**Elif Yıldız[1], Hasan Çabuk[1]* and Atakan Toprak[2]**

[1]Bülent Ecevit University, Faculty of Science and Letters, Department of Chemistry, 67100, Zonguldak, Turkey
[2]Bülent Ecevit University, Devrek Vocational School, Department of Chemistry and Chemical Processing Technologies, 67100, Zonguldak, Turkey

*E-mail: ozdalelif@gmail.com*

Environmental samples are very complex materials for research. Solid-phase extraction (SPE) has commonly used isolation and enrichment technique for analytes from environmental samples [1]. In recent years, a new procedure has been developed for SPE based on the use of magnetically or magnetically modified adsorbents called magnetic solid phase extraction (MSPE) [2]. MSPE can be applied environmental samples without centrifugation or filtration steps and makes separation easy and fast [3]. A carbon coated $Fe_3O_4$ ($Fe_3O_4$/C) magnetic nanoparticles as an adsorbent was prepared for magnetic solid phase extraction (MSPE) of herbicides (prometryn (PR), propachlor (PC) and hexazinone (HX)) from environmental water samples. The carbon coated $Fe_3O_4$ was obtained by a hydrothermal method using ferric nitrate nonahydrate and activated carbon that was prepared from laurel stone with chemical activation methods. The experimental parameters affecting the extraction efficiency of herbicides, including adsorbent amount, elution solvent, elution solvent volume, sample pH, ionic strength and extraction time were investigated and optimized. Under the optimum experimental conditions, LODs and LOQs were achieved 0.05- 0.11 ng/mL and 0.18–0.37 ng/mL, respectively. Relative standard deviations based on five replicate extraction of 0,02 µg/mL of each herbicide were less than 4.5 % for intra-day and 5.2 % for inter-days precision. The proposed method was successfully applied in the analysis of herbicides in environmental water samples.

## References

[1] M. Wierucka and M. Biziuk, Trends in Analytical Chemistry, 59 (2014) 50-58.
[2] M. Safarikova, I. Safarik and J. Magn. Magn. Mater. 194 (1999) 108-112.
[3] Z. Sabatkovaa, M. Safarikovaa and I. Safarik, Biochem. Eng. J., 40 (2008) 542-545.

---

* Corresponding author, *E-mail: cabukhasan@hotmail.com*

P-67

# Determination of Cadmium and Selenium in Food Samples by Electrothermal Atomic Absorption Spectrometry

**Orhan Acar*, Tuğba Nur Akbaba and A. Rehber Türker**

Gazi University, Faculty of Science, Department of Chemistry, 06500, Ankara, Turkey

*E-mail: tugba.nur.25@gmail.com*

Wheat, starch, powdered sugar is necessary foods in many parts of the world gastronomy. Especially, breads, cakes, baklava and etc. products are consumed by the people and they are important for human health. Selenium is an essential element for human as a potent antioxidant. It strengthens the immune system and reduces cancer risk. Selenium has been shown to counteract the toxicity of heavy metals such as cadmium. Cadmium is a toxic element. Cadmium is easily absorbed by food samples such as wheat [1,2].

Determination of trace amounts of Se and Cd in biological and food samples (wheat, starch and etc) was performed by electrothermal atomic absorption spectrometry (ETAAS). Optimization of heating program, pyrolysis-atomization temperatures and atomization-background absorption profiles were carried out by using solutions of AAS standards and standard reference materials. Determinations of Se and Cd in the samples will be performed by using direct analysis, standard addition technique, and hydride generation with enrichment methods. The results obtained will be compared with each other for the accuracy of the methods [3].

**References**

[1] C. Almela, M.J. Clemente, D. Velez and R. Montoro, Food Chem. Toxicol., 11 (2006), 1901-1908.
[2] L. Lin, W. Zhou, H. Dai, F. Cao, G. Zhang and F. Wu, Journal of Hazardous Materials, 235-236 (2012) 343-351.
[3] O. Acar, Talanta, 55 (2001) 613-622.

---

* Corresponding author, *E-mail: oacar@gazi.edu.tr*

P-68

# Removal of Reactive Blue 19 from Aqueous Solution Using Low Cost Banana Peel: Optimization by Box Behnken Experimental Design

**Peknur Şanslı and Elçin Demirhan***

Yıldız Technical University, Department of Chemical Engineering, 34210, Esenler, İstanbul, Turkey

*E-mail: peknursansli1@gmail.com*

Water is really important for human life and economy. Water is used for consumption, personal hygiene and it is required for the development of industry, farming and other sectors [1]. Water pollution is a big problem in our modern society. Increased industrial and agricultural activities resulted in the generation of various types of toxic pollutants. Dyes are an important class of pollutants which came in large amounts from textile, dyeing, paper and pulp, tannery and paint industries [2]. Many of these dyes are also toxic and even carcinogenic and this poses a serious hazard to aquatic living organisms [3]. Various methods such as adsorption, coagulation, advanced oxidation, and membrane separation are used in the removal of dyes from wastewater. However, adsorption is one of the most effective processes of advanced wastewater treatment [2]. Activated carbon is a preferred sorbent, its widespread use is restricted due to high cost. Therefore, attempts have been made to find inexpensive alternative adsorbents including natural and waste materials from agriculture for dye removal [3].

Therefore, in the present work, it was aimed to investigate the potential use of banana peel for dye removal from aqueous solutions. The effect of several parameters such as pH, adsorbent dose and dye concentration was studied by using Box Behnken design and adsorption mechanisms were evaluated. Moreover, according to the data obtained from the adsorption experiments, the most suitable adsorption kinetic models were examined. Based on the results, banana peel has found as an effective and eco-friendly alternative for the cleanup of dye-polluted aqueous media as a new natural sorbent with desirable absorption capacity.

## References

[1] E.Tomczak and M. Blus, Ecol Chem Eng S., 23(1) (2016) 175-185.
[2] I. Anastopoulos and G.Z. Kyzas, Journal of Molecular Liquids, 200 (2014) 381-389.
[3] G. Crini, Bioresource Technology, 97 (2006) 1061-1085.

---

* Corresponding author, *E-mail: demirhan@yildiz.edu.tr*

P-69

# Investigation of Reactive Blue 19 Dye Removal Using Corncorb as an Eco-Friendly Biosorbent

**Peknur Şanslı** and **Elçin Demirhan***

Yıldız Technical University, Department of Chemical Engineering, 34210, Esenler, İstanbul, Turkey

*E-mail: peknursansli1@gmail.com*

Water is essential for life and the economy. It is used for consumption, personal hygiene and it is required for the development of industry, farming and other sectors [1]. Water pollution has become a major problem day by day because the scarcity of drinking water source, increasing population and the diversity of pollutant substances [2]. One of the water pollutants is dyes which are extensively used in various industries, particularly in textile, paper, rubber, plastic, leather, cosmetics, food, and drug industries. Dye wastewater discharged from various industries creates certain hazards and environmental problems [3]. Many methods are reported to remove dyes from effluents and adsorption has been found to be superior to other techniques in terms of initial cost, flexibility and simplicity of design, ease of operation and insensitivity to toxic pollutants [2]. Activated carbon is the most commonly used adsorbent but that process has highly cost [3]. Therefore, some investigations have been reported using non-conventional low-cost adsorbents including natural and waste materials from agriculture for dye removal [2].

In the present study, it was aimed to investigate the potential use of corncorb for Reactive Blue19 removal from aqueous solutions. The effect of several parameters such as pH, adsorbent dose and dye concentration was studied by using Box Behnken Design and adsorption mechanisms were evaluated. In conclusion, the present study demonstrated that the corncob as a biosorbent could be employed as an effective and eco-friendly alternative for the cleanup of dye-polluted aqueous media.

## References

[1] E. Tomczak and M. Blus, Ecol. Chem. Eng. S., 23(1) (2016) 175-185.
[2] A. Azizi, M.R.A. Moghaddam and M. Arami, Fresenius Environmental Bulletin, 20(4) (2011) 929-938.
[3] A. Sohair, S. Ahmed, L.B. Khalil and T. El-Nabarawy, Carbon Letters, 13(4) (2012) 212-220.

---

* Corresponding author, *E-mail: demirhan@yildiz.edu.tr*

P-70

# Experimental Treatment of Sunflower Oil Refinery Wastewater by Means of Electrochemical Methods

**Şule Camcıoğlu, Baran Özyurt, Mert Fırtın and Hale Hapoğlu***

Ankara University, Faculty of Engineering, Department of Chemical Engineering,
06100, Ankara, Turkey

*E-mail: camcioglu@eng.ankara.edu.tr*

Vegetable oil production sources include soybean, peanut, rapeseed, sunflower, safflower, cotton, sesame, coconut, palm, mustard, rice cork, watermelon, neem, mahuwa etc. [1]. Refining crude vegetable oils produce waste water in large quantities. Wastewater characteristics vary depending on the type of oil processed and the process applied. High chemical oxygen demand (COD), oil and grease, sulphate and phosphate contents create high inorganic and organic pollution loads in wastewater treatment plants. In order to treat a wastewater by conventional methods such as aerobic or anaerobic digestion, the ratio of biochemical oxygen demand (BOD) to COD should be greater than 0.6 [2]. However, the BOD/COD ratio of the waste water from the vegetable oil industry is usually 0.2, which causes destruction of microorganisms which are useful for biological degradation [3]. Other methods such as evaporation or incineration are not economical due to high energy requirements. These disadvantages emphasize the need for further research using new treatment methods [3]. In this study, batch treatment of real sunflower oil refinery wastewater was performed by means of 4 different methods including chemical coagulation, electrocoagulation (EC), electro-oxidation (EO) and consecutive EC-EO. Treatment studies were carried out under 25ºC temperature, pH 5 and 5 mS/cm electrical conductivity conditions. In electrochemical treatment studies, 3 mA/cm$^2$ current density was applied by using 6 aluminum electrodes for EC and 6 graphite electrodes for EO. Samples were collected at regular intervals throughout the treatment and analyzed for COD, color and turbidity according to Standard Methods [4]. Among the treatment methods examined, consecutive EC-EO was considered to be more effective in removing COD from sunflower oil refinery wastewater. Although there was a significant COD reduction in the coagulation method, the high amount of sludge formation during treatment was considered as a disadvantage. EO was observed to provide the least COD, color, turbidity remediation in the treatment of sunflower oil wastewater. EC has the ability of removing pollutants quickly but not completely. EO is able to remove pollutants slowly but consistently. Complete turbidity and color removal with over 95% COD removal was achieved using EC-EO by combining the best abilities of EC and EO processes with fast and complete pollutant removal.

## References

[1] U.T. Un, A.S. Koparal and U.B. Ogutveren, Journal of Environmental Management, 90(1) (2009) 428-433.
[2] E.S.K. Chian and F.B. DeWalle, Water Research, 11(3) (1977) 295-304.
[3] S. Sridhar, A.Kale and A.A. Khan, Journal of Membrane Science, 205(1) (2002) 83-90.
[4] APHA, Standard Methods for the Examination of Water and Wastewater, 21st Ed., American Public Health Association, American Water Works Association, Water Environment Federation, Washington, DC, USA (2005).

---

* Corresponding author, *E-mail: hapoglu@eng.ankara.edu.tr*

P-71

# Chemometric Evaluation of Effective Process Parameters on Electrocoagulation Treatment of Pulp and Paper Mill Wastewater

**Şule Camcıoğlu, Baran Özyurt, Mert Fırtın and Hale Hapoğlu***

Ankara University, Faculty of Engineering, Department of Chemical Engineering,
06100, Ankara, Turkey

*E-mail: camcioglu@eng.ankara.edu.tr*

Since the amount of water used during paper production is high and the wastewater generated during production stages contains non-biodegradable organic and inorganic contaminants, this industry becomes an environmental concern [1-3]. Wastewater generation and characteristics vary depending on the type of paper produced and the process applied. Pulp and paper mill wastewater contains high amounts of pollutants classified by biochemical oxygen demand (BOD), chemical oxygen demand (COD), suspended solids, color, turbidity and sludge formation in the receiving environment. Turbidity which is caused by the presence of suspended solids and colloidal particles in wastewater cannot be removed by conventional methods such as filtration and sedimentation [3]. It has been verified by many researchers [1-3] that electrocoagulation (EC) process is effective in destabilizing colloidal particles and removing color. EC treatment of pulp and paper mill wastewater is a complex process that is influenced by many factors such as electrode configuration and material, current density, electrolysis time, stirring speed, electrical conductivity, pH and temperature. The first step in the optimization of the process parameters is to determine the factors which are considered to have a significant impact on the response. In this study, the Plackett - Burman method is used as an experimental design to determine the significant factors that affect the process. The advantage of the Plackett-Burman design over the other statistical-experimental methods is to investigate the effect of the large number of factors with the smallest number of trials possible and to determine the least significant factors [4]. In this study, the effects of current intensity, electrolysis time, electrical conductivity, initial pH, temperature, electrode material and stirring speed on turbidity removal and power consumption responses were investigated by using Plackett-Burman experimental design for EC treatment of pulp and paper industry wastewater. According to analysis of variance (ANOVA) results, it was concluded that current intensity, electrolysis time and electrode material for power consumption and initial pH for turbidity removal have significant effects.

## References

[1] R. Katal and H. Pahlavanzadeh, Desalination, 265 (2011) 199-205.
[2] K.P.S. Kalyani, N. Balasubramanian and C. Srinivasakannan, Chemical Engineering Journal, 151 (2009) 97-104.
[3] E. Terrazas, A. Vázquez, R. Briones, I. Lázaro and I. Rodríguez, Journal of Hazardous Materials, 181 (2010) 809-816.
[4] D.C. Montgomery, Design and Analysis of Experiments, 5th Edition, John Wiley & Sons, USA (2001).

---

* Corresponding author, *E-mail: hapoglu@eng.ankara.edu.tr*

# Reaction Kinetics of Electrochemical Sunflower Oil Refinery Wastewater Treatment

**Baran Özyurt, Şule Camcıoğlu, Mert Fırtın and Hale Hapoğlu***

Ankara University, Faculty of Engineering, Department of Chemical Engineering,
06100, Ankara, Turkey

*E-mail: bozyurt@ankara.edu.tr*

Refining crude vegetable oils produce wastewater in large quantities [1]. Wastewater characteristics vary depending on the type of oil processed and the process applied [2]. High chemical oxygen demand (COD), oil and grease, sulphate and phosphate contents create high inorganic and organic pollution loads in wastewater treatment plants [1]. When discharged to the environment, oily wastewater causes the formation of surface films and shoreline deposits, which impact ecological resources and functions [3]. The biodegradability of oil in the natural ecosystem is low and the oily components prevent long-term biological functions in the environment. For this reason, it is essential that the oil in the wastewater to be treated before discharge [3]. Some available technologies such as gravity separation, cyclone separation, chemical precipitation, sorption, membrane filtration and chemical oxidation have been used for oil removal [3]. Although many advantages of these technologies have been reported, there are some disadvantages associated with these treatment applications (i.e. low efficiency, long processing time, secondary pollution and high costs. In this study, reaction kinetics of electrochemical treatment of sunflower oil refinery wastewater were investigated using graphite electrodes in a batch electrochemical reactor under pH 6, 5 mS/cm electrical conductivity, 7 mA/cm$^2$ current density conditions. In a batch electrochemical reactor, linearized overall electrochemical conversion rate of pollutants can be generally expressed based on COD concentration as in Equation (1) given below [4].

$$\ln\left(\frac{-dC_{COD}}{dt}\right)=\ln\left(A\right)-\frac{E_A}{RT}+\alpha.\ln\left(C_{COD}\right) \qquad (1)$$

Where $C_{COD}$ represents chemical oxygen demand concentration in mg/L, t is the reaction time in min, A is the Arrhenius constant in min$^{-1}$, $E_A$ is the activation energy in kJ/mole, T is the reaction temperature in K, α is the reaction order. The rate constant at different temperatures was calculated from batch runs and plotted against 1/T. Linear regression of data yielded the activation energy and Arrhenius constant from its slope and from its intersection point, respectively.

## References

[1] U.T. Un, A.S. Koparal and U.B. Ogutveren, Journal of Environmental Management, 90 (2009) 428-433.
[2] S. Sridhar, A. Kale and A.A. Khan, Journal of Membrane Science, 205 (2002) 83-90.
[3] C. An, G. Huang, Y. Yao and S. Zhao, Science of the Total Environment, 579 (2017) 537-556.
[4] B.K. Körbahtı and K. Artut, Desalination, 258 (2010) 219-228.

---

* Corresponding author, *E-mail: hapoglu@eng.ankara.edu.tr*

P-73

# Effect of Initial pH on Boron Removal from Industrial Wastewater by Means of Consecutive Chemical and Electrochemical Coagulation

**Baran Özyurt, Çağlar Ateş, Şule Camcıoğlu and Hale Hapoğlu***

Ankara University, Faculty of Engineering, Department of Chemical Engineering,
06100, Ankara, Turkey

*E-mail: bozyurt@ankara.edu.tr*

Boron is present in the form of calcium, sodium and magnesium salts and is a basic micro-nutrient for plants and animals [1,2]. In order to avoid adverse effects on plants and humans due to excessive use of the boron, it is necessary to control the amount of boron in various water resources [3]. Various treatment processes have been developed for boron removal from water, including adsorption, ion exchange, reverse osmosis, electrocoagulation, membrane filtration and precipitation [1]. In the literature, successful results have been achieved with the use of synthetic low amount of boron containing solutions. Since the amount of boron in the wastewater generated by boron industry is very high, these treatment methods do not find a wide use area for themselves. In this study, removal of boron from industrial wastewater was studied by means of consecutive chemical and electrochemical coagulation method. Experimental conditions of chemical and electrochemical treatment methods are given below in Table 1. Results show that water has been obtained in a dischargeable quality according to Water Pollution Control Regulation of Turkish Authorities [4] with 88.7% $B_2O_3$ removal.

**Table 1.** Experimental Conditions of Chemical Coagulation

| Method | Parameter | Unit | Value |
|---|---|---|---|
| Chemical Coagulation | Initial Temperature | °C | 25 |
| | Initial pH | - | 9.43 |
| | Initial $B_2O_3$ Content | g/L | 10.81 |
| | Coagulant Dosage | g $Ca(OH)_2$ | 30.27 |
| | Duration | h | 1 |
| | Agitation speed | rpm | 750 |
| | Working Volume | L | 2.7 |
| Electrocoagulation | Electrode Material | - | Al |
| | Active Surface Area | $m^2$ | 0.084 |
| | Electrolysis Duration | h | 1 |
| | Initial Temperature | °C | 25 |
| | Current Intensity | A | 2 |
| | Inter-electrode Distance | mm | 3 |
| | Agitation speed | rpm | 200 |
| | Initial pH | - | 2.43-5.05-7.04-8.16-13.36 |
| | Working Volume | L | 0.4 |

## References

[1] A.E. Yilmaz, R. Boncukcuoğlu, S. Bayar, B. A. Fil and M.M. Kocakerim, Korean Journal of Chemical Engineering, 29 (2012) 1382-1387.
[2] R. Boncukcuoğlu, M.M. Kocakerim, E. Kocadağistan and M.T. Yilmaz, Resources, Conservation and Recycling, 37 (2003) 147-157.
[3] D. Uygan and Ö. Çetin, II. International Boron Symposia, (2004) 22-25.
[4] Turkish Water Pollution Control Regulation, 2008. Official Gazette No. 26786, 13 February.

---

* Corresponding author, *E-mail: hapoglu@eng.ankara.edu.tr*

# The Formation Pathways of Aroma and Aromatic Components in Fish and Crustaceans

**İlknur Meriç Turgut[1]* and Merve Onay[2]**

[1]Ankara University, Faculty of Agriculture, Department of Fisheries and Aquaculture Engineering, 06110, Dışkapı, Ankara, Turkey
[2]Republic of Turkey Ministry of Food, Agriculture and Livestock, Department of Fisheries, Eskisehir Road 9th Km Lodumlu, Ankara, Turkey

*E-mail: meric@agri.ankara.edu.tr*

Pleasing tastes of the nutriments emerge when flavor and aroma of the products' chemical structures are combined. Today, modern instrumental analysis techniques allow distinguishing and defining various flavors [1]. Subjective evaluation together with sensory evaluation lets the producers develop new flavors in order to improve the quality of their products. The most important characteristics of the flavor materials of which quantities range between nanogram and milligram are that they are sensated even when in small concentrations and that they play a great role in the quality [2]. Even though the nutriments contain hundreds of different aroma mediums [3], only a small amount of these mediums provide the smell of the nutriment. Therefore, determining these effective aroma ingredients is a significant subject for aroma studies.

Despite being a significant quality indicator, studies on the aroma ingredients of the fish species and distinctive aroma active ingredients of each specie are limited. This study aims to provide a compilation of the studies in our country and worldwide.

**References**
[1] T.H. Acree, J. Barnard and D.G. Cunningham, Food Chem., 14 (1984) 273-286.
[2] D.B. Josephson and R.C. Lindsay, Enzymic Generation of Volatile Aroma Compounds from Fresh Fish. In T.H. Parliament and R. Croteau (Eds.), Biogeneration of Aromas, ACS Symposium Series 317. Washington D.C: American Chemical Society, pp 201-219 (1986).
[3] H.H. Baek and K.R. Cadwallader, Character-impact Aroma Compounds of Crustaceans. In F. Shadidi and K.R. Cadwallader (Eds.), Flavor and Lipid Chemistry of Seafoods, ACS Symposium Series 674. Washington, DC: American Chemical Society, pp 85-94 (1997).

---

* Corresponding author, *E-mail: meric@agri.ankara.edu.tr*

# Assessment of Some Bio-chemical Parameters Associated with Quality Loss Under Different Storage Temperatures of Whiting (*Gadus merlangus euxinus* N. 1840)

**İlknur Meriç Turgut***

Ankara University, Faculty of Agriculture, Department of Fisheries and Aquaculture Engineering, 06110, Dışkapı, Ankara, Turkey

*E-mail: meric@agri.ankara.edu.tr*

As the world's fastest on-growing sector in food production, seafood and aquaculture has remarkable priority and gained attention from the consumer due to a great deal of nutritional characteristics. Freezing and frozen storage are the best methods to preserve the flesh and to obtain a product with a minimum loss of quality. Therefore, the determination of the parameters that reflect quality loss during frozen storage in filleted whiting (*Gadus merlangus euxinus* N. 1840) at three different temperatures (-12ºC, -18ºC and -24ºC) over a period of 10 months frozen storage was the aim of this study. Fresh whiting, a total number of 360 fish with mean body weight of 94.49±10.70 g, were obtained from the main fish market in Ankara, Turkey. Samples were immediately filleted by hand and blast frozen -30ºC for 6 h followed by a storage period of 300 days at -12, -18 and -24ºC. All analysis were performed from six replicates ($n$=6). The fillet samples were analyzed for moisture, crude ash, crude protein and crude fat, according to standard procedures following AOAC [1]. The fillet yield [100x(weight after filleting/total weight)] was calculated as described in Gülyavuz and Ünlüsayın [2]. Total volatile base nitrogen (TVB-N) values were determined with slight modification according to Pearson and Cox [3]. The measurement of trimethylamine nitrogen (TMA-N) was performed spectrophotometrically according to AOAC [1]. Thiobarbituric acid (TBA) values, expressed in mg malonaldehyde/kg was assessed using the method described by Tarladgis et al. [4]. Free fatty acid (FFA) content was determined by titration of lipid extract with 0.1N NAOH solution using phenolphtalein as an indicator and the results are expressed as % oleic acid [1]. One and two-way analysis of variance (ANOVA) were applied using statistical software SPSS 15.0 and the comparison of means was performed by DUNCAN multiple comparison test ($p<0.05$). It was found that the quantities of TVB-N, TMA–N, TBA and amount of FFA increased corresponding to the accelerated period of frozen storage. The variations of parameters between different storage temperatures were statistically significant ($p<0.05$) and acceptable limits of those were determined at -24º C.

**References**

[1] AOAC. Official Methods of Analysis. 16th Edition, (1995) Virginia, USA.
[2] H. Gülyavuz and M. Ünlüsayın. Su Ürünleri İşleme Teknolojisi. Süleyman Demirel Üniversitesi Eğirdir Su Ürünleri Fakültesi, Isparta, Türkiye, (1999) 366 p.
[3] D. Pearson and H.E. Cox. Determination of Total Volatile Bases in Flesh Foods. The Chemical Analyses Inc, New York, USA, (1962) 320 p.
[4] B.G. Tarladgis, B. M. Watts, M.T. Younathan and T.R.L. Dugan., J. Am. Oil Chem. Soc., 37 (1960) 44-48.

---

* Corresponding author, *E-mail: meric@agri.ankara.edu.tr*

# The Effect of Deep Eutectic Solvents on the Lipase Catalyzed Esterification of Lactic Acid

**Azime Arıkaya, Ayşe Ezgi Ünlü and Serpil Takaç***

Ankara University, Faculty of Engineering, Department of Chemical Engineering,
06100, Ankara, Turkey

*E-mail: azimearikaya@gmail.com*

Deep eutectic solvents (DESs) are regarded as green solvents that have taken considerable attention in the past few decades. They are studied extensively to replace toxic components of the processes with eco-friendly constituents. Especially biocatalytic processes are under research because of the compatibility of enzymes with DESs. Lipases, as one of the most widely used enzymes in different industrial bioprocesses, were reported to be utilized at various reactions using DESs [1]. Some examples are, lipophilization of methyl p-coumarate [2], alcoholysis of vinyl laurate [3], the transesterification of ethyl valerate [4], hydrolysis of *para*-nitrophenyl palmitate [5] and esterification of butyl acetate [6]. In this study, various choline chloride (ChCl) based DESs were investigated on the lipase catalyzed esterification reaction of lactic acid. For this purpose, ChCl: glucose (Glu) (1:1), ChCl:Glu (5:2), ChCl: fructose (Fru) (1:1), ChCl: sucrose (Suc) (1:1), ChCl: maltose (Malt) (4:1), ChCl: xylose (Xyl) (2:1), ChCl:Xyl (3:1), ChCl: galactose (Ga) (5:2), ChCl: glycerol (Gly) (1:2), ChCl:Gly (1:1), ChCl:Gly (3:2), ChCl:Urea (1:2) and ChCl: Ethylene glycol (EG) (1:2) were prepared [7]. Among them, ChCl:Suc (1:1), ChCl:Xyl (2:1), ChCl:Xyl (3:1) and ChCl:Ga (5:2) were unstable. The rest of the DESs were used in the esterification reaction of lactic acid with ethanol. The reactions were conducted at 0.8 M lactic acid and 6.7 M ethanol concentrations with 30 mg/mL lipase enzyme at 50°C and 200 rpm, in the presence of DES. The samples were analyzed using HPLC after 24 h of reaction. Among the DESs used, ChCl-Gly (1:2), ChCl-Glu (1:1) provided the highest conversion values. Sugar containing DESs; ChCl-Glu (5:2) and ChCl-Malt (4:1) also provided high conversion values that were nearly two fold higher than ChCl-Gly (3:2). When enzyme amount was increased to 110 mg/ml, the reaction rate was found to increase by 3.2 fold. On the other hand, when the reaction temperature was 30°C, the reaction rate decreased by nearly threefold.

## References

[1] B. Andualema and A. Gessesse, Biotechnology, 11(3) (2012) 100-118.
[2] E. Durand, J. Lecomte, B. Baréa, E. Dubreucq, R. Lortie, and P. Villeneuve, Green Chemistry, 15(8) (2013) 2275-2282
[3] E. Durand, J. Lecomte, B. Baréa, G. Piombo, E. Dubreucq and P. Villeneuve, Process Biochemistry, 47(12) (2012) 2081-2089.
[4] J.T. Gorke, F. Srienc and R.J. Kazlauskas, Ionic Liquid Applications: Pharmaceuticals, Therapeutics, and Biotechnology, American Chemical Society, 14 (2010) 169-180.
[5] I. Juneidi, M. Hayyan, M.A. Hashim and A. Hayyan, Biochemical Engineering Journal, 117 (2017) 129-138.
[6] M.C. Bubalo, A.J. Tušek, M. Vinković, K. Radošević, V.G. Srček, and I.R. Redovniković, Journal of Molecular Catalysis B: Enzymatic, 122 (2015) 188-198.
[7] Y. Dai, J. van Spronsen, G.J. Witkamp, R. Verpoorte and Y.H. Choi, Analytica Chimica Acta, 766 (2013) 61-68.

---

* Corresponding author, *E-mail: takac@eng.ankara.edu.tr*

P-77

# Modification of Apricot Kernel Shells to Remove Cr(VI) Ions in Aquatic Medium

**Hafize Nagehan Köysüren**[1]*, **Özcan Köysüren**[2] **and Şükrü Dursun**[3]

[1]Ahi Evran University, Faculty of Engineering and Architecture, Department of Environmental Engineering, 40100, Kırşehir, Turkey
[2]Ankara University, Faculty of Engineering, Department of Energy Engineering, 06830, Ankara, Turkey
[3]Selçuk University, Faculty of Engineering, Department of Environmental Engineering, 42075, Konya, Turkey

*E-mail: hnkoysuren@gmail.com*

In this study, apricot kernel shells were used for Cr(VI) ions adsorption. For this purpose, chemical modifications were applied to apricot kernel shells. Several chemicals (Fenton, HCl and NaOH) were used for the modification processes. The structure of the apricot kernel shells before and after the modification was analyzed by FTIR and SEM. As well as, kinetic, isotherm and thermodynamic parameters were worked for HCl, NaOH and Fenton modified apricot kernel shells. Additional costs resulted from the applied modification processes were calculated and compared with the general methods. Modification methods were improved the adsorption capacity of Cr(VI) ions. Removal efficiency changed with Cr(VI) ion concentration in the water sample and increased up to 75 % removal. Adsorption capacities were found out between 1.8 mg/g and 2.7 mg/g depending on the adsorbent and modification methods (Figure 1). In conclusion, the adsorption capacity of apricot kernel shells can confront with conventional adsorbents and apricot kernel shells can be used in the Cr(VI) ions waste-treatment economically [1].

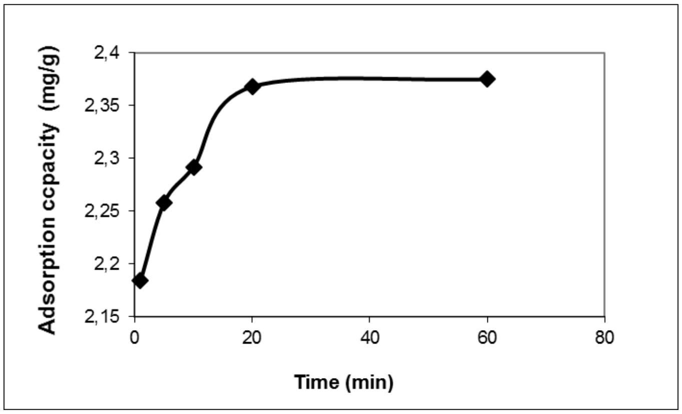


**Figure 1.** Cr(VI) ions adsorption capacity of apricot kernel shells modified with Fenton

## References

[1] H.N. Koysuren and S. Dursun, Journal of the Faculty of Engineering and Architecture of Gazi University, 28 (2013) 427-436.

---

* Corresponding author, *E-mail: hnkoysuren@gmail.com*

# Treatment of Herbicide Contaminated Water

**Ülküye Dudu Gül[1] and Hülya Silah[2]***

[1]Bilecik Seyh Edebali University, Vocational School of Health Services, Bilecik, Turkey
[2]Bilecik Seyh Edebali University, Faculty of Art and Science, Department of Chemistry, Bilecik, Turkey

*E-mail: ulkuyedudu.gul@bilecik.edu.tr*

Herbicides are commonly used in agricultural activities. Although they ensure some benefits such as controling unwanted plants which damaged crops, they form toxic residues for crops and become environmental pollutants. For example, 2,4-dichlorophenoxy acetic acid (2,4 D) is used to increase crop yield at low concentrations but high concentrations of 2,4 D inhibits crop growth because acidic herbisides like 2,4 D has toxic effects in metabolism of living organisms [1]. The treatment of herbicide contaminated water is a hot point in literature. Biosorption is an efficient and economic way to handle with water pollution [2]. Researchers are focused on usage of fungal biomass in biosorption process because fungal biomass is easily available as industrial waste products and shows exxcellent pollutant binding [3]. The aim of this study was to determine the usage of fungal biomass in biosorption of 2,4 D herbicide from aqueous solutions as a potential biosorbent. The effect of pH and pesticide concentration on 2,4 D biosorption properties of *A. versicolor* was examined. Electrochemical methods were used to analyze 2,4 D concentration. According to the results of this study, *Aspergillus versicolor* removed 2,4 D succefuly. Since the removal of herbicides is an important issue to control water pollution, the findings of this study are important sources of information to cope with water pollution.

## References

[1] V. Singh, K.Singh, Environ. Process., 2 (2015) 251-260.
[2] A.S. Ayangbenro and O.O. Babalola, Int. J. Environ. Res. Public Health, 14(94) (2017) 1-16.
[3] Y. Fu and T. Viraraghavan, Bioresource Technology, 79 (2001) 251-262.

## Acknowlegement

This study was supported by Bilecik Seyh Edebali University Research Foundation (Project No: 2012-02.BİL.12-01) and The Scientific and Technical Research Council of Turkey (TÜBİTAK-ARDEP, Project No: 113Y590).

---

* Corresponding author, *E-mail: ulkuyedudu.gul@bilecik.edu.tr*

# Ecological Risk Assessment and Seasonal-Spatial Distribution of Some Trace Elements from Surface Sediment: Eutrophic-Shallow Mogan Lake, Turkey

**Akasya Topçu* and Doğukan Kaya**

Ankara University, Faculty of Agriculture, Department of Fisheries and Aquaculture Engineering, 06110, Dışkapı, Ankara, Turkey

*Email: atopcu@ankara.edu.tr*

Trace metals in aquatic environments accumulate primarily in the upper sections of sediment due to biological-geochemical mechanisms. The extent of metal pollution is determined by comparing metal concentrations in surface sediments to the TEL (threshold effects level) and PEL (probable effects level) of the SQGs (Sediment Quality Guidelines) [1,2]. Mogan Lake, shallow-eutrophic and a popular recreational area, is under the environmental protection status as ‘Golbasi Specially Protected Area’. Several studies [3,4] have been undertaken regarding the eutrophication-sediment interaction in Mogan Lake. The objectives of this research were to assess: (1) the seasonal and spatial concentrations of some mineralogical characters with the use of X-ray fluorescence (XRF) spectrometry; (2) the environmental risk associated with the metal contents of the sediments using available TEL, PEL and SQGs. (3) the contamination levels according to the Igeo and EF. Based on their mean content, the components of the surface sediment were arranged in the following decreasing order: Ca>Zn>Al>Cu>TFe>K>Na>Mg>Mn. According to the applied TEL/PEL SQGs both Cu and Zn concentrations were lower than the Avarage Continental Crust, Avarage Shale and SQGs (Low-High) values in general according to [1,2,5,6] in Mogan Lake. The results of the geoaccumulation index revealed that Mogan Lake, Igeo values for Cu, Mn and Zn were lower than zero, indicating that sediment pollution level remained at a very low degree. The calculation of enrichment factors in the Mogan Lake for the two stations showed that: For Zn concentrations EF values were <1 in general, showing low pollution levels. Comparison with sediment quality guidelines revealed that in general there is not an adverse biological effect. In conclusion, trace elements does not currently pose a threat to the environment and the data from this study regarding metal levels should be used as a baseline reference for future metal pollution monitoring programs in Mogan Lake which will be a useful tool for authorities in charge of sustainable management.

## References

[1] D.D. MacDonald, C.G. Ingersoll and T.A. Berger, Archives of Environmental and Contamination Toxicology, 39 (2000) 20-31.
[2] D.D. MacDonald, C.G. Ingersoll, E.S. Dawn, A.L. Rebecca, Development and Applications of Sediment Quality Criteria for Managing Contaminated Sediment in British Columbia. MacDonald Environmental Sciences Ltd. # 24-4800 Island Highway North Nanaimo, British Columbia V9T1W6 (2003).
[3] S. Pulatsü, A. Topçu, M. Kırkağaç and G. Köksal, Lakes and Reservoirs: Research and Management, 13 (2008) 197-205.
[4] A. Topçu and S. Pulatsu, Fresenius Environmental Bulletin, 17(2) (2008) 164-172.
[5] K. Loska and D. Wiechula, Chemosphere, 51(8) (2003) 723-733.

---

* Corresponding author, *E-mail: atopcu@ankara.edu.tr*

# Food Chemistry

P-80

# The Importance of Inorganic Ingredients in Fermented Beverages

**Zülal Taçar** and Nilgün Kalaycıoğlu Özpozan*

Erciyes University, Faculty of Science, Department of Chemistry, Kayseri, Turkey

*E-mail: zulaltacarr@hotmail.com*

Especially there are many factors that effect the amount of the phenol components in fermented beverages, for example potassium bicarbonate, potassium metabisulfite, potassium sorbate, sodium carbonate, sodium percarbonate, sodium metabisulfite, etc. We study fermented beverage components and anthocyanin substances necessary for dealing with the research after doing some research on the trail of this components, increasing of the amount and inorganic substances that have different effective properties that are used in the production process.

We are investigating these effects on our most important work in our research. Considering the consumption of organic food has grown recently, organic grape and non-organic wines produced from grapes are to study the amounts and types of antioxidants. The other important factor is the wines that have the same region, same production conditions. Phenol components are different each year due to seasonal, rainfall, nutrition and other effects. The changes in the phenolic components will be included in the scope of this study by selecting the same region and production conditions and the antioxidant amounts in different years. It is considered that the studies related to the positive and negative effects of the wine on the health and the chemistry and the examination of the effects of the inorganic substances, will contribute to the related studies in the literature [1,2].

## References

[1] A.V. Akman and T. Yazıcıoğlu, Fermantasyon Teknolojisi, Cilt 2, Şarap Kimyası ve Teknolojisi, A.Ü. Ziraat Fakültesi Yayınları. No: 160, Ankara (1960).
[2] S. Koundouras, S., V. Marinos, A. Gkoulioti, Y. Kotseridis and C. Vanleeuwen, J. Agric. Food Chem., 54 (2006) 5077-5086.

## Acknowledgment

We acknowledge the financial support granted by Erciyes University (ERUBAP), ((FYL-2017-7446).

---

* Corresponding author, *E-mail: nozpozan@gmail.com*

# The Effect of the Phenol Component in the Wine

**Nilgün Kalaycıoğlu Özpozan* and Zülal Taçar**

Erciyes University, Faculty of Science, Department of Chemistry, Kayseri, Turkey

*E-mail: zulaltacarr@hotmail.com*

The antioxidant phenol-structured compounds in fermented beverages are important substances for human health and wine with fermented alcoholic beverage. Antioxidant in wine and the reaction of phenolic-structured compounds reduce the risk of paralysis cause of preventing vascular stiffness formation, increase the HDL cholesterol level due to preserve blood fat ratio, reduce the cholesterol level so reducing heart disease risks, prevent the blood clot due to reduce the clot protein formation, digestive system Configurator, germicidal, prevent the cancer for many cancer types have a positive effect for human health. Therefore, it is lead for all research about this field. The phenol compounds with antioxidant are substances that influence chemistry of wine [1,2]. This researching is important to follow a conscious path about health. In recent years, characterization of analysis is easier due to the rapid development of chemistry and chromatography methods (GC-MS, HPLC).

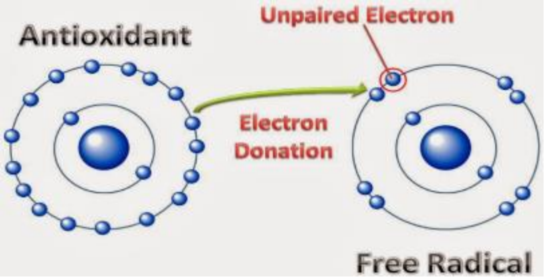


**Figure 1.** Antioxidant substances and free radikal molecules

**References**
[1] A.V. Akman and T. Yazıcıoğlu, Fermantasyon Teknolojisi, Cilt 2, Şarap Kimyası ve Teknolojisi, A.Ü. Ziraat Fakültesi Yayınları. No: 160, Ankara (1960).
[2] H. Kelebek, Değişik Bölgelerde Yetiştirilen Öküzgözü, Boğazkere ve Kalecik Karası Üzümlerinin ve Bu üzümlerden Elde Edilen Şarapların Fenol Bileşikleri Profili Üzerine Araştırmalar, Ç.Ü. Fen Bilimleri Enstitüsü, Gıda Mühendisliği Anabilim Dalı Doktara Tezi, Adana (2009).

**Acknowledgement**
We acknowledge the financial support granted by Erciyes University (ERUBAP), (FYL-2017-7446).

---

* Corresponding author, *E-mail: nozpozan@gmail.com*

# Materials Science

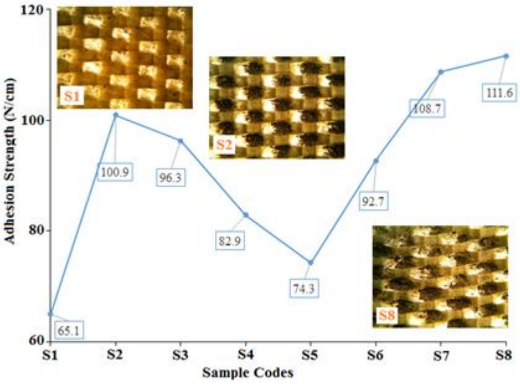
# Preparation of Dual-Curable Adhesive Formulations by Composition of Acrylic Reactive Diluents for Cord/Rubber Applications

**Zehra Yıldız[1,2,3], Hacer Ayşen Önen[4]*, Atilla Güngör[5], Youjiang Wang[3], and Karl Jacob[3]**

[1]Marmara Univ., Faculty of Technology, Dept. of Textile Eng., Istanbul, Turkey
[2]Istanbul Technical Univ., Inst. of Sci. and Tech., Dept. of Polymer Sci. and Tech., Turkey
[3]Georgia Institute of Technology, School of Materials Science and Eng., Atlanta, USA
[4]Istanbul Technical Univ., Faculty of Arts and Sciences, Dept. of Chemistry, Turkey
[5]Marmara University, Faculty of Arts and Sciences, Dept. of Chemistry, Istanbul, Turkey

*E-mail: zehra.yildiz@marmara.edu.tr*

Cord fabric/rubber composites are widely used in industrial applications such as conveyor belts, hoses, bicycle and car tires, etc. The adhesion is an important issue considering the differences in polarity and functionality of cord fabric and rubber surfaces [1,2]. In this study dual-curable (UV+thermal) formaldehyde-free adhesive formulations were prepared by using the reaction of toluene 2,4-diisocyanate (TDI) and 2-hydroxyethyl methacrylate (HEMA) in the presence of a catalyst (T12). Then the TDI-HEMA adduct was reacted with polyvinyl butyral (PVB) to increase the functionality of the oligomer and wettability of the polyester cord fabric. The obtained oligomer was characterized by $^1$H NMR spectroscopy. In order to adjust the viscosity of the oligomer and enhance the mechanical properties, tricyclodecane dimethanol diacrylate (TCDDA) and trimethylolpropane trimethacrylate (TMPTMA) were used as reactive diluents. The effect of reactive diluent combinations on the adhesion strength between cord/rubber surfaces was investigated (Figure 1).



| Sample Codes | Reactive Diluent Compositions (TCDDA/TMPTMA) |
|---|---|
| S1 | -- |
| S2 | 0/100 |
| S3 | 25/75 |
| S4 | 40/60 |
| S5 | 50/50 |
| S6 | 60/40 |
| S7 | 75/25 |
| S8 | 100/0 |

**Figure 1.** Sample codes, compositions and adhesion strength values between cord/rubber surfaces with optical microscopy images

## References

[1] S.S. Choi and O.B. Kim, Journal of Industrial and Engineering Chemistry, 20 (2014) 202-207.
[2] A. Louis, J. Noordermeer, W. Dierkes and A. Blume, 186th Technical Meeting of Rubber Division (2014).

## Acknowledgement

This study has been financially supported by the Marmara University, Faculty of Technology, the Istanbul Technical University Research Foundation, and the Scientific and Technological Research Council of Turkey (TUBITAK BIDEB-2214).

---

* Corresponding author: *E-mail:onen@itu.edu.tr*

P-83

# Corrosion Properties of Ti-6Al-4V Alloy Coated with a Novel Nanobiocomposite

**Umut Beskan** and Aylin Aytaç*

Gazi University, Faculty of Science, Department of Chemistry, 06500, Ankara, Turkey

*E-mail: umut.beskan@gazi.edu.tr*

Biomaterials are widely employed in order to heal or replace traumatized or failed tissues and organs so that they improve life quality of patients. Biomaterials should have mechanical strength enough to endure mechanical force to which they are exposed in the human body, more importantly exhibit good corrosion resistance in the hostile body environment [1]. Corrosion is a slow degradation of materials. Especially when a metallic material placed in a human body, it generates high importance because of corrosive anions, cations, proteins and other substances in body fluids. Surface modification methods can give improved corrosion and biocompatibility properties of biomaterials. In this study, the most widely used titanium implant material in orthopedic and dental surgery Ti-6Al-4V was coated with chitosan/hydroxyapatite/ceramic nanocomposite by electrophoretic deposition technique (EPD) after hydroxyapatite and ceramic nanoparticles were synthesized by wet precipitation method. According to the open circuit, anodic polarization and electrochemical impedance spectroscopy (EIS) measurements of the bare and coated electrodes, obtained nanobiocomposite increases the corrosion resistance of the titanium alloy Ti-6Al-4V thanks to its barrier effect, thus the possibility for the migration of metal ions from substrate into biological environment is reduced (Figure 1). Using chitosan/hydroxyapatite/ceramic nanobiocomposite which contains natural ingredients, a pre-treatment method applied before implant materials being put in a package has been achieved.

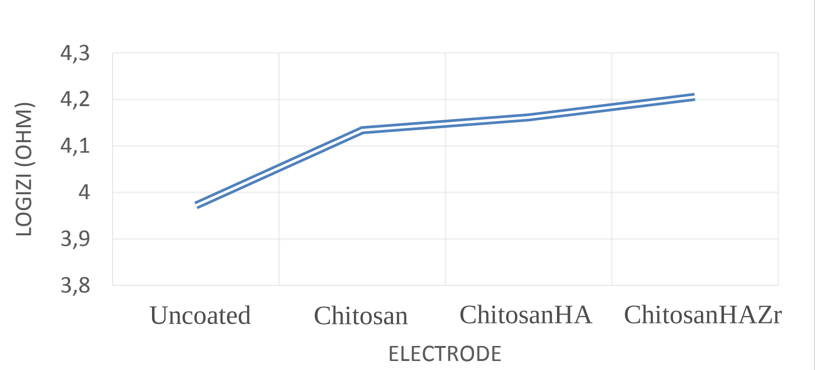


**Figure 1.** Low frequency impedances at 72 hours

## References

[1] R.A. Ahmed, A.M. Fekry and R.A. Farghali, Applied Surface Science, 285P (2013) 309-316.

## Acknowledgement

This study was supported by TUBITAK with Project 116M015.

---

* Corresponding author, *E-mail:* aytaca@*gazi.edu.tr*

P-84

# A Novel Nanobiocomposite for Improved Hydroxyapatite Coatings on Ti-6Al-4V Alloy

**Umut Beskan and Aylin Aytaç***

Gazi University, Faculty of Science, Department of Chemistry, 06500, Ankara, Turkey

*E-mail: umut.beskan@gazi.edu.tr*

Hydroxyapatite [$Ca_5(PO_4)_3OH$] is the main mineral compound of the inorganic part of human bone. When it is used to coat biomaterials such as hip and dental implants, it can increase the bonding strength of bone to implant thanks to its osteoconductive properties, thus improve the osseointegration process, healing time and load stress distribution to surrounding bone resulting in more biocompatible materials [1]. Although these advantages, hydroxyapatite coatings suffer from poor mechanical properties like brittleness, toughness and low fatigue resistance which reduce its adhesion strength and prevent it from load bearing applications. Moreover, due to high sintering temperatures, hydroxyapatite coatings react with the substrate material so that different phases such as β-tricalciumphosphate (β-TCP) which accelerates corrosion phenomena can occur. To overcome these problems, composites that bring good properties of different materials together can be prepared. Chitosan as a biopolymer and some ceramic material can provide better biocompatibility and mechanical properties by increasing the adhesion strength of hydroxyapatite coatings. Besides, chitosan eliminates sintering process. In this study, hydroxyapatite and some ceramic nanoparticles were obtained by wet precipitation method. Afterwards, these obtained nanoparticles and chitosan were co-deposited by electrophoretic deposition technique (EPD) on Ti-6Al-4V implant materials. Surface morphology and characterization of coatings were analyzed by scanning electron microscopy (SEM), x-ray diffraction (XRD), fourier transform infrared spectroscopy (FTIR) and optical micrometer. Adhesion strength of coatings was determined by universal testing machine. The obtained coatings are suitable for using in a pre-treatment process applied to implant biomaterials before they being put in packages.

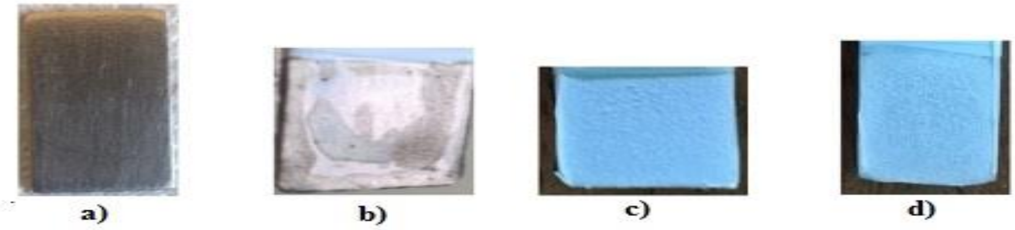


**Figure 1.** a) Bare and coated implants b) chitosan c) chitosan/HA, and d) chitosan/HA/ceramic material

## References

[1] X. Pang and I. Zhitomirsky, Materials Characterization, 58 (2007) 339-348.

## Acknowledgements

This study was supported by TUBITAK with Project 116M015.

---

* Corresponding author, *E-mail: aytaca@gazi.edu.tr*

# Characterization and Preparation Free-Standing and Flexible Pt-MoS2/rGO Paper Electrode for Hydrogen Evolution Reaction

**Kader Dağcı Kıranşan***, Ezgi Topçu and Elif Erçarıkcı

Atatürk University, Faculty of Science, Department of Chemistry, Erzurum, Turkey

*E-mail: kdagci@atauni.edu.tr*

Highly flexible $MoS_2$-rGO composite paper was successfully prepared for Hydrogen Evolution Reaction (HER). For this purpose, a dispersion including graphene oxide (GO) and molybdenum sulfur ($MoS_2$) was prepared and $MoS_2$/GO paper was acquired by vacuum-filtration of this dispersion through a suitable membrane [1]. After peeling it off from the membrane, it was transformed to $MoS_2$/rGO paper by performing reduction with hydriodic acid [2]. The PtNPs-loaded $MoS_2$/rGO paper (Pt-$MoS_2$/rGO) was efficiently prepared by electrochemical deposition at a constant potential using PtCl solution without any surfactant [3] or hydrothermal process [4]. Structural, chemical and morphological characterization of the $MoS_2$/rGO composite papers was investigated by using (i) scanning electron microscopy (SEM), (ii) energy-dispersive X-ray spectroscopy (EDS), (iii) X-ray photoelectron spectroscopy (XPS), (iv) X-ray diffraction spectroscopy (XRD), (v) Raman spectroscopy, (vi) electrochemical impedance spectroscopy (EIS) and (vii) linear sweep voltammetry (LSV) techniques. The catalytic performance of Pt-$MoS_2$/rGO, $MoS_2$/rGO and rGO for HER was evaluated by using LSV recorded from 0.0 to -250 mV vs. SHE in 0.1 M $H_2SO_4$ at a sweep rate of 5 mV $s^{-1}$. It is noted that the overpotential of Pt-$MoS_2$/rGO catalyst is 75 mV (vs. SHE), which is much lower than that of $MoS_2$/rGO and rGO.

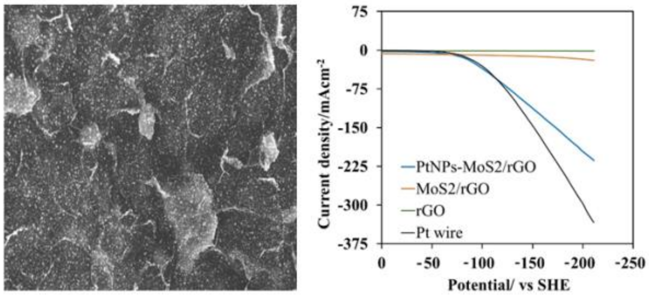


**Figure 1.** (a) SEM image Pt-$MoS_2$/rGO paper electrode, (b) Polarization curves for Pt-$MoS_2$/rGO paper, $MoS_2$/rGO paper, rGO paper and Pt wire electrodes in 0.5 M $H_2SO_4$. Scan rate: 5 mV $s^{-1}$

**References**
[1] Y. Zhang, J. Yan and X. Ren, International Journal of Hydrogen Eergy, 42 (2017) 5472-5477.
[2] Y. Zhao, X. Bo and L. Guo, International Journal of Hydrogen Energy, 42 (2017) 5569-5576.
[3] D. Liu, L. Li and T. You, Journal of Colloid and Interface Science, 487 (2017) 330-335.
[4] X. Zhang, D. Wu, D. Cheng, Electrochimica Acta, 246 (2017) 572-579.

---

* Corresponding author, *E-mail: kdagci@atauni.edu.tr*

P-86

# Comparative Study for Water Resistance and Strength of Pure and Hydrophobic Coated Corrugated CardBoard

**Betül Gök**[1,2*], Duygu Akpınar[1], Sefa Selçuk[1] and Özge Taşkan[1]

[1]Ankutsan R & D Center Antalya Organize Sanayi Bölgesi 22. Cad. Osb 2nd Section, 07190, Döşemealtı, Antalya, Turkey
[2]Akdeniz Üniversity, Faculty of Science, Department of Chemistry, 07058, Antalya, Turkey

*E-mail: Betul.GOK@ankutsan.com*

Paper is widely used in packaging applications and is environmentally safe as it is biodegradable. The hydrophilic nature of cellulose in paper, due to the -OH sites in the basic unit of cellulose ($C_6H_{10}O_5$), limits the water-vapor-barrier properties of paper [1]**.** The corrugated cardboard used in fresh fruits and vegetables packaging readily absorbs moisture from the environment or from the food, especially when stored under high humidity conditions [2]. To avoid the deterioration of the packing material either due to the high humidity conditions, various chemicals are being applied to corrugated cardboard. Some types of coatings such as resins, polymers, copolymers, inorganic and organic compounds are commonly used for paper and board [3].

In this study, the effect of the hydrophobic coating (barrier) to water resistance and strength of corrugated cardboard were investigated. For this purpose weight, thickness, edge crush test (ECT), box compression test (BCT) and Cobb test were performed. According to the Cobb test results, the applied barrier increased the water resistance of the board. Table 1 shows pure and coated corrugated cardboard strength test results. This demonstrates that the hydrophobic coating also enhances the strength of the corrugated cardboard.

**Tablo 1.** Strength test results of hydrophobic coated and pure corrugated cardboards

| Properties | Flute type | Thickness (mm) | BST (kPa) | ECT (kN/m) | BCT (kgf) | %Increase of strenght |
|---|---|---|---|---|---|---|
| **Pure** | C | 3,78 | 589 | 4,60 | 218 | - |
| **Hydrophobic coated** | C | 3,8 | 687 | 5,48 | 260 | 19 |

**References**
[1] K. Khwaldia, E. Arab-Tehrany and S. Desobry, Comprehensive Reviews in Food Science and Food Safety, 9 (2010) 82-91.
[2] A. Taboada-Rodríguez, I. García-García and R. Cava-Rod, Journal of Coatings Technology and Research, 10 (2013) 749-755.
[3] S.A.D.C.V. Sigma Alimentos.Patent: EP 2837736 A1, 2015.

---

[*] Corresponding author, *E-mail: Betul.GOK@ankutsan.com*

P-87

# Investigation for Factors Influencing Corrugated Cardboard Strength

**Betül Gök**[1,2*], **Sefa Selçuk**[1], **Serhat Bayık**[1] **and Ebru Kalaycıoğlu**[1]

[1]Ankutsan R & D Center Antalya Organize Sanayi Bölgesi 22. Cad. Osb 2nd Section,
07190, Döşemealtı, Antalya, Turkey
[2]Akdeniz Üniversity, Faculty of Science, Department of Chemistry, 07058, Antalya,
Turkey

*E-mail: Betul.GOK@ankutsan.com*

Corrugated cardboard is a high-performance packaging material designed to protect and present a variety of products [1]. A corrugated cardboard consisting of a single corrugated layer sandwiched between two liner layers (Figure 1). This product consists of a combination of the three layers stronger than each layer is individually owned. The weight, type and properties of the outer, inner and intermediate papers forming the corrugated cardboard are of great importance as they are directly related to the box performance. In addition to the papers used, the type of glue and additives should be chosen appropriately [2].

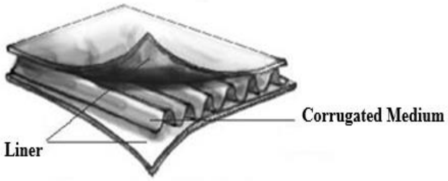


**Figure 1.** Schematic representation of corrugated cardboard

In this study, the effects of starch glue thickness and glue-cellulose reaction time on product quality were investigated. For this purpose weight, thickness, edge crush test (ECT), box compression test (BCT) tests were performed. Also water resistance of the hydrophobic coated product was investigated. Table 1 shows corrugated cardboard strength changes with different time reveal. As shown in Table 1, ECT and BCT test results increased systematically with time. So that as the reaction time increases the strength of the cardboard increases.

**Tablo 1.** Effect of reaction time on product strength

| Rxn time (min) | Flute type | Thickness (mm) | ECT (kN/m) | BCT (kgf) | %Increase of Strenght |
|---|---|---|---|---|---|
| 10 | BC | 6,37 | 10,4 | 640 | 0 |
| 90 | BC | 6,37 | 10,9 | 671 | 4,84 |
| 1440 | BC | 6,37 | 12,6 | 777 | 21,40 |

**References**

[1] M.O. Önen, Oluklu Mukavva Ambalaj Ürünleri, Türkiye Kalkınma Bankası A.Ş.-Sektörel Araştırmalar, 2 (2002) 2-5.
[2] M. Vishnuvarthanan and N. Rajeswari, Alexandria Engineering Journal, 52 (2013) 137-140.

---

* Corresponding author, *E-mail: Betul.GOK@ankutsan.com*

P-88

# The Effect of Electrode Materials on The Gas Sensing Properties of Ni-doped ZnO Films

**Hakan Sürel[1], Ali Orkun Çağırtekin[1]*, Baktiyar Soltabayev[1], Memet Ali Yıldırım[2], Aytunç Ateş[3] and Selim Acar[1]**

[1]Gazi University, Faculty of Science, Department of Physics, Ankara, Turkey
[2]Erzincan University, Engineering Faculty, Department of Electric Electronics Engineering, Erzincan, Turkey
[3]Yıldırım Beyazıt University, Faculty of Engineering and Natural Sciences, Department of Material Engineering, Ankara, Turkey

*E-mail: orkunbjk1903@gmail.com*

Along with people enhancing the consciousness of environmental protection, it is more and more important to realize the detection of toxic gases. Hence, an increasing number of researchers are interested in all sorts of gas sensing materials [1]. In recent years, researchers have found that complex oxides also have good gas sensing properties. A vast amount of research papers, regarding the gas sensing properties of ZnO thick and thin films or nanostructures, have been published in recent years [2]. The role of electrode material on the sensing properties of ZnO, was intensively investigated. In the current study, $Zn_{0.9}Ni_{0.1}O$ sensor materials were grown by Successive Ionic Layer Adsorption and Reaction (SILAR) method and evaporated two different electrode metals; Pt and Au. The effects of electrode material on the gas sensing properties were investigated. The responses of sensing materials to NO, hydrogen, ammonia and methane were examined and the factors influencing the gas sensing performance were investigated. The sensor with Au electrode exhibited higher response compared to sensor with Pt electrode to NO gas (Figure 1).

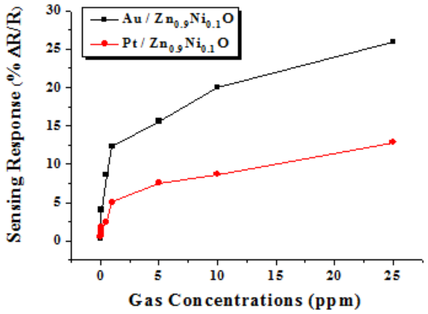


**Figure 1.** The response of $Zn_{0.9}Ni_{0.1}O$ sensor with Au and Pt electrode exposed to different NO gas concentrations

## References

[1] A.P. Rambu, L. Ursu, N. Iftimie, V. Nica, M. Dobromir and F. Iacomi, Appl. Surf. Sci., 280 (2013) 598-604.
[2] S. Ghosh, P. Srivastava, B. Pandey, S. Maurav, P. Bharadwaj, D.K. Avasthi, D. Kabiraj and S.M. Shivaprasad, Appl. Phys. A, 90 (2008) 765-769.

## Acknowledgement

This work is supported by TUBITAK Project No. 115M658 and Gazi University Scientific Research Fund Project No. 05/2016-21.

---

* Corresponding author, *E-mail: orkunbjk1903@gmail.com*

P-89

# Impedance Spectroscopy Analysis of Sn-Doped ZnO Sensors for NO Gas Detection

**Tuğba Çorlu[1], Irmak Karaduman[1], Ali Orkun Çağırtekin[1]*, Memet Ali Yıldırım[2], Aytunç Ateş[3] and Selim Acar[1]**

[1]Gazi University, Faculty of Science, Department of Physics, Ankara, Turkey
[2]Erzincan University, Engineering Faculty, Department of Electric Electronics Engineering, Erzincan, Turkey
[3]Yıldırım Beyazıt University, Faculty of Engineering and Natural Sciences, Department of Material Engineering, Ankara, Turkey

*E-mail: orkunbjk1903@gmail.com*

Chemical gas sensors find extensive applications in toxic and combustible gas monitoring, automobile combustion control, medical analysis, and energy and drying operations markets. In contrast to the conventional equipment for gas separation and detection such as gas chromatography, ion mobility spectroscopy, and mass spectroscopy; gas sensors are more cost effective and have a simpler instrumentation operation especially for real-time and in situ applications [1]. The interaction of the gas with the sensing layer of a chemical gas sensor leads to physical parameter changes such currents, electrical conductance; capacitance, absorbance, mass or acoustic variables, which are, all correlated with the gas concentrations [2]. In this study, Sn-doped ZnO thin films with different tin-doping levels were deposited on glass substrates by employing an inexpensive, simplified Successive Ionic Layer Adsorption and Reaction (SILAR) method at room temperature. The effect of Sn doping on the AC and DC conductivity and gas sensor application were investigated. Also, deposited thin films were studied by means of complex impedance spectroscopy and frequency dependence of conductivity measured from the impedance data at a range of frequency intervals between 20 Hz and 1.5 MHz at 530 K. Impedance spectroscopy analysis indicates that grain boundary resistance increases with the increasing NO concentration up to 25 ppm. The results showed that the resistance due to grain boundaries significantly contributed to the characteristics of the gas sensor (Figure 1).

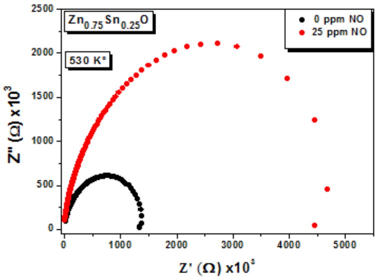


**Figure 1.** The Cole-Cole plots of $Zn_{0.75}Sn_{0.25}O$ sensor with and without NO gas

## References

[1] S. Homayoonnia and S. Zeinali, Sensors and Actuators B, 237 (2016) 776-786.
[2] M. Madou, S. Morrison, Academic Press Inc., San Diego, 1989.

## Acknowledgement

This work is supported by TUBITAK Project No. 115M658 and Gazi University Scientific Research Fund Project No. 05/2016-21.

---

* Corresponding author, *E-mail: orkunbjk1903@gmail.com*

# Effect of Annealing Procedure on the Electrical and NO Gas Sensing Properties of Ni Doped ZnO Nanostructured Thin Films

**Hakan Sürel[1]*, Irmak Karaduman[1], Tuğba Çorlu[1], Memet Ali Yıldırım[2], Aytunç Ateş[3] and Selim Acar[1]**

[1]Gazi University, Faculty of Science, Department of Physics, Ankara, Turkey
[2]Erzincan University, Engineering Faculty, Department of Electric Electronics Engineering, Erzincan, Turkey
[3]Yıldırım Beyazıt University, Faculty of Engineering and Natural Sciences, Department of Material Engineering, Ankara, Turkey

*E-mail: hakan.surel@hotmail.com*

In the current study, Ni doped ZnO nanostructured thin films ($Zn_{0.95}Ni_{0.05}O$) have been deposited by Successive Ionic Layer Adsorption and Reaction method (SILAR) and annealed at 300 °C in $N_2$ environment. The measurements of electrical conductivity of the fabricated sensors carried out in the temperature range 300-500 K using the two-point-probe method under dark media. The gas sensing properties of fabricated sensors investigated as a function of operating temperature and gas concentrations. The optimum temperature from 85 °C shifted to 55 °C and displays lower response and recovery times than those as-grown sensors. The result indicates that the gas sensing properties are strongly related to annealing procedure and renders the reason for the utilization of ZnO nanostructured thin films in gas sensors and other expanding devices [1]. This improvement in response is beneficial for environmental sensors. This work is supported by.

**References**

[1] T. Corlu, I. Karaduman, M. Alı, Yıldırım, A. Ates and S. Acar, J. Electron. Mater., 46(7) (2017) 3995-4002.

**Acknowledgement**

TUBITAK Project No. 115M658 and Gazi University Scientific Research Fund Project No. 05/2016-21.

---

* Corresponding author, *E-mail: hakan.surel@hotmail.com*

P-91

# Effect of Film Thickness on No Gas Sensing Properties of Ni-Doped Zno Thin Film Grown by Successive Ionic Layer Adsorption and Reaction Method

**Hakan Sürel[1]*, Irmak Karaduman[1], Tuğba Çorlu[1], Memet Ali Yıldırım[2], Aytunç Ateş[3] and Selim Acar[1]**

[1]Gazi University, Faculty of Science, Department of Physics, Ankara, Turkey
[2]Erzincan University, Engineering Faculty, Department of Electric Electronics Engineering, Erzincan, Turkey
[3]Yıldırım Beyazıt University, Faculty of Engineering and Natural Sciences, Department of Material Engineering, Ankara, Turkey

*E-mail: hakan.surel@hotmail.com*

In the present work, Ni-doped ZnO thin films have been successfully grown onto the glass substrates using Successive Ionic Layer Adsorption And Reaction Method (SILAR) at room temperature [1]. The effect of film thickness on the physicochemical properties such as structural, surface morphological, elemental and optical has been reported. Finally, the gas sensing properties of Ni-doped ZnO thin films are studied at different operating temperatures and NO gas concentrations. 40-cycle Ni-doped ZnO thin film shows rapid response and reproducibility towards 25 ppm NO gas concentration at 55 ºC. The present gas sensor exhibits good sensing properties such as high response, quick response-recovery times and reproducibility.

**References**

[1] T. Corlu, I. Karaduman, M. Alı, Yıldırım, A. Ates and S. Acar, J. Electron. Mater., 46(7) (2017) 3995-4002.

**Acknowledgement**

This work is supported by TUBITAK Project No. 115M658 and Gazi University Scientific Research Fund Project No. 05/2016-21.

---

* Corresponding author, *E-mail: hakan.surel@hotmail.com*

P-92

# Study of Magnetoresistance Property on Rare-earth Doped Layered Manganites with the Same A-site Ionic Radius

**Nevin Soylu Koç***, **Sevgi Polat Altıntaş and Cabir Terzioğlu**

AIB University, Faculty of Arts and Science, Department of Physics, Bolu Turkey

*E-mail: nevinsoylu@ibu.edu.tr*

We studied the relationship between the effect of rare-earth doping and magnetoresistance (MR) on layered manganites [1]. A series of $(La_{1-\delta}Re_{\delta})_{1.4}Ca_{1.6}Mn_2O_7$ (Re:Gd, Sm, Nd, Pr) have been prepared by the solid state reaction method and fractional occupancies (δ) of rare earth elements were determined according to the calculation made to obtain the same A-site ionic radius (≈1.3213 Å). The chemical compositions of the layered manganites are as follows: $(La_{0.6}Gd_{0.4})_{1.4}Ca_{1.6}Mn_2O_7$, $(La_{0.5}Sm_{0.5})_{1.4}Ca_{1.6}Mn_2O_7$, $(La_{0.34}Nd_{0.66})_{1.4}Ca_{1.6}Mn_2O_7$, $(La_{0.142}Pr_{0.857})_{1.4}Ca_{1.6}Mn_2O_7$. This study was completed through the measurement of X-ray (XRD) diffraction patterns, scanning electron microscope (SEM) images, resistivity-temperature (ρ-T) curves and magnetoresistance–temperature (MR-T) curves. The MR was defined as $MR\ \% = \{[\rho(H) - \rho(0)]/\rho(0)\}\times 100\%$ [1] and where ρ(H) and ρ(0) are the resistivities measured in a magnetic field of 1T and in the absence of an applied magnetic field, respectively.

**References**

[1] C. Zener, Phys. Rev., 82 (1951) 403-405.

---

* Corresponding author, *E-mail: nevinsoylu@ibu.edu.tr*

# Impact of A-site Cation Size Disorder on Electronic Properties of Perovskite Manganites

**Sevgi Polat Altıntaş[1]* and Nabil Mahamdioua[2]**

[1]Abant Izzet Baysal University, Department of Physics, Bolu, Turkey
[2]Lend, Universite´ de Jijel, B. P 98 Jijel, Algeria

*E-mail: sevgialtintas@ibu.edu.tr*

We investigate the influence of size mismatch effect of a series of $La_{2/3-x}RE_xCa_{1/3-y}Sr_yMnO_3$ with RE: Y, Gd and Ce. A-site cationic size mismatch, $\sigma^2$, is kept constant while the average cationic radius $<r_A>$ is varied. After characterizing the samples by X-ray diffraction, scanning electron microscope and energy dispersive X-ray spectrometer, a systematic investigation of electrical and magneto-transport properties were investigated. Also, electrical resistivity data were carried out using theoretical models to understand the conduction mechanism [1].

**References**

[1] G. Li, H.D. Zhou, S.J. Feng, X.J. Fan and X.G. Li, Journal of Applied Physics, 92 (2002) 1406-1410.

---

* Corresponding author, *E-mail: sevgialtintas@ibu.edu.tr*

P-94

# Metal- and Carbon-Based Materials as Heterogeneous Electrocatalysts for $CO_2$ Reduction

**Azam Khan[1], Haseeb Ullah[1], Jamal Abdul Nasir[1], Wei Chen[2], Abdullah Khan[3], Zia-Ur-Rehman[1]* and Suzanne Shuda[2]**

[1]Quaid-i-Azam University, Department of Chemistry, 45320, Islamabad, Pakistan
[2]University of Texas at Arlington, Department of Physics, Arlington, 76019, Texas, USA
[3]National University of Science and Technology, Center for Advanced Studies in Energy (CAS-E), Islamabad, Pakistan

*E-mail: chemist.ktk.06@gmail.com*

Climate change is caused by the continuous rising level of $CO_2$ and the depletion of fossil fuel reserves has made it highly desirable to electrochemically convert $CO_2$ into fuels and commodity chemicals. Implementing this approach will close the carbon cycle by recycling $CO_2$ providing a sustainable way to store energy in the chemical bonds of portable molecular fuels [1]. In order to make the process commercially viable, the challenge of the slow kinetics of $CO_2$ electroreduction and low energy efficiency of the process needs to be addressed. To this end, this review summarizes the progress made in the past few years in the development of heterogeneous electrocatalysts with a focus on nanostructured material for $CO_2$ reduction to CO, $HCOOH/HCOO^-$, $CH_2O$, $CH_4$, $H_2C_2O_4/HC_2O_4^-$, $C_2H_4$, $CH_3OH$, $CH_3CH_2OH$, etc. The electrocatalysts presented here are classified into metals, metal alloys, metal oxides, metal chalcogenides and carbon based materials on the basis of their elemental composition, whose performance is discussed in light of catalyst activity, product selectivity, Faradaic efficiency (FE), catalytic durability and in selected cases mechanism of $CO_2$ electroreduction. The effect of particle size, morphology and solution-electrolyte type and composition on the catalyst property/activity is also discussed and finally some strategies are proposed for the development of $CO_2$ electroreduction catalysts. The aim of this article is to review the recent advances in the field of $CO_2$ electroreduction in order to further facilitate research and development in this area.

## References

[1] A. Khan, H. Ullah, J.A. Nasir, W. Chen, A. Khan, Z.U. Rehman and S. Shuda, Reviews in Nanoscience and Nanotechnology, 6 (2017) 1-20.

---

* Corresponding author, *E-mail: zrehman@qau.edu.pk*

P-95

# $TiO_2$ Supported Bimetallic PdAg Nanoparticles as Highly Active, Selective, and Reusable Catalyst for The Photocatalytic Decomposition of Formic Acid

**Kadir Karakaş[1], Senem Karahan[2], Mehmet Zahmakıran[1]* and Mehmet Tunç[1]**

[1]YüzüncüYılUniversity, Faculty of Science, Department of Chemistry, Van, Turkey
[2]Dokuz Eylül University, Faculty of Science, Department of Chemistry, İzmir, Turkey

*E-mail: kadirkarakash@gmail.com*

The current worldwide problem of air pollution induced by the excessive use of fossil fuels has become an increasingly serious issue for all people in modern society. Hydrogen gas has gained acceptance as both a clean and renewable energy source to replace fossil fuels for the sustainable future [1,2]. In this study, we report the high-yield hydrogen production through selective photocatalytic decomposition of formic acid (FA) by using $TiO_2$ supported PdAg bimetallic alloy nanoparticles under simulated UV irradiation.$TiO_2$ supported bimetallic catalyst was simply and reproducibly prepared by wet-impregnation technique in water at room temperature (Figure 1). The results showed that bimetallic catalysts with various molar ratios of Ag/Pd absorbed UV lightstrongly and their activities increased remarkably under UV irradiation compared with the PdAg nanoparticles in the dark. $Pd_{0,75}$ $Ag_{0,25}/TiO_2$ exhibited the highest activity under mild conditions at 295 K. ICP-MS, XRD, XPS, BFTEM, HR-TEM, STEM and HAADF-STEM-line analysis were used for the characterization of PdAg nanoparticles. The study also includes the compilation of kinetic data for thePdAg/$TiO_2$ catalyzed decomposition of FA depending on the catalyst [PdAg], substrate [HCOOH], promoter [HCOONa] concentrations and temperature to determine the rate law and the activation parameters ($E_a$, $\Delta H^{\#}$and $\Delta S^{\#}$) of the catalytic reaction.

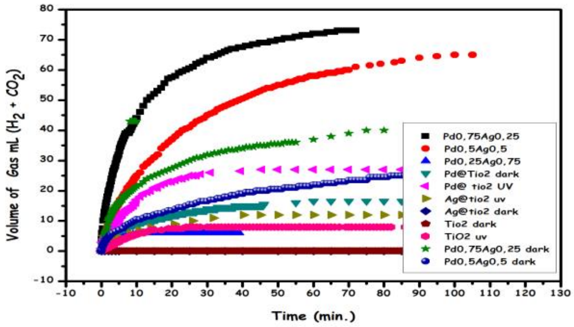


**Figure 1.** Amount of gas released in a UV environment: Nearly two times that of the amount released in an environment not subject to any light

**References**
[1] M. Grasemann and G. Laurenczy, Energy Environ. Sci., 5 (2012) 8171–8181.
[2] S. Park, J.M. Vohs and R.J. Gorte, Nature, 404 (2000) 265-267.

---

* Corresponding author, *E-mail: zmehmet@yyu.edu.tr*

P-96

# Mechanical and Microstructure Properties of $Si_3N_4$ Ceramics Prepared by Direct Coagulation Casting

**Hande Marulcuoğlu and Ferhat Kara***

Anadolu University, Faculty of Engineering, Department of Materials Science and Engineering, 26480, Eskişehir, Turkey

*E-mail: handemarulcuoglu@anadolu.edu.tr*

Green shaping of complex ceramic parts requires extensive green machining which may be rather costly. Depending on the shaping technique, particularly injection moulding for complex parts, also require long binder removal cycles. Therefore, slurry based methods such as direct coagulation casting and gel casting have been developed as alternative shaping processes. With these methods, complex shaped parts can be easily produced with the requirement of no or minimal machining processes. Direct coagulation casting relies on coagulation of a stable colloidal suspension by using a suitable additive in the suspension which leads to its destabilization [1]. In this way, the suspension is gelled to a rigid structure that take the shape of the mould with any complexity. In this study, concentrated and low viscosity $Si_3N_4$ slurries, stabilized with TMAH is destabilized by using glycerol diacetate. Glycerol diacetate reacts with TMAH to reduce pH. After shaping of silicon nitride ceramic parts using these slurries, drying and sintering behaviour of shape parts, their microstructure and mechanical properties are evaluated.

## References

[1] K. Gan, J. Xu, X. Zhang, W. Huo, M. Yang, Y. Qu and J. Yang, Ceram. Int., 42 (2016) 4347-4353.

---

* Corresponding author, *E-mail: fkara@anadolu.edu.tr*

P-97

# Synthesized of New Pt(II) / Pt(IV) Complexes and Investigation of Charge Effective on Inhbition of AChE

**Elvan Hasanoğlu Özkan***, Meryem Çat, Fatma Arslan and Nurşen Sarı

Gazi University, Faculty of Science, Department of Chemistry, 06500, Ankara, Turkey

*E-mail: elvanelvan_06@hotmail.com*

Alzheimer's disease (AD) is a neurodegenerative disease and main cause of dementia in the elderly (especially people >65 years-old). AChE inhibitors including donepezil and galantamine are given top priorities in the therapeutic treatment of AD. Donepezil and galantamine are resemble piperazine's structure [1]. In the current study, two novel 1,4-Bis(3-aminopropyl) piperazine including Pt(II) / Pt(IV) complexes were synthesized and evaluated as inhibitors of acetylcholinesterase (AChE). The Pt(II) or Pt(IV) complexes were synthesized according to the template method [2]. Structures of the newly synthesized complexes were confirmed using elemental analysis, FT-IR and LC-MS spectra. Among the platinum complexes, 1,4-Bis(3-aminopropyl) piperazine including Pt(II) (Figure 1) showed very good inhibition on AChE enzyme.

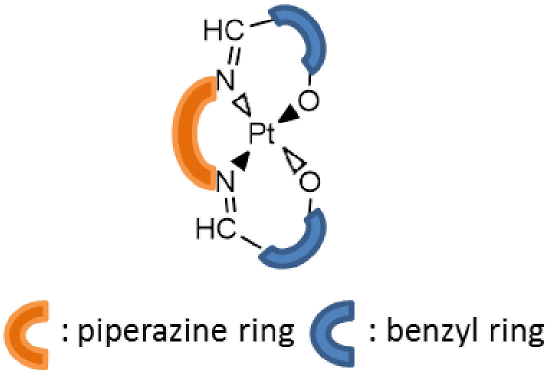


**Figure 1.** Structure of studied Pt(II) complex

**References**

[1] T. D. Tran, T.C.V. Nguyen, N.S. Nguyen, D.M. Nguyen, T.T.H. Nguyen, M.T. Le and K.M. Thai, Appl. Sci., 6 (2016) 198-212.

[2] H. Öğütçü, N. Kurnaz Yetim, E. Hasanoğlu Özkan, O. Eren, G. Kaya, N. Sarı and A.Dişli, Polish J. Chem. Tech., 19 (2017) 74-80.

---

* Corresponding author, *E-mail: elvanelvan_06@hotmail.com*

P-98

# Study on the Structural, Optical and Electrical Properties of Erbium and Ytterbium Doped ZnO Nanostructures

**Sevim Demirözü Şenol***

Abant İzzet Baysal University, Faculty of Science, Department of Chemistry, 14280, Bolu, Turkey

*E-mail: sevimdemirozu@gmail.com*

In recent years, semiconductors doped with trivalent rare earth ($RE^{3+}$) ions are technologically important materials in optoelectronic devices and have received great research interest [1]. In this study the effect of Er and Yb doping with at 5% concentration on structural, optical and electrical properties of zinc oxide nanopowder synthesized by a hydrothermal method has been reported. We have performed X-Ray Diffraction (XRD), Scanning Electron Microscopy (SEM), optical, Hall and resistivity measurements on the samples. X-ray diffraction (XRD) studies show the hexagonal wurtzite phase structure of prepared Er and Yb doped ZnO nanopowders. Scanning Electron Microscopy (SEM) indicated that the growth of dopants with different radii affected the surface morphology of ZnO nanostructures. Further, the presence of Er and Yb ions doping in ZnO matrix has been confirmed by EDS measurement. Optical properties were examined by UV–VIS absorption/diffuse reflectance spectroscopy. We have obtained band gap values of ZnO, $Zn_{0.95}Er_{0.05}O$ and $Zn_{0.95}Yb_{0.05}O$ as 3.24, 3.23, 3.22 eV, respectively. To investigate the electrical properties of the samples, the carrier concentration (n), Hall mobility (μH) and electrical resistivity (ρ) are measured using a Hall effect measurement system based on the Van der Pauw method. The carrier concentration of ZnO decreases, while the mobility and resistivity increases with Er and Yb doping at room temperature. Yb doped ZnO showed characteristic semiconductor behavior while temperature dependent resistivity measurements of Er doped ZnO showed a metal–semiconductor transition at about 295 K.

## References

[1] Y. Yauguang, C. Gang, Z. Yansong and H. Zhonghui**,** Journal of Rare Earths, 33(5) (2015) 453.

---

* Corresponding author, *E-mail: sevimdemirozu@gmail.com*

P-99

# Synthesis, Structural and Optical Properties of Li-Mg co-doped ZnO Nanoparticles by Solid State Reaction Method

**Sevim Demirözü Şenol***

Abant İzzet Baysal University, Faculty of Science, Department of Chemistry, 14280, Bolu, Turkey

*E-mail: sevimdemirozu@gmail.com*

Zinc oxide (ZnO) has attracted much attention of the scientific and industrial communities as future material, which has been under study since 1935 [1]. ZnO has a wide band gap (3.4 eV) semiconductor which has a broad range of potential uses in optical and electrical applications such as; nonlinear optics, gas sensors, transparent conducting oxides (TCOs) for solar photovoltaic (PV) devices, solar energy conversion, e.g, laser diodes [2]. In this work, Lithium (Li) and magnesium (Mg) co-doped zinc oxide nanoparticles have been prepared by solid state reactions.The effects of Li co-doping for x=0.0,0.01,0.02,0.03 on structural, morphological and optical properties of the $Zn_{0.98-x}Mg_{0.02}Li_xO$ nanoparticles were investigated by X-Ray Diffraction (XRD), Scanning Electron Microscopy (SEM)-energy dispersive X-ray analysis (EDX) and UV–VIS absorption/diffuse reflectance spectroscopy, respectively. XRD analysis revealed that all the nanoparticles a hexagonal wurtzite structure. The surface morphological properties of the samples show that without Li has homocentric bundles like ZnO structure. Addition of Li causes hexagonal pyramid like of nanoparticles. The composition of $Zn_{0.98-x}Mg_{0.02}Li_xO$ nanoparticles was detected by energy dispersive X-ray analysis. EDS results indicated that the existence of Zn, O, Li and Mg. The optical measurements exhibited blue-shift of optical band edge and widening of the band gap.

## References

[1] C.W. Bunn, Proc. Phys. Soc., London, 47 (1935) 835-842.
[2] C. Abinaya, M. Marikkannan, M. Manikandan, J. Mayandi, P. Suresh, V. Shanmugaiah, C. Ekstrum and J.M. Pearce, Material Chem. and Phys., 184 (2016) 172-182.

---

* Corresponding author, *E-mail: sevimdemirozu@gmail.com*

# Preperation and Characterization of Antibacterial Polymer Fibers Containing the Transition Metal Complexes of 2-Amino-5-bromopyridine

**Derya Kılıç[1], Fatih Mehmet Emen[2]*, Ruken Esra Demirdöğen[3], Tuncay Yeşilkaynak[4], Zehra Gülten Altın[5] and Şinasi Aşkar[6]**

[1]Department of Material Technologies, Faculty of Engineering, Mehmet Akif Ersoy University, TR 15030, Burdur, Turkey
[2]Mehmet Akif Ersoy University, Faculty of Arts and Science, Department of Chemistry, 15100, Burdur, Turkey
[3]Çankırı Karatekin University, Faculty of Science, Department of Chemistry, 18100, Çankırı, Turkey
[4]Sütçü İmam University, Afsin Vocational High School, 46500, Kahramanmaraş, Turkey
[5]Çankırı Karatekin University, Faculty of Engineering, Department of Chemical Engineering, 18100, Çankırı, Turkey
[6]Çankırı Karatekin University, Faculty of Health Science, Department of Dietetic and Food, 18100, Çankırı, Turkey

*E-mail:klc.derya13@gmail.com*

There is an increase in the number of patients infected with methyciline resistant *S. aureus* and 95% of these patients do not respond to first class antibiotics such as penicillin or ampicillin [1]. Antimicrobial drugs are considered to be the most effective tool in terms of both cost and drug efficacy [2]. It is important to develop new antibacterial products to prevent MRSA based infections [3]. Thus, for an effective struggle mixed pyridine derivative of metal halogen complexes, which show antibacterial activity, and textiles functioned with these complexes have gained importance both with respect to cost effectiveness and drug activity. The micro-fibers were obtained by incorporating the transition metal ion [Cu(II), Co(II), Ni(II)] complexes of 2-amino-5-bromopyridine into cellulose acetate polymer via electrospinning and also characterized by $^1$H-NMR, FE-SEM, FT-IR techniques.

## References

[1] H.C. Neu, Science, 257(5073) (1992) 1064-1073.
[2] R.D. Scott, 2nd, S.L. Solomon and J.E. McGowan, Jr., Emerging Infectious Diseases, 7(2) (2001) 282-285.
[3] K.K. Govarthanam, S.C. Anand and S. Rajendran, Journal of Industrial Textiles, 40(3) (2011) 281-296.

## Acknowledgement

This study was supported by TUBITAK The Scientific and Technological Research Council of Turkey (Project Number: 116Z295).

---

* Corresponding author, *E-mail: femen106@gmail.com*

P-101

# A Novel Luminescent Mesoporous Composite: $Ca_2MoO_5$:Eu@MCM-41

**Ali İhsan Karaçolak[1], Fatih Mehmet Emen[1]*, Ruken Esra Demirdöğen[2], Zeynep Yıldırım[1], Derya Kılıç[3], Göktürk Avşar[4] and Tuncay Yeşilkaynak[5]**

[1]Mehmet Akif Ersoy University, Faculty of Arts and Science, Department of Chemistry, 15100, Burdur, Turkey
[2]Çankırı Karatekin University, Faculty of Science, Department of Chemistry, 18100, Çankırı, Turkey
[3]Mehmet Akif Ersoy University, Faculty of Engineering, Department of Material Technologies, 15030, Burdur, Turkey
[4]Mersin University, Faculty of Arts and Science, Department of Chemistry, 33100, Mersin, Turkey
[5]Sütçü İmam University, Afsin Vocational High School, 46500, Kahramanmaraş, Turkey

*E-mail: alikaracolak@hotmail.com*

MCM-41 is the most popular member of the M41S family of mesoporous silicate materials. MCM-41 has a regular pore system consists of a hexagonal array of one-dimensional shaped pores. The pore diameter of MCM-41 can be varied systematically from 2 to 10nm [1]. Other interesting physical properties of MCM-41 include a high specific surface of up to 1500m2 $g^{-1}$, and a specific pore volume of up to 1.3 ml $g^{-1}$. Mesoporous materials which show photoluminescence property upon functionalization are of potential in the drug storage/release fields [2,3]. The design and preparation of non-toxic, stable systems with luminescence property have key role in realizing this application. In this study, $SrMO_4$:Eu@MCM-41 composite was prepared by a sol-gel process. The obtained composites were characterized via XRD, FT-IR and PL techniques.

## References

[1] J.S. Beck, J.C. Vartuli, W.J. Roth, M.E. Leonowicz, C.T. Kresge, K.D. Schmitt, C.T. Chu, D.H. Olson, E.W. Sheppard, S.B. McCullen, J.B. Higgins and J.L. Schlenker, J. Am. Chem. Soc., 114 (1992) 10834-10843.
[2] D.L. Shi, J. Lian, W. Wang, G.K. Liu, P. He, Z.Y. Dong, L.M. Wang and R.C. Ewing, Adv. Mater., 18 (2006) 189-193.
[3] J. Sauer, F. Marlow, B. Spliethoff and F. Schuth, Chem. Mater., 14 (2002) 217-224.

## Acknowledgement

This study was supported by TUBITAK The Scientific and Technological Research Council of Turkey (Project Number: 116Z402).

---

* Corresponding author, *E-mail: femen106@gmail.com*

P-102

# Surface Modification of Nanofibers with Boron Nitride for Remediation of Effluent Waters Contaminated with Grease

**Zehra Gülten Altın[1]*, Ruken Esra Demirdöğen[2] and Fatih Mehmet Emen[3]**

[1]Çankırı Karatekin University, Faculty of Engineering, Department of Chemical Engineering, 18100, Çankırı, Turkey
[2]Çankırı Karatekin University, Faculty of Science, Department of Chemistry, 18100, Çankırı, Turkey
[3]Mehmet Akif Ersoy University, Faculty of Arts and Science, Department of Chemical Engineering, 15030, Burdur, Turkey

*E-mail: zaltin@karatekin.edu.tr*

Effluent water from textile, pulp and leather industries are known to be primary pollutants of water resources [1]. Today the most effective adsorbents used are: activated carbon, zeolite and natural fibers. However, they have low selectivity and adsorption capacity. Other than these, adsorbant materials are expected to have favourable capacity and kinetic properties. They should have facile water purification properties. Boron nitride, which is also called white graphene, have similar properties with graphene. Wide energy band, electrical insulation, UV Photoluminescence, high thermal conductivity and high resistance toward oxidation [2]. In this study, boron nitride (BN) nanofibers were obtained via electrospinning. Cellulose acetate of Da 30 000 and 50 000 were dissolved in acetone. BN powder was added and the solutions were rigorously stirred before loading into the syringe. The optimum fibers were obtained when the potential difference was 15.5 kV and the spinneret and the earthed electrode were placed at a distance of 10 cm apart from each other. The optimum flow rate was 0.51 mL/min. The BN nanofibers thus obtained were characterized via 1H-NMR and their FE-SEM images, TG/DSC and FT-IR spectra were also taken. The FT-IR spectra of the BN nanofibers and pure cellulose acetate were similar. The vibration bands observed at (1380-810 cm-1) (1300-1700 cm-1) in the FT-IR spectra of the nanofibers thus obtained appear to overlap with those of the cellulose acetate. The thermal degradation analysis of the nanofibers was made via DTA-TG in N2 atmosphere and the cycles were taken at a rate of 10 °C/min and the DTA-TG curves were obtained. Degradation reactions were assumed upon taking into consideration the mass losses. Melting started at about 50°C. At about 300°C evaporation started and at about 400°C evaporation was completed. According to the results obtained the BN nanofibers were successfully obtained and used in oil sorption.

**References**

[1] T. Dalton and D. Jin, Mar. Pollut. Bull., 60 (2010) 1939-1945.
[2] C. Lee, Q. Li, W. Kalb, H. Berger, R.W. Carpick and J. Hone, Science 328 (2010) 76-80.

**Acknowledgement**

This study was funded by Çankırı Karatekin University BAP unit. Project No: MF060416822).

---

* Corresponding author, *E-mail: zaltin@karatekin.edu.tr*

P-103

# Photopolymerization of 2-Vinylpyridine with Type I Photoinitiators

**Elif Karacan Yeldir**[1]* and Ayhan Oral[1,2]

[1]Çanakkale Onsekiz Mart University, Faculty of Science, Department of Chemistry, 17100, Çanakkale, Turkey
[2]Çanakkale Onsekiz Mart University, Science Technology Application and Research Center, 17100, Çanakkale, Turkey

*E-mail: elifkaracan@comu.edu.tr*

Photopolymerization is one of the remarkable polymerization technique due to ambient polymerization temperature and also high rates of polymerization [1]. There are two types of photoinitiation mechanism, which are photofragmentation (Type I) and hydrogen abstraction chromophores (Type II) [2,3].

Poly(2-vinylpyridine) has a great potential as an adsorbant resin to remove pollutants from aquous solutions because of hydrophilic properties [4]. In this study 2-vinylpyridine was polymerized by photopolymerization by Type I photoinitiator. Benzoyl peroxide (BPO) and Benzoin (BN) were used as a Type I photoinitiator, dry tetrahydrofuran (THF) was used as solvent during polymerization. Initiator was placed into quartz tube and applied vacuum. After that, THF and monomer were added into the tube under $N_2$ atmosphere. Photopolymerization occurred in 360 nm wavelenght for BPO and 310 nm for BN (Figure 1). The contains of the tube was dissolved in methanol when polymerization is over. Polymer solution was precipitated in diethylether and washed three times with ether. NMR and IR spectrums were obtained.

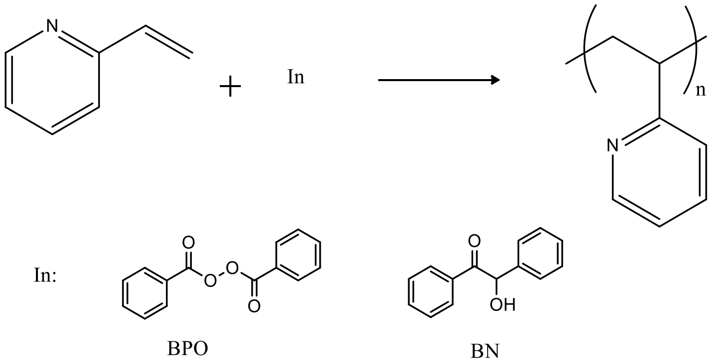


**Figure 1.** Photopolymerization of 2-VP

**References**
[1] G. Oster and N.L. Yang, Chem. Rev., 68 (1968) 125-151.
[2] K. Wang, K. Yang and Q. Yu, Prog. Org. Coatings, 77 (2014) 1929-1934.
[3] X. Jiang, X. Luo and J. Yin, J. Photochem. Photobiol. A Chem., 174 (2005) 165-170.
[4] W.H. Tao, A.M. Li, C. Long and H.M. Qian, Chin. Chem. Lett., 20 (2009) 604-607.

---

* Corresponding author, *E-mail: elifkaracan@comu.edu.tr*

P-104

# Effect of [$RuCl_2$(*p*-cymene)(L)] (L=N-coordinate Aromatic sulfonamide ligands) as Catalysts in the Reduction of Nitroarenes and Reductive Amination Reactions

**Nilgün Kalaycıoğlu Özpozan***, **Nilgün Kayacı and Serkan Dayan**

Erciyes University, Faculty of Science, Department of Chemistry, 38039, Kayseri, Turkey

*E-mail: nozpozan@gmail.com*

Reductive amination (RA), the coupling of ketones or aldehydes with amines in the presence of a reducing agent, is one of the most powerful methods for one-step synthesis of substituted amines. This method is extremely valuable from a synthetic point of view, since it avoids the isolation of in situ generated imine products, which is not easy due to the limited stability of imines. In most of the RA procedures developed, stoichiometric boron hydride reduction and heterogeneous hydrogenation dominate the scene [1,2]. Nitro compounds are a widely found organic pollutant in waste water. Thus, the removal of the nitroarenes is an important issue. Various processes have been developed, including adsorption, photocatalysis, electrochemical treatment, the electro-Fenton method, electrocoagulation, catalytic hydrogenation etc. [3-5].Additionally, nitroaniline derivatives have been used as precursors in the chemical synthesis of azo dyes, antioxidant compounds, poultry medicine, antiseptic agents etc. [6]. However, avoiding the use of organic solvents and the improvement of suitable pro-cesses for hydrogenation of nitroarenes in aqueous media under the mild conditions are still necessary. At the same time, some quite remarkable studies have been carried out with compounds containing ruthenium in the reduction of nitroarenes. Herein, we chose to prepare $Ru^{II}$ complexes prepared from *N*-arenesulfonyl-*o*-phenylenediamines and then the complexes were used as catalysts in the hydrogenation of nitroarenes in aqueous media at ambient temperature in the presence of NaBH4 by UV–vis spectrophotometer. Then, the new complexes were found to be an active catalyst for transfer hydrogenative reductive amination under aqueous conditions with sodium formate as a hydrogen source. Various carbonyl compounds such as aromatic aldehydes were successfully reacted with amines to gives new amines. All the [$RuCl_2$(*p*-cymene)(L)] type complexes were found as a good catalyst in the reductive amination reaction.

## References

[1] S. Gomez, J.A.Peters, T. Maschmeyer, Adv. Synth. Catal., 344 (2002) 1037-1057.
[2] D. Gulcemal, S. Gulcemal, M.C. Robertson and J. Xiao, Organometallics, 34 (2015) 4394-4400.
[3] O.A. O'Connor and L.Y. Young, Environ. Toxicol. Chem., 8 (1989) 8853–8862.
[4] P. Canizares, C. Saez, J. Lobato and M.A. Rodrigo, Ind. Eng. Chem. Res., 43 (2004) 1944-1951.
[5] F. Khan, J. Pandey, S. Vikram, D. Pal, S.S. Cameotra and J. Hazard. Mater., 254-255 (2013) 72-78.
[6] J.H. Sun, S.P. Sun, M.H. Fan, H.Q. Guo, L.P. Qiao and R.X. Sun, J. Hazard. Mater., 148 (2007) 172-177.

## Acknowledgment

We acknowledge the financial support granted by Erciyes University (ERUBAP), (FDK-2015-6143).

---

* Corresponding author, *E-mail: nozpozan@gmail.com*

P-105

# Ru$^{II}$ Complexes Containing 8-Aminoquinoline Backbone Bearing Imine Bond and *p*-Cymene Ligands as Effective Photoactive Dye in DSSC

**Serkan Dayan and Nilgün Kalaycıoğlu Özpozan***

Erciyes University, Faculty of Science, Department of Chemistry, 38039, Kayseri, Turkey

*E-mail: nozpozan@gmail.com*

Since the first report on dye-sensitized solar cells (DSSCs) introduced by M. Grätzel at 1990, too much attention has been attracted to the development of new and ever more performing materials as this technology fulfills many requirements concerning the cost of the materials and cells, low energy expenditure and ease of preparation. Their maximum conversion efficiency of over 12 % suggests that they are a promising type of next generation solar cells. For their commercial application, it is important to develop low-cost materials and to achieve maximum efficiency for the cells [1-3]. Herein, we chose to prepare Ru$^{II}$ complexes prepared from *N*-R-benzylidenequinoline-8-amine and [RuCl$_2$(*p*-cymene)] as starting complex and then the complexes were used as photoactive dye in DSSC (Figure 1). The structural elucidations of the *N*-coordinate ruthenium(II) were characterized by different methods such as infrared spectroscopy, elemental analysis, cyclic voltammetry, nuclear magnetic resonance and UV-VIS spectrophotometer. Moreover, the effect of different substituents on the aromatic ring on the photophysical properties and photovoltaic performance is investigated.

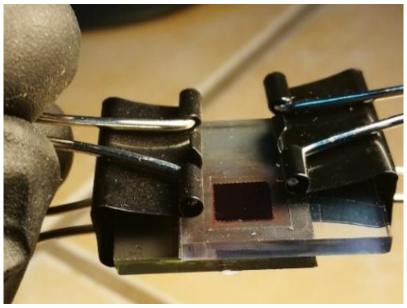


**Figure1.** Dye-Sensitized Solar Cell (DSSC) containing *N*-Coordinate Ru$^{II}$ complex as dye

**References**

[1] B. O’Regan and M. Grätzel, Nature 353 (1991) 737-740.
[2] A. Hagfeldt, G. Boschloo, L. Sun, L. Kloo and H. Pettersson, Chemical Reviews, 110 (2010) 6595–6663.
[3] K. Kakiage, Y. Aoyama, T. Yano, T. Otsuka, T. Kyomen, M. Unno and M. Hanaya, Chem. Commun., 50 (2014) 6379-6381.

**Acknowledgment**

We acknowledge the financial support granted by Erciyes University (ERUBAP), (FDK-2015-6013).

---

* Corresponding author, *E-mail:nozpozan@gmail.com*

P-106

# Highly Transparent and Conducting F-doped ZnO Thin Films Prepared by Ultrasonic Spray Pyrolysis

Seniye Karakaya*

Eskişehir Osmangazi University, Faculty of Arts and Sciences, Department of Physics, 26480, Eskişehir, Turkey

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

Zinc oxide (ZnO), a wide band gap (3.37 eV) and a large excition binding energy of 60 meV semiconductor, has attracted much attention for possible applications in optoelectronic devices and solar cells [1,2]. F-doped ZnO (FZO) thin films were deposited on glass substrates with Ultrasonic Spray Pyrolysis method. The effects of F doping content on microstructure, optical and electrical properties of FZO films were systematically investigated by XRD, SEM, AFM, UV-VIS spectrophotometer. The transmittance of the FZO films is revealed to be 85% in the visible region. Structural investigations revealed that, in both cases, high-quality films were grown with the wurtzite structure and c-axis preferred crystalline orientation. The surface morphology and grain structure depended on the deposition process as well as the physical properties induced by F-doping. The analyses of the deposited FZO thin films tested in the Hall measurements at room temperature show that these thin films are p-type electrical conductivity.

**References**

[1] A. Douayar, R. Diaz, F. Cherkaoui El Moursli, G. Schmerber, A. Dinia and M. Abd-Lefdil, Eur. Phys. J. Appl. Phys., 53(2) (2011) 20501-20504.
[2] A. Sanchez-Juarez, A. Tiburcio-Silver, A. Ortiz, E.P. Zironi and J. Rickards, Thin Solid Films, 333 (1998) 196-202.

---

* Corresponding author, *E-mail: seniyek@ogu.edu.tr*

# Nanotechnology

P-107

# Preparation and Characterization of ZnO Nanostructured Thin Films

**Seniye Karakaya***

Eskişehir Osmangazi University, Faculty of Arts and Sciences, Department of Physics, 26480, Eskişehir, Turkey

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

Nano-sized semiconductor materials have received considerable attention mainly due to their important potential applications, which include photovoltaic solar cells, transparent electrodes, gas sensors as well as other optoelectronic devices [1]. Especially, ZnO has attracted considerable attention to the fabrication of short wavelength optoelectronic applications such as solar cells. ZnO thin films have been prepared by the ultrasonic spray pyrolysis (USP) technique. The deposited ZnO films were subjected to annealing treatment in air at 500˚C for 3 h. The effects of the annealing process on the surface and optical properties have been investigated. The values of the direct band gap Eg decreased with annealing treatment from 3.28 eV to 3.21 eV. All films had an average optical transparency over 80% in the visible range. Due to its relatively high transmittance characteristics and promising properties of converting both UV and NIR light to visible light, the developed film is considered to have a potential application in solar cells.

## References

[1] Z.L. Wang, J. Phys.: Condens. Matter, 16 (2004) 829-858.

---

* Corresponding author, *E-mail: seniyek@ogu.edu.tr*

**P-108**

# Biosynthesis, Structural Characterization and Cytotoxicity Activity of Silver Nanoparticles Produced by Bacteria: *Lysinibacillus* sp. NOSK

**Nalan Oya San Keskin[1]*, Esra Yaylacı[2] and Selen Güçlü Durgun[2]**

[1]Gazi University, Polatlı Faculty of Arts and Science, Department of Biology, Ankara, Turkey
[2]Gazi University, Faculty of Medicine, Department of Medical Biology and Genetics, Ankara, Turkey

*E-mail: oyasan@gazi.edu.tr*

Metallic nanoparticles are generated by a variety of methods such as physical and chemical methods but these methods have low productivities and the chemical methods lead to contamination and the formation of dangerous by-products [1,2]. To this end, biosynthesis methods have appeared as an easy, clean, and applicable choice of physical and chemical methods. In the present study, the biosynthesis of silver nanoparticles using the cell-free extract of bacteria was investigated. The synthesized nanoparticles were characterized using UV-Vis Spectroscopy and ATR-Fourier Transform Infrared Spectroscopy (ATR-FTIR). The particle size was viewed by using dynamic light scattering (DLS). The cytotoxicity activity of AgNPs was researched on Hela cancer cell lines using MTT assay. Fig. 1a shows the UV-Vis absorption spectra recorded from aqueous $AgNO_3$-the cell free extract of the *Lysinibacillus* sp. NOSK culture medium as a function of time of reaction. After 6 h incubation, the color change of the reaction mixture was observed and it indicates that more than 6 h required for the synthesis of detectable amounts of AgNPs (Figure 1b). The average particle size distribution of AgNPs in colloidal solution for 24 h was found to be 42 nm and polydispersity index (PDI) were obtained as 0.166. The average size values recorded for 48 h and 72 h is 61 nm and 76 nm, respectively. The FTIR spectrum of the sample for 24 h shows the presence of two bands at 1646 cm$^{-1}$ and 1541.6 cm$^{-1}$ corresponding to the bending vibrations of the amide I and amide II bands of the proteins, respectively. It was noticed from cytotoxicity tests that 50% of the cells lose their viability at 120 µg/ml of AgNPs, this dosage has been considered as IC50 for Hela cells. In conclusion, the current approach offers a green chemistry methodology for the production of silver nanoparticles.

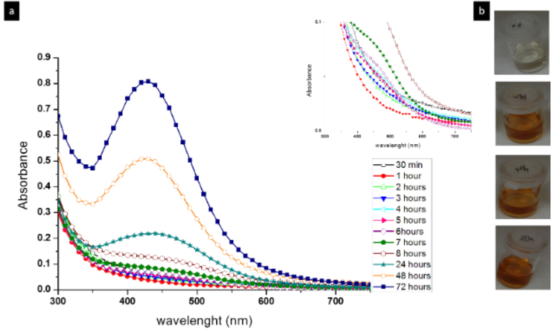


**Figure 1.** UV-Vis measurements of materials

**References**

[1] D. Hebbalalu, M. Nadagouda and R.S Varma, ACS Sustainable Chemistry Engineering, (2013) 703-712.
[2] N.O. San Keskin, G. Dönmez, N. Kocberber Kilic and T. Tekinay, Journal of Nano Research, 40 (2016) 120-127.

---

* Corresponding author, *E-mail: oyasan@gazi.edu.tr*

P-109

# New Magnetic Nanoparticle-Supported Ferrocene, Synthesis and Image Optical Microscope

**Ali Dişli***, **Elvan Hasanoğlu Özkan and Nurşen Sarı**

Gazi University, Faculty of Science, Department of Chemistry, 06500, Ankara, Turkey

*E-mail: adisli@gazi.edu.tr*

The last twenty years, there has been increasing syntheses in the design of new magnetic nanoparticles [1]. They are widely used in numerous fields of nanotechnology. Redox-active macromolecules, particularly those containing late transition-metal sandwich complexes have been studied in various fields. The ferrocenyl sandwich complexes are the most common ones because of their stability in different oxidation states ($Fe^{II}$ and $Fe^{III}$) on the electrochemical time scale [2]. The convergent synthesis [3] of the nanoparticles that were used herein involved the template reactions of ferrocenealdehyde with 2,4,6-triamino-1,3,5-triazine (Figure 1A).

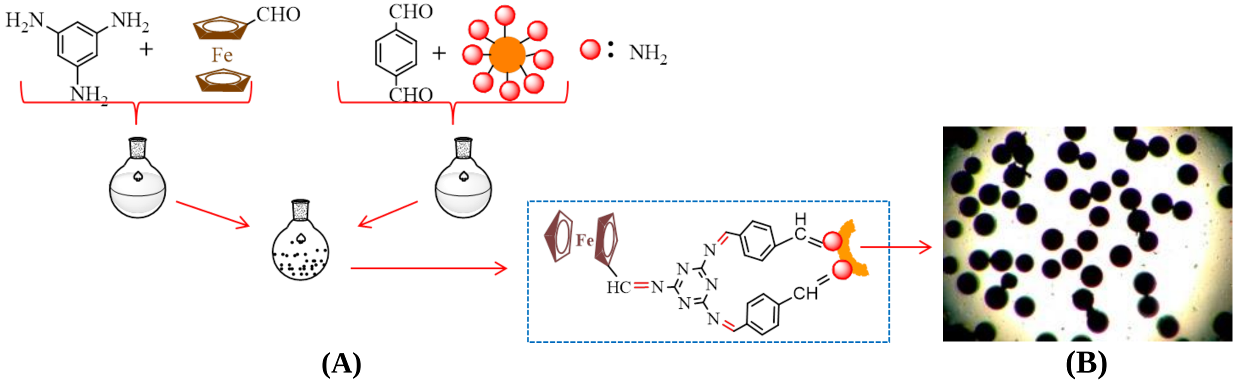


**Figure 1.** Rotation convergent synthesis of the nanoparticles (A) and image optical microscope of their (B)

New magnetic nanoparticles were characterized using various techniques such as SEM-EDS, GPC, FTIR, and Optical microscope.

**References**
[1] V. Mereacre, M. Schlageter and A. K.Powell, J. Magn. and Magnetic Mat., 381 (2015) 478-480.
[2] A.K. Diallo, J. Ruiz and D. Astruc, Chem. Eur. J., 19 (2013) 8913-8921.
[3] A. Armstrong and D. Craig, Organic Synthesis, Part 3, Synthetic Strategy, 1-3, 2003-2004.

---

* Corresponding author, *E-mail: adisli@gazi.edu.tr*

P-110

# Synthesis of Polyurethane (PU) Nanopolymers with Different Structures

**Erdem Babaarslan[1], Ceren Atila Dinçer[2], Ayşe Karakeçili[2] and Nuray Yıldız[2]***

[1]Turkish Ministry of Labor and Social Security, Occupational Health and Safety Institution, Ankara, Turkey
[2] Ankara University, Faculty of Engineering, Department of Chemical Engineering, 06100, Ankara, Turkey

*E-mail: nyildiz@eng.ankara.edu.tr*

Nanopolymers are used in several application fields such as textile, drug release, food, medical and composite technology. Polymer nanostructures could be synthesized as particle or fiber depending on the purpose of the application. Polymer nanoparticles were synthesized by top-down or bottom-up methods. Electrospinning is one of synthesis methods of polymer nanofibers [1,2]. In this study, polyurethane (PU) polymers were synthesized as nanoparticle and nanofiber by miniemulsion polymerization and electrospinning methods, respectively. The effect of surfactant amount (sodium dodecylsulfate, SDS; wt % 0.1, 0.25, 0.5) on the polymer nanoparticles and voltage (15-24 kV), collector distance (15-20 cm) and solution feed rate (0.5-2 mL/h) on the polymer nanofibers were investigated. Polymer nanostructures were analyzed by scanning electron microscope (SEM), transmission electron microscope (TEM), dynamic light scattering (DLS) and differential centrifugal sedimentation (DCS). Experimental setups for miniemulsion polymerization and DLS results were given in Table 1. The average particle size and the fiber diameter of PU nanoparticles from TEM and SEM images were found as 78 nm and between 400-1000 nm, respectively. However, it was determined that the nanoparticles and nanofibers were agglomerated.

**Table 1.** Experimental setups for miniemulsion polymerization and DLS results

| Reaction setup | Monomer (g) | SDS (wt.-%) | Particle diameter (nm) | Polydispersity index (PDI) |
|---|---|---|---|---|
| PU-1 | IPDI (3,4), Di-ol (3)<br>HD (0,2) | 0.5 | 283 | 0.32 |
| PU-2 | IPDI (3,4), Di-ol (3)<br>HD (0,2) | 0.25 | 312 | 0.24 |
| PU-3 | IPDI (3,4), Di-ol (3)<br>HD (0,2) | 0.1 | 261 | 0.2 |

## References

[1] A. Musyanovych., J. Dausend, M. Dass, P. Walther, V. Mailander and K. Landfester, Acta Biomaterialia, 7 (2011) 4160-4168.
[2] R.N. Wijesena, N. Tissera, Y.Y. Kannangara, Y. Lin, G.A. Amaratunga and K.N. de Silva, Carbohydrate Polymers, 117 (2015) 731-738.

## Acknowledgement

This study was supported by the EU FP-7 funded Quality Nano Transnational access infrastructure (UCD-TAF-178).

---

* Corresponding author, *E-mail: nyildiz@eng.ankara.edu.tr*

# The Effects of Exfoliation Techniques on the Electrical Conductivity of SiAlON-Graphene Nanoplatelets Composites

**Sinem Baskut*, Alper Çınar and Servet Turan**

Anadolu University, Faculty of Engineering, Department of Materials Science and Engineering, 26480, Eskisehir, Turkey

*E-mail: skayhan@anadolu.edu.tr*

SiAlON ceramics are widely used in high temperature industrial applications such as high speed cutting tools, wear components, metal forming tools and gas turbine engine components. [1,2] However, the inability to produce these materials in complex shapes leads to restrictions on their application areas. In addition, although the electric discharge machining (EDM) technique allows the complex shapes to be easily obtained, it requires the electrical conductive materials in certain amount. Recently, graphene is used extensively as the second phase to increase the electrical conductivity of ceramic matrix materials due to their superior charge carrier mobility (exceeding 200,000 $cm^2V^{-1}s^{-1}$) [3,4].

In this study, graphene platelets (GNPs) were exfoliated in two different ways: sonication and microfluidization techniques. Then, different amounts (2, 4 and 8 wt %) of graphene nanoplatelets after microfluidization or sonication process were added into SiAlON forming powders. The prepared compositions were sintered by using SPS furnace at 1875°C under 50 MPa for 15 minutes. Morphologic images of GNPs indicated that the exfoliation of platelets was more successfully achieved by microfluidization than by sonication technique. Furthermore, it was observed that microfluidized GNPs were distributed more homogeneously than sonicated GNPs in the microstructure of composites. The electrical conductivity values were higher in the all composites containing microfluidized GNPs than in sonicated GNPs added composites. The conductivity difference tended to increase as the amount of added GNP increased from 2 to 8 wt %. The microfluidized GNPs with higher aspect ratio caused an increase in electrical conductivity in the composites at lower percolation values compared to the sonicated GNPs.

## References

[1] T. Ekström and M. Nygren, J. Amer. Ceram. Soc., 75 (1992) 259-276.
[2] V.A. Izhevskiy. L.A. Genova. J.C. Bressiani and F. Aldinger, J. Eur. Ceram. Soc., 20 (2000) 2275-2295.
[3] A.K. Geim and K.S. Novoselov, Nat. Mater., 6 (2007), 183-191.
[4] S.V. Morozov, K.S. Novoselov, M.I. Katsnelson, F. Schedin, D.C. Elias, J.A. Jaszczak and A.K. Geim, Phys. Rev. Lett., 100 (2008) 016602-016604.

---

* Corresponding author, *E-mail: skayhan@anadolu.edu.tr*

P-112

# Preparation and characterization of Quince Seed Mucilage/Poly (vinyl alcohol) Blend Nanofiber Membranes by Electrospinning Method

**Merve Dağcı, Ümran Zeren and Orhan Murat Kalfa***

Dumlupınar University, Faculty of Science and Art, Department of Chemistry, 43000, Kütahya, Turkey

*E-mail: merve.dagci@dpu.edu.tr*

Recently, electrospinning has been a versatile method for making nanometer to micrometer size range fibers for a variety of natural polysaccharides and their blends with synthetic polymers such as chitosan, chitin, poly (vinyl alcohol) (PVA)/carboxymethyl chitin, PVA/chitosan, chitin/silk fibroin, hyaluronic acid, alginate [1]. The mucilage of quince seeds to be a mixture of cellulose and water soluble polysaccharides [2]. In this study, PVA-quince seed mucilage (QSM) nanofiber membranes were synthesized by electrospinning technique (Table 1). Crosslinking of PVA with QSM was achieved with glutaraldehyde (GA). The morphology of nanofiber was characterized by scanning electron microscope (SEM) (Figure 1).

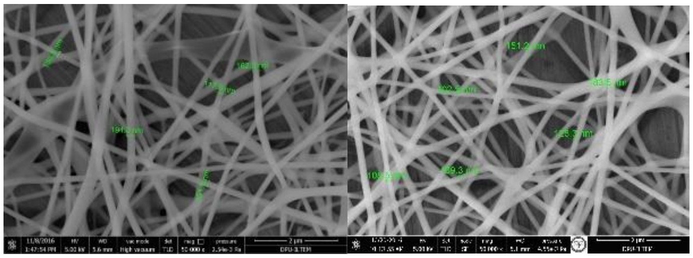


**Figure 1.** SEM images of the QSM/PVA nanofiber membrane

**Table 1.** Details of the electrospinnig experiments concerning the fabrication of QSM/PVA

| Parameters | Values |
|---|---|
| PVA concentration (wt%) | 10 |
| QSM/PVA ratio | 60/40 |
| Volume (mL) | 5 |
| Flow rate (mL/h) | 0.5 |
| Voltage (kV) | 20 |

**References**

[1] K.S. Novoselov, A.K. Geim, S. V. Morozov, D. Jiang, Y. Zhang, S.V. Dubonos, I.V. Grigorieva and A.A. Firsov, Science, 306 (2004) 666-669.

[2] M. Jouki, S.A. Mortazavi, F.T. Yazdi, and Koocheki, International Journal of Biological Macromolecules, 66, (2014) 113-124.

---

* Corresponding author, *E-mail: orhanmurat.kalfa@dpu.edu.tr*

P-113

# Poly (Acrylonitrile) Nanofibers for the Solid Phase Extraction of $Cu^{2+}$ from Aqueous Solutions

**Merve Dağcı, Ümran Zeren and Orhan Murat Kalfa***

Dumlupınar University, Faculty of Science and Art, Department of Chemistry, 43000, Kütahya, Turkey

*E-mail: merve.dagci@dpu.edu.tr*

Electrospinning is a feasible and simple technique for the production of nanofibers. The electrospun nanofibers exhibit increased surface to volume ratio with improved and controlled porosity allowing their use in various applications including tissue engineering, drug delivery, wound healing, filtration, energy storage, defense, and security. Recently, electrospun nanofibers based on synthetic polymers have been used for the preconcentration of metal ions from water [1,2]. In this study, poly (acrylonitrile) (PAN) nanofibers were synthesized by electrospinning technique. The morphology of electrospun nanofibers was characterized by scanning electron microscope (SEM). The method is developed for the preconcentration of ions by using columns containing the adsorption capabilities of PAN nanofibers completed characterization operations and determined by atomic absorption spectrometry. Several factors affecting the extraction of $Cu^{2+}$ metal ions including pH, the element type and concentration, flow rate, sample volume were investigated (Table 1).

**Table 1.** Optimum condition of the methods

| Parameters | Values |
|---|---|
| pH | 5.0-10.0 |
| Concentration and Type of Eluent | 0.5 mol/L HCl |
| Flow Rate | 3 mL/min |
| Sample Volume | 100 mL |
| Preconcentration Factor | 20 |
| Recovery (%) | 98.14±0.22 |

## References

[1] F.E. Ahmed, B.S. Lalia and R. Hashaikeh, Desalination, 356 (2015) 15-30.
[2] W.A. Sarhan, H.M. Azzazy and I.M. El-Sherbiny, Materials Science and Engineering C, 67 (2016) 276-284.

---

* Corresponding author, *E-mail: orhanmurat.kalfa@dpu.edu.tr*

P-114

# A Novel Magnetic Graphene Oxide Composite Adsorbent for Removing Trace of As(III) in Water

**Şerife Saçmacı[1]*, Cansu Kök[1] and Mustafa Saçmacı[2]**

[1]Erciyes University, Faculty of Science, Dep. of Chemistry, Kayseri, Turkey
[2]Bozok University, Faculty of Science, Department of Chemistry, Yozgat, Turkey

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

Carbon nanotubes and graphene oxide (GOx) are a class of electron-rich carbon adsorbents with a large delocalized π-electron system, which shows promising applications in water treatment [1]. Due to graphene oxide's unique plate structure and properties, including large specific surface area, excellent stability and rich functionalities [2], organic compounds with a benzene ring can be strongly adsorbed on GOx. However, a major defect comes from the difficulties that are associated with the separation of water-insoluble GOx from water solutions after absorption procedures. Magnetic composite materials also have many advantages, such as simple separation, high adsorption capacity and cyclic utilization, which can greatly expand their application in environmental purification. Magnetic separation has been developed to facilitate the collection of GOx [3].

The purpose of the study was to develop a facile method for the removal a stable and reusable magnetic graphene composite adsorbent to remove trace levels of As(III) in water treatment. Thus, the $Fe_3O_4$@GOx@ DL (Dithiothreitol) composite adsorbent was prepared. Its performance was tested by disperse solid phase extraction and Zetasizer used for the determination for removing As(III) in the water. The removal percentages of several real samples for As(III) at the ng/mL order of magnitude were in the range of 96%–99%. The removal percentage still reached 99% when the adsorbent was reused at least 100 times. The results suggested that the magnetic adsorbent can obviously remove trace levels of As(III) from large volumes of aqueous solutions in environmental pollution cleanup with high removal efficiency.

## References

[1] J.W. Hu, Y. Zhuang, J. Luo, X. Wei, and X.F. Huang, Int. J. Mol. Sci., 13 (2012) 9332-9342.
[2] R.A. Hites, Environ. Sci. Technol., 38 (2004) 945-956.
[3] H.B. Moon, K. Kannan, M. Choi, J. Yu, H.G. Choi, Y.R. An, S.G. Choi, J.Y. Park and Z.G. Kim, J. Hazard. Mater., 179 (2010) 35-41.

## Acknowledgement

The author is grateful for the financial support provided by the Unit of Scientific Research Projects of Erciyes University (Project no. FBA-2016-6135).

---

* Corresponding author, *E-mail: sacmaci@erciyes.edu.tr*

P-115

# Removal of As(III)/As(V) from Aqueous Solution Using Magnetic Graphene Oxide Nanocomposite as an Adsorbent

**Şerife Saçmacı[1]*, Aylin Hasdıraz[1] and Mustafa Saçmacı[2]**

[1]Erciyes University, Faculty of Science, Dep. of Chemistry, Kayseri, Turkey
[2]Bozok University, Faculty of Science, Department of Chemistry, Yozgat, Turkey

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

Graphene oxide (GO), also called graphite oxide sheet, is a two dimensional nanomaterial prepared from chemical oxidation of natural graphite [1]. In contrast to pristine graphite, the graphene oxide sheets are heavily oxygenated, bearing hydroxyl and epoxide functional groups on their basal planes, in addition to carbonyl and carboxyl groups located at the sheet edges [2]. These groups and the large surface area of GO hold great promise for removal and recovery of metals from aqueous solutions [3].

As(III)/(V) commonly toxic metal and constitute the most important and dangerous source of environmental pollution. Graphene oxide has received worldwide attention due to its exceptional physicochemical properties. Herein, the $Fe_3O_4$@GOx@GSH (Glutathione) composite adsorbent was prepared and was used as an adsorbent for removing As(III)/(V) ions from aqueous solution. It can be separated and recovered easily using magnetic separation technology. The effects of operating parameters such as pH, As(III) concentration and temperature on the As(III) adsorption were investigated by using a response surface methodology (RSM). Optimum As(III) uptake of 96 mg $g^{-1}$ was achieved at pH 1, As(III) concentrations 0.1 mg $L^{-1}$, and temperature 25 °C. All results indicate that the $Fe_3O_4$@GOx@GSH is a promising adsorbent for the efficient removal of As(III) ions from wastewater.

## References

[1] J.W. Hu, Y. Zhuang, J. Luo, X. Wei and X.F. Huang, Int. J. Mol. Sci., 13 (2012) 9332-9342.
[2] M.J. Allen, V.C. Tung and R.B. Kaner, Chem. Rev., 110 (2010) 132-145.
[3] G. Chen, S. Zhai, Y. Zhai, K. Zhang, Q. Yue, L. Wang, J. Zhao, H. Wang, J. Liu and J. Jia, Biosens. Bioelectron., 26 (2011) 3136-3141.
[4] S. Stankovich, D.A. Dikin, G.H.B. Dommett, K.M. Kohlhaas, E.J. Zimney, E.A. Stach, R.D. Piner, S.T. Nguyen and R.S. Ruoff, Nature, 442 (2006) 282-286.

## Acknowledgement

The author is grateful for the financial support provided by the Unit of Scientific Research Projects of Erciyes University (Project no. FBA-2016-6135).

---

* Corresponding author, *E-mail: sacmaci@erciyes.edu.tr*

# Synthesis and Characterization of Polyurethane/CuMOF Nanocomposite Films Derived from Vegetable Oil Based Polyols

**Sevilay Nigar and Sennur Deniz***

Yıldız Technical University, Chemical Engineering Department, Davutpasa cd.,
34210, Esenler, İstanbul, Turkey

*E-mail: sevilay.nigar@gmail.com*

The replacement of petroleum-derived chemicals with biorenewable chemicals offers significant advantages [1]. Vegetable oils are very important resources for polyols, they have been widely used for the production of various polymers including polyol and polyurethanes (PUs). The unsaturated vegetable oils, having double bonds but without hydroxyl groups, are transformed by various chemical reactions into polyols, which by reaction with isocyanates are transformed into PUs [2]. Several approaches have been used to make polyols from epoxidized soybean oil (ESBO) by ring opening reactions involving the epoxide groups [1]. Vegetable oil based polyols, which are relatively cheap, renewable and environmentally friendly, have been used to replace or partially replace conventional polyols derived from petroleum in many fields such as the polyurethane manufacture and fine chemicals [3]. ESBO based polyols are a great alternative for the polyurethane industry with their excellent properties. In this study, the epoxidized soybean oil based polyols with a range of hydroxyl numbers was prepared using commercial epoxidized soybean oil by ring opening reactions with methyl ethyl ketone (MEK) in the presence of a catalyst. Flexible PU films were prepared via the mixing of poly(tetramethylene glycol) (PTMG1000) and ESBO polyols by reacting them with diphenylmethane diisocyanate (MDI). Also, in this work, PU/CuMOF nanocomposite films were prepared using Cu based metal organic framework (CuMOF). CuMOF was synthesized by combining an organic ligand and metal salt using a room temperature solvothermal synthesis route. CuMOF was characterized in terms of structure, $N_2$ adsorption isotherms and surface area by BET, SEM, FT-IR analyses. Synthesized ESBO based polyols and PU films were characterized by FT-IR spectroscopy. Mechanical properties of PU and PU/CuMOF nanocomposite films which are elongation at break, tensile strength and tear strength were measured.

## References

[1] L.C. Bailosky, L.M. Bender, D. Bode, R.A. Choudhery, G.P. Craun, K.J. Gardner, C.R. Michalski, J.T. Rademacher, G.J. Stella and D.J. Telford, Progress in Organic Coatings, 76 (2013) 1712-1719.
[2] M. Ionescu, Chemistry and Technology of Polyols for Polyurethanes, Rapra Technology Limited (2005) First Edition, p:443.
[3] L.K. Jia, L.X. Gong, W.J. Ji and C.Y. Kan, Chinese Chemical Letters, 22 (2011) 1289-1292.

## Acknowledgements

This work was supported by the Yıldız Technical University (No: 2014-07-01-DOP05).

---

* Corresponding author, *E-mail: sennurdeniz@gmail.com*

# Synthesis & Characterization

P -117

# Synthesis of Tin(ıv) α-benzoin Oxime Compounds and Their Catalytic Activity over Polymerization of ε-caprolactone

**Begüm Canan Yıldız*** and Asgar Kayan

Kocaeli University, Science and Art Faculty, Chemistry Department, Umuttepe, 41380, Kocaeli, Turkey

*E-mail: begum.yildiz@kocaeli.edu.tr*

In this work, tin(IV) α-benzoin oximate compounds were synthesized (Figure 1), characterized and tested for catalytic activity. Firstly, α-benzoin oxime reacted with KOBu$^t$ and then butyltin trichloride ($BuSnCl_3$) was added to this solution and was let to react for 6 h at 70° C temperature [1,2]. Then it was cooled at room temperature and washed two times with toluene. After that, it was dried under reduced pressure and white solid was obtained. Secondly, same precursor was prepared another chemical method and ratio. In order to see their catalytic activity, these compounds were tested in polymerization of ε-caprolactone and were effective. All these compounds were characterized by $^1H$, $^{13}C$ NMR, FTIR spectroscopies, mass spectroscopy and elemental analysis. Addition to these, poly-caprolactone (PCL) was also characterized by gel permeation chromatography (GPC) [3].

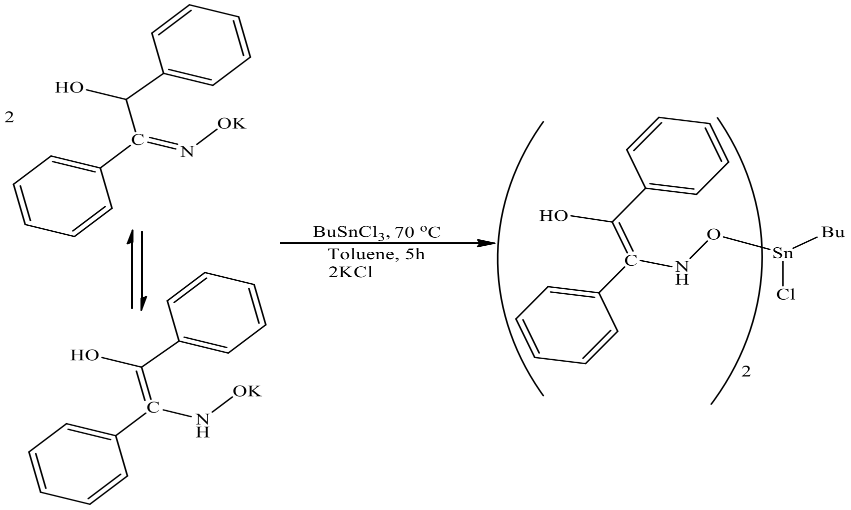


**Figure 1.** Reaction of α-benzoin oximate with $BuSnCl_3$

**References**
[1] B.C. Yildiz and A. Kayan, Designed Monomers and Polymers, 20 (2017) 89-96.
[2] M.H. Chisholm, J.C. Gallucci and C. Krempner, Polyhedron, 26 (2007) 4436-4444.
[3] L.S. Mopes, A.L. Jardini and R.M. Filho, Chemical Engineering Transactions, 28 (2014) 331-336.

---

* Corresponding author, *E-mail: begum.yildiz@kocaeli.edu.tr*

# Studies on the Absorption and Fluorescence Properties of Cholesterol-Curcumin and Cholesterol-Coumarin Conjugates

**Sevinç İlkar Erdağı***

Kocaeli University, Faculty of Science, Department of Chemistry, 41380, Kocaeli, Turkey

*E-mail: sevinc.ilkar@kocaeli.edu.tr*

In recent years, natural products have drawn a great deal of attention both from researchers and the public. Because they are valuable sources of bioactive compounds and have the potential ability to suppress cancers as well as reduce the risk of cancer development. Curcumin and coumarin, naturally occurring phytochemicals, have effective therapeutic and medical properties such as anti-inflammatory, anti-oxidant, anti-inflammatory, anti-carcinogenic, anti-bacterial agent [1,2] and anti-Alzheimer's disease activity [3,4]. On the other hand, cholesterol is an essential lipid in all mammalian cells as a component of cell membrane and as a precursor of steroid hormones and bile acids at high concentrations in cellular plasma membranes and certain intracellular organelles, as well as in plasma lipoproteins [5]. In this study, novel curcumin and coumarin conjugated cholesterol compounds were synthesized by using "click" chemistry techniques (Figure 1). Absorption and fluorescence properties of compounds were studied (Table 1).

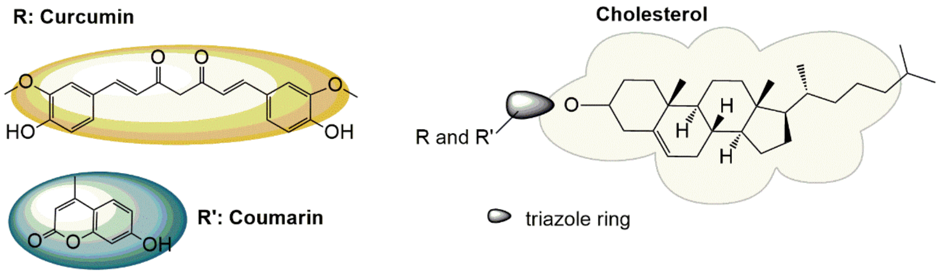


**Figure 1.** Schematic illustration of cholesterol-curcumin and cholesterol-coumarin conjugates

**Table 1.** Absorption and emission values of conjugates in DMF

| Compound | $\lambda^{abs}_{max}{}^{1}$ | $\lambda^{abs}_{max}{}^{2}$ | $\varepsilon_{max}{}^{1}$ | $\varepsilon_{max}{}^{2}$ | $\lambda^{ems.}_{max}{}^{1}$ | $E_s{}^{1}$ | $\Delta\lambda$ |
|---|---|---|---|---|---|---|---|
| Curcumin mono alkyne | 430 | 456 | 81300 | 63900 | 506 | 56.4 | 76 |
| Cholesterol-Curcumin | 435 | 460 | 78000 | 58500 | 497 | 57.4 | 62 |
| Coumarin mono alkyne | 320 | 380 | 45000 | 75000 | 395 | 72.2 | 75 |
| Cholesterol-Coumarin | 325 | 390 | 25000 | 38000 | 406 | 70.2 | 81 |

## References

[1] B. Gogoi and N.S. Sarma, ACS Appl. Mater. Interfaces, 7 (2015) 11195-11202.
[2] Y. Erez, R. Simkovitch, S. Shomer, R. Gepshtein and D. Huppert, J. Phys. Chem. A, 118 (2014) 872-884.
[3] P. Anand, B. Singh and N. Singh, Bioorganic and Medicinal Chemistry, 20 (2012) 1175-1180.
[4] M.Y. Ali, S. Jannat, H.A. Jung, R.J. Choi, A. Roy and J.S. Choi, Asian Pac. J. of Trop. Med., 9 (2016) 103-111.
[5] V.M. Olkkonena, H. Gylling , E. Ikonen, Jour of Steroid Biochemistry and Molecular Biology, 169 (2017) 4-9.

---

* Corresponding author, *E-mail: sevinc.ilkar@kocaeli.edu.tr*

# Monopodal Complexes of Iron(III) Salen Schiff Bases with Bridging 2,4-Dichloro-6-(4-carboxyanilino)-1,3,5-triazine

**Ziya Erdem Koç***

Selçuk University, Department of Chemistry, Konya 42075, Turkey

*E-mail:zerdemkoc@gmail.com*

Sophisticated s-triazine derivatives can be easily prepared from the cheap and readily available cyanuric chloride (2,4,6-trichloro-1,3,5-triazine) [1,2]. Cyanuric chloride is definitely an excellent starting compound for the straightforward preparation of highly structured multitopic molecules. Indeed, each chloride atom of 2,4,6-trichloro-1,3,5-triazine can be substituted by any nucleophilic reactant (Figure 1) [3]. The first substitution is exothermic. Therefore, the temperature of the reaction mixture has to be maintained to $^{o}$C.

We were reported here that a cyanuric chloride and its Schiff bases were syntheses to be a new template. The reaction of cyanuric chloride with 1 equiv of 4-aminobenzoic acid in acetone has given the desired monocarboxy in a single step, coded to be **MONOPOD**. Aromatic carboxy was then reacted under -5 $^{o}$C with 4-aminobenzoic acid and 2,4-dichloro-6-(4-carboxyanilino)-1,3,5-triazine. [3] It may be useful to stress at this point that the new products mentioned above are the main result of this work. These are the first in the literature and we call them "Oxy-Schiff Bases Bridging Metal Complexes" due to literature [4]. The magnetochemical properties of the µ-oxo-bridged complexes [{Fe(salen)}]$O_2$ [5].

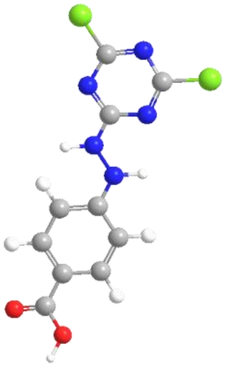


**Figure 1.** 2,4-Dichloro-6-(4-carboxyanilino)-1,3,5-triazine

**References**

[1] Z.E. Koc and H.I. Ucan, Trans. Met. Chem., 32 (2007) 597-602.
[2] H.S. Patel and V.C. Patel, J. Eur. Polym., 37 (2001) 2263-2271.
[3] D.C. Tahmassebi and T. Sasaki, J. Org. Chem., 63 (1998) 728-731.
[4] P. Kopel, Z. Sindelar and R. Klicka, Transition Met. Chem., 23 (1998) 139-142.
[5] Z.E. Koc, J. Heterocyclic Chem., 48 (2011) 769-775.

---

* Corresponding author, *E-mail: zerdemkoc@gmail.com*

# Tripodal Complexes of Manganese(III) Salen Schiff Bases with Bridging 2,4,6-(4-Carboxyanilino)-1,3,5-triazine Derived Multidirectional Ligands

**Ziya Erdem Koç***

Selçuk University, Department of Chemistry, Konya 42075, Turkey

*E-mail:zerdemkoc@gmail.com*

Cyanuric chloride is definitely an excellent starting compound for the straightforward preparation of highly structured multitopic molecules [1,2]. Indeed, each chloride atom of 2,4,6-trichloro-1,3,5-triazine can be substituted by any nucleophilic reactant (Figure 1). The third position is functionalized under refiux of the solvent. As a result, a careful control of the temperature during the substitution reactions will allow the synthesis of 2,4,6-trisubstituted-triazines by sequential and very selective addition of amines.

We were reported here that a cyanuric chloride and its Schiff bases were syntheses to be a new template. The reaction of cyanuric chloride with 3 equiv of 4-aminobenzoic acid in acetone has given the desired dicarboxy in a single step, coded to be **TRIPOD**. Aromatic carboxy was then reacted under room temperature with 4-aminobenzoic acid and 2,4,6-(4-carboxyanilino)-1,3,5-triazine [3]. It may be useful to stress at this point that the new products mentioned above are the main result of this work. These are the first in the literature and we call them “Oxy-Schiff Bases Bridging Metal Complexes” due to literature [4]. The magnetochemical properties of the µ-oxo-bridged complexes [{Mn(salen)}]$O_2$ [5].

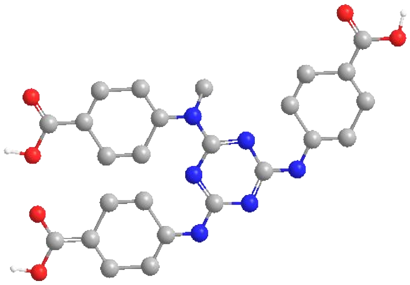


**Figure 1.** 2,4,6-(4-Carboxyanilino)-1,3,5-triazine

**References**
[1] Z.E. Koc and H.I. Ucan, Trans. Met. Chem., 32 (2007) 597-602.
[2] H.S. Patel and V.C. Patel, J. Eur. Polym., 37 (2001) 2263-2271.
[3] D.C. Tahmassebi and T. Sasaki, J. Org. Chem., 63 (1998) 728-731.
[4] P. Kopel, Z. Sindelar and R. Klicka, Transition Met. Chem., 23 (1998) 139-142.
[5] Z.E. Koc, J. Heterocyclic Chem., 48 (2011) 769-775.

---

* Corresponding author, *E-mail: zerdemkoc@gmail.com*

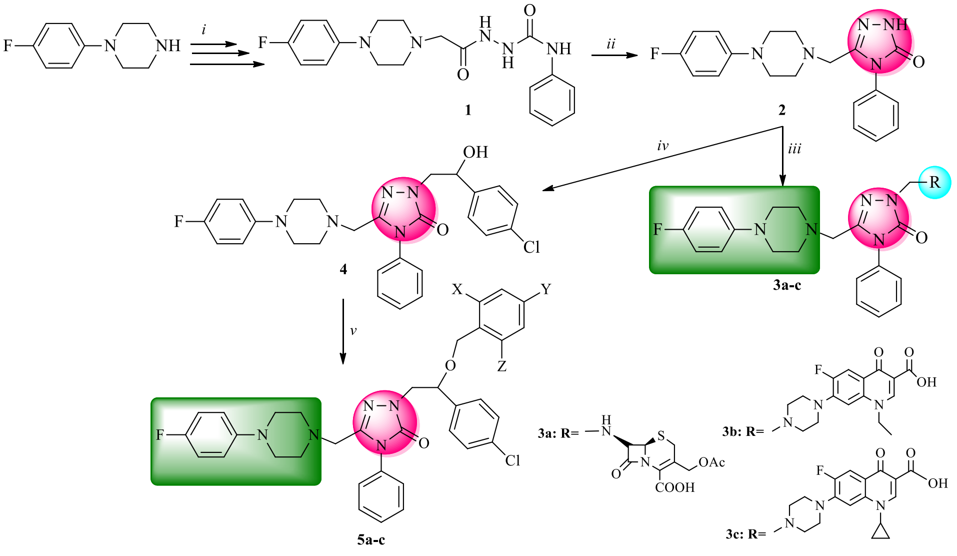
# Synthesis and Characterization of Some Novel 1,2,4-Triazole Derivatives Bearing Fluorophenyl and Piperazine Moieties as Promising Heterocycles

**Neslihan Demirbaş***, Serap Başoğlu Özdemir and Ahmet Demirbaş

Karadeniz Technical University, Faculty of Science, Department of Chemistry, 61080, Trabzon, Turkey

*E-mail: neslihan@ktu.edu.tr*

1,2,4-Triazoles are well-known as promising antimicrobial agents. Compounds of the said structure often exhibit higher activity than standard antibiotics: penicillin G, ampicillin, and gentamicin. On the other hand, many authors reveal that the introduction of halogen atoms into the pharmacophore structure can, in many cases, be useful for antimicrobial activity [1]. *N*-Mannich bases have been used successfully to obtain prodrugs of amine as well as amide-containing drugs. Some Mannich bases derived from 1,2,4-triazole nucleus have been reported to possess protozocidal and antibacterial activity [2]. In this study, the Mannich reactions of 1,2,4-triazole moieties containing fluorophenyl piperazine ring was studied and antimicrobial activities were investigated. All the newly synthesized compounds were characterized by $^1$H NMR, $^{13}$C NMR, FT IR, EI MS spectroscopic techniques.



**5a:** X, Z=H, Y= Cl; **5b:** X, Y= Cl, Z=H; **5c**: X, Z= Cl; Y= H

**Reagent and Conditions**: *i:* a: $BrCH_2COOEt$, $Et_3N$, THF, rt; b: $H_2NNH_2$.EtOH, reflux; c: PhNCO, DCM, rt; *ii:* NaOH, reflux; *iii:* HCHO, amine, DMF, rt; *iv*: a: $BrCH_2C_6H_4Cl$, EtOH, reflux; b: $NaBH_4$, EtOH, reflux; *v*: NaH, $ClCH_2C_6H_4X$, THF, reflux.

## References

[1] T. Plech, M. Wujec, A. Siwek, U. Kosikowska, A. Malm, European Journal of Medicinal Chemistry, 46 (2011) 241-248.
[2] S. Basoglu, S. Ulker, S. Alpay-Karaoglu, N. Demirbas, Med. Chem. Res., 23 (2014) 3128-3143.

---

* Corresponding author, *E-mail: neslihan@ktu.edu.tr*

# Synthesis, Biological Assessment and Molecular Docking Studies of Novel Quinolone Derivatives

**Arif Mermer**, **Neslihan Demirbaş*** **and Ahmet Demirbaş**

Karadeniz Technical University, Faculty of Science, Department of Chemistry, 61080, Trabzon, Turkey

*E-mail: arfmermer@hotmail.com*

Alzheimer's disease (AD), the first most common form of senile dementia, affects nearly 50% of adults over the age of 85. The average survival time after being diagnosed with this illness is about 8-10 years [1]. One of the current therapeutic strategies is to decrease the oxidative stress involved in cellular death. Another therapeutic strategy is to remedy the brain acetylcholine (ACh) level, as this neurotransmitter is important for the regulation of the memory and the learning process [2]. Quinolone moiety is found in a large variety of naturally occurring compounds possessing diverse biological activities. Quinolone derivatives have been used as antimalarial, anti-inflammatory, anticancer, antibiotic, antihypertensive and anti HIV [3]. Quinolone scaffold has also been effectively used for design of dual AChE inhibitor. It is well accepted by now that microwaves and ultrasound produce superior results in many chemical syntheses attributed to both thermal and specific non-thermal effects induced by these irradiations [4]. Our aim here is to introduce new acetylcholinesterase inhibitors, whose structures include a quinolone and a triazole moiety by using microwave and ultrasound irradiation methods (Figure 1).

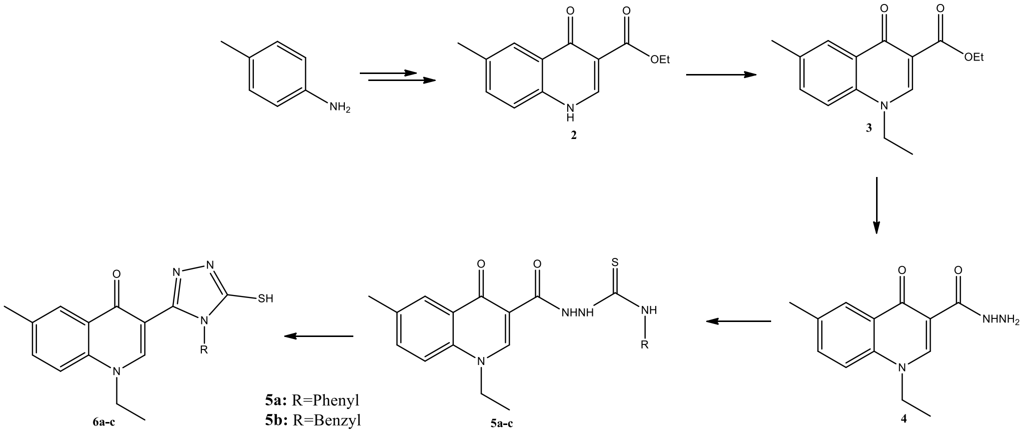


**Figure 1.** Synthesis of substituted quinolone derivatives

**References**

[1] L.F. Lau and M.A. Brodney, Alzheimer's Disease, Vol. 2, Springer, 2008.
[2] A. Andreani, S. Burnelli, M. Granaiola, M. Guardigli, A. Leoni, A. Locatelli, R. Morigi, M. Rambaldi, M. Rizzoli, L. Varoli and A. Roda, Eur. J. Med. Chem., 43 (2008) 657-661.
[3] S.S. Panda, S.C. Jain, Bioorg. Med. Chem. Lett., 23 (2013) 3225-3229.
[4] E.M. Guerra and V.G. Gude, Fuel, 137 (2014) 100-108.

---

* Corresponding author, *E-mail: neslihan@ktu.edu.tr*

# Methylation of 2-Methyl Naphthalene to 2,6-Dimetyl Naphthalene over Pd/Zr Bimetal Loaded Ferrierite Zeolite Catalyst

**Aysima Tunç and Ali Karaduman***

Ankara University, Faculty of Science, Department of Chemical Engineering, 06100, Ankara, Turkey

*E-mail: tuncaysima@gmail.com*

Zeolites have very high surface area and adsorption capacity. Therefore, zeolites are the most widely used as catalyst for oil refining, petrochemistry, and organic synthesis [1]. In this study, Pd and Zr metals were loaded on ferrierite zeolite and it was used as catalyst for methylation of 2-methylnaphthalene (2-MN) to produce 2,6-dimethylnaphthalene (2,6-DMN). 2,6-DMN uses for the production of polyethylene naphthalate (PEN) which is important material because it has better qualities than polyethylene terephthalate (PET) [2]. Bimetal loaded ferrierite zeolite catalysts were prepared by means of the Wet Impregnation Method. The prepared catalysts were tested in a fixed bed tubular reactor system. The catalysts were activated at 500°C temperature and 5 ml/min $N_2$ flow rate. The feed was consisted of 2-MN, methanol and 1,3,5 trimethyl benzene (1:5:5 molar ratio). Experimental studies were carried out at three different temperatures (300, 350, 400 °C) and weight hourly space velocities (1 $st^{-1}$, 2$st^{-1}$, 3$st^{-1}$). The methylation products were analyzed by GC-MS. The effect of bimetal loaded on ferrierite catalyst, reaction temperature and weight hourly space velocity on 2-MN conversion, 2,6-DMN yield and 2,6-DMN/2,7-DMN ratios were investigated.

**References**

[1] W. Vermeiren and J.P. Gilson, Topics in Catalysis, 52(9) (2009) 1131-1161.
[2] G. Watanabe, Y. Nakasaka, T. Taniguchi, T. Yoshikawa, T. Tago and T. Masuda, Chemical Engineering Journal, 312 (2017) 288-295.

---

* Corresponding author, *E-mail: ali.karaduman@ankara.edu.tr*

P -124

# Effect of Metal Loaded Ferrierite Zeolite Catalists on Methylation of Coal Tar Naphthalene Oil Fraction

**Sümeyye Tol and Ali Karaduman***

Ankara University, Faculty of Engineering, Department of Chemical Engineering,
06100, Ankara, Turkey

*E-mail: smyyetol@gmail.com*

Coal Tar Naphthalene Oil Fraction (CTNOF) was produced in coke formation of coals as by-product. CTNOF has important naphthalene and its derivatives such as 1-Methylnaphthalene (1-MN), 2-Methylnaphthalene (2-MN) and Dimethylnaphthalenes (DMNS). In this naphthalene derivatives such as 2-MN and 2,6-DMN have commercial prescription [1]. 2-MN is used in the production of Vitamin-K and 2,6-DMN. Also 2,6-DMN, which is one of the most important substances in synthesis of polyethylene naphthalate (PEN) [2]. In this study, the methylation of CTNOF has been studied to increase the ratio of 2-MN and 2,6-DMN in CTNOF. To produce 2,6-DMN and 2-MN, methylation of CTNOF was investigated over H-Ferrierite, 0.1 Pd-Ferrierite and 0.1 Ni-Ferrierite zeolite catalysts. The methylation reactions of CTNOF with methanol were carried out in a fixed bed reactor operating at a range of 300 – 400 °C, and weight hourly space velocity (WHSV) ranging from $1h^{-1}$ to $3h^{-1}$. In the experiments feed composition (mass ratio) was 1:5:5 (CTNOF: Methanol: 1,2,4-Trimetilbenzene) was used. Methylation liquid products of CTNOF were analyzed by using GC-MS system with 60 meters ZB-1ms capillary column. The catalysts were characterized by FTIR, SEM and BET analysis methods. The results of the CTNOF methylation over metal loaded Ferrieite catalyst showed that 2-MN and 2,6-DMN contents of CTNOF increased by using metal loaded catalysts.

**References**

[1] G.P. Hagen and D.T. Hung. "Selective Production of 2,6-Dimethylnaphthalene, U.S. Patent No. 5,670,704 (1997).
[2] L. Zhao, H. Wang, M. Liu, X. Guo, X. Wang, C. Song and H. Liu, Chemical Engineering Science, 63(21) (2008) 5298-5303.

---

* Corresponding author, *E-mail: karaduman@ankara.edu.tr*

P -125

# Synthesis of New Pyrazoline Derivatives as Antibacterial Agents

**Adnan Çetin*** **and Sedat Bozarı**

Muş Alparslan University, Faculty of Education, Department of Science, 49250, Muş, Turkey

*E-mail: a.cetin@alparslan.edu.tr*

Synthetic organic and pharmaceutical chemistry is growing very rapidly the in the development of synthetic methods and investigation of the bioactive properties. The pyrazoline compounds are used in the development of agricultural products and in drug research. Because heterocyclic compounds containing substitute pyrazole and pyrazoline rings were important goal molecules in the field of synthetic and medicinal chemistry. These compounds are reported to possess a broad spectrum of biological activities such as antimicrobial, antidepressant, neuroprotective, anticonvulsant, anti-inflammatory *ie.* [1-3] Firstly, starting material was prepared by result coupling reaction ethyl benzoylacetate and 4-bromoaniline with sodium nitrite solution in the ice bath in Figure 1. Then, the pyrazoline derivatives were synthesized via various hydrazines and starting material. The structures of these synthesized compounds were determined by spectroscopic methods.

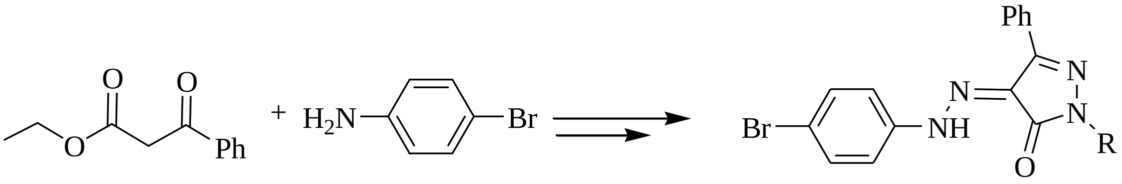


**Figure 1.** Synthesis of pyrazoline compounds

## References

[1] M. Amir, H. Kumar and S.A. Khan, Bioorg. Med. Chem. Lett., 18(3) (2008) 918-922.
[2] S. Bhandari, A.C. Tripathi and S.K. Saraf, Med. Chem. Research, 22(11) (2013) 5290-5296.
[3] V. Monga, K. Goyal, M. Steindel, M. Malhotra, D.P. Rajani and S.D. Rajani, Med. Chem. Research, 23(4), (2014) 2019-2032.

## Acknowledgements

The authors thank to the Management Unit of Scientific Research Projects of Mus Alparslan University (MSÜBAP) for financial support under Project MSÜ15-EMF-G05.

---

* Corresponding author, *E-mail:* s.bozari*@alparslan.edu.tr*

# Organogelation Properties of 1,3-bPBis[n-(*p*-aryl)-carbamoyloxy]-2-Methyl-2-propylpropane Derivatives

**Murat Gürel** and **Öznur Demir Ordu***

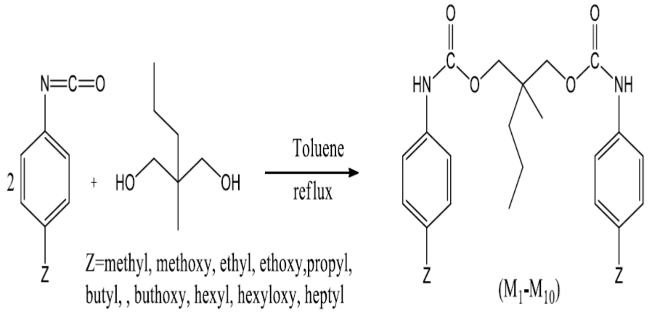
Abant İzzet Baysal University, Faculty of Arts and Science, Department of Chemistry, 14100, Bolu, Turkey

*E-mail: 1muratgurel@gmail.com*

Low molecular weight supramolecular gels belong to an important class of soft materials with a wide range of applications. In organogels, small molecules are self-assembled into long fiber-like by intermolecular non-covalent interactions such as hydrogen bonds, π-π stacking, van der Waals forces, charge-transfer interactions and others. These fibres then entangle to form a three-dimensional network, which entraps the solvents within the pores through capillary forces [1].

The self-assembly process is influenced by a variety of factors, including solvent type, concentration, temperature and especially molecular structure. It is believed that structural and substituent variations provide a basis for a better understanding of the relation between aggregate gel properties and the chemical structure of gelators, thus may lead to the development of new nano fibrillar materials.

With this aim, ten derivatives of bis-carbamates (1,3-Bis [N-*p*-aryl) carbamoyloxy]-2-methyl-2-propyl propanes) were synthesized by the reaction of *p*-arylisocyanates and 2-methyl-2-propyl-1,3-propanediol in tolüene (Figure 1) [2], and their organogelation properties in organic solvents were investigated (Figure 2). It was found that the gelation ability of the compounds was affected by the para-substitution (*p*-alkyl, *p*-alkoxy) on the aryl ring. Introduction of para-alkoxy groups changed the gelation ability compared to *para*-alkyl substituted derivatives. The length of *p*-alkyl and *p*-alkoxy tail also had an influence on organogel formation.



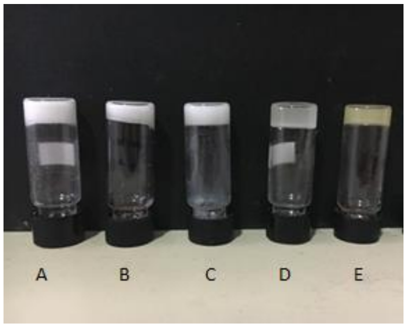


**Figure 1.** General synthesis for ($M_1$-$M_{10}$) derivatives

**Figure 2.** Organogels of bis-carbamates

**References**
[1] D.K. Smith, Tetrahedron, 63 (2007) 7283-7284.
[2] O. Demir Ordu, H. Simsir and K. Alper, Tetrahedron, 71 (2015) 1529-1539.

---

* Corresponding author, *E-mail: demirordu@ibu.edu.tr*

# Morphological Studies on Self-assembling 1,3-Bis [N-*p*-aryl) carbamoyloxy]-2-methyl-2-propyl propanes by Optical Microscopy

**Murat Gürel and Öznur Demir Ordu***

Abant İzzet Baysal University, Faculty of Arts and Science, Department of Chemistry, 14100, Bolu, Turkey

*E-mail: 1muratgurel@gmail.com*

Thermoreversible supramolecular gels constructed from low molecular weight organogelators (LMWOs) are forms of soft matter which have attracted great attention due to their potential applications in cosmetics, liquid crystals, development of separation processes, drug delivery and controlled release. Molecules of LMWOs create entangled supramolecular networks through non-covalent interactions such as hydrogen bonding, p-p stacking, van der Waals interactions and other weak interactions. These non-covalent interactions give rise to the formation of fibrous, spherulite, tubular or helical aggregates of gelators, which subsequently results in the immobilization of the solvent molecules.

Structural units like aromaticity, hydrogen bonding groups and aliphatic chains are known to be responsible for gel assembly. Generally, low molecular weight organogelators with double hydrogen bonding sites (bis-ureas, bis-amides) are known to have intermolecular hydrogen bondings with two adjacent molecules. A number of bis-carbamates also exhibited self-assembling properties [1] through hydrogen bonding between carbamate groups. Recently, we have reported [2] that the driving force for gel formation in bis[N-(*p*-aryl)-carbamoyloxy]alkanes is found to be hydrogen bonding, p-p stacking, van der Waals interactions.

The aim of the study is to study gel structures obtained from (1,3-Bis [N-*p*-aryl) carbamoyloxy]-2-methyl-2-propyl propanes) (Figure 1) in organic solvents using optical microscopy. There is a potential of these gel materials to be used as sorbents in environmental applications. In this project, with the knowledge of the types of fiber growth in 3D, materials having high surface area will be obtained.

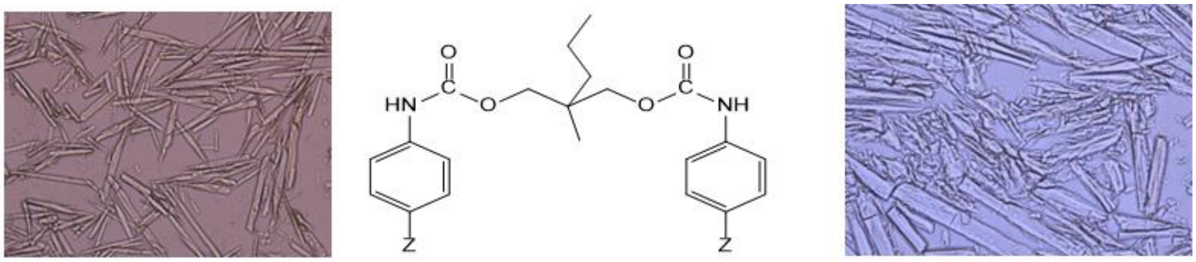


**Figure 1.** Optical micrographs of nut oil gel of *p*-ethoxy derivative (20X (left) and 50X (right))

**References**
[1] S. Khanna, M. Moniruzzaman and P.R. Sundararajan, J. Phys. Chem. B., 110 (2006) 15251-15260.
[2] O. Demir Ordu, H. Simsir and K. Alper, Tetrahedron, 71 (2015) 1529-1539.

---

* Corresponding author, *E-mail: demirordu@ibu.edu.tr*

# Structural Characterization of Cu(II)-1,2-di(pyridin-4-yl)ethene Coordination Polymer

**Hakan Erer, <u>İlknur Özdemir</u>, Büşra Salun and Okan Zafer Yeşilel***

Eskişehir Osmangazi University, Faculty of Arts and Sciences, Department of Chemistry, 26480, Eskişehir, Turkey

*E-mail: nihalkucukoglu@hotmail.com*

In the past two decades, coordination polymers (CPs) with interesting structural topologies and potential applications such as sorption, gas storage/separation, magnetism, non-linear optics, sensors, luminescence and catalysis have been extensively explored in the fields of crystal engineering. To design and synthesize CPs with the desired structure and specified properties, many structural and experimental factors such as the coordination geometry of metal centers, organic linkers, counter ions, pH, temperature, solvent and metal/ligand ratio play important roles in the self-assembly process of CPs [1]. In the coordination polymer synthesis, glutaric acid was used as the aliphatic dicarboxylic acid and nitrogen donor 1,2-di(pyridin-4-yl)ethene ligand was used as the secondary ligand. The structure of the synthesized $\{[Cu(\mu\text{-dpeten})_2Cu(\mu\text{-}SO_4)_2](H_2O)_2(\mu\text{-dpeten})]_2\cdot H_2O\}_n$ (**1**) (dpeten=1,2-di(pyridin-4-yl)ethene) complex was characterized by elemental analysis, FT-IR, TG / DTA and X-ray single crystal studies. There are two different copper centers with two different coordination environments. Cu1 ion is coordinated with the four oxygen atoms of the two sulphates and the two aqua ligands and two nitrogen atoms of the two dpeten ligands. Cu2 centers are coordinated by two oxygen atoms of the two sulphates and four nitrogen atoms belonging to four different dpeten ligands. And both centers have octahedral geometry (Figure 1). 1D zigzag chain was formed by bridging sulphate ligand between Cu centers. Three-dimensional porous coordination polymer (PCP) structure has been formed by bonding adjacent 1D chain with the dpeten ligands.

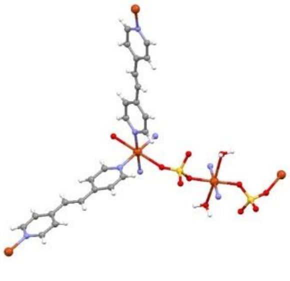


**Figure 1.** Molecular structure of complex **1**

**References**
[1] H.C. Kim, S. Huh, J.Y. Kim, H.R. Moon, D.N. Lee and Y. Kim, CrystEngComm., 19 (2017) 99-109.

**Acknowledgement**
This study was supported by TUBITAK 2209/A program.

---

* Corresponding author, *E-mail: yesilel@ogu.edu.tr*

# Synthesis, Crystal Structure, Spectroscopic and Thermal Properties of N-Ethylimidazole Complex of Cd(II)-Squarate

**Hakan Erer, Nihal Küçükoğlu and Okan Zafer Yeşilel***

Eskişehir Osmangazi University, Faculty of Arts and Sciences, Department of Chemistry, 26480, Eskişehir, Turkey

*E-mail: nihalkucukoglu@hotmail.com*

In the past decade, the rational design and synthesis of polymeric coordination frameworks have gained considerable attention due to their attractive structures and promising applications for magnetism, conductivity, catalysis, gas storage, host–guest chemistry. Recently, increasing investigations have been focused on the constructions of coordination polymers using oxocarbons such as squaric acid as building blocks. Oxocarbons have been extensively used to design polynuclear complexes and supramolecular compounds with unique structures and interesting magnetic behaviors. Squaric acid (3,4-dihydroxy-3-cyclobutene-1,2-dione) is a member of oxocarbons. Squarate dianion ($C_4O_4^{2-}$, sq) is an excellent bridging ligand and can link the metal ions in bis(monodentate) coordination through oxygen atom forming trans-(μ-O1,O3) or cis-(μ-O1,O2) [1,2]. The structure of the synthesized $[Cd(\mu_{1,3}\text{-sq})(H_2O)_2(\text{N-etim})_2]_n$ (**1**) ($H_2sq$=squaric acid, $sq^{2-}$=dianionic squarate, N-etim=N-ethylimidazole) complex was characterized by elemental analysis, FT-IR, TG / DTA and X-ray single crystal studies. Complex **1** was synthesized under hydrothermal conditions (120 °C and 96 hours). According to X-ray diffraction analysis result, the structure of $[Cd(\mu_{1,3}\text{-sq})(H_2O)_2(\text{N-etim})_2]_n$ was obtained with crystallization of two Cd(II) centered molecular structures in the monoclinic crystal system with the space group $P2_1/c$. The squarate ligand is coordinated to the Cd(II) ion as the bridge ligand from the oxygen atoms at trans-1,3 positions. The distorted octahedral geometry of the complex is complemented by two N-etim ligands in axial position and two aqua ligands in the equatorial position (Figure 1). Dianionic sq ligand coordinates to Cd(II) ions to form a one-dimensional (1D) chain structure.

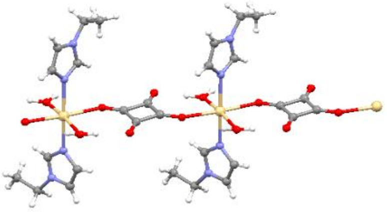


**Figure 1.** 1D polymeric structure of complex **1**

**References**

[1] R. Köferstein and C. Robl, Z. Anorg. Allg. Chem., 642 (2009) 560-565.
[2] X. Solons, M. Aguilõ, A. Gleizes, J. Faus, M. Julve and M. Verdaguer, Inorg. Chem., 29 (1990) 775-780.

**Acknowledgement**

This study was supported by TUBITAK 2209/A program.

---

* Corresponding author, *E-mail: yesilel@ogu.edu.tr*

# Synthesis, Crystal Structure, Spectroscopic and Thermal Properties of 2-Methylimidazole Complex of Co(II)-Squarate

**Hakan Erer, Nihal Küçükoğlu and Okan Zafer Yeşilel***

Eskişehir Osmangazi University, Faculty of Arts and Sciences, Department of Chemistry, 26480, Eskişehir, Turkey

*E-mail: nihalkucukoglu@hotmail.com*

In recent years, rational design and synthesis of polymeric coordination compounds have attracted great interest due to their interesting structures and applications such as magnetism, conductivity, catalysis, gas storage, drug release. The coordination chemistry of cyclic carboxylates and oxocarbons has been widely studied as squarate containing compounds since they have varied structural features and applications in biological and magneto chemistry. Squaric acid (3,4-dihydroxy-3-cyclobutene-1,2-dione) is a useful tool for constructing crystalline architectures because of its rigidity and flat four-membered ring framework, and its proton donating and accepting capabilities for hydrogen bonding. Squarate dianion ($C_4O_4^{2-}$, sq) is an excellent bridging ligand and can link metal ions in a bis(monodentate) coordination through the oxygen atoms forming trans-(μ-O1,O3) or cis-(μ-O1,O2) [1]. The structure of the synthesized $[Co(\mu_{1,3}\text{-sq})(H_2O)_2(2\text{-meim})_2]_n$ (**1**) ($H_2sq$ = squaric acid, $sq^{2-}$=dianionic squarate, 2-meim=2-methylimidazole) complex was characterized by elemental analysis, FT-IR, TG / DTA and X-ray single crystal studies. The complex was prepared by adding the 2-meim ligand to the aqueous solution of $Cosq \cdot H_2O$ at 60 ºC in a 1:4 molar ratio. According to the results of single crystal X-ray diffraction analysis, one dimensional (1D) structure of $[Co(\mu_{1,3}\text{-sq})(H_2O)_2(2\text{-meim})_2]_n$ was obtained by Co(II) centered molecular structures in monoclinic system with $P2_1$ space group. The squarate ligand is coordinated to the Co(II) ion as the bridge ligand from the oxygen atoms at trans-1,3 positions. The distorted octahedral geometry of the complex is complemented by two 2-meim ligands in axial position and two aqua ligands in equatorial position (Figure 1).

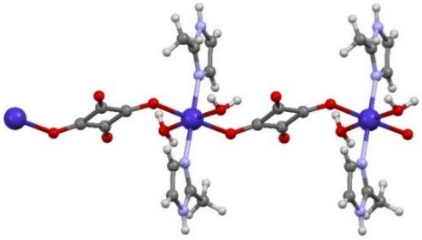


**Figure 1.** 1D polymeric structure of complex **1**

## References

[1] O. Kovalchukova and S. Strashnova, Rev. Inorg. Chem., 34 (2014) 1-24.

## Acknowledgement

This study was supported by TUBITAK 2209/A program.

---

* Corresponding author, *E-mail: yesilel@ogu.edu.tr*

# Synthesis and Structural Characterization of Cd(II)-Glutarate Coordination Polymer

**Hakan Erer, Büşra Salun, İlknur Özdemir and Okan Zafer Yeşilel***

Eskişehir Osmangazi University, Faculty of Arts and Sciences, Department of Chemistry, 26480, Eskişehir, Turkey

*E-mail: salunbusra@gmail.com*

The design and synthesis of coordination polymers (CPs) have received much attention in recent years owing to their diverse topologies and potential applications in various areas such as sorption, separation, catalysis, luminescence, biological applications, and magnetism and so on. It is well-known that the organic ligands and metal ions play important roles in the design and synthesis of desirable CPs. In the construction of complexes, polycarboxylate ligands, especially dicarboxylate ligands, have often been used as a molecular building block to afford a variety of new functional coordination polymers with high dimensionality due to their versatile coordination modes [1]. In the coordination polymer synthesis, glutaric acid was used as the aliphatic dicarboxylic acid and nitrogen donor N,N'-dimethylethylenediamine ligand was used as the secondary ligand. The structure of the synthesized $\{[Cd(\mu\text{-glu})(H_2O)_3]\cdot 2H_2O\}_n$ (1) ($H_2glu$=glutaric acid) complex was characterized by elemental analysis, FT-IR, TG/DTA and X-ray single crystal studies. The complex was prepared by adding N,N'-dimethylethylenediamine ligand (1:1) to the aqueous solution of the Cd(glu)EtOH compound at 50ºC. The Cd(II) ion exhibited seven coordinated pentagonal bipyramidal geometries. The four oxygen atoms of the glutarate ligand and the three aqua ligands are coordinated to Cd(II) ion. The one-dimensional straight chain structure was formed by bridging glutarate ligand (Figure 1). Neighboring chains have expanded to three-dimensional supramolecular structure with O-H···O hydrogen bond.

**Figure 1.** 1D straight chain structure of complex **1**

## References

[1] K. Zhang, Z.W. Qao and J.W. Jiang, Cryst. Growth. Des., 17 (2017) 543-549.

## Acknowlegment

This study was supported by TUBITAK 2209/A program.

---

* Corresponding author, *E-mail: yesilel@ogu.edu.tr*

P -132

# Insoluble Metal-Organic Frameworks Including Lanthanide Metals: Hydrothermal Synthesis, Characterization and Investigation of Their Luminescence Properties

**Burak Ay[1]*, Emel Yıldız[1] and İbrahim Kani[2]**

[1]Çukurova University, Faculty of Science, Department of Chemistry, Adana, Turkey
[2]Anadolu University, Faculty of Science, Department of Chemistry, Eskişehir, Turkey

*E-mail: bay@cu.edu.tr*

In the field of coordination polymers, much work has been focused on metal-organic frameworks (MOFs) based on lanthanides and multifunctional carboxylic acid ligands because of their interesting structures and their many varied of applications. The design possibilities of organic ligands, the coordination tendencies of metal ions, and the variety of possible crystallization conditions have led to a large number of open framework structures [1]. Multidentate N-and O-donor bridging pyridine or pyrazine carboxylic acid ligands have been extensively used for the construction of new MOF systems. Among these ligands, pyridine- 2,6-dicarboxylate is suitable for preparing multifunctional MOF properties such as the ability to deprotonate, high symmetry, considerable structural flexibility, and a variety of modes forco- ordination of metal atoms [2-5]. Herein, we describe the hydrothermal synthesis of two coordination polymers $(H_2pip)_n[Ln_2(pydc)_4(H_2O)_2]_n$ (Ln=La (**1**) and Nd **(2)**, $H_2$pydc=2,6-pyridinedicarboxylic acid, $H_2$pip=piperazine). They have been successfully synthesized and structurally characterized by the elemental analysis, ICP-OES, IR spectroscopy, TGA, single- crystal X-ray diffraction and powder X-ray diffraction (PXRD) analysis. MOFs are isomorphous, showing three-dimensional Ln-O-Ln chains. Ln(III) ions in **1-2** adopt a nine-coordinated mode to construct a tricapped trigonal prism coordination environments. The synthesized lanthanide frameworks are insoluble all organic, inorganic and mixed solvents. The luminescence properties of **1-2** have been investigated.

**References**

[1] A. Aijaz, E.C. Sañudo and P.K. Bharadwaj, Cryst. Growth Des., 11 (2011) 1122-1134.
[2] H.D. Yin, F.H. Li and C.H. Wang, Inorg. Chim. Acta, 360 (2007) 2797-2808.
[3] L.-F. Chen, Z.-J. Li, Y.-Y. Qin, J.-K. Cheng and Y.-G. Yao, J. Mol. Struct., 892 (2008) 278-282.
[4] D. Deng, P. Liu, W. Fu, L. Li, F. Yang and B. Ji, Inorg. Chim. Acta, 363 (2010) 891-898.
[5] L. Duan, Y. Li, Y. Liu, E. Wang, X. Wang, C. Hu and L. Xu, J. Mol. Struct., 689 (3) (2004) 269-274.

---

* Corresponding author, *E-mail: bay@cu.edu.tr*

P -133

# Hydrothermal Synthesis of Cu(I) Nanopolymer Structure and Investigation of Its Catalytic Activity on the Oxidation of Thymol

**Burak Ay[1], Emel Yıldız[1]* and Jon Zubieta[2]**

[1]Çukurova University, Faculty of Science, Department of Chemistry, Adana, Turkey
[2]Syracuse University, Faculty of Science, Department of Chemistry, NY, Syracuse, USA

*E-mail: eeyildiz@cu.edu.tr*

The design and synthesis of metal-organic frameworks (MOFs) is one of the most important research areas in crystal engineering [1]. MOFs exhibiting interesting structures and topologies are of great interest not only for their unique structural and functional properties, but also for their potential applications in a variety of areas. The hydrothermal method provides an efficient technique for synthesizing MOFs [2]. Furthermore, while multidentate carboxylic acid ligands can easily decarboxylate under hydrothermal conditions [3], decarboxylation reactions of multiple carboxyl groups are rarely encountered. We observed multiple decarboxylation during the synthesis of the complex in the absence of catalyst under hydrothermal conditions as reported in this work (Figure 1).

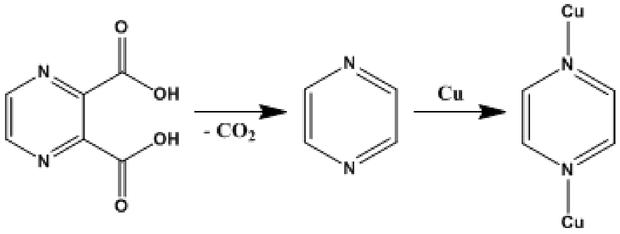


**Figure 1.** Multiple decarboxylation reaction of $H_2$pzdc and its coordination mode in **1**.

In this study, inorganic-organic hybrid system including metal-polymer, $[Cu_2Cl_2(pyrz)]_n$ (**1**) $H_2$pzdc=2,3-pyrazinedicarboxylic acid, pyrz = pyrazine), has been synthesized under hydrothermal conditions.The catalytic activity of the synthesized nanopolymer was investigated on the oxidation of thymol to thymoquinone.

**References**
[1] C. Yuste-Vivas, M. Ramos Silva, P. Martín-Ramos, L.C.J. Pereira, J. Ferrando-Soria, P. Amorós and M. Julve, Polyhedron, 87 (2015) 220-225.
[2] T.M. Smith, A. Lau and J. Zubieta, Inorg. Chim. Acta, 409 (2014) 296-301.
[3] B. Ay, G. Yağ, E. Yildiz and A.L. Rheingold, Polyhedron, 88 (2015) 164-169.

---

* Corresponding author, *E-mail: eeyildiz@cu.edu.tr*

# Synthesis of Environmentally Friendly and Efficient Lewis Acid-Type Calix[4]arene Catalyst for the Mannich Reaction

Serkan Sayın[1]* and Mustafa Yılmaz[2]

[1]Giresun University, Department of Environmental Engineering, Giresun, Turkey
[2]Selcuk University, Department of Chemistry, Konya, Turkey

*E-mail: serkan.sayin@giresun.edu.tr*

Production of β-amino carbonyl compounds by using Mannich reaction is highly desirable because they are potential intermediates of pharmaceutical agents [1,2]. However, a catalyst, which is produced in a high yield and soluble in aqueous solution as well as it may easily recovered and reused, is required to obtain β-amino carbonyl derivatives. For this goal, numerous catalysts have been developed to catalyze Mannich-type reactions [1,3]. However, most of them are drastically soluble in water but well soluble in organic solvent. Taking into account on the toxicological effects of any organic solvent to the environment [1], development a catalyst that is well soluble in water or could catalyze without any organic solvents is highly respected.

In this study, a Lewis acid-type calix[4]arene derivative was synthesized (Figure 1), and characterized. Moreover, the calixarene derivative was grafted onto an epoxysilica-coated magnetite nanoparticle surface in order to provide it easily recyclable, environmentally benign, cost effective and reusable catalyst. The catalytic efficacy of calixarene-grafted magnetite nanoparticles was also evaluated in the three component Mannich reaction of benzaldehyde with aniline and acetophenone in water without co-solvents.

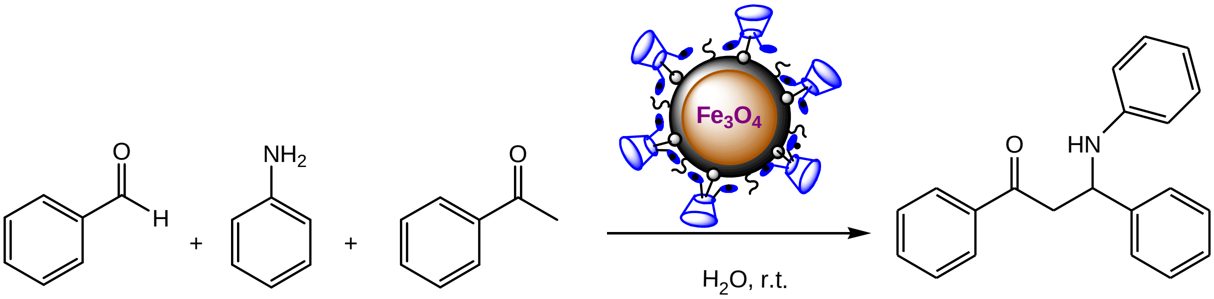


**Figure 1.** The catalytic abilities of calixarene derivative in three component Mannich reactions of benzaldehyde with aniline and acetophenone in an aqueous media

## References

[1] S. Sayin and M. Yilmaz, RSC Adv., 7 (2017) 10748-10756.
[2] P. Hermange, M. E. T. H. Dau, P. Retailleau and R. H. Dodd, Org. Lett., 11 (2009) 4044-4047.
[3] T. Akiyama, J. Takaya and H. Kagoshima, Adv. Synth. Catal., 344 (2002) 338-347.

---

* Corresponding author, *E-mail: serkan.sayin@giresun.edu.tr*

P-135

# Cr(VI)/As(V) Binding Properties of the Calix[4]arene Substituted Chitosan

**Serkan Sayın***

Giresun University, Department of Environmental Engineering, Giresun, Turkey

*E-mail: serkan.sayin@giresun.edu.tr*

In recent years, oxyanions such as As (V) and Cr (VI) being two substances among the top 20 most hazardous substances have spread all over the world. (1) People whom in touch with those oxyanions suffer serious health hazard such as lung, bladder, kidney, and skin cancers, etc. Fabricating a convenient and efficient way for the removal of these oxyanions from their contaminant is a prominent task. For this aim, researchers have been applied numerous methods such as chemical precipitation, ion exchange, membrane separation, and sorption. (2,3) Among these techniques, the sorption technique is widely used.

Chitosan obtained from naturally abundant chitin has been widely used in various applications such as pharmaceutics, medicine, textiles, agriculture and other industrial applications due to its low toxicity, good biocompatibility, biodegradability and economical advantages. (4) In view of that, in this study, the calix[4]arene derivative bearing convenient binding arms was substituted to the chitosan. The structure of the calix[4]arene-substituted chitosan (Figure 1) was well characterized using NMR, FTIR, TGA, SEM and elemental analyses techniques. In addition, the binding efficacy of the calix[4]arene-substituted chitosan towards arsenate and dichromate anions was also investigated by using solid-liquid extraction.

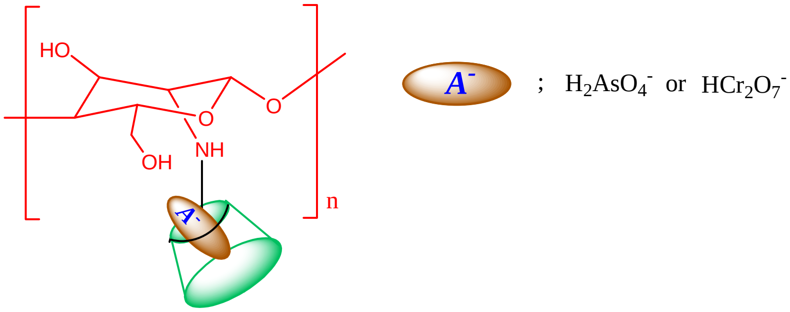


**Figure 1.** The suggested complexation phenomena of arsenate and dichromate ion with the calix[4]arene-substituted chitosan

**References**
[1] Q. Guo, Y. Cao, Y. Zhuang, Y. Yang, M. Wang and Y. Wang, Appl. Geochem., 77 (2017) 206-212.
[2] S. Sayin, F. Ozcan and M. Yilmaz, Mater. Sci. Eng. C, 33 (2013) 2433-2439.
[3] Y. Masue, R.H. Loeppert and T.A. Kramer, Environ. Sci. Technol., 41 (2007) 837-842.
[4] T. Yan, H. Zhang, D. Huang, S. Feng, M. Fujita and X.-D. Gao, Nanomater., 7 (2017) 59-68.

---

* Corresponding author, *E-mail: serkan.sayin@giresun.edu.tr*

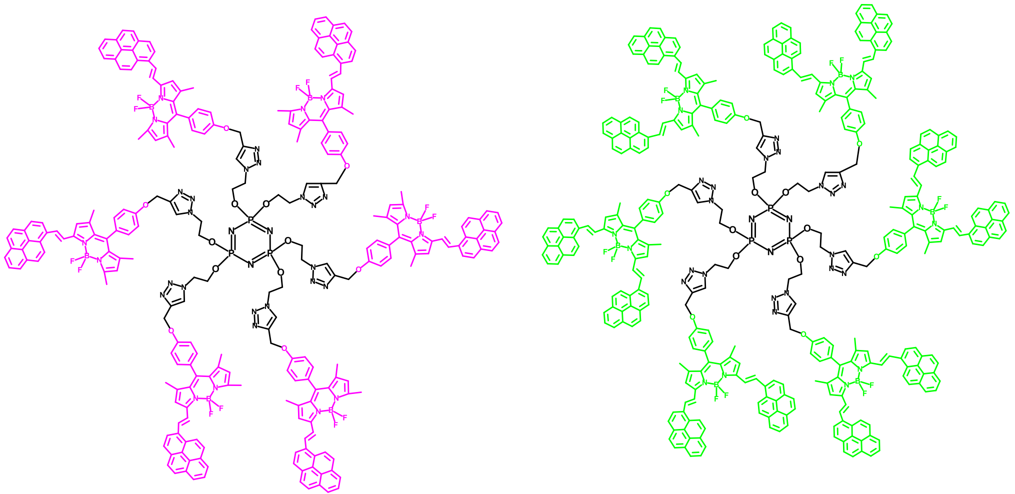
P-136

# Synthesis and Characterization of mono- and distyryl Bodipy Substituted Cyclophosphazene Compounds and Investigation of Their Fluorescence Properties

**<u>Seda Çetindere</u>, Süreyya Oğuz Tümay, Mahmut Durmuş, Adem Kılıç and Serkan Yeşilot***

Gebze Technical University, Faculty of Science, Department of Chemistry, Kocaeli, Turkey

Phosphazene compounds have a very wide application area because they exhibit different physical and chemical properties depending on the organic, inorganic or organometallic groups which are substituted into the phosphazene core [1]. On the other hand, boradiazaindasen (Bodipy) compounds known as fluorescent dyes which have interesting spectral properties such as high quantum yields (0.6-1.0), large extinction coefficients (60000-80000 $M^{-1}cm^{-1}$) and narrow emission bands. Absorption and emission properties of these compounds can be adjusted by substitution of different groups into the bodipy core [2]. In this study, new cyclotriphosphazene compounds (Psz-1 and Psz-2) bearing mono- and distyryl pyrene contained Bodipy substituents (Figure 1) were designed, synthesized and characterized for the first time. Synthesized compounds were fully characterized by FT-IR, mass spectrometry, $^{1}H$, $^{13}C$ and $^{31}P$ NMR spectroscopies and elemental analysis as well. Additionally, fluorescence properties of these compounds were investigated by using UV-vis and fluorescence spectrophotometer.



(Psz-1) (Psz-2)

**Figure 1.** Chemical structures of compounds (Psz-1 and Psz-2)

**References**

[1] H.R. Allcock, Phosphorus Nitrogen Vompounds: Cyclic, Linear and High Polymeric Systems. Academic Press, (1972).

[2] A. Loudet and K. Burgess, Chem. Rev., 107 (2007) 4891-4932.

---

* Corresponding author, *E-mail: yesil@gtu.edu.tr*

P-137

# Synthesis and Photophysical Properties of Pyrene Substituted Cyclotriphosphazenes

**Hüsnüye Ardıç Alidağı, Süreyya Oğuz Tümay, Ahmet Şenocak,
Ömer Faruk Çiftbudak and Serkan Yeşilot***

Gebze Technical University, Faculty of Science, Department of Chemistry, 41400, Kocaeli, Turkey

*Email: hardic@gtu.edu.tr*

Cyclic phosphazenes which physical and chemical properties can be adjusted according to the feature of the substituted groups are an important class of inorganic heterocyclic ring systems. Phosphazenes can be easily functionalized, functionalized cyclic phosphazene core is stable under harsh chemical conditions and show a three-dimensional global orientation, etc. that increases the potential to be used in their electroluminescence device [1]. Electron enriched pyrene derivatives play an important role in the development of electroluminescence device due to easy workability, having a good thermal stability, high luminescence efficiency [2]. In this study, the conjugated pyrene derivative substituted dendrimeric cyclotriphosphazene compounds which have potential use as advanced materials were synthesized (Figure 1). Structural determinations of the obtained products were studied by MALDI-TOF mass spectrometry, FT-IR, $^{1}H$, and $^{31}P$ NMR. Thermal stability, photophysical properties and electroluminescence measurements of the synthesized compounds have been made and it has reached the conclusion that there is potential used in electroluminescence devices. Also, the theoretical calculations of compounds are studied.

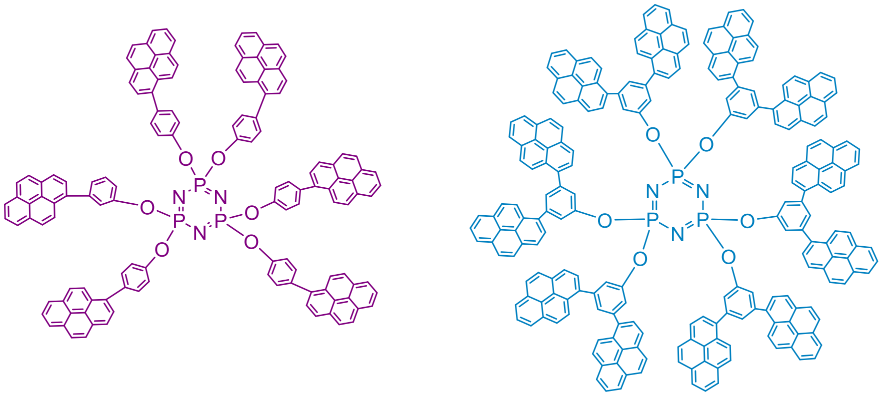


**Figure 1.** Pyrene substituted cyclotriphosphazenes

**References**
[1] J.K.P. Ng, C.M. Cho, J.M. Chin, K.L. Ke and C. He, J. Xu, Eur. Polym. J., 49 (2013) 2404-2414.
[2] Z. Wang, C. Xu, W. Wang, X. Dong, B. Zhao and B. Ji, Dyes and Pigm., 92 (2011) 732-736.

---

* Corresponding author, *E-mail: yesil@gtu.edu.tr*

P-138

# Investigation of Effects Anti-microbial against Pathogenic Microorganisms of Some Schiff Bases

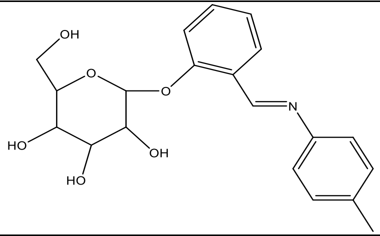
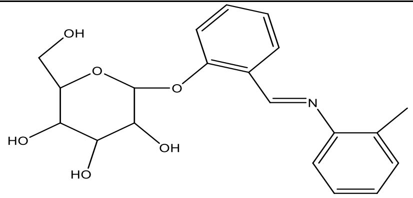
**Hatice Ögütcü[1]*, Seher Meral[2], Selçuk Çeker[3], Ayşen Alaman Ağar[2], Güleray Ağar[4] and Ferhat Kantar[1]**

[1]Ahi Evran University, Faculty of Science and Art, Department of Biology, Kırşehir, Turkey
[2]Ondokuzmayıs University, Faculty of Science and Art, Department of Chemistry, Samsun, Turkey
[3]Department of Basic Pharmaceutical Sciences, Faculty of Pharmacy, Ağrı İbrahim Çeçen University, Ağrı, Turkey
[4]Atatürk University, Faculty of Science, Department of Biology, Erzurum, Turkey

*E-mail:hogutcu@gmail.com*

In this study, we aimed to investigate for the first time anti-microbial activities new two Schiff bases, containing a primary amine and an aldehyde or a ketone. Antimicrobial activity of Schiff bases has been demonstrated for antibacterial activity against 10 pathogenic four Gram-positive bacteria and four Gram-negative bacteria and two yeasts (for their antimicrobial activity by the well-diffusion method) [1]. On the other hand, both of studied compounds were found effective against pathogenic bacteria and yeasts. Compound I exhibited more activity against *P. aeroginosa, S aureus, S.typhi H and C. albicans* comparable to Compound II and standard antibiotics (Table 1). Additionally, Compound II showed better activity *C. albicans* and *Br. abortus* (Compound I). Therefore, these compounds can be used inphytotherapeutic due to their antimicrobial activities.

**Table 1.** Structures and abbreviations of synthesized Schiff bases

| Compounds | Name of compounds | Structure of compounds |
|---|---|---|
| I | (*E*)-2-(hydroxymethyl)-6-(2-((*p*-tolylimino)methyl) phenoxy) tetrahydro-2*H*-pyran-3,4,5-triol |  |
| II | (*E*)-2-(hydroxymethyl)-6-(2-((*o*-tolylimino)methyl) phenoxy)tetrahydro-2*H*-pyran-3,4,5-triol |  |

**References**
[1] N. Sarı , N. Pişkin, H. Öğütcü and N. Kurnaz, Medicinal Chemistry Research, 22(2) (2013) 580-587.

---

[*] Corresponding author, *E-mail: hogutcu@gmail.com*

P -139

# Synthesis, Anti-Microbıal Activities of Some Schiff Bases Derivatives Containing Thiophene Group

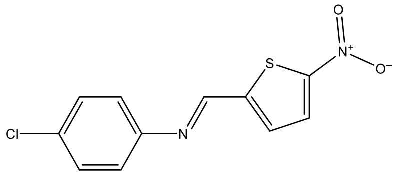
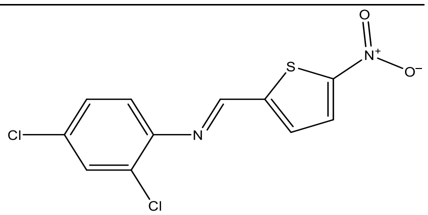
**Hatice Ögütcü[1]*, Selçuk Çeker[2], Seher Meral[3], Ayşen Alaman Ağar[3], GülerayAğar[4] and Hülya Avşar[1]**

[1]Ahi Evran University, Faculty of Science and Art, Department of Biology, Kırşehir, Turkey
[2]Department of Basic Pharmaceutical Sciences, Faculty of Pharmacy, Ağrı İbrahim Çeçen University, Ağrı, Turkey
[3]Ondokuzmayıs University, Faculty of Science and Art, Department of Chemistry, Samsun, Turkey
[4]Atatürk University, Faculty of Science, Department of Biology, Erzurum, Turkey

*E-mail:hogutcu@gmail.com*

The aim of this study is to investigate for the first time *in vitro* antimicrobial activities of Schiff bases included the azomethine group (Compound I and Compound II) (Table 1). These groups have been examined for antibacterial activity against 10 pathogenic strains (for their antimicrobial activity by the well-diffusion method) [1]. On the other hand, these compounds were also found to possess antimicrobial activity against some test bacteria and yeast. The antimicrobial test results of these Schiff bases included the azomethine group exhibited better activity than some known antibiotics. In particular, Compound I was more potent bactericides than all of the substances synthesized. In conclusion, these Schiff bases included the azomethine group can be used pharmacy industries as recognized with their antimicrobial.

**Table 1.** Structures and abbreviations of synthesized Schiff bases

| Compounds | Name of compounds | Structure of compounds |
|---|---|---|
| I | (E)-N-(4-chlorophenyl)-1-(5-nitrothiophen-2-yl) methanimine |  |
| II | (E)-N-(2,4-dichlorophenyl)-1-(5-nitrothiophen-2-yl) methanimine |  |

**References**
[1] N. Sarı, N. Pişkin, H. Öğütcü and N. Kurnaz, Medicinal Chemistry Research, 22**(**2) (2013) 580-587.

---

* Corresponding author, *E-mail: hogutcu@gmail.com*

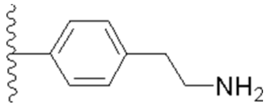
# Synthesis and Characterization of Novel Schiff Base Attached Polymers

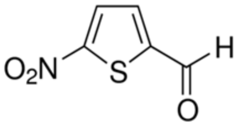
**Dilek Nartop**[1]* **and Erkan Tokmak**[2]

[1]Düzce University, Faculty of Technology, Department of Polymer Engineering, Düzce, Turkey
[2]Nevşehir Hacı Bektaş Veli University, Faculty of Arts and Science, Department of Chemistry, Nevşehir, Turkey

*E-mail: dileknartop@duzce.edu.tr*

Polymers containing imine (-CH=N-) group are called as polymeric-Schiff bases. Studies of Schiff base polymers have become important in recent years due to their antimicrobial properties, chemical resistance, semi-conductor /conductor properties, thermal stability, optical, electrical and catalytic properties [1,2]. In this paper, two novel Schiff base attached polymers are reported. The polymer-bound Schiff bases were prepared from condensation reaction of polystyrene-A-$NH_2$ and 5-nitro-2-thiophenecarboxaldehyde (or 5-(2-nitrophenylfurfural)) and characterized by elemental analyses, FT-IR, GPC and TGA analyses (Table 1).





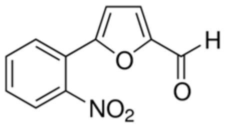


**Table 1.** FT-IR, GPS and analytical data of the modified polymers

| Chemical formula<br>Colour, $M_w$[a] | ($M_w$, $M_n$), PDI | ν(CH)$_{arom.}$ | ν(CH)$_{aliph.}$ | ν(C=N) | ν(C=C)$_{arom.}$ | ν(CSC) | ν(CO)$_{furan}$ | δ(CO)$_{furan}$ |
|---|---|---|---|---|---|---|---|---|
| $[(C_8H_8)_4(C_{15}H_{14}N_2O_2S)]$<br>Yellow, 702 | (763, 647), 1.18 | 3015 | 2889 | 1600 | 1546 | 697 | - | - |
| $[(C_8H_8)_5(C_{21}H_{18}N_2O_3)]$<br>Yellow, 866 | (876, 595), 1.47 | 3031 | 2892 | 1602 | 1544 | - | 1502 | 856 |

* Determined by elemental analyses

## References

[1] E. Dyer and C.C. Anderson, J. Polym. Sci., Polym. Chem., 5 (1967) 1659-1669.
[2] P. Phatak, V.S. Jolly and K.P. Sharma, Orient. J. Chem., 16 (3) (2000) 493-494.

---

* Corresponding author, *E-mail: dileknartop@duzce.edu.tr*

P-141

# Synthesis of New Indole Containing Polymeric-Schiff Bases

**Dilek Nartop[1]*, Mehmet Gündem[2], Elvan Hasanoğlu Özkan[3],**
**Nurdan Kurnaz Yetim[4] and Nurşen Sarı[3]**

[1]Düzce University, Faculty of Technology, Department of Polymer Engineering, 81620 Konuralp, Düzce, Turkey
[2]Nevşehir Hacı Bektaş Veli University, Faculty of Arts and Science, Department of Chemistry, 50300 Nevşehir, Turkey
[3]Gazi University, Faculty of Science, Department of Chemistry, Ankara, Turkey
[4]Kırklareli University, Faculty of Arts and Science, Department of Chemistry, Kırklareli

*E-mail: dileknartop@duzce.edu.tr*

Polymers including Schiff base and their metal complexes have been studied widely due to their high chemical activity, thermal stability, high ion selectivity, heat resistance and biological activity [1,2]. Furthermore, immobilization of enzymes onto this type polymeric nanoplatforms have attracted considerable attention due to their applications. This is the most useful strategy to improve the operational stability of biocatalysts [3]. In this research, two novel polymeric-Schiff bases were obtained from the condensation of (aminomethyl)polystyrene and indole-3-carboxaldehyde (or 2-methylindole-3-carboxaldehyde). Then, the polymeric-Schiff bases containing indol were characterized using elemental analyses, FT-IR, GPC and TGA analyses (Table 1).

**Table 1.** IR spectra, GPS and some analytical data and physical properties of the poylmeric-Schiff bases

| Chemical formula<br>Colour, $M_w$$^a$ | ($M_w$, $M_n$), PDI | ν(CH)$_{arom.}$ | ν(CH)$_{aliph.}$ | ν(C=N) | ν(C=C)$_{arom.}$ |
|---|---|---|---|---|---|
| $[(C_8H_8)_{10}(C_{18}H_{16}N)]$<br>Yellow, 1286 | (1385, 1087), 1.27 | 3043 | 2909 | 1651 | 1585 |
| $[(C_8H_8)_{10}(C_{19}H_{18}N_2)]$<br>Yellow, 1314 | (1329, 1201), 1.11 | 3014 | 2915 | 1614 | 1571 |

*Determined by elemental analyses

**References**
[1] T. Kaliyappan and P. Kannan, Prog. Polym. Sci., 25(3) (2000) 343-370.
[2] S. Banerjee and C. Saxena, J. Polym. Sci. Part A: Polym. Chem., 34(17) (1996) 3565-3572.
[3] S. Kayhan, N. Sarı and D. Nartop, Artif. Cells. Nanomed. Biotechnol., 43(4) (2015) 224-229.

---

* Corresponding author, *E-mail: dileknartop@duzce.edu.tr*

P -142

# Synthesis and Antibacterial Activity Evaluation of L-Aminoacid-Schiff Bases

**Elvan Hasanoğlu Özkan[1], İffet Şakıyan[2], Hatice Öğütcü[3] and Nurşen Sarı[1]***

[1]Gazi University, Faculty of Science, Department of Chemistry, Ankara, Turkey
[2]Ankara University, Faculty of Science, Department of Chemistry, Ankara, Turkey
[3]Ahi-Evran University, Faculty of Science, Department of Chemistry, Kırşehir, Turkey

*E-mail: nursens@gazi.edu.tr*

Amino acid-Schiff bases exhibit a wide range of biological activities and applications as [1] a marker in the study of biological processes: decarboxylation, transamination, electron transfer, *etc*. N and O containing ligands have become important due to their wide biological activity such as anti-HIV activities [2]. Over the recent decade, there has been a growing interest in the correlation between biological activities and molecule structures. This has been partially the result of reports concerned with the interaction of various chemicals including molecules and their some properties [3]. These properties can be of importance to understand biological activities on molecular structure. The aim of this work was to investigate the antibacterial and antifungal activities of L-amino acid-Schiff bases (L-a.a; L-Arginine, L-Glutamic Acid, L-Lysine). All these substances have been examined for antibacterial activity against pathogenic strains *L. monocytogenes* 4b ATCC19115, *S. aureus*, *E. coli*, *S. typhi H*, *B. abortus*, *S. epidermis*, *M. luteus* ATCC9341), and *Shigella dysenteria typ* 10 NCTC 9351.The antimicrobial test results of these amino acid-Schiff base exhibited better activity than some known antibiotics (Table 1).

**Table 1.** Antimicrobial activity of studied compounds (0.25 μg/ml) and standard reagents [diameter of zone inhibition (mm)]

| Microorganisms | | (Arg-NSch) | (Glu-NSch) | (Lys-NSch) | control |
|---|---|---|---|---|---|
| Gram (+) | *L.monocytogenes 4b* | 11 | 14 | 12 | - |
| | *B.cereus* | 12 | 11 | 17 | - |
| | *S.aureus* | - | 12 | 12 | - |
| | *S.epidermis* | 11 | - | 12 | - |
| | *M.luteus* | 12 | - | 12 | - |
| Gram (-) | *Sh.dys. typ 7* | 19 | 20 | 17 | - |
| | *P.putida* | 12 | 11 | 24 | - |
| | *S.typhi H* | 15 | 16 | 13 | - |
| | *Br. abortus* | 22 | 20 | 13 | - |
| | *E.coli* | 12 | 16 | 12 | - |

**References**
[1] M. Nath and R. Yadov, Bull. Chem. Soc. Jpn., 70 (1987) 1331-1337.
[2] S.S Kandil, G.Y Ali and A. El-Dissouky, Transition Met. Chem., 27 (2002) 398-406.
[3] N. Sarı, N. Pişkin, H. Öğütcü and N. Kurnaz, Med. Chem. Research, 22, (2013) 580-587.

---

* Corresponding author, *E-mail: nursens@gazi.edu.tr*

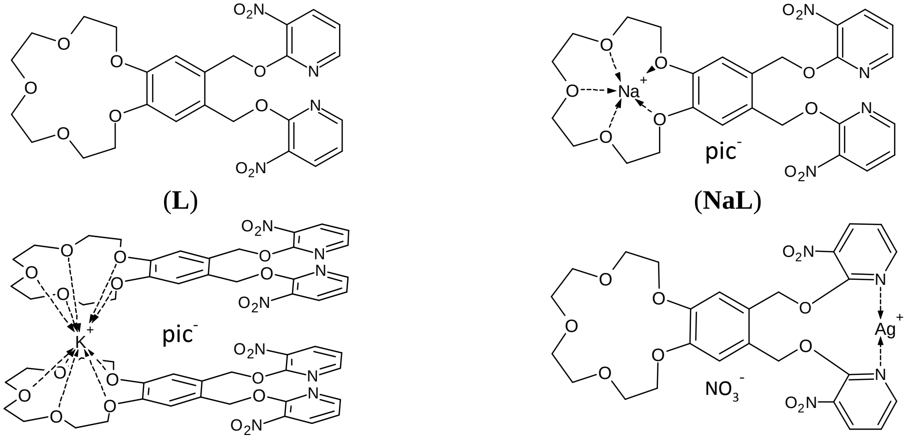
# Synthesis, Characterization and Antimicrobial Activities of New Crown Ether Compounds

**Serhat Koçoğlu**[1,2], **Hatice Ögütcü**[3], **Zeliha Hayvalı**[1]* **and Murat Güler**[3]

[1]Department of Chemistry, Ankara University, Faculty of Science, 06100, Ankara, Turkey
[2]Bozok University, Science and Technology Application and Research Center, Yozgat, Turkey
[3]Department of Biology, Faculty of Arts and Science, Ahi Evran University, Kırşehir, Turkey

*E-mail: skocoglu@outlook.com*

The best known and most striking characteristic of crown ethers is that they give stable complexes within the crown ether ring due to ionic-dipole interaction with alkali and alkaline earth metals, depending on the size of the cavities. In addition, crown ethers coordinate with other group metals, transition metals, lanthanides and actinide ions, by coordinating the substitute side groups [1]. In recent years, crown ether derivatives, which contain substituted side groups have shown great interest in chemistry because of spectroscopic properties, and biochemistry due to such applications like antimicrobial activities and DNA interactions [2-4]. In this study, new benzo-15-crown-5 ligand and its $Na^+$, $K^+$ and $Ag^+$ complexes which substituted with 2-hydroxy-3-nitro-pyridine were synthesized (Figure 1) and were characterized by spectroscopic methods (FT-IR, HR/MS, $^1$H-NMR and $^{13}$C-NMR). In addition to these, the synthesized compounds were examined for their antimicrobial activity against 12 pathogenic microorganism by the well-diffusion method. All the synthesized compounds and antibiotic exhibited varying degree of inhibitory effects on the growth of different tested strains.



(**L**) (**NaL**)

(**KL**$_2$) (**AgL**)

**Figure 1.** Synthesized ligand (**L**), sodium (**NaL**), potassium (**KL**$_2$) and silver (**AgL**) complexes

## References

[1] D. Liu, K. Tang, W. Liu, C. Su, X. Yan, M. Tan and Y. Tang, Dalton Transactions, 39 (2010) 9763-9765.
[2] D. Şahin, S. Koçoğlu, Ö. Şener, C. Şenol, H. Dal, T. Hökelek and Z. Hayvalı, J. Mol. Struct., 102 (2015) 302-313.
[3] Z. Hayvalı, H. Güler and H. Öğütçü, Med. Chem. Res., 23 (2014) 3652-3661.
[4] G.W. Gokel, W.M. Leevy and M.E. Weber, Chem. Rev., 104 (2004) 2723-2750.

---

* Corresponding author, *E-mail: zhayvali@science.ankara.edu.tr*

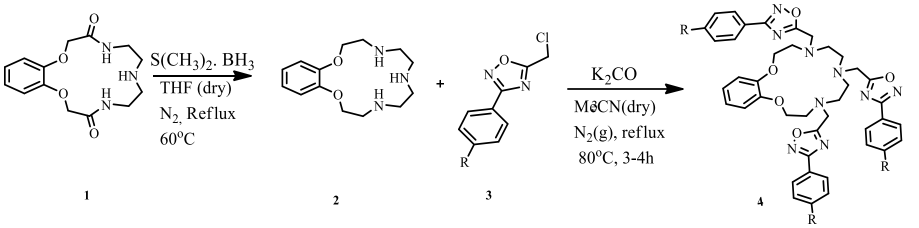
# Synthesis of Novel Aza-Crown Ethers Carrying 1,2,4-Oxadiazole Scaffold

**Besra Özer** and Yaşar Dürüst*

Abant İzzet Baysal University, Faculty of Science and Art, Department of Chemistry, 14030, Bolu, Turkey

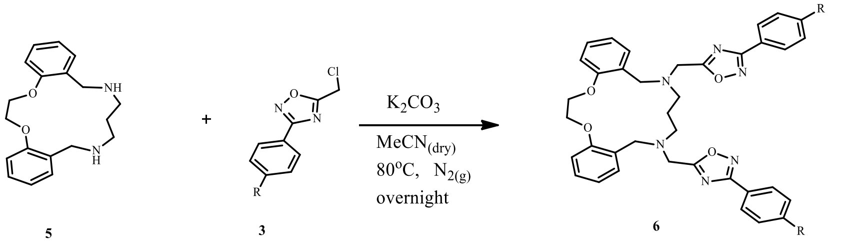
*E-mail: besrazer0454@gmail.com*

During the recent decades, a developing interest has been directed on the chemistry of nitrogen, oxygen-macrocycles and heterocycles bearing 1,2,4-oxadiazole as the publications showed. Because a great number of these compounds have been found to exhibit various biological activities and to serve as an ion, metal sensing capability [1-7]. We were inspired to conduct a synthetic sequence in order to prepare two series of 1,2,4-oxadiazolylmethyl-substituted benzodioxadetriaza (Figure 1) and benzodioxadiaza-crowns (Figure 2). Structures of the new macrocycles were identified by means of spectral/physical characteristics.



| | R | Yield(%) |
|---|---|---|
| a | H | 43 |
| b | $CH_3$ | 41 |
| c | $OCH_3$ | 48 |
| d | I | 48 |
| e | F | 51 |
| f | CI | 80 |
| g | Br | 67 |
| h | $SCH_3$ | 38 |

**Figure 1.** The synthesis of *p*-phenylsubstituted 1,2,4-oxadiazolylbenzodioxatriaza crowns (**4a-h**)



| | R | Yield(%) |
|---|---|---|
| a | H | 92 |
| b | CH3 | 95 |
| c | F | 89 |
| d | Cl | 84 |
| e | Br | 42 |
| f | $NO_2$ | 22 |
| g | $OCH_3$ | 70 |
| h | $SCH_3$ | 44 |

**Figure 2.** Synthesis of the *p*-phenylsubstituted 1,2,4,-oxadiazolylbenzodioxadiaza crowns (**6a-h**)

## References

[1] R. Krishnakumar and R. S. Swathi, ACS Appl Mater Interfaces, 9 (2017) 999-1010.
[2] M. Marjanović, M. Kralj, F. Supek, L.Frkanec, I. Piantanida,T. Šmuc and L. Tušek-Božić, J. Med. Chem., 50 (2007) 1007-1018.
[3] L. Nezbedova, M. Hesse, K. Drandarov and C. Werner, Tetrahedron Lett., 42 (2001) 4139-4141.
[4] W. Li, X. Yu and X. Wang, J Phys Chem C, 121 (2017) 1436-1441.
[5] Y.-F. Zhang, X.-P. Cao, H.-F. Chow and D. Kuck, J. Org. Chem., 82 (2017) 179-187.
[6] P. Bühlmann, E. Pretsch and E. Bakker, Chem. Rev., 98 (1998) 1593-1687.
[7] G.D. Diana, D.L.Volkots, T.J. Nitz, T.R. Bailey, M.A. Long, N.Vescio, S. Aldous, D.C. Pevear and F.J. Dutko, J. Med. Chem., 37 (1994) 2421-2436.

---

* Corresponding author, *E-mail: yasardurust@ibu.edu.tr*

P -145

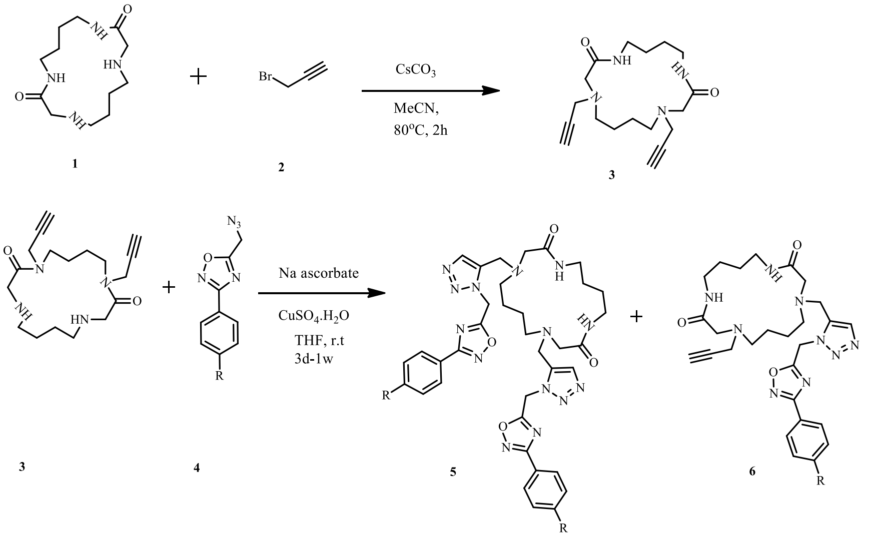
# 1,3-Dipolar Cycloadditions of Azamacrocycles Carrying Acetylenic Side Chain with Azidomethyl 1,2,4-Oxadiazoles

**Besra Özer** and Yaşar Dürüst*

Abant İzzet Baysal University, Faculty of Science and Art, Department of Chemistry, 14030, Bolu, Turkey

*E-mail: besrazer0454@gmail.com*

Azacrowns, that contain one or more nitrogen, have attracted remarkable attention due to their biological and environmental properties [1-4]. On the other hand, 1,2,4-oxadiazole and 1,2,3-triazole containing heterocyclic compounds exhibit various biological activities [5-8]. In this study, 1,3 dipolar cycloaddition reactions of 3-aryl substituted 5-azidomethyl 1,2,4-oxadiazoles 4 with the tetraza macrocycle 3 afforded fourteen novel cycloadducts (Figure 1). Their structures were elucidated by means of IR, NMR ($^1$H,$^{13}$C), LC-MS spectra.



| R | | Yield(%) | |
|---|---|---|---|
| | | **5** | **6** |
| **a** | H | 73 | 38 |
| **b** | CH$_3$ | 53 | 44 |
| **c** | F | 61 | 43 |
| **d** | Cl | 42 | 40 |
| **e** | Br | 71 | 38 |
| **f** | NO$_2$ | 41 | 35 |
| **g** | OCH$_3$ | 46 | 36 |
| **h** | SCH$_3$ | 41 | 38 |

**Figure 1.** Synthesis and cycloadditions of macrotetrazacycles **3** leading to cycloadducts **5** and **6**

## References

[1] P. Bühlmann, E. Pretsch and E. Bakker, Chem. Rev., 98 (1998) 1593-1687.
[2] L. Nezbedova, M. Hesse, K. Drandarov and C. Werner, Tetrahedron Lett., 42 (2001) 4139-414.
[3] B. Valeur and I. Leray, Coord. Chem. Rev., 205 (2000) 3–4.
[4] T.P. Quinn, P.D. Atwood, J.M. Tanski, T.F. Moore and J.F. Folmer-Andersen, J. Org. Chem., 76 (2011) 10020-10030.
[5] N. Takayuki, N. Susumu, T. Kiyoshi, M. Kenji, F. Kei-Ichi, K. Hiroshi and J. Antibiot, 21 (1998) 300-305.
[6] C. Lamberth, Heterocycles, 71 (2007) 1467-1502.
[7] M. Yıldırım and Y. Dürüst, Tetrahedron, 6 (2011) 3209-3215.
[8] B.E. Fink, D.S. Mortensen, S.R. Stauffer, Z.D. Aron and J.A. Katzenellenbogen, Chem. Biol., 6 (1999) 205-219.

---

* Corresponding author, *E-mail: yasardurust@ibu.edu.tr*

# Synthesis of Significant New Mannich Bases Containing Antipyrine, Triazole, Ciprofloxacin and Norfloxacin Groups - Biological Activity Studies

**Hacer Bayrak**[1]*, **Yıldız Uygun Cebeci**[2], **Arif Mermer**[2] **and Neslihan Demirbaş**[2]

[1]Karadeniz Technical University, Maçka Vocational School, Department of Chemistry and Chemical Processing Technology, 61750, Trabzon, Turkey
[2]Karadeniz Technical University, Faculty of Science, Department of Chemistry, 61080, Trabzon, Turkey

*E-mail: h.bayrak@ktu.edu.tr*

In recent years, the concept of hybrid molecules which contain two or more pharmacophores bound together covalently in one molecular framework has been introduced. It has been suggested that such compounds may inhibit two or more conventional targets simultaneously. This multiple target strategy has already resulted in the development of a number of bioactive hybrid molecules [1]. Triazoles have considerable biological importance and are effective as antibacterial, antifungal, antimycobacterial, antiviral, anti-inflammatory, anticonvulsant, antidepressant, antitubercular, antitumoral, antihypertensive and analgesic activities, respectively [2]. Mannich bases have gained importance due to their application in pharmaceutical chemistry. Mannich bases have been found to possess antibacterial, antifungal, anticancer, antitubercular, analgesic and anti-inflammatory properties. With all these Based on all these data, new hybrid compounds shown in Figure 1 were synthesized and their biological activities were examined.

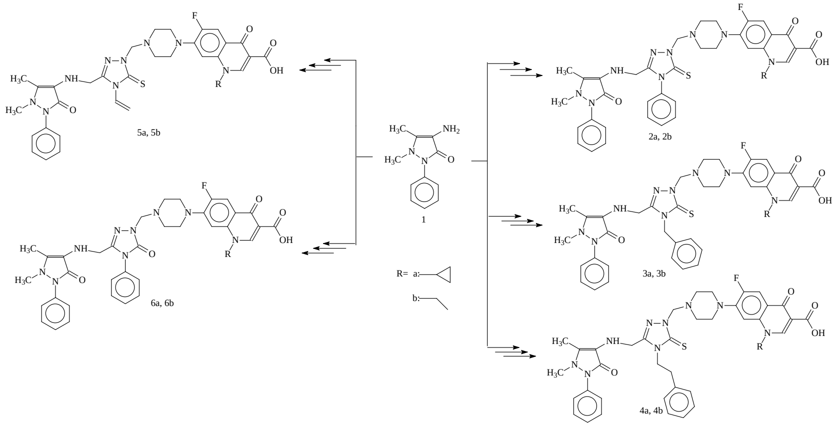


**Figure 1.** Synthetic route for the new Mannich Bases containing antipyrine, triazole, ciprofloxacin and norfloxacin groups

## References

[1] S.B. Özdemir, Y.U. Cebeci, H. Bayrak, A. Mermer, S. Ceylan., A. Demirbas, S.A. Karaoglu and N. Demirbas, Heterocycl. Commun., 23(1) (2017) 43-54.
[2] H. Bayrak, A. Demirbas, N. Demirbas and S.A. Karaoglu, Eur. J. Med. Chem., 44 (2009) 4362-4366.

## Acknowledgement

This study is supported by a grant (Project Number: KTU-BAP-FBB-2015-5289) from Karadeniz Technical University Scientific Research Project.

---

* Corresponding author, *E-mail: h.bayrak@ktu.edu.tr*

P -147

# Synthesis of Some New Schiff Bases Containing Azole Rings Starting from Phenylpiperazine and Investigating Their Antimicrobial and Antioxidant Activity

**Hacer Bayrak**[1]*, Arif Mermer[2], Neslihan Demirbaş[2] and Yakup Şirin[2]

[1] Karadeniz Technical University, Maçka Vocational School, Department of Chemistry and Chemical Processing Technology, 61750, Trabzon, Turkey
[2] Karadeniz Technical University, Faculty of Science, Department of Chemistry, 61080, Trabzon, Turkey

*E-mail: h.bayrak@ktu.edu.tr*

Azoles have considerable biological importance such as 1,3,4-thiadiazoles and 1,3,4-oxadiazoles both have been reported as antibacterial, antifungal, antimycobacterial, antiviral, anti-inflammatory, anticonvulsant, antidepressant, antitubercular, antitumoral, antihypertensive and analgesic activities, respectively [1]. Linezolid and Eperezolid are currently used antibiotics against microbial infections and they contain Piperazine ring in their structure [2]. Schiff base derivatives of azoles are also important molecules and have a large biological activity [2]. In this study we have synthesized new compounds starting from phenylpiperazine to afford different Schiff bases containing different heterocyclic groups in one molecule (Figure 1). All newly synthesised compouns were screened or their antimicrobial and antioxidant activity.

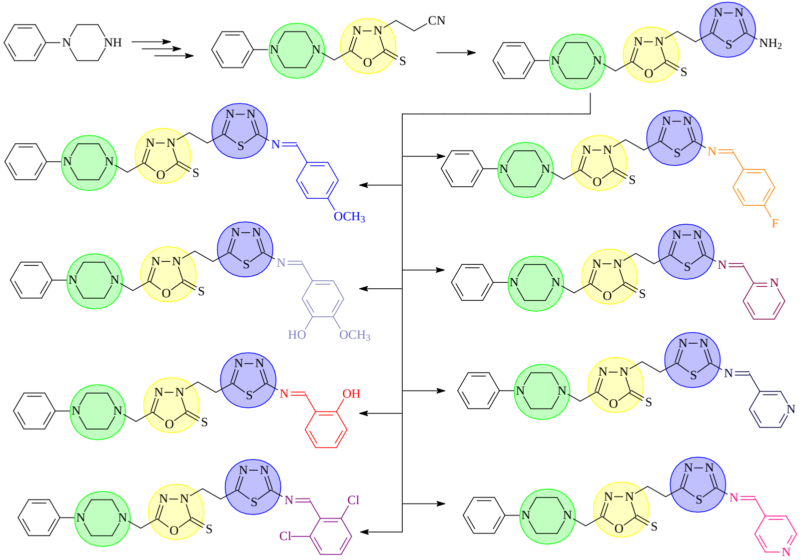


**Figure 1.** Synthetic route of new Schiff Bases

**References**
[1] N.C. Desai, G.M. Kotadiya, A.R. Trivedi, V.M. Khedkar and P.C. Jha, Med. Chem. Res., 25 (2016) 712-727.
[2] H. Bayrak, A. Demirbaş, S.A. Karaoglu and N. Demirbaş, Eur. J. Med. Chem., 44 (2009) 1057-1066.

**Acknowledgement**
This study is supported by a grant from Scientific and Technological Research Council of Turkey (TUBITAK) (Project Number: 115Z770).

---

* Corresponding author, *E-mail: h.bayrak@ktu.edu.tr*

P -148

# Investigation of Herbicide Effects on Cress (*Lepidium sativum L.*) Seeds of Some Disubstituted-imidazole and Disubstituted-imidazo[1,2-a]pyrazine Compounds

**İsmail Kayağil* and Leyla Çakıcı**

Mehmet Akif Ersoy University, Faculty of Science and Arts, Department of Chemistry, 15030, Burdur, Turkey

*E-mail: ikayagil@mehmetakif.edu.tr*

Today, there are many developments related to agricultural products. The term "organic farming" is replaced by the term "good agricultural product". The recommended method for this is to apply the appropriate amount of medication at the appropriate time. For this purpose, agrochemicals (pesticides) are used to combat harmful grasses, harmful insects, harmful rodents and plant diseases. One of the most common among the pesticides is herbicides. Herbicides are used to combat weeds [1]. In this study, 18 imidazoles (Figure 1) and 18 imidazo[1,2-a]pyrazine compounds (Figure 2) derived therefrom, which are thought to be herbicides, have been selected. These 36 compounds were previously synthesized and published [2]. Herbicide studies were carried out by germinating cress (*Lepidium sativum L.*) seeds. This survey, which is made according to the lengths of the roots of the seeds, is a common method used in the literature. Biological activity results are given as $TD_{50}$.

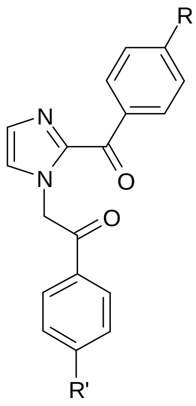


**Figure 1.** The imidazoles

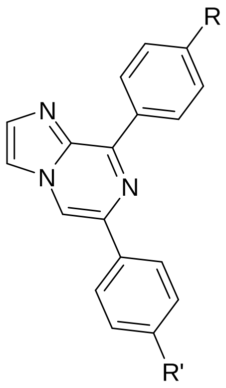


**Figure 2.** The imidazo[1,2-a]pyrazines

**References**

[1] N.E. Zazueta, O.O. Acosta, L.M. Herrera, R.A. Vazquez, E.L. Lopez, A.G. Zuniga and A.R. Dorantes, American Journal of Plant Sciences, 4 (2013) 2199-2205.
[2] İ. Kayağil and Ş. Demirayak, Journal of Heterocyclic Chemistry, 42 (2005) 319-325.

**Acknowledgement**

This study was supported by the project numbered 1919B011400418 under The TÜBİTAK 2209-A program.

---

* Corresponding author, *E-mail: ikayagil@mehmetakif.edu.tr*

# Investigation of Herbicide Effects on Cress (*Lepidium sativum L.*) Seeds of Some Tetrasubstituted-imidazo[1,2-a]pyrazine Compounds

**İsmail Kayağil*** **and Caner Baltacı**

Mehmet Akif Ersoy University, Faculty of Science and Arts, Department of Chemistry, 15030, Burdur, Turkey

*E-mail: ikayagil@mehmetakif.edu.tr*

The method which is applied nowadays to obtain quality agricultural product medicates with the right dose on the right time. Agricultural medicines are generally known as pesticides. The mostly used one of them is herbicides without doubt. The weed is also very important for agriculture [1]. In this study, the cress (*Lepidium sativum L.*) seeds were chosen as a model organism to weed. The 27 synthesized and published compounds [2] (Figure 1) were tested on the seeds and the results according to the root growth were reported.

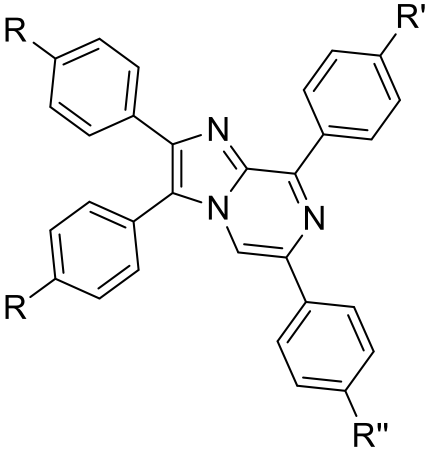


**Figure 1.** The synthesized and published compounds

**References**

[1] N.E. Zazueta, O.O. Acosta, L.M. Herrera, R.A. Vazquez, E.L. Lopez, A.G. Zuniga and A.R. Dorantes, American Journal of Plant Sciences, 4 (2013) 2199-2205.
[2] İ. Kayağil and Ş. Demirayak, Turkish Journal of Chemistry, 35 (2011) 13-24.

**Acknowledgement**

This study was supported by the project numbered 1919B011400348 under The TÜBİTAK 2209-A program.

---

* Corresponding author, *E-mail: ikayagil@mehmetakif.edu.tr*

P -150

# *N*-(Allylcarbamothioyl)thiophene-2-carboxamide Ligand and Its Transition Metal Complexes: Synthesis, Characterization and Thermal Properties

**Ali İhsan Karaçolak[1], Fatih Mehmet Emen[1]*, Ruken Esra Demirdöğen[2], Zeynep Yıldırım[1], Derya Kılıç[1], Göktürk Avşar[3], Zehra Gülten Altın[2] and Tuncay Yeşilkaynak[4]**

[1]Mehmet Akif Ersoy University, Faculty of Arts and Science, Department of Chemistry, 15100, Burdur, Turkey
[2]Çankırı Karatekin University, Faculty of Science, Department of Chemistry, 18100, Çankırı, Turkey
[3]Mersin University, Faculty of Arts and Science, Department of Chemistry, 33100, Mersin, Turkey
[4]Afsin Vocational High School, Sütçü İmam University, TR46500, Kahramanmaraş, Turkey

*E-mail: alikaracolak@hotmail.com*

Study of the thiourea derivatives has recently attracted interest in view of the potential use of these compounds as highly selective reagents for the concentration and separation of metal cations. These derivatives have also been implemented in a solid supported liquid membrane system for the selective transport of palladium and gold ions [1]. In this study, we synthesized new thiourea derivative ligand, *N*-(allylcarbamothioyl)thiophene-2-carboxamide, and it's Ni(II), Cu(II) and Co(II) complexes according to literature [2]. The synthesis steps are given in Figure 1. The obtained ligand and complexes were characterized by $^1$H-NMR and FT-IR spectrometers. Thermal behaviors of the compounds were also investigated DTA/TG techniques.

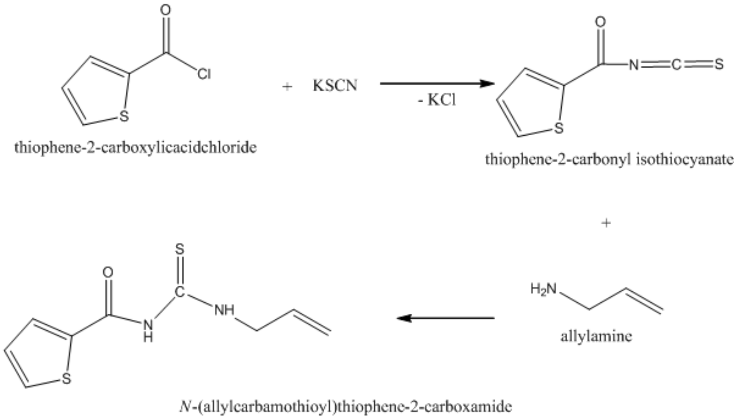


**Figure 1.** The synthesis reactions of the ligand.

**References**
[1] E. Anticó, A. Masana, M. Hidalgo, V. Salvadó and M. Valiente, Hydrometallurgy, 35 (1994) 343-352.
[2] F.Z. El Aamrani, A. Kumar, L. Beyer, J.L. Cortina and A.M. Sastre, Hydrometallurgy, 50 (1998) 315-330.

---

* Corresponding author, *E-mail: femen@mehmetakif.edu.tr*

P-151

# Electrophilic Amination of Arylcadmium Iodides with Ketoximes

**Tahir Daşkapan[1] and Adem Korkmaz[2]***

[1]Ankara University, Science Faculty, Department of Chemistry, Ankara-Turkey
[2]Muş Alparslan University, Technical College Vocational School, Muş-Turkey

*E-mail: a.korkmaz@alparslan.edu.tr*

A number of methods have been developed for the synthesis of arylamines. Among these methods, the electrophilic amination method is an important and frequently used because of suitable reaction conditions [1-3].

In this work, an easily applicable method was developed for electrophilic amination of arylcadmium iodides with oximes. The applicability of this method from the view of arylcadmium reagent using various functionalized arylcadmium iodides and from the view of oxime using acetone *o*-(4-fluorophenylsulfonyl)oxime and acetone *o*-(methylsulfonyl)oxime, as electrophilic amination reagents (Figure 1). Corresponding functionalized aryl amines were obtained in good yields.

$$\mathrm{ArCdI} + (\mathrm{CH_3})_2\mathrm{C{=}NOSO_2LG} \xrightarrow{\mathrm{CuCN}} \left[(\mathrm{CH_3})_2\mathrm{C{=}NAr}\right] \xrightarrow{\mathrm{Conc.\ HCl}} \mathrm{ArNH_2}$$

Ar : Phenyl, 4-methylthiophenyl, 4-methoxyphenyl, 3-methoxyphenyl, 4-chlorophenyl,
3-chlorophenyl, 3,5-dichlorophenyl, 3,5-dimethoxyphenyl, 4-methylphenyl,
2,5-Dimethylphenyl, 4-fluorophenyl, 4-chloro-2-methylphenyl, 1-naphtyl.

LG : 4-Fluorophenyl, Methyl

**Figure 1.** Aryl C-N bond formation by electrophilic amination of arylcadmium reagents

All reactions involving organocadmium reagents were performed in flame-dried glassware with standard syringe/cannula techniques under an atmosphere of dry, oxygen-free argon. Arylamines as the final products were isolated as their *N*-benzoyl derivatives and these known compounds were identified from their melting points and $^1$H NMR spectra.

## References

[1] T. Daşkapan, Arkivoc, (2011) 230-262.
[2] A. Ricci, Amino Group Chemistry, From Synthesis to the Life Sciences; Wiley-VCH: Weinheim, (2007).
[3] E. Ciganek, Organic Reactions, (Editor: S.E. Denmark), John Wiley and Sons, Inc., 72 (2009).

## Acknowledgements

Financial supports from Ankara University Research Fund (grant no. 15L0430009) and Turkish Higher Education Council (ÖYP Program) are greatly acknowledged by the authors

---

* Corresponding author, *E-mail: a.korkmaz@alparslan.edu.tr*

P-152

# Reaction of Rhodamine 6G with Indole-3-carbaldehyde Derivatives

**Ayşegül Atmaca, İbrahim Evren Kıbrız* and Mustafa Saçmacı**

Bozok University, Faculty of Arts and Science, Department of Chemistry, 66100, Yozgat, Turkey

*E-mail:e.kibriz@hotmail.com*

Rhodamine dyes are widely used as laser dyes [1], fluorescence standards [2], single-molecule imaging agents [3], fluorescent markers in biological studies [4,5] and chemosensors [6,7] due to their excellent photophysical properties, such as long absorption and emission wavelength, high fluorescence quantum yield, large extinction coefficient and high photostability. In this study, a new Rhodamine 6G compound was synthesized from the reaction of Rhodamine 6G with indole-3-carbaldehyde derivatives (Figure 1). The product was characterized with molecular spectroscopic techniques (FT-IR, $^1$H-NMR and $^{13}$C-NMR) and HRMS analysis.

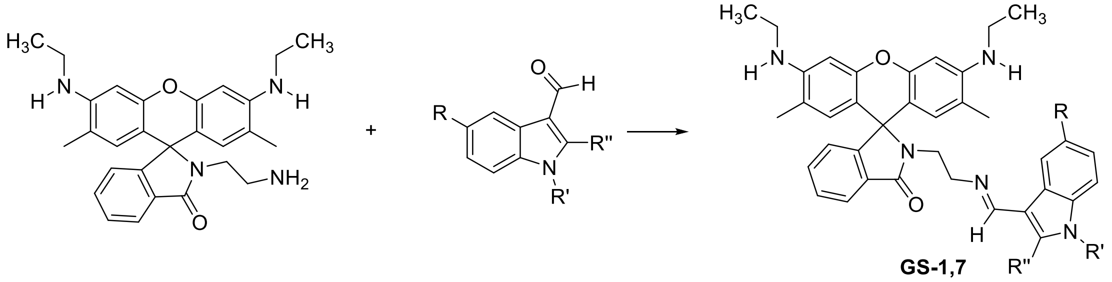


**Figure 1.** Synthesis GS-1,7 Compounds

**References**

[1] K.H. Drexhage, Laser Focus, 9 (1973) 35-39.
[2] T. Karstens and K. Kobs, J. Phys. Chem., 84 (1980) 1871-1872.
[3] M. Bossi, J. Folling, V.N. Belov, V.P. Boyarskiy, R. Medda, A. Egner, C. Eggeling, A. Schonle and S.W. Hell, Nano Lett., 8 (2008) 2463-2468.
[4] Z. Zhou, M Yu, H. Yang, K. Huang, F. Li, T. Yi and C. Huang, Chem. Commun., 29 (2008) 3387-3389.
[5] W. Liu, M. Howarth, A.B. Greytak, Y. Zheng, D.G. Nocera, A.Y. Ting AY and M.G. Bawendi, J. Am. Chem. Soc., 130 (2008) 1274-1284.
[6] V. Dujols, F. Ford and A.W. Czarnik, J. Am. Chem. Soc., 119 (1997) 7386-7387.
[7] M. Beija, C.A.M. Afonso, Chem. Soc. Rev., 38 (2009) 2410-2433.

---

* Corresponding author, *E-mail: e.kibriz@hotmail.com*

# 5-*endo*-dig Cyclisations of *N*-alkynyl Proline Ester Derivatives

**Muhammet Yıldırım**[1]*, **Hamza Karakuş**[2] **and Garba Suleiman**[1]

[1]Abant İzzet Baysal University, Faculty of Arts and Sciences, Department of Chemistry, 14030, Gölköy, Bolu, Turkey
[2]Abant İzzet Baysal University, Technology Transfer Application and Research Center, Bolu, Turkey

*Email: muhammetyildirim@ibu.edu.tr*

Sonogashira coupling is one of the best methods for constructing new C-C bonds [1] and the examples of copper co-catalyzed Sonogashira cross-coupling reactions have been well-described in the literature [2]. The mechanisms controlling the formation of different heterocycles (or carbocycles) are known as the Baldwin's rules which describe and classify ring closure steps by geometric and orbital overlapping manner to predict the favored products [3]. The cyclisations of alkyne systems to give 5- or 6-membered rings are all favorable over 5-(or 6-)endo-dig and 5-(or 6-)exo-dig mechanisms by Baldwin's rules. Furthermore, carbocyclization reactions give the ring formation of a system by either in intra- or inter-molecular pattern affording new C-C or C-heteroatom bonds [4]. Fused ring systems can be obtained from unactivated alkynes by an intramolecular alkyne carbocyclization by strong non-nucleophilic bases such as KHDMS or LiHDMS [5]. In the current work, the terminal alkynes **3** on proline esters were coupled with aryl iodides to generate aryl substituted *N*-alkynyl proline esters (**5**) in very mild conditions. Then, new pyrrolizine derivatives were obtained via LiHMDS or KHMDS-mediated carbocyclizations of *N*-alkynyl prolines (**5**) and the variety of new pyrrolizines (**6**) were obtained in good to excellent yields.

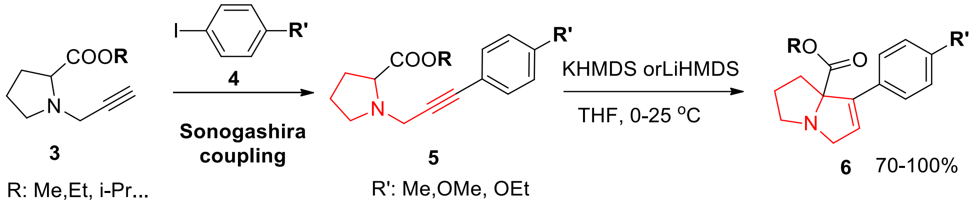


**Figure 1.** Route for preparation of aryl substituted pyrrolizine esters

The cyclisation products (**6**) have been isolated by the FCC and after the purification they were fully characterized by means of IR, proton and carbon NMR and HRMS analyses. In HRMS spectra of all products (**6**), the molecular ions have been found as $MH^+$ accurately by ESI-TOF-MS, which were in accordance with calculated accurate masses.

## References

[1] K. Bera, S. Sarkar, S. Biswas, S. Maiti and U. Jana, Eur. J. Org. Chem., 76 (2011) 3539-3544.
[2] M. Alami, F. Ferri and G. Linstrumelle, Tetrahedron Lett., 34 (1993) 6403-6406.
[3] J.E. Baldwin, Journal of the Chemical Society, Chemical Communications, 18 (1976) 734-736.
[4] O. Kitagawa, T. Suzuki, T. Inoue, Y. Watanabe and T. Taguchi, J. Org. Chem., 63 (1998) 9470-9475.
[5] C. Kourra, F. Klotter, F.Sladojevich and D.J. Dixon, Org. Lett., 14 (2012) 1016-1019.

---

* Corresponding author, *E-mail: muhammetyildirim@ibu.edu.tr*

P-154

# Synthesis and Characterization of New Ferrocene Substituted Compounds

**Hakan Aslan*** and Atilla Öktemer

Ankara University, Faculty of Science, Department of Chemistry, 06100, Ankara, Turkey

*E-mail: haslan@science.ankara.edu.tr*

Ferrocene has attracted very much attention due to the presence of both organic and inorganic properties, high thermal stability, good solubility in organic solvents, easy synthesis, and reversible redox properties. Ferrocene derivatives are used as homogeneous catalysts, chemo- and biosensors, asymmetric ligands, non-linear optical materials, conductive polymers. In addition, ferrocene compounds and ferrocenium salts have strong antitumor activities [1]. Furan, benzofuran and pyrimidine derivatives form the basic structure of many natural compounds and show a wide range of biological activities. Besides, these compounds are used as substrates for the synthesis of many polyfunctional organic compounds [2,3]. Furan compounds can easily prepare by the oxidative cyclization reaction of an active methylene compound and an unsaturated system mediated by transition metal salts ($Mn^{3+}$, $Ce^{4+}$, $Cu^{2+}$, etc.). Manganese(III) acetate has introduced differences in the field of free radical chemistry, due to its selectivity, specificity, mild and efficient reaction conditions [4]. In this study, manganese(III) acetate mediated oxidative cyclization reactions of ferrocene substituted alkene and active methylene compounds have been carried out. As a result, ferrocene substituted dihydrofuran, benzofuran and pyrimidine derivatives with a potential of showing biological activity were obtained. The uses of ferrocene substituted alkenes in the manganese(III) acetate mediated radical reactions is the first example in this field as far as we know.

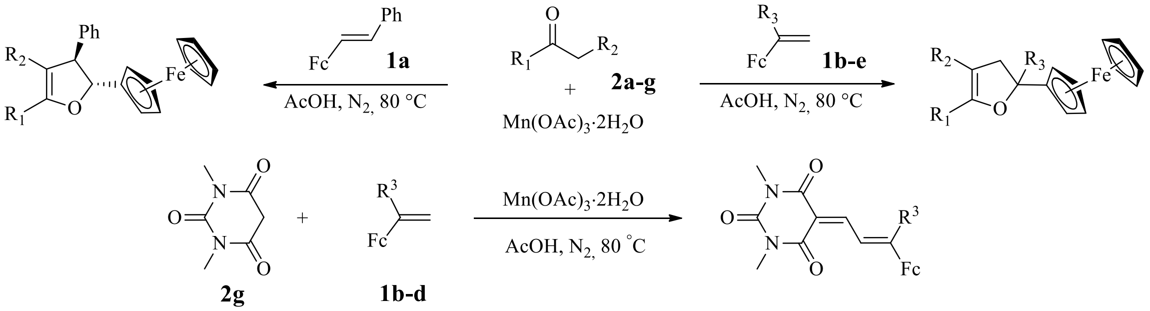


**Figure 1.** Synthesis of new ferrocene substituted compounds

## References

[1] S.S. Braga and A.M.S. Silva, Organometallics, 32 (2013) 5626-5639.
[2] X. Jiang, W. Liu, W. Zhang, F. Jiang, Z. Gao, H. Zhuang and L. Fu, Eur. J. Med. Chem., 46 (2011) 3526-3530.
[3] C. Kao and J. Chern, J. Org. Chem., 67 (2002) 6772-6787.
[4] A.S. Demir and M. Emrullahoglu, Curr. Org. Synth., 4 (2007) 223-237.

## Acknowledgement

We gratefully acknowledge financial support from the Scientific and Technical Research Council of Turkey (TUBITAK) (No: 115Z079).

---

* Corresponding author, *E-mail: haslan@science.ankara.edu.tr*

P-155

# The Synthesis and Cytotoxic Activities of *N(1)*, *N(4)*-Di-substitue-salicylidene-S-methyl- isothiosemicarbazidato Nickel(II) Complexes

**Tülay Bal Demirci[1]*, Serap Erdem Kuruca[2] and Bahri Ülküseven[1]**

[1]İstanbul University, Faculty of Engineering, Department of Chemistry, 34320 Avcılar, İstanbul, Turkey
[2]İstanbul University, İstanbul Medical Faculty, Physiology Department, İstanbul, Turkey

*E-mail: tulaybal@istanbul.edu.tr*

Thiosemicarbazones have a wide range of pharmacological activities. These biological effects were observed as early as the 1950s. After the antibacterial effect of thiosemicarbazide derivatives were reported, thiosemicarbazones have raised considerable interest, and so numerous articles on the biologic potential of various thiosemicarbazones have been published. In the last 20 years, several thiosemicarbazone complexes having biological activity were synthesized. It is known that S-methyl thiosemicarbazone complexes have cytotoxic effects. [1-3].

In this work, Ni (II) template complexes of *ONNO* type are presented (Figure 1). The template products were characterized by elemental analysis, magnetic susceptibility, $^{1}$H-NMR and FT-IR spectroscopy.

The cytotoxic effects of the complexes and thiosemicarbazon ligands were evaluated by MTT test for K562 chronic myeloid leukemia cell line. The complexes have shown significantly cytotoxic effects by reducing cell viability.

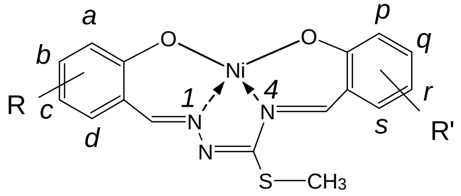


**Figure 1.** The general formula of nickel (II) complexes

**References**

[1] T.S. Lobana, R. Sharma, G. Bawa and S. Khanna, Coord. Chem. Rev., 253(7–8) (2009) 977-1055.
[2] T. Bal-Demirci, M. Sahin, E. Kondakçı, M. Ozyürek, B. Ulküseven and R. Apak, Spectrochim. Acta A, 138 (2015) 866-872.
[3] T. Bal, B. Atasever, Z. Solakoğlu, S. Erdem-Kuruca and B. Ulkuseven, Eur. J. Med. Chem., 42(2) (2007) 161-167.

---

* Corresponding author, *E-mail: tulaybal@istanbul.edu.tr*

# Solid-Phase Photocatalytic Degradation of PMMA/$TiO_2$ Composite Nanofiber Film

**Özcan Köysüren**[1]* **and Hafize Nagehan Köysüren**[2]

[1]Ankara University, Faculty of Engineering, Department of Energy Engineering, 06830, Ankara, Turkey
[2]Ahi Evran University, Faculty of Engineering and Architecture, Department of Environmental Engineering, 40100, Kırşehir, Turkey

*E-mail: koysuren@ankara.edu.tr*

Pure poly(methyl methacrylate) (PMMA) nanofiber and PMMA/titanium dioxide ($TiO_2$) composite nanofiber films were prepared by electrospinning method and the photocatalytic degradation of solid-phase PMMA was investigated. $TiO_2$ nanoparticles were first prepared by sol-gel process [1] and then embedded into the commercial PMMA through the electrospinning. The as-prepared films were characterized by scanning electron microscopy, FTIR and the photoinduced weight loss. The weight loss of the as-prepared films depended on the irradiation time. The weight loss percent of the composite nanofiber mat reached about 4% after 192 h irradiation, while pure PMMA nanofiber mat presented only about 1% of weight loss at the same experimental condition (Figure 1).

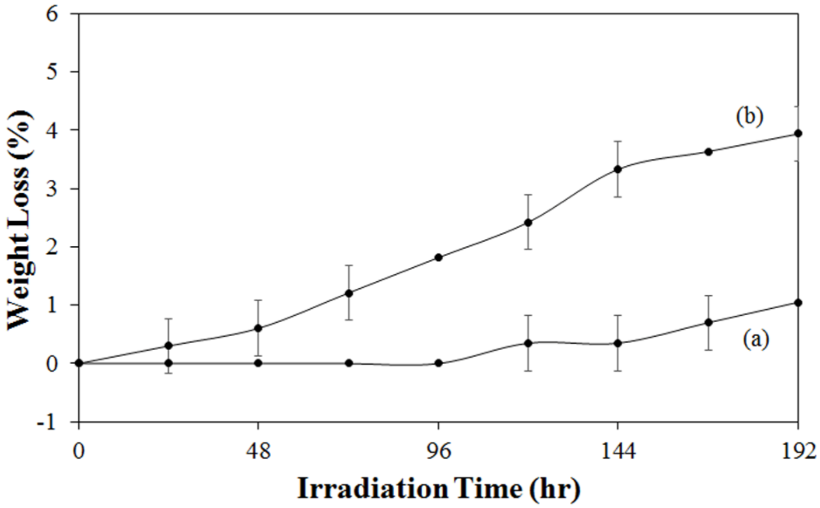


**Figure 1.** Weight loss curve of a) pure PMMA nanofiber film and b) PMMA/$TiO_2$ composite nanofiber film under UV illumination in air

**References**

[1] N. Agoudjil and T. Benkacem, Desalination, 206 (2007) 531-537.

---

* Corresponding author, *E-mail: koysuren@ankara.edu.tr*