

# POSTER PRESENTATIONS

Physical and Theoretical Chemistry

(PTC)





## **Influence of preparation process on viscoelastic properties of two emulsion formulations**

**Elezović A.<sup>a</sup>, Kostić S.<sup>b</sup>, Hadžiabdić J.<sup>a</sup>, Rahić O.<sup>a</sup>, Vranić E.<sup>a</sup>, Vehabović M.<sup>b</sup>**

<sup>a</sup>*Department of Pharmaceutical Technology, Faculty of Pharmacy, University of Sarajevo, Zmaja od Bosne 8, 71000*

*Sarajevo*

<sup>b</sup>*Bosnalijek, d.d. Sarajevo, Jukićeva 53, 71000 Sarajevo*

### **Keywords:**

rheology,  
viscoelastic properties,  
cosmetic emulsions

**Abstract:** Rheological properties are crucial for cosmetic formulations, determining product's properties during production and application. O/W emulsions (pH 6.86–7.10) were prepared with decyl-oleate as internal phase. A-formulations contained K-stearate, while N-formulations contained polyglyceryl-stearate and -behenate as principal emulsifiers. The formulations were prepared by adding the water to the oil phase (NA and AA) or vice versa (NB and AB). Oscillatory measurements were performed on Haake RheoStress using double gap cylinder. In amplitude sweep at low stresses all samples behaved as viscoelastic solids. With increasing stress, phase angles increased to  $>80^\circ$ . Crossover of storage and loss moduli for AA happened at nine times higher stress compared to the other formulations, forming lamellar crystalline gel network. Linear viscoelastic region showed that AA was much more stabile. Frequency sweep showed NA and AB to be liquid-like, but crossover of storage and loss moduli and decrease of phase angle indicate poor spreadability at faster rubbing rates. In NB and AA decrease in complex viscosity indicates better spreadability. Stability of phase angles and storage and loss moduli indicate more elastic behavior. New nonionic emulsifier was more independent of processing, unlike anionic emulsifier. However, AA formulation gives much better feel properties, needed in cosmetic formulations.

### **Corresponding author:**

Alisa Elezović

### **E-mail:**

alisa.elezovic@ffsa.unsa.ba

Tel: +38733586173

Fax:

### **Sažetak**

Reološke osobine su ključne za kozmetičke formulacije, budući da određuju osobine proizvoda tokom njegove proizvodnje i aplikacije. A-formulacije su sadržavale K-stearat, a N-formulacije poligliceril-stearat i -behenat, kao glavne emulgatore. Formulacije su pripremljene dodajući vodu u masnu fazu (NA i AA) ili obrnuto (NB i AB). Oscilatorna mjerenja su izvršena na Haake RheoStress korištenjem cilindra sa duplim zazorom. Pri promjeni amplitude, kod niskih napona smicanja svi uzorci su se ponašali kao viskoelastična čvrsta tijela. Povećanjem napona smicanja, fazni uglovi su se povećali do  $>80^\circ$ . Križanje modula elastičnosti i viskoznosti za AA se desilo pri devet puta većem naponu smicanja u poređenju sa ostalim formulacijama, te formira lamelarnu kristalnu gel mrežu. Linearni viskoelastični region je pokazao da je AA mnogo stabilnija. Promjena frekvencije je pokazala da su NA i AB slične tečnostima, ali križanje modula elastičnosti i viskoznosti i smanjenje faznog ugla ukazuju na slabu razmazivost pri višim brzinama nanošenja. Kod NB i AA smanjenje kompleksnog viskoziteta indicira bolju razmazivost. Stabilnost faznog ugla i moduli elastičnosti i viskoznosti ukazuju na više elastično ponašanje. Novi neionski emulgator je bio više neovisan o metodi izrade za razliku od anionskog emulgatora. Međutim, AA formulacija daje mnogo bolje osjetne osobine potrebne u kozmetičkim formulacijama.



## DFT study of guaiazulene

Špirtović-Halilović S.<sup>a</sup>, Salihović M.<sup>b</sup>, Osmanović A.<sup>a</sup>, Veljović E.<sup>a</sup>, Trifunović S.<sup>c</sup>, Roca S.<sup>d</sup>,  
Ašimović Z.<sup>e</sup>, Završnik D.<sup>a</sup>

<sup>a</sup>Department of Pharmaceutical Chemistry, Faculty of Pharmacy, University of Sarajevo, Zmaja od Bosne 8, 71000 Sarajevo, Bosnia and Herzegovina

<sup>b</sup>Department of Organic Chemistry, Faculty of Pharmacy, University of Sarajevo, Zmaja od Bosne 8, 71000 Sarajevo, Bosnia and Herzegovina

<sup>c</sup>Faculty of Chemistry, University of Belgrade, Studentski trg 12-16, 11000 Belgrade, Serbia

<sup>d</sup>NMR Centre, Ruđer Bošković Institute, Bijenička cesta 54, 10000 Zagreb, Croatia

<sup>e</sup>Department of Chemistry and Biochemistry, PAM Institute, Faculty of Agriculture and Food science, University of Sarajevo, Zmaja od Bosne 8, 71000 Sarajevo, Bosnia and Herzegovina

**Keywords:**  
guaiazulene,  
chemical reactivity descriptors

**Corresponding author:**  
Amar Osmanović

**E-mail:**  
amar.ffsa@gmail.com

Tel: +38761256848  
Fax:

**Abstract:** Quantum mechanics provides the mathematical apparatus for determining numerous properties of chemical systems, whereas computer programs carry out the necessary calculations. Guaiazulene is starting compound in many reactions for obtaining azulene derivatives with significant pharmacological activity. Calculations for guaiazulene were done using software Spartan 10. The guaiazulene molecule was optimized by B3LYP/6-31G\* method. Chemical hardness, total energy, electronic chemical potential and electrophilicity were calculated and used to predict relative stability and reactivity of guaiazulene. Results of DFT study showed that guaiazulene possess good reactivity and behaves as nucleophile. These results were in good accordance with former experimental research about this compound.

### Sažetak

Kvantna mehanika obezbjeđuje matematički aparat za određivanje brojnih osobina hemijskih sistema, gdje računarski programi izvršavaju neophodne proračune. Gvajazulen je početna supstanca u mnogim reakcijama za dobivanje azulenskih derivata koji imaju značajna farmakološka djelovanja. Proračuni za gvajazulen su dobiveni korištenjem programa Spartan 10. Molekula gvajazulena je optimizirana metodom B3LYP/6-31G\*. Hemijska tvrdoća, totalna energija, elektronski hemijski potencijal i elektrofilnost su izračunati i iskorišteni za predviđanje relativne stabilnosti i reaktivnosti gvajazulena. Rezultati DFT studije su pokazali da gvajazulen posjeduje dobru reaktivnost i da se u reakcijama ponaša kao nukleofil. Ovi rezultati se dobro slažu s dosadašnjim eksperimentalnim istraživanjima na ovom spoju.



## **Chemical reactivity and stability predictions of some coumarins using Spartan software**

**Špirtović-Halilović S.<sup>a</sup>, Salihović M.<sup>b</sup>, Veljović E.<sup>a</sup>, Osmanović A.<sup>a</sup>, Trifunović S.<sup>c</sup>, Završnik D.<sup>a</sup>**

<sup>a</sup>*Department of Pharmaceutical Chemistry, Faculty of Pharmacy, University of Sarajevo, Zmaja od Bosne 8, 71000*

*Sarajevo, Bosnia and Herzegovina*

<sup>b</sup>*Department of Organic Chemistry, Faculty of Pharmacy, University of Sarajevo, Zmaja od Bosne 8, 71000 Sarajevo,*

*Bosnia and Herzegovina*

<sup>c</sup>*Faculty of Chemistry, University of Belgrade, Studentski trg 12-16, 11000 Belgrade, Serbia*

### **Keywords:**

coumarins,  
chemical reactivity descriptors,  
Spartan software

### **Corresponding author:**

Amar Osmanović

### **E-mail:**

amar.ffsa@gmail.com

Tel: +38761256848

Fax:

**Abstract:** Three synthesized coumarin derivatives were studied for their quantum-chemical properties. These compounds are commonly used as starting material for many chemical reactions. In order to explore the theoretical-experimental consistency, DFT global chemical reactivity descriptors (chemical hardness, total energy, electronic chemical potential and electrophilicity) were calculated for these compounds using standard Spartan 10 software. Complete geometry optimization was carried out by B3LYP/6-31G\* level of theory.

Some quantum-chemical calculations correlated well with experimental work; mechanisms of reactions with these compounds as starting material were partially explained by these calculated parameters. These calculations were once more proof that by means of mathematical models it is possible to describe chemical interactions and simulate the behavior of chemical systems – molecules and reactions.

### **Sažetak**

Za tri sintetizirana kumarinska derivata ispitana su njihova kvantno-hemijska svojstva. Ispitivani spojevi polazne su komponente u mnogim hemijskim reakcijama. U svrhu istraživanja teoretsko-eksperimentalne dosljednosti, DFT deskriptori globalne hemijske reaktivnosti (hemijska tvrdoća, totalna energija, elektronski hemijski potencijal i elektrofilnost) su izračunati za ove supstance koristeći standardni Spartan 10 program. Kompletna geometrijska optimizacija je urađena na B3LYP/6-31G\* teorijskom nivou.

Neke kvantno-hemijske kalkulacije se dobro slažu s eksperimentalnim istraživanjima na ovim spojevima. Mehanizmi reakcija u kojima su ovi spojevi početni reaktanti mogu se djelimično objasniti rezultatima ovih proračuna. Ovo izračunavanje je još jedan u nizu dokaza da je pomoću matematičkih modela moguće opisati hemijske interakcije i simulirati ponašanje hemijskih sistema – molekula i reakcija.



## **TD-DFT Studies of Poly(Oxyethylene)-Substituted Zinc Phthalocyanines in Photodynamic Therapy of Cancer**

**Türker Acar E.<sup>a</sup>, Can H.<sup>b</sup>, Gül Gürek A.<sup>b</sup>**

<sup>a</sup> *Istanbul University, Engineering Faculty, Department of Chemistry, Avcılar 34320, Istanbul, Turkey*

<sup>b</sup> *Gebze Institute of Technology, Department of Chemistry, Gebze 41400, Kocaeli, Turkey*

**Keywords:**

Phthalocyanine,  
TD-DFT,  
Photodynamic Therapy,  
Photosensitizer.

**Abstract:** The interaction of light with the metallophthalocyanine molecule accompanying of the oxygen in the cancer cell lead to photodynamic therapy (PDT) of cancer as a photosensitizer. Therefore, the electronic structure, the photophysical and excited state properties of metallophthalocyanine should be clarified as much detail as possible. Especially for the large molecules such as metallophthalocyanines, time-dependent density functional theory (TDDFT) is a very powerful tool for precisely calculation of excited state energies and many related response properties.

An accurate description of the molecular structures, molecular orbitals and UV-vis spectra of tetra- and octa- Poly(oxyethylene) substituted zinc phthalocyanines have been provided DFT and TD-DFT calculations to explore the effects of tetra-chlor substitution on the electronic structure and the excited state properties. The calculated results are in good agreement with the experimental data, indicating that the method and the basis set selected are feasible for calculating such a large molecule as tetra- and octa- Poly(oxyethylene) substituted zinc phthalocyanines. The results of photophysical and photochemical measurements indicates zinc phthalocyanines have a potential as photosensitizers in applications where singlet oxygen is required.

**Corresponding author:**

Elif TÜRKER ACAR

**E-mail:**

elifacar@istanbul.edu.tr

Tel: +90 212 473 7070

Fax: +90 212 473 7180

### **Sažetak**

Interakcija svjetla sa molekulom metaloftalocijanina koja prati kisik u ćelijama kancera predstavlja fotodinamičnu terapiju („photodynamic therapy”- PDT). Ova interakcija u PDT terapiji predstavlja fotopojivač. Zbog toga, elektronska struktura, fotofizičke osobine i osobine pobuđenog stanja metaloftalocijanina moraju biti potpuno definisane. Vremenski ovisna funkcionala teorija gustoće (“time-dependent density functional theory”-TDDFT) je jako važno sredstvo za preciznu kalkulaciju energija pobuđenih stanja i drugih osobina vezanih za ova energetska stanja, naročito kod velikih molekula kakve su metaloftalocijanini<sup>1</sup>.

Precizan i tačan opis molekularnih struktura, molekulskih orbitala I UV-Vis spektara tetra- i okta-poli(oksietilenom) substituiranih cink ftalocijanina je dat sa DFT I TD-DFT proračunima da bi se ispitao uticaj tetra-hlor substituenata na elektronsku strukturu i osobine pobuđenih stanja. Izračunate vrijednosti se slažu sa eksperimentalnim podacima, pokazujući da se metoda i postavljena baza za kalkulaciju mogu primjeniti na velike molekule kao što su tetra- i okta-poli(oksietilenom) substituiranih cink ftalocijanina. Rezultati fotofizičkih i fotohemijskih određivanja pokazuju da se cink ftalocijanini mogu koristiti kao fotopojivači u primjenama koje zahtjevaju prisustvo singletnog kisika<sup>2</sup>.



## Comparison of acid and basic dyes sorption ability onto Bottom Ash

Türker Acar E., Ortaboy S., Atun G.<sup>a</sup>

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

### Keywords:

bottom ash,  
adsorption, acid dye,  
basic dye,  
sorption ability

### Corresponding author:

Elif TÜRKER ACAR

### E-mail:

elifacar@istanbul.edu.tr

Tel: +90 212 473 7070

Fax: +90 212 473 7180

**Abstract:** In recent years, removal of dyes from wastewaters has received great attention because estimated amount of dye stuffs annually released in environment is  $10^5$  ton. Some low cost adsorbents have been developed from industrial waste products such as activated slugs, baggase fly ash and coal fly ash. The bottom ash (BA) is a coarse, granular, incombustible by-product of power plants. It is an undesired collected material, whose disposal has always been a matter of concern. It can be evaluated as adsorbent for dye removal from colored effluents. Sorption ability of eight textile dyes on the bottom ash were compared and correlated with their chemical structures. In general, acid dyes were more preferred by the sorbent than the basic dyes. The removal efficiency for acid dyes follows the order Lanaset Green B > Acid Black 63 > Lanaset Red 2B > Acid Brilliant Yellow G > Lanaset Red G. The results showed that bottom ash had higher affinity for anthraquinone dyes than the azodyes but metal complex dyes could not be adsorbed. On the other hand, sorption efficiency of the BA for basic dyes decreased in the order Victoria Blue (tri aryl methane dye) > Methylene Blue (thi-azin dye) > Safranin T (di-azin dye).

### Sažetak

Posljednjih godina velika pažnja se poklanja procesu uklanjanja boja iz otpadnih voda zbog toga što prosječna dozvoljena količina boja otpuštenih u okoliš godišnje iznosi  $10^5$  tona. Adsorbenti niskih cijena nabavke proizvedeni iz industrijskih otpadnih produkata kao što su aktivni mulj, otpad iz industrije šećera, i pepeo nastao sagorjevanjem uglja se danas sve više primjenjuju za uklanjanje boja. Pepeo koji nastaje kao grubi, granularni, negorljivi nusprodukt u elektranama ("bottom ash" - BA) se može koristiti za uklanjanje boja iz otpadnih voda. To je otpadni materijal, čije je uklanjanje uvijek bilo problem.

Sposobnost sorpcije osam tekstilnih boja na BA je poređena sa njihovim hemijskim strukturama. Općenito, kisele boje imaju boje sorptivne osobine od baznih boja. Efikasnost uklanjanja kiselih boja slijedi niz Lanaset Green B > Acid Black 63 > Lanaset Red 2B > Acid Brilliant Yellow G > Lanaset Red G. Rezultati su pokazali da BA ima veći afinitet za antrakinolne boje nego za azoboje dok se metalni kompleksi boja nisu mogli apsorbovati. Sa druge strane, sorptivna efikasnost BA za bazne boje se smanjivala u nizu Victoria Blue (tri aril metan boja) > metilen plavo (ti-azin boja) > Safranin T (di-azin boja).



## Investigation of Cisplatin on the Activity of Catalase

**Herenda S.<sup>\*</sup>, Ostojić J., Gojak-Salimović S., Galić B.**

*Faculty of Science, Department of Chemistry, Zmaja od Bosne 33-35, Bosnia and Herzegovina, 71000 Sarajevo*

**Keywords:** Cisplatin, catalase, inhibition

**Abstract:** The inhibitory effect of cis platinum (II) diammine dichloride was tested in an *in vitro* experiment on the activity of the enzyme catalase. It is known that certain salts of platinum affect the cells of a living organism in various ways. Cis-platinum (II) diammine dichloride or cisplatin is an effective anti-cancer drug, and chloroplatinic acid elicits strong allergy. It is expected that these salts have influence to other parts of the human organism and their influence on the activity of the enzymes is particularly significant. We opted for the enzyme catalase, whose role in the body is very important especially in relation to the occurrence and level of free radicals. Manometric method, using a modified method by Schubert-in, measured by the amount of released O<sub>2</sub> generated by the interaction of the substrate H<sub>2</sub>O<sub>2</sub> and catalase, with and without the presence of cisplatin. Assuming that the true Michaelis-Menten's model, the value of K<sub>m</sub>, V<sub>max</sub> and type of inhibition were calculated over Lineweaver-Burk's diagrams and inhibition constant K<sub>i</sub> over Dixon's diagram, on the basis of certain initial velocity of corresponding substrate concentration and cisplatin. In this paper, it is shown that cisplatin is a weak inhibitor of the enzyme catalase and the type of inhibition is non-competitive.

**Corresponding author:**  
Safija Herenda  
**E-mail:**  
islamovic.safija@gmail.com

Tel: +38733279918  
Fax:

### Sažetak

Ispitan je, u *in vitro* eksperimentu, inhibitorni uticaj cis platina (II) diamindihlorida na aktivnost enzima katalaze. Poznato je da neke soli platine utiču na ćelije živog organizma na razne načine. Cis platina (II) diamindihlorid ili cisplatin je efikasan antikancer lijek, a heksahloroplatinatna (IV) kiselina izaziva snažnu alergiju. Za očekivati je da ove soli utiču i na druge dijelove organizma a posebno je značajno poznavanje njihovog uticaja na aktivnost enzima. U ovom radu koristili smo enzim katalazu čija je uloga u organizmu veoma važna zbog pojave slobodnih radikala. Gasometrijskom metodom, korištenjem modifikovane metode po Schubert-u, mjerena je količina izdvojenog O<sub>2</sub> nastalog interakcijom supstrata H<sub>2</sub>O<sub>2</sub> i katalaze, bez i u prisustvu cisplatin. Uz pretpostavku da vrijedi Michaelis-Menten-ov model, vrijednosti K<sub>m</sub>, V<sub>max</sub> i tip inhibicije su računane preko Lineweaver-Burk-ovog dijagrama a konstanta inhibicije K<sub>i</sub> preko Dixon-ovog dijagrama, na osnovu određenih početnih brzina u funkciji odgovarajućih koncentracija supstrata i cisplatin. U ovom radu je pokazano da je cisplatin slab inhibitor enzima katalaze i da je tip inhibicije nekompetitivan.



## **Mathematical models of release kinetics of diazepam from solid dispersions**

**Hadžiabdić J.<sup>a</sup>, Elezović A.<sup>a</sup>, Rahić O.<sup>a</sup>, Vranić E.<sup>a</sup>**

*<sup>a</sup>Department of Pharmaceutical Technology, Faculty of Pharmacy, University of Sarajevo, Zmaja od Bosne 8, 71000 Sarajevo, Bosnia and Herzegovina*

### **Keywords:**

diazepam solid dispersions, release models

**Abstract:** According to the biopharmaceutics classification system diazepam belongs in the class II drugs. Inadequate dissolution rate of diazepam can be the limiting factor for its absorption rate. The aim of the present study was preparation of diazepam solid dispersions using various carriers like polyethylene glycol 2000, polyethylene glycol 4000 and polyvinylpyrrolidone K30, estimation of solubility and dissolution rate of prepared diazepam solid dispersions and comparison of these data to that of pure diazepam. The solid dispersions were prepared by solvent evaporation method. Phosphate buffer pH 6.8 was used as dissolution medium. Solid dispersions of diazepam with polymers resulted in increased solubility and dissolution rate of diazepam (highest with polyvinylpyrrolidone K30). The rate release kinetics of diazepam from the solid dispersions followed Hixson-Crowell cube root law. The correlation coefficient ( $r^2$ ) values of the Hixson-Crowell's cube root model were slightly higher (0.9665 to 0.9977) when compared to the zero and first order release model. The high values of regression coefficients suggested that all formulations followed Korsmeyer-Peppas model of release kinetics. The low values of the release exponent ( $< 0.45$ ) indicated that the mechanism of diazepam release from all the formulations could be described as a Fickian diffusion mechanism.

### **Corresponding author:**

Jasmina Hadžiabdić

### **E-mail:**

[jasmina.hadziabdic@ffsa.unsa.ba](mailto:jasmina.hadziabdic@ffsa.unsa.ba)

Tel: 033 586 173

Fax:

### **Sažetak**

Prema biofarmaceutskom sistemu klasifikacije diazepam spada u lijekove klase II. Neadekvatna brzina otapanja diazepama može biti ograničavajući faktor za njegovu brzinu apsorpcije. Cilj ovog istraživanja je bio da se pripreme čvrste disperzije diazepama koristeći razne nosače kao što su polietilenglikol 2000, polietilenglikol 4000 i polivinilpirolidon K30, procijeni topivosti i brzina otapanja pripremljenih čvrstih disperzija diazepama i uporede podaci sa podacima čistog diazepama. Čvrste disperzije su izrađene metodom evaporacije otapala. Kao disolucijski medij korišten je fosfatni pufer pH 6.8. Čvrste disperzije diazepama s polimerima pokazuju povećanu topivost i brzinu otapanja diazepama (najviše disperzija sa polivinilpirolidonom K30). Brzina kinetike oslobađanja diazepama iz čvrstih disperzija slijedi Hixson-Crowell-ov zakon kubnog korijena. Vrijednosti koeficijenta korelacije ( $r^2$ ) Hixson-Crowell-ovog modela kubnog korijena su nešto više (0,9667-0,9977) u odnosu na modele oslobađanja nultog i prvog reda. Visoke vrijednosti koeficijenta regresije sugerišu da sve formulacije slijede Korsmeyer-Peppas model kinetike oslobađanja. Niske vrijednosti eksponenta oslobađanja ( $< 0,45$ ) ukazuju da se mehanizam oslobađanja diazepama iz svih formulacija može opisati Fick-ovim mehanizmom difuzije.





## **Ionic strength and counteranion type influence on formation of PAH/PSS multilayers and correlation with polyelectrolyte complex formation in solution**

**Salopek J, Požar J., Kovačević D.**

*Division of Physical Chemistry, Department of Chemistry, Faculty of Science, University of Zagreb, Horvatovac 102a,  
10000 Zagreb, Croatia*

### **Keywords:**

polyelectrolyte multilayers,  
polyelectrolyte complexes,  
quartz crystal microbalance,  
Hofmeister series.

### **Corresponding author:**

Jasmina Salopek

### **E-mail:**

jsalopek@chem.pmf.hr

Tel: +385 14606 149

Fax:

**Abstract:** The formation of polyelectrolyte multilayers of polyallylammonium cation (PAH) and polystyrenesulfonate anion (PSS) was investigated in aqueous solutions of sodium electrolytes (NaX, X = F, Cl, Br, I, NO<sub>3</sub>, ClO<sub>4</sub>) at 25 °C by means of quartz crystal microbalance with dissipation monitoring (QCM-D). The obtained results were compared with the results of polyelectrolyte complexation in solution. The QCM-D measurements indicated that increase in ionic strength led to larger thickness of deposited layers and assymmetric incorporation of polymers into nanoassemblies (the amount of polycation was higher than that of polyanion). Anions influenced the film thickness at higher ionic strengths considerably. The largest deposition of material was noticed in the case of nitrate and perchlorate anions. This is in accordance with DLS and spectrophotometric experiments in which anion specific aggregation of positive colloid complexes and the formation of precipitates containing larger amount of PAH with respect to PSS was observed. The complexation enthalpies were also correlated with the thickness of deposited films, following the Hofmeister series. The more enthalpically disfavoured complexation process in solution was, the larger was the amount of material deposited. The results can be explained by different counteranion distributions around polycation, caused by differences in the corresponding hydration enthalpies.

### **Sažetak**

Nastajanje polielektrolitnih višeslojeva polialilamonijevog kationa (PAH) i polistirensulfonatnog aniona (PSS) istraženo je u vodenim otopinama natrijevih soli (NaX, X = F, Cl, Br, I, NO<sub>3</sub>, ClO<sub>4</sub>) pri 25 °C upotrebom kvarc-kristalne mikrovage uz praćenje disipacije (QCM-D). Dobiveni rezultati su uspoređeni s rezultatima kompleksiranja polielektrolita u otopini. QCM-D mjerenja pokazala su da porast ionske jakosti dovodi do porasta debljine slojeva i asimetrične ugradnje polimera u nanokompozite (količina vezanih polikationa je veća od količine vezanih polianiona). Pri višim ionskim jakostima pokazan je izrazit utjecaj aniona na debljinu filma. Najviše polielektrolita u višeslojevima vezano je u prisustvu nitratnih i perkloratnih aniona. Rezultati su u skladu s DLS i spektrofotometrijskim mjerenjima kod kojih je uočena anion specifična agregacija pozitivnih koloidnih kompleksa i nastajanje taloga koji sadrži veću količinu PAH-a prema PSS-u. Entalpije kompleksiranja polielektrolita u otopini su također povezane s debljinom filma u prisutnosti odgovarajućih aniona te slijede Hofmeisterovu seriju. Što je entalpijski nepovoljnije kompleksiranje u otopini, to je veća količina polielektrolita vezana u višeslojevima. Rezultati se mogu objasniti različitom raspodjelom protuaniona oko lanca polikationa uzrokovanom razlikama u odgovarajućim entalpijama hidratacije.



## **Inhibition of Iron Corrosion with Lavender Extracts as Eco-acceptable Inhibitors**

**Veletovac I., Ostojić J.\*, Korać F., Gutić S., Herenda S., Vidic D.**

*Faculty of Science, Department of Chemistry, Zmaja od Bosne 33-35, 71000 Sarajevo, Bosnia and Herzegovina*

**Keywords:**

Inhibition  
Lavander  
Iron Corrosion

**Corresponding author:**

Ostojić Jelena

**E-mail:**

ostojic.jelena@live.com

Tel: +387 61 789 487

Fax:

**Abstract:** Inhibition of iron corrosion with lavender extracts in seawater as corrosion media has been studied using *Lavandula hybrida* Reverchon from Istria peninsula (Croatia). One lavender extract is prepared by ultrasonic extraction with water as a solvent, and the second is used as a water extract after hydrodistillation. The total phenolic content of the extracts was determined spectrophotometrically according to the Folin-Ciocalteu method. Extract prepared with ultrasound extraction had higher content of phenolic compounds and it was used for corrosion tests.

Inhibition efficiency was studied using potentiodynamic polarization technique. Values calculated from potentiodynamic polarization and polarization curves showed that lavender extracts behaves as a mixed-type inhibitor in seawater. The results obtained showed that the lavender extracts *Lavandula hybrida* Reverchon could serve as an effective inhibitor of the corrosion of iron in seawater solution.

### **Sažetak**

Inhibicija korozije željeza sa ekstraktima lavande u morskoj vodi kao korozionom mediju je proučavana korištenjem uzorka *Lavandula hybrida* Reverchon iz Istre (Hrvatska). Jedan ekstrakt lavande je pripremljen ultrazvučnom ekstrakcijom uz vodu kao rastvarač, a drugi je uzet kao vodeni ekstrakt nakon hidrodestilacije. Ukupan sadržaj fenola je određen spektrofotometrijski Folin-Ciocalteu metodom. Ekstrakt pripremljen ultrazvučnom ekstrakcijom je imao veći sadržaj fenolskih spojeva i korišten je za koroziona ispitivanja. Efikasnost inhibicije je određena potenciodinamičkom metodom. Vrijednosti dobivene potenciodinamičkom polarizacijom kao i polarizacione krive su pokazale da se ekstrakt lavande ponaša kao mješoviti inhibitor u morskoj vodi. Dobiveni rezultati su pokazali da testirani uzorci ekstrakata *Lavandula hybrida* Reverchon mogu poslužiti kao inhibitori korozije željeza u morskoj vodi.



Glasnik hemičara i  
tehnologa  
Bosne i Hercegovine

## Investigation of potentially contaminated areas in the FBiH with depleted uranium

Nuhanović M.<sup>a</sup>, Vidic A.<sup>b</sup>, Ilić Z.<sup>b</sup>, Kaldžija N.<sup>a</sup>, Pušina N.<sup>a</sup>

<sup>a</sup>University of Sarajevo, Faculty of Science, Department of Chemistry, Zmaja od Bosne 33-35,

71000 Sarajevo, Bosnia and Herzegovina

<sup>b</sup>Institute for Public Health of FBiH, M.Tita 9, 71000 Sarajevo, Bosnia and Herzegovina

### Keywords:

ammunition depleted uranium, contamination, alpha-spectrometry, determination of uranium

### Corresponding author:

Mirza Nuhanović

### E-mail:

mirza.nuhanovic@yahoo.com

Tel: +387/33/279-865

Fax:

**Abstract:** During the war in Bosnia, depleted uranium was used on several locations in Bosnia and Herzegovina, including the area Hadžici. Estimated amount of used ammunition is close to three tons. Only a fraction of depleted uranium penetrator, detected in the surface ground layer was removed. A certain number of ground, moss and subterranean water samples have been collected in december 2013, for the purpose of evaluation of two decade long contamination from depleted uranium ammo usage. The collected samples were subjected to radiochemical separation and alpha- spectrometric analysis. The results of the examination showed that the uranium was present in the amount of 0,6 to 1,8 µg/kg in the ground samples, 0,2 to 7,0 µg/kg in the moss samples and 0,36 to 1,04 µg/L in the subterranean water. The activity ratio of U-234/U-238 in three moss samples, as well as one ground sample, showed the presence of depleted uranium. Analyzed water samples indicated a natural relation of uranium isotopes. Tests shows that the presence of depleted uranium deserves detailed examination of radioactivity, radioecology assessment and evaluation of population exposure

### Sažetak

Tokom rata u BiH, osiromašeni uran je upotrebljen na nekoliko lokacija u BiH, uključujući područje Hadžića. Procjenjena količina upotrebljene municije iznosi približno 3 tone. Samo dio penetratora od osiromašenog urana, detektovan u površinskom sloju tla, je uklonjen. U decembru 2013. godine je prikupljen određen broj uzoraka tla, mahovina i podzemnih voda, u cilju procjene kontaminacije dvije decenije nakon upotrebe municije od osiromašenog urana. Prikupljeni uzorci su podvrgnuti radiohemijskoj separaciji i alfa spektrometrijskoj analizi. Rezultati ispitivanja pokazuju da sadržaj urana u uzorcima tla iznosi od 0.6 do 1.8 mg/kg, u uzorcima mahovina od 0.2 do 7.0 mg/kg, i uzorcima vode od 0.36 do 1.04 µg/L. Odnos aktivnosti <sup>234</sup>U/<sup>238</sup>U u tri uzorka mahovina, kao i jednom uzorku tla ukazuje na prisustvo osiromašenog urana. Analizirani uzorci vode pokazuju prirodan odnos uranovih izotopa. Ispitivanja pokazuju da prisustvo osiromašenog urana zavređuje detaljno ispitivanje radioaktivnosti, radioekološku procjenu i procjenu izloženosti stanovništva.



## **Spectrophotometric Analysis of Caffeine in Energy Drinks**

**Halilović, N., Bašić, A., Omanović, R., Gojak-Salimović, S.**

*University of Sarajevo, Faculty of Science, Department of Chemistry, Zmaja od Bosne 33-35, 71000 Sarajevo,  
Bosnia and Herzegovina*

### **Keywords:**

caffeine,  
extraction,  
energy drinks,  
spectrophotometry

### **Corresponding author:**

Namir Halilović

### **E-mail:**

namir.halilovic@live.com

Tel: +387 61 495 311

Fax:

**Abstract:** Young people, especially students, are the major consumers of energy drinks that contain caffeine because of its pronounced stimulatory effect on the central nervous system. However, excessive consumption of caffeine can cause a range of adverse health effects such as insomnia, headache, gastrointestinal complaints, heart palpitations. Harmful effects of caffeine is classified as a form of the disease (World Health Organization's International Classification of Diseases, ICD-10). Although there are no regulatory requirements to control or label food products with their caffeine content, numerous studies have been conducted to determine the caffeine content in the most frequently consumed beverages using different methods. This work was done by quantification of caffeine in energy drinks available in the local market by UV/Vis spectrophotometry. UV/Vis spectrum of caffeine was recorded in different solvents. The best agreement with literature data were obtained by UV/Vis spectrum of caffeine in dichloromethane. Extraction of caffeine from energy drinks was performed with dichloromethane. In accordance with the Lambert-Beer law, the absorbance was measured at a wavelength of 274 nm at room temperature. For most samples obtained values of caffeine content are higher than declared.

### **Sažetak**

Mladi ljudi, pogotovo studenti, su danas glavni konzumenti energetske pića, koji sadrže kofein zbog njegovog izraženog stimulatornog efekta na centralni nervni sistem. Pretjerana konzumacija kofeina može prouzročiti niz neželjenih posljedica po zdravlje, kao što su nesanicu, glavobolju, probavne smetnje, lupanje srca. Štetno djelovanje kofeina je klasificirano kao vid bolesti (World Health Organization's International Classification of Diseases, ICD-10). Iako ne postoje regulatorni zahtjevi za kontrolu ili oznaku prehrambenih proizvoda na sadržaj kofeina, brojna istraživanja su provedena kako bi se odredio sadržaj kofeina u najčešće konzumiranim pićima pomoću različitih metoda. U ovom radu je vršena kvantifikacija kofeina u energetskim pićima dostupnim u lokalnim marketima primjenom UV/VIS spektrofotometrije. UV/VIS spektar kofeina sniman je u različitim rastvaračima. Najbolje slaganje sa literaturnim podacima dobijeno je za UV/VIS spektar kofeina u dihlometanu. Ekstrakcija kofeina iz energetske pića vršena je sa dihlometanom. Sukladno Lambert-Beerovom zakonu, apsorbancija je mjerena na talasnoj dužini od 274 nm na sobnoj temperaturi. Za većinu ispitivanih uzoraka dobijene vrijednosti sadržaja kofeina su više od deklariranih.



---

## **Activity Coefficients for CdCl<sub>2</sub> in 2-Methylpropan-2-ol (5 mass %) + Water Mixed Solvent from Potentiometric Measurements with Cadmium-Selective Electrode**

**Tomaš R., Bajlo B.**

*Department of Physical Chemistry, Faculty of Chemistry and Technology, University of Split, Nikole Tesle 10/V,  
HR-21000 Split, Croatia;*

---

**Keywords:**

cadmium chloride,  
activity coefficients,  
cadmium-selective electrode,  
aqueous mixture of 2-  
methylpropan-2-ol

**Corresponding author:**

Renato Tomaš

**E-mail:**

rtomas@ktf-split.hr

Tel: 00385 21 329 448

Fax:

**Abstract:** The potential difference (pd),  $E$ , of the galvanic cell without a liquid junction: Cd-ISE|CdCl<sub>2</sub>( $b$ ) in Z|AgCl(s)|Ag(s), where ISE stands for ion-selective electrode, was measured at different temperatures (20, 25, 30, and 35 °C) and various CdCl<sub>2</sub> molalities,  $b$ , in aqueous mixture with 5 mass % 2-methylpropan-2-ol (Z). From these values and using literature data for stability constants of the chlorocadmium complexes, the values for the standard pd,  $E^{\circ}$  (molal scale), were obtained at each temperature. The standard pd data are served to calculate the stoichiometric mean molal activity coefficients of CdCl<sub>2</sub>. The agreement between the results for the activity coefficient obtained with cadmium-selective electrode in the present work with those obtained using amalgam electrode, are discussed.

---

**Sažetak**

U ovom radu mjerena je elektromotivnost ( $E$ ) galvanskog članka bez prijenosa: Cd-ISE|CdCl<sub>2</sub>( $b$ ) u Z|AgCl(s)|Ag(s) pri raznim molalitetima CdCl<sub>2</sub> ( $b$ ) u Z (Z označava korišteno miješano otapalo), te pri raznim temperaturama od 20, 25, 30 i 35 °C. Potenciometrijski podaci su obrađeni korištenjem podataka za konstante stabilnosti klorokadmijevih kompleksa. Rezultat te obrade je standardna molalna elektromotivnost članka ( $E^{\circ}$ ) za pojedinu temperaturu. Iz vrijednosti  $E^{\circ}$  dobiveni su srednji stehiometrijski koeficijenti aktiviteta CdCl<sub>2</sub> u Z. Te su vrijednosti uspoređene s onima koje su dobivene potenciometrijski korištenjem zasićene kadmij-amalgamske electrode, Cd(Hg), u istom ili sličnom sustavu.



## The Effect of $H_2PtCl_6$ on the Belousov-Zhabotinsky Reaction

**Gojak-Salimović S., Ostojić J., Herenda S., Galić B.**

*University of Sarajevo, Faculty of Science, Department of Chemistry, Zmaja od Bosne 33-35, 71000 Sarajevo,  
Bosnia and Herzegovina*

### Keywords:

Belousov-Zhabotinsky reaction  
Oscillation  
Ferriin  
Catalyst

### Corresponding author:

Sabina Gojak-Salimović

### E-mail:

sgojak@pmf.unsa.ba

Tel: +387/33/279-907

Fax: +387/33/649-359

**Abstract:** Oscillating reactions are insufficiently studied in relation to the known catalytic effects of noble metals. In this work, the effect of concentration  $H_2PtCl_6$  on the reaction system Belousov-Zhabotinsky reaction, which was comprised of malonic acid, potassium bromate, sulfuric acid and ferriin, was investigated. The reaction was performed in a thermostated, stationary, closed, constantly stirred reactor, with a accurately defined concentrations of reactants, at constant temperature of 25°C. Simultaneously, potentiometric method with platinum and saturated calomel electrode, and gasometric method were used. Change in the system potential, volume of evolved  $CO_2$ , number, amplitude and time of oscillations were monitored. The volume of evolved  $CO_2$  during the time followed the rate law of first-order reaction. Oxidation rate constants of malonic acid were calculated using Guggenheim method. It was found that  $H_2PtCl_6$  does not affect the order of the reaction but affects the value of the rate constant. Increasing concentration of  $H_2PtCl_6$ , number of oscillations increases, oscillations amplitude decreases, and time of the oscillating period extends.

### Sažetak

Oscilirajuće reakcije su nedovoljno istražene u odnosu na poznate katalitičke efekte plemenitih metala. U ovom radu ispitivan je uticaj koncentracije  $H_2PtCl_6$  na reakcioni sistem reakcije Belousov-Zhabotinsky, koga su činili malonska kiselina, kalijum bromat, sulfatna kiselina i ferriin. Reakcija je izvođena u stacionarnom, zatvorenom reakcionom sudu koji je termostatiran na 25 °C, uz stalno miješanje reaktanata tačno definisanih koncentracija. Simultano su korištene potenciometrijska metoda, uz platinsku i zasićenu kalomelovu elektrodu i gasometrijska metoda. Istovremeno je mjerjen potencijal reakcionog sistema, volumen izdvojenog  $CO_2$ , broj, amplituda i vrijeme trajanja oscilacija. Volumen izdvojenog  $CO_2$  u toku vremena je slijedio zakon za brzinu reakcije I reda. Konstante brzine oksidacije malonske kiseline računane su Guggenheimovom metodom. Nađeno je da  $H_2PtCl_6$  ne utiče na red reakcije, ali utiče na vrijednost konstante brzine reakcije. Porastom koncentracije  $H_2PtCl_6$  povećava se broj oscilacija, smanjuje amplituda oscilacija i produžava vrijeme trajanja oscilirajućeg perioda.



## **Temperature Influence on the Extent of the Belousov-Zhabotinsky Reaction**

**Gotovac N., Gojak-Salimović S., Galić B.**

*University of Sarajevo, Faculty of Science, Department of Chemistry, Zmaja od Bosne 33-35, 71000 Sarajevo,  
Bosnia and Herzegovina*

**Keywords:**

Belousov-Zhabotinsky reaction  
Oscillation  
Catalyst  
Activation energy

**Abstract:** One of the most historically significant and studied oscillating reaction is the Belousov-Zhabotinsky reaction which reaction system involves oxidation of organic substrates bromate ion in acidic media and with various catalysts. In this work, the effect of temperature on the reaction system Belousov-Zhabotinsky containing malonic acid as a substrate, and catalyst cerium(IV)sulfate or ferroin was investigated. The reaction were performed in a thermostated, stationary, closed, constantly stirred reactor with a accurately defined concentrations of reactants at different temperatures ( $25^{\circ}\text{C} \leq T \leq 40^{\circ}\text{C}$ ). Simultaneously, potentiometric method with platinum and saturated calomel electrode and gasometric method were used. At the same time, change in the system potential, volume of evolved  $\text{CO}_2$ , and time of oscillations were monitored. Extent of Belousov-Zhabotinsky reaction is defined as the percent of malonic acid reacted. Oxidation rate constant of malonic acid were calculated using Guggenheim method based on the volume of evolved  $\text{CO}_2$ . Values of the activation energy were calculated using the Arrhenius equation. Lower values of activation energy, extent and time of oscillations were obtained for ferroin in relation to cerium(IV)sulfate catalyst used.

**Corresponding author:**

Sabina Gojak-Salimović

**E-mail:**

sgojak@pmf.unsa.ba

Tel: +387/33/279-907

Fax: +387/33/649-359

### **Sažetak**

Jedna od istorijski najznačajnih i najviše istraživanih oscilirajućih reakcija je reakcija Belousov-Zhabotinsky čiji reakcioni sistem predstavlja oksidaciju organskog supstrata bromatnim jonom, u kiseloj sredini i uz razne katalizatore. U ovom radu je određivan uticaj temperature na reakcioni sistem Belousov-Zhabotinsky koji je sadržavao malonsku kiselinu kao supstrat i katalizatore cer(IV) sulfat ili ferroin. Reakcija je izvođena u termostatiranom, stacionarnom, zatvorenom reakcionom sudu, uz stalno miješanje tačno definisanih koncentracija reaktanata, na različitim temperaturama ( $25^{\circ}\text{C} \leq T \leq 40^{\circ}\text{C}$ ). Simultano su korištene potenciometrijska metoda uz platinsku i zasićenu kalomelovu elektrodu i gasometrijska metoda. Istovremeno je vršeno mjerenje potencijala sistema, volumen izdvojenog  $\text{CO}_2$  i vrijeme trajanja oscilacija. Doseg Belousov-Zhabotinsky reakcije definisan je preko procenta izreagovane malonske kiseline. Konstante brzine oksidacije malonske kiseline računane su Guggenheimovom metodom na osnovu volumena izdvojenog  $\text{CO}_2$ . Izračunate su vrijednosti energije aktivacije preko Arrheniusove jednačine. Niže vrijednosti energije aktivacije, dosega i vremena trajanja oscilacija su dobijene za ferroin u odnosu na korišteni katalizator, cer(IV) sulfat.



## **Competitive Sorption of Thionine with Cs and Sr on zeolites**

**Ortaboy S., Türker Acar E., Atun G.**

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

**Keywords:**

Zeolite, thionine,  
adsorption,  
Cesium,  
Strontium

**Corresponding author:**

Sinem Ortaboy

**E-mail:**

ortaboy@istanbul.edu.tr

Tel: +90 212 473 7070

Fax: +90 212 473 7180

**Abstract:** The natural and synthetic zeolites are candidate buffer materials for geological disposal sites to inhibit groundwater flow and thus retard the movement of radionuclides. The radionuclides of Cs and Sr are main fission products stored in geological formations. The presence of competing inorganic and organic cations in groundwater may control the interaction of the radionuclides with surrounding solid phases. Although competition of inorganic cations with the radionuclides for sorption on the solid phases has been extensively studied limited researches are reported on the influence of organic cations. Thionine (TH) is the smallest cationic thiazin dye which may replace with Cs and Sr on sorbent material. In this work, sorption of TH on natural and synthetic zeolites was investigated in the presence of  $\text{Cs}^+$  and  $\text{Sr}^{2+}$  cations. The natural zeolite consisted of mainly clinoptilolite whilst the synthetic zeolite produced from fly ash composed of analcime and sodalite. The data obtained from long term equilibration upto two months well fit with the homogeneous surface diffusion and pseudo-second-order kinetic models. Distribution coefficients ( $K_D$ ) were nearly the same on both zeolite and were not influenced by  $\text{Cs}^+$  and  $\text{Sr}^{2+}$  ions.

### **Sažetak**

Prirodni i sintetski zeoliti su kandidati za puferski materijal na geološkim odlagalištima, radi usporavanja toka podzemnih voda, čime usporavaju i pomjeranja radionuklida. Radionuklidi Cs i Sr su glavni fisioni produkti koji su pohranjeni u geološke formacije. Prisustvo kompetirajućih neorganskih i organskih kationa u podzemnim vodama može kontrolisati interakciju radionuklida sa okolnim čvrstim fazama. Iako je opsežno istražena kompeticija neorganskih kationa sa radionuklidima za sorpciju na čvrstoj fazi, postoji ograničen broj objavljenih istraživanja o uticaju organskih kationa.

Thionin (TH) je najmanja kationska tiazin boja koja može da se zamjeni sa Cs i Sr na sorpcijskom materijalu. U ovom radu je ispitana sorpcija TH na prirodne i sintetske zeolite u prisustvu  $\text{Cs}^+$  i  $\text{Sr}^{2+}$  kationa. Prirodni zeoliti su uglavnom bili sačinjeni od klinoptilolita dok je sintetički zeolit proizveden od pepela koji je sačinjen od analcita i sodalita. Prikupljeni podaci tokom dugoročnog uravnoteženja (u toku dva mjeseca), se dobro slažu sa modelom homogene površinske difuzije i kinetičkim modelom pseudo-drugog-reda. Distribicioni koeficijenti ( $K_D$ ) su bili gotovo isti na oba zeolita i nisu bili pod uticajem  $\text{Cs}^+$  i  $\text{Sr}^{2+}$  jona.





## **Retention of Eosin Yellow onto aluminium modified Fuller's Earth**

**Ortaboy S.<sup>a</sup>, Obay F.<sup>b</sup>, Atun G.<sup>a</sup>**

<sup>a</sup> *Istanbul University, Engineering Faculty, Department of Chemistry, 34320 Avcilar, Istanbul, Turkey*

<sup>b</sup> *Environment And Clean Production Institute, TUBITAK, Kocaeli, 41400, Turkey*

### **Keywords:**

Adsorption,  
Eosin Y,  
Fuller's Earth,  
Aluminum,  
Surface modification.

**Abstract:** Eosin Y, which is bromine derivative of fluorescein, a yellow fluorescence dye with slightly acidic, highly water-soluble properties. They are widely used in dyeing textiles, ink manufacturing and coloring cosmetics. This anionic organic substance is one of the problematic contaminants in industrial waste water. Thus, removal of these substances from the effluent to the desired level is required before they are discharged into large bodies of water. The removal by adsorption process is an economical method when locally available low cost materials are used as adsorbents. Clays minerals, modified with inorganic cations may be alternative adsorbent for acid dye removal due to abundance of the material and low cost compared with other natural adsorbents. In this study, Al-modified Fuller's Earth were prepared by adding Al-chlorhydrol solution to the clay suspension using conductometric titration method. The adsorbents were obtained by changing amount of clay and the volume of acetone of 50%. The effects of adsorbent dosage, initial dye concentration and sequential adsorption on adsorption capacity were investigated. Adsorption data were analyzed by using Freundlich and Dubinin-Radushkevich (D-R) isotherms. Gibbs free energy changes were calculated using equilibrium constants derived from distribution coefficients consistent with the mean adsorption energies calculated from D-R parameters.

### **Corresponding author:**

Sinem Ortaboy

### **E-mail:**

ortaboy@istanbul.edu.tr

Tel: +90 212 473 7070

Fax: +90 212 473 7180

### **Sažetak**

Eozinsko žuto, koji je bromni derivat fluorescina je žuta fluorescirajuća boja sa neznatnim kiselim svojstvima i izraženom rastvorljivošću u vodi. Naširoko se koristi za bojenje tekstila, u proizvodnji tinte i proizvodnji šminke. Ova anionska organska supstanca je jedan od problematičnih zagađivača koji se nalazi u industrijskim otpadnim vodama. Prema tome, potrebno je uklanjanje ove tvari iz otpadne vode do željene razine prije nego što se ispusti u veće vodene mase. Uklanjanje procesom apsorpcije je ekonomična metoda, kada se koriste jeftini, trenutno dostupni materijali kao adsorbenti. U poređenju sa drugim prirodnim adsorbentima minerali gline, modifikovani sa neorganskim kationima, mogu biti alternativni adsorbenti za odstranjivanje kiselih boja zbog zastupljenosti materijala i niske cijene u poređenju sa drugim prirodnim adsorbentima. U ovom radu, Al-modificirana Fullerova zemlja je pripremljena dodavanjem Al-hlorhidrol rastvora u suspenziju gline korištenjem konduktometrijske metode titracije. Adsorbenti su dobiveni mijenjanjem količine gline i zapremine acetona od 50%. Ispitani su efekti doziranja adsorbenta, početna koncentracija boje i sekvencijalna adsorpcija na adsorbcijski kapacitet. Podaci o adsorpciji su analizirani korištenjem Freundlich i Dubinin-Radushkevich (D-R) izoterma. Promjena slobodne Gibbsove energije je izračunata korištenjem konstante ravnoteže, derivirane iz distribucionog koeficijenta u skladu sa prosječnim apsorpcijskim energijama, izračunatim iz DR parametara.



## **Electrochemical characterization of (1E)-1-N-{{4-(4-{{(E)-N-(3-aminophenyl)carboxyimidoyl}phenoxy}butoxy) phenyl} methylidene} benzene -1,3-diamine**

**Anamarija Šter, Tomislav Balić, Berislav Marković, Martina Medvidović-Kosanović**

*Department of Chemistry, J. J. Strossmayer University of Osijek, Cara Hadrijana 8/A, HR-31000*

*Osijek*

**Keywords:**

Schiff base,  
electrochemistry,  
oxidation,  
voltammetry

**Abstract:** Oxido-reduction properties of a newly synthesized Schiff base were investigated by cyclic voltammetry and differential pulse voltammetry. Measurements were conducted in a three electrode voltammetric cell in a non-aqueous media. Glassy carbon was used as a working electrode, platinum wire as counter electrode and non-aqueous Ag/Ag<sup>+</sup> electrode as a reference electrode. Inert atmosphere was accomplished by system purging with high purity argon Ar 5 ( $\phi_{Ar} = 99,999\%$ ) before each measurement. Cyclic voltammograms revealed one oxidation peak of the investigated Schiff base ( $E_{p,a} = 0,69$ ), which increased with increasing concentration ( $c = 3,1 \cdot 10^{-5} \text{ mol dm}^{-3} \dots 1,25 \cdot 10^{-4} \text{ mol dm}^{-3}$ ) and scan rate ( $v = 50 \dots 300 \text{ mV/s}$ ). Differential pulse voltammetry showed one oxidation peak  $E_{p,a} = 0,69 \text{ V}$ , which also increased with increasing concentration.

**Corresponding author:**

Martina Medvidović-Kosanović

**e-mail:** [mmkosano@kemija.unios.hr](mailto:mmkosano@kemija.unios.hr)

**Tel:** ++385 31 399 959

**Fax:** ++385 31 399 969

**Sažetak**

Ispitivana su oksido-redukcijska svojstva novosintetizirane Schiffove baze uporabom cikličke i diferencijalne pulsne voltametrije. Mjerenja su izvedena u troelektrodnoj ćeliji u nevodenom mediju pri sobnoj temperaturi, a inertna atmosfera je postignuta propuhivanjem sustava argonom visoke čistoće Ar 5 ( $\phi_{Ar} = 99,999\%$ ), prije svakog mjerenja. Kao radna elektroda korištena je elektroda od staklastog ugljika, protuelektroda je bila platinska žica, a kao referentna elektroda je korištena Ag/Ag<sup>+</sup> elektroda za nevodeni medij. Rezultati cikličke voltametrije su pokazali da se ispitivana Schiffova baza oksidira (uočen je jedan oksidacijski strujni vrh u anodnom dijelu voltamograma na potencijalu  $E_{p,a} = 0,69 \text{ V}$ , a visina oksidacijskog strujnog vrha raste s povećanjem koncentracije ( $c = 3,1 \cdot 10^{-5} \text{ mol dm}^{-3} \dots 1,25 \cdot 10^{-4} \text{ mol dm}^{-3}$ ) i brzine promjene potencijala ( $v = 50 \dots 300 \text{ mV/s}$ ). Diferencijalnom pulsnom voltametrijom je također uočen jedan oksidacijski strujni vrh pri  $E_{p,a} = 0,69 \text{ V}$ , koji se povećavao s povećanjem koncentracije ispitivane Schiffove baze.



## **Conductivity of ammonium bromide in aqueous butan-2-ol of lower mass fraction**

**Sokol V.<sup>a</sup>, Bošković P.<sup>a</sup>, Prkić A.<sup>b</sup>, Giljanović J.<sup>b</sup>**

<sup>a</sup>*Department of Physical Chemistry, Faculty of Chemistry and Technology, University of Split, Teslina 10, 21000 Split, Croatia*

<sup>b</sup>*Department of Analytical Chemistry, Faculty of Chemistry and Technology, University of Split, Teslina 10, 21000 Split, Croatia*

### **Keywords:**

butan-2-ol + water mixtures, NH<sub>4</sub>Br, association to ion-pairs, thermodynamic quantities

### **Corresponding author:**

Vesna Sokol

### **E-mail:**

vsokol@ktf-split.hr

Tel: +385-21-329 448

Fax: +385-21-329 461

**Abstract:** Molar conductivity of dilute solutions of ammonium bromide in binary mixture of butan-2-ol and water with 10 mass. % of alcohol were measured in the temperature range from 15 °C to 35 °C. Data were processed using conductivity model based on the Lee-Wheaton equation. A three-parameter adjustment did not give uniform values for the association distance  $R$ . Therefore, the Bjerrum critical distance was chosen as a fixed value of that parameter ( $R = q$ ). By repeated treatment, the limiting molar conductivity ( $\Lambda_0$ ) and the ion-pair formation constant ( $K_A$ ) were solved at each temperature, and the thermodynamic quantities of the association reaction ( $\Delta G^\circ$ ,  $\Delta H^\circ$  and  $\Delta S^\circ$ ) were derived at 25 °C. The obtained thermodynamic quantities, together with Walden product, were compared with literature data for ammonium bromide in mixtures with butan-2-ol mass fraction ( $w$ ) 70, 80, 90 and 95 %. From the thermodynamic quantities it is seen that the association reaction is spontaneous, endothermic and leads to an increased disorder in the system; all these features are more pronounced in mixtures with a higher alcohol content.

### **Sažetak**

Mjerena je vodljivost razrijeđenih otopina amonijevog bromida u smjesi butan-2-ola i vode s 10 mas. % alkohola pri pet temperatura u području od 15 °C do 35 °C. U obradi je korišten model provodnosti utemeljen na jednadžbi Lee-Wheaton. Podešavanje triju parametara nije dalo ujednačene vrijednosti asocijacijskog razmaka  $R$ . Stoga je za fiksnu vrijednost tog parametra odabran Bjerrumov kritični razmak ( $R = q$ ). Ponovljenom obradom dobivena su rješenja za graničnu molarnu provodnost ( $\Lambda_0$ ) i konstantu asocijacije ( $K_A$ ) pri svakoj temperaturi, te su izvedene termodinamičke veličine za reakciju asocijacije ( $\Delta G^\circ$ ,  $\Delta H^\circ$  i  $\Delta S^\circ$ ) pri 25 °C. Dobivene termodinamičke veličine, skupa s Waldenovim produktom, uspoređene su s onima za amonijev bromid u 70, 80, 90 i 95 mas. %-tnom butan-2-olu iz literature. Termodinamičke veličine pokazuju da je asocijacijska reakcija spontana, endotermna i vodi ka povećanju nereda u sustavu; sve te osobine više su izražene u smjesama s većim sadržajem alkohola.