

DAY 1

Scientific Tracks & Abstracts



Euroscicon Conference on

Physical Chemistry and Analytical Separation Techniques 2018

October 08-09, 2018 | Amsterdam, Netherlands

DAY 1

October 08, 2018

Sessions

Computational Chemistry | Physical Chemistry | Polymer Chemistry | Nanosciences | Surface Chemistry | Spectroscopic Methods in Separation Techniques | Process Analytical Chemistry

Session Chair

Amin A. El-Meligi

AMA International University Bahrain, Bahrain

Session Co-Chair

Bart Reuvers

DSM Resins, Netherlands

Session Introduction

Title: Corrosion resistance: impact of toothpastes on orthodontic wires

Amit Chattree, Sam Higginbottom Institute of Agriculture, Science and Technology, India

Title: Computational and empiric considerations regarding the electro catalytic reduction of CO₂ by water soluble cobalt porphyrins

Yeshayahu Ben Eliyahu, Ben-Gurion University of the Negev, Israel

Title: Modelling ion diffusion over hydroxylated support surfaces

Manuel J Louwerse, Utrecht University, Netherlands

Title: Sorption of fluoride using chemically modified Moringa oleifera leaves

Shabnam Dan, Sam Higginbottom Institute of Agriculture, Science and Technology, India

Title: Temperature and pH responsive double hydrophilic betaine copolymer: synthesis and investigation of the behaviour

Jongmin Lim, Kyoto University, Japan

Title: Development of bio-based polymers based on agroforestry waste extractions of lignins cured and reinforced with antimicrobial agents delaying fungal and bacterial activity by increasing the period of life of a food on the shelf

Luis Eduardo Gonzalez Granados, UACH, Mexico

Title: Cytotoxic pyran based cembranoids from Sarcophyton glaucum

Zahra Alsaihati, King Abdulaziz University, Saudi Arabia

Title: Spectral resolution and simultaneous quantification of levodopa, carbidopa and entacapone by artificial neural networks

Mahsa Khalili, IAU, IRAN

EuroSciCon

Physical Chemistry and Analytical Separation Techniques 2018

October 08-09, 2018
Amsterdam, NetherlandsAmit Chattree, J Org Inorg Chem 2018 Volume: 4
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CORROSION RESISTANCE: IMPACT OF TOOTHPASTES ON ORTHODONTIC WIRES

Amit Chattree

Sam Higginbottom University of Agriculture, Technology and Sciences (SHUATS), India

The inhibition potentials of five toothpastes (Vicco, Dant Kanti, Sparkle Fresh, Emoform R and Colgate Visible White) was investigated by evaluating the corrosion behaviour of orthodontic wires made of 18 ct gold, SS 316 L, 22 ct gold, SS 18/8 and NiTi shape memory alloy immersed in artificial saliva solution containing 1% toothpaste. Linear polarization resistance, corrosion current, charge transfer resistance, double layer capacitance and impedance were utilized to evaluate the corrosion resistance and adsorption properties of the toothpaste. UV-visible absorption spectroscopy, Fourier transform infrared spectroscopy, fluorescence spectroscopy, scanning electron microscopic studies, electron dispersive X-ray spectroscopy and atomic force microscopy provided the confirmatory evidence of improved surface condition due to adsorption for the corrosion protection. The impedance measurement has shown that the change in the impedance parameters like charge transfer resistance with the addition of extract is due to the adsorption of active molecules leading to the formation of a protective layer on the surface of the orthodontic wire. NiTi shape memory alloy has shown highest percentage of inhibition efficiency ($\eta\%$ of 98% and 97%) in the electrochemical analysis in the presence of Colgate Visible White toothpaste. Sparkle Fresh toothpaste has offered highest corrosion resistance to three of the alloys namely SS 316L, 22ct gold and SS 18/8

Biography

Amit Chattree has graduated from the University of Allahabad in 1994 and completed his MSc in Chemistry (specialization in Analytical and Environmental Chemistry) from the University of Allahabad in 1996. He obtained first position in his Post-graduation and then he completed his PhD in Environmental Chemistry in 2002. His area of research includes environmental chemistry, corrosion chemistry and synthetic organic chemistry. Since July 2012, he is serving as an Associate Professor and the Head of the Department of Chemistry, Sam Higginbottom University of Agriculture, Technology and Sciences, Allahabad. He has been in the teaching and research profession for more than 17 years. He has supervised about 28 MSc theses and at present, 8 PhD students are registered under him for their Doctoral program. He has more than 60 research publications in various peer reviewed national and international Journals. In addition to his responsibilities as the Head of the department, he is also the Member of the Editorial Board of a Journal *The Allahabad Farmer* published by the University. He is also a Referee in the *Arabian Journal of Chemistry* and the *Turkish Journal of Chemistry*. He is the Fellow of the Indian Chemical Society and a Member of the National Environmental Science Academy. He is also the Research Coordinator of the Faculty of Science, School Coordinator of the Directorate of Innovations, Patenting and Consultancy, Joint Secretary of the SHUATS Natural History Society and also a Member of the special events committee of the University. At present, he is working as a Co-Principal Investigator in a joint ISRO Project on "Assessment of Spatial and Temporal Variation of Water Quality in River Ganga using Remote Sensing Techniques".

amit.chattree@shiats.edu.in

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Amsterdam, NetherlandsYeshayahu Ben Eliyahu et al., J Org Inorg Chem 2018 Volume: 4
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COMPUTATIONAL AND EMPIRIC CONSIDERATIONS REGARDING THE ELECTRO CATALYTIC REDUCTION OF CO₂ BY WATER SOLUBLE COBALT PORPHYRINS

Yeshayahu Ben Eliyahu^{1,2}, Y Bochlin¹, S Kozuch¹, E Korin¹
and A Bettelheim

¹Ben-Gurion University of the Negev, Israel

²Nuclear Research Center NEGEV, Israel

The electrochemical reduction of CO₂ offers one of the possible solutions to current energy and sustainability issues since it can sequester carbon from the atmosphere and can be used to produce fuels and useful chemicals. In this respect, some metalloporphyrins have been reported to catalyse the electro reduction of CO₂. However, key issues still remain in regard to the elucidation of the effect of the porphyrin structure on the reaction mechanism and catalyst activity. An essential and necessary stage in the proposed mechanism for the catalytic reduction of CO₂ by the Co(II)/Co(I) porphyrin redox couple is the formation of an intermediate Co(II)porphyrin-CO₂⁻ complex. In an attempt to examine the effect of positively and negatively charged porphyrin substituents on the catalytic activity, we report here on a combined density functional theory (DFT) and empirical study regarding the electrochemical reduction of CO in the presence of the Cobalt(II) 5,10,15,20-(tetra-N-methyl-4-pyridyl) porphyrin - Co(II)TMPyP and Cobalt(II) 5,10,15,20-(tetra-4-sulfonatophenyl) porphyrin - Co(II)TPPS complexes, with charges of +4 and -4, respectively. The lower catalytic activity of the CoTPPS complex as compared to that of CoTMPyP, both dissolved in aqueous alkaline solutions, as demonstrated by cyclic voltammetry experiments, are in agreement with the DFT study. Columbic interactions seem to dictate the cobalt-carbon bond length and strength in the porphyrin-CO₂ intermediate, and consequently have an impact on its stability and on the overall catalytic activity towards CO₂ reduction

Biography

Yeshayahu Ben Eliyahu has received all his degrees in Chemistry from the Hebrew University of Jerusalem. His MSc and PhD theses were done under the supervision of the late Prof Yehuda Haas from the Physical Chemistry Department. He is working in the NRCN, Department of Chemistry since 1995. He has served as the Head of Department of Chemistry in NRCN from 2010-2013 and as the Head of Nuclear Engineering Department in the IAEC from 2013-2018. Now he is on Sabbatical in the Department of Chemical Engineering in Ben-Gurion University of the Negev in Israel.

beneliye@post.bgu.ac.il

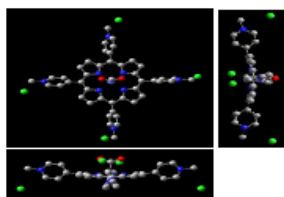


Figure 1: Calculated CoTMPyP-CO₂ complex, top and side views

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MODELLING ION DIFFUSION OVER HYDROXYLATED SUPPORT SURFACES

Manuel J Louwerse

Debye Institute for Nanomaterials Science-Utrecht University, The Netherlands

For many processes in chemistry and in catalysis, diffusion plays an important role. Specifically, for forming nanoparticles during the preparation of solid catalysts and for sintering during their use, controlling the diffusion of metal atoms or ions is the key. The diffusion of metal atoms over the surface of metallic nanoparticles, pristine support surfaces, and hydroxylated support surfaces has been studied before by others. However, the diffusion of metal ions over (hydroxylated) support surfaces has not yet received any attention. Nonetheless, especially during catalyst preparation it is ions that diffuse, so the mobility of ions needs to be studied as well. For the diffusion of ions, everything revolves around the behaviour of counter-charges: displacements of charged ions without any charge compensation would lead to charge separation resulting in high diffusion barriers. However, co-diffusion of counter-ions is not trivial, since these are often incorporated in the hydroxylation layer and are strongly bound by hydrogen bonds. For the co-diffusion of OH^- ions, we have observed that there are two possible mechanisms: adjustments of the hydrogen bond network to allow OH^- co-diffusion, or counter-diffusion of protons, or a combination of these two mechanisms. Using density functional theory (DFT), we studied the diffusion of Cu^{2+} and Cu^+ ions over the surface of γ -alumina at varied hydration states. Apart from setting up a methodology to overcome the challenges of sampling, the many possible adjustments of the hydrogen bond network, we have found interesting trends in the balance between the two possible charge-compensation mechanisms depending on the hydration state of the surface and the charge of the metal ion. We anticipate that many of our conclusions can be translated to other metal ions and types of supports as well, based on the hydrophilicity of the support and the net charge of the metal ion involved

Biography

Manuel J Louwerse has completed his PhD from the Free University Amsterdam. He has worked as Researcher at Organon and TNO and had several postdoctoral positions at the University of Amsterdam and Utrecht University. His research focusses on the Application of Molecular Modelling in several fields of Chemistry. He has published more than 15 papers in reputed journals.

m.j.louwerse@uu.nl

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SORPTION OF FLUORIDE USING CHEMICALLY MODIFIED MORINGA OLEIFERA LEAVES

Shabnam Dan and Amit Chattree

Sam Higginbottom Institute of Agriculture, Science and Technology (SHIATS), India

Contamination of drinking water due to fluoride is a severe health hazard problem. Excess of fluoride (>1.5 mg/L) in drinking water is harmful to human health. Various treatment technologies for removing fluoride from groundwater have been investigated. The present study showed that the leaves of *Moringa oleifera*, an herbal plant are an effective adsorbent for the removal of fluoride from aqueous solution. Acid treated *Moringa oleifera* leaves powder showed good adsorption capacity than alkali treated *Moringa oleifera* leaves powder. Batch sorptive defluoridation was conducted under variable experimental condition such as pH, contact time, adsorbent dose and initial fluoride ion concentration. Maximum defluoridation was achieved at pH 1. The percentage of fluoride removal increases with adsorbent dose. The equilibrium sorption data were fitted into Langmuir, Freundlich and Temkin isotherms. Of the three adsorption isotherms, the R^2 value of Langmuir isotherm model was the highest. The maximum monolayer coverage (Q_{max}) from Langmuir isotherm model was determined to be 1.1441 mg/g, the separation factor indicating a favourable sorption experiment is 0.035. It was also discovered that the adsorption did not conform to the Freundlich adsorption isotherm. The heat of sorption process was estimated from Temkin isotherm model to be -0.042 J/mol which vividly proved that the adsorption experiment followed a physical process

Biography

Shabnam Dan is a Research Scholar in the Department of Chemistry at Sam Higginbottom University of Agriculture, Technology and Sciences, Allahabad, India. Currently, she is working on Nanoadsorbents, trying to incorporate a few aspects of polymer chemistry. Her research interest lies in the area of surface chemistry especially adsorption. She has a good research aptitude. Her past research works focuses on defluoridation using chemically modified biosorbent, under which she has two research publications, one of which is published in a Springer journal of high repute. She also has an experience of teaching as a Guest Lecturer in Department of Chemistry, Ewing Christian College which is one of the oldest and good colleges of the city. She is also serving as a Reviewer in one of the Springer journal and has also been invited by a journal to be a part of the Editorial Board.

shabnamjasmine@gmail.com

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TEMPERATURE AND PH RESPONSIVE DOUBLE HYDROPHILIC BETAINE COPOLYMER: SYNTHESIS AND INVESTIGATION OF THE BEHAVIOUR

Jongmin Lim¹, Hideki Matsuoka¹ and Yoshiyuki Saruwatari²¹Kyoto University, Japan²Osaka Organic Chemical Industry Ltd, Japan

The polycarboxybetaine polysulfobetaine double hydrophilic block copolymer, poly (2-((2-(methacryloyloxy) ethyl) dimethylammonio) acetate)-*b*-poly (3-((2-(methacryloyloxy) ethyl) di-methylammonio) propane-1-sulfonate) (PGLBT-*b*-PSPE), was synthesized by reversible addition fragmentation chain transfer (RAFT) polymerization. The block copolymer was designed for responding to both temperature and pH. The temperature dependent behaviours in aqueous solution of PGLBT-*b*-PSPEs were revealed by observing transmittance variation at $\lambda=400$ nm. The transmittance of solutions was gradually increase/decreased over 20 °C, unlike polysulfobetaine homopolymers or other temperature responsive non-ionic polymers that usually show abrupt transition within only a few °C. Dynamic light scattering studies at transparent or translucent state elucidated that the block copolymer chains created monodisperse particles (hydrodynamic radius $R_h = 40-60$ nm, depended on the chain length) although the both are hydrophilic components, and the particles turned into individual chains when the solution was transparent. At the intermediate temperature, highly expanded particles and unimer like small particles were detected simultaneously. (Fig. 1) ¹H NMR measurement showed disappearances of some signals of PSPE at low temperatures and reappearances by temperature increase, which suggested that the UCST-type PSPE segments aggregate each other to form core and the PGLBT segments form corona on the particle surface. Consequently, PGLBT-*b*-PSPE forms polymeric micelles below certain temperature, then gradually disassembled upon heating, and eventually turned into single chains while the transmittance rises to almost 100%. The structure of particles was identified by comparing radius of gyration to hydrodynamic radius, R_g/R_h . In micellar region, the shape factor was approximately 0.77 which anticipates spherical particles and closed to unity just before disassociation which implies hollow or anisotropic structure. Particle images obtained by TEM met in a good agreement with the light scattering results. Under acidic (pH ~2) condition, zeta potentials of the particle surface turned into positive from near neutral by protonation of carboxylate unit on PGLBT chains, and large aggregates made the solution more turbid

Biography

Jongmin Lim is currently pursuing his PhD degree at Kyoto University under the supervision of Prof Hideki Matsuoka. His current research interests focus on the synthesis and characterizing stimuli responsive double betaine block copolymers. He has received his MS degree in Chemical Engineering in 2011 from KAIST, South Korea under the guidance of Prof Bumjoon J Kim before working several years at LG Household and Health Care.

lim.jongmin.33a@st.kyoto-u.ac.jp

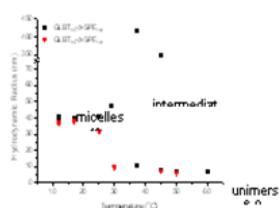


Figure 1: Variations of hydrodynamic radii of GLBT86 derivative PGLBT-*b*-PSPEs

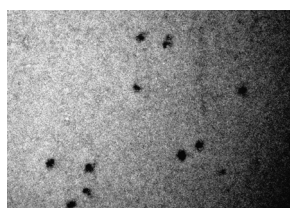


Figure 2: TEM image of GLBT86-*b*-SPE164 (scale bar: 1 μ m)

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DEVELOPMENT OF BIO-BASED POLYMERS BASED ON AGROFORESTRY WASTE EXTRACTIONS OF LIGNINS CURED AND REINFORCED WITH ANTIMICROBIAL AGENTS DELAYING FUNGAL AND BACTERIAL ACTIVITY BY INCREASING THE PERIOD OF LIFE OF A FOOD ON THE SHELF

Luis Eduardo Gonzalez, Juan P Palomares and Eduardo V Gomez

The Autonomous University of Chihuahua (UACH), Mexico

In this work we evaluated the characteristics of a new material made of lignin in different molecular weights (high, medium and low molecular weight) in the development of films made of lignin incorporating essential oils and extracts functional previously analyzed, peppermint (*Mentha piperita*), oregano (*Oreganum vulgare L.*) garlic (*Allium Sativum*) and cinnamon (*Cinnamomun zeylanicum*) as antimicrobial agents. Our main goal is to limit the production of hydrocarbon based polymers in our country to decrease the burning of these and take advantage of the agroforestry waste as the main source of raw material for extraction of lignin: water hyacinth, wheat, maize, walnut shells, coconut fiber and wood (sawdust) of Alamo where it was demonstrated that these have a 20% to 45% lignin that resource where in the future we create in order to remove any residue both forestry and industrial. The antimicrobial activity of the essential oils and extracts functional was evaluated through the determination of the minimum inhibitory concentration and minimum bactericidal concentrations (CMB) against: *Escherichia coli* O157:H7 (ATCC 43888), *Salmonella typhimurium* (ATCC 14028), *Staphylococcus aureus* (ATCC 25923), the essential oils and extracts functional based on the results of microbiological, were incorporated in a polymer matrix of lignin to different molecular weights, and the antimicrobial activity of the films was evaluated by the diffusion technique in Mueller-Hinton agar and blood agar. The molecular weights were characterized by infrared through different processes of removal of lignin thus obtaining various types of lignin however the methodology being a bit orthodox organosolv processes of drag in fractions and retention of oxidant gases. It is a material with such characteristics that has a high temperature degradation that was determined by a term ogavimetrico TGA analysis , with antimicrobial and antifungal agent that slows down this growth

Biography

Luis Eduardo Gonzalez is currently a student at the Autonomous University of Chihuahua. He has been working on different research projects within the scope of developing innovative projects based in the environment and its improvement. In this research, he has studied the effect of the land within molecular arrays that help inhibit a very large proportion of microorganisms, as well as polymer matrices.

Luis.cimav@gmail.com

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CYTOTOXIC PYRAN BASED CEMBRANOIDS FROM SARCOPHYTON GLAUCUM

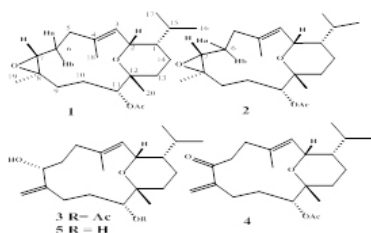
Zahra A Alsaihati¹, Walied M Alarif¹, Mohamed H PH¹, Ahmed Abdel Lateff^{1,2}, Mahmoud A Elfaky², Nahed O Bawakid¹, Najla A Alburae¹ and Hajer S Alorfi¹¹King Abdulaziz University, Saudi Arabia²Minia University, Egypt

Four new pyran-based cembranoidal diterpenes were isolated from the Red Sea soft-bodied coral *Sarcophyton glaucum*. Sarcoglauphine A (1) and B (2) are conformers with respect to the dihedral angle between H-7 and the pair of H-6a, 6b, while sarcotrocheliol-B acetate (3) and sarcotrochelione (4) are bicyclic cembranoids. The chemical structures of the isolated compounds were elucidated using spectroscopic methods. The cytotoxicity of the isolated compounds was evaluated against HepG2, MCF-7 and HCT116 cell lines by employing Sulphorhodamine B (SRB) method. Compounds 1 and 2 showed significant activities toward HCT116

Biography

ZahraA Alsaihati has completed her Master of Sciences in Chemistry from King Abdulaziz University at Saudi Arabia. She holds BSc in Biochemistry from King Abdulaziz University. She was awarded a second prize for the best poster in the 4th international conference and exhibition on Laboratory Technology Conference, which was held in Kingdom of Bahrain. Her research interests include organic analytical separation techniques.

Zahraa.alsaihati@gmail.com

Figure 1: Compounds isolated from *Sarcophyton glaucum*

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SPECTRAL RESOLUTION AND SIMULTANEOUS QUANTIFICATION OF LEVODOPA, CARBIDOPA AND ENTACAPONE BY ARTIFICIAL NEURAL NETWORKS

Mahsa Khalili, M R Sohrabi and V Mirzabeyg

Islamis Azad University (IAU), North Tehran Branch, Iran

Levodopa, carbidopa and entacapone in pharmaceutical formulation were simultaneously quantified by UV-Vis spectrophotometric studies and artificial neural networks (ANN). Absorption spectra of three components were recorded in 200-400 nm spectral region with an interval of 1 nm. The calibration models were thoroughly evaluated at several concentration levels using the spectra of synthetic ternary mixture. Two layer feed-forward neural networks using the back-propagation algorithm (BP) has been employed for building and testing models. The number of neurons in the hidden layer was optimized. The relative standard deviation (RSD) for each component in the real sample was calculated as 0.045, 0.486 and 0.214 for levodopa, carbidopa and entacapone, respectively. The results showed a very good agreement between true values and predicted concentration values and were compared with the standard chromatographic method results. The proposed procedure is a simple, precise and convenient method for the simultaneous determination of levodopa, carbidopa and entacapone in commercial tablets

Biography

Mahsa khalili has completed her BSc in Applied Chemistry, in 2007 from IAU (Karaj Branch). She followed her education at Chemistry and Chemical Engineering Research Center of IRAN and received her MSc degree in Analytical Chemistry. Due to her motivation, she has experienced a vast range of quality control and research activities in the field of Food and Drug. She has started her PhD education in 2014. She also has job experience as a QC Supervisor in a pharmaceutical company. She is Chair of the Board of Directors in NAPLAB, her own R&D Laboratory as well. She has published two ISI papers until now.

chem.khalili@gmail.com

DAY 1

Video Presentation



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PLANT MODIFICATION TO REUSE THE PRODUCED WATER FROM THE DEHYDRATION UNIT IN NGL PLANT IN IRRIGATION

Mohamed A Saad Mahmoud

Suez Canal University, Egypt

Simple modification of NGL plant process flow to treat the produced water in oil and gas industry. If produced water meets appropriate water quality criteria, it may be used beneficially for purposes such as irrigation, livestock watering, aquifer storage, stream flow augmentation, and municipal and industrial uses. Treatment may be required to improve the quality of produced water so that it can be put to beneficial use as in our paper as the produced water was injected to the sewage treatment unit with different ratios to digest the oil and glycols by the microorganisms using additional nutrient, continual monitoring for oil content and the glycols concentration using oil in water instrument and gas chromatograph to monitor the progress to know the optimum injection rate of the produced water to the sewage treatment unit which was 100:900 respectively.

Biography

Mohamed A Saad Mahmoud is an Egyptian Scientist. He has completed his Masters and PhD in Organic Chemistry from Suez Canal University, Ismailia, Egypt. He has worked as Laboratory Chemist in United Gas Derivatives Company and developed the presented invention to save 400,000\$ annually to the company; then he joined Saudi Vision Company in April 2013 and introduced several innovative ideas and alternative analytical techniques in oil and gas analytical techniques, such as mercury determination in range of 5 ppb using ICP-OES without auxiliary unit. He became the Laboratory Manager in 2015. He has been recruited by Saudi Aramco Oil Company in 2017, and became the Youngest Lab Scientist, with the highest employee grade code. He became the Laboratory Technical Leader of the NATSD and filed two patents related to glycols in water determination and general aerobic bacteria alternative medias for quantification in the first year with the company.

saad_chemist2010@yahoo.com