

2014

# Chemistry Abstracts

Second Annual International  
Conference on **Chemistry**, 21-24  
July 2014, Athens, Greece

Edited by Gregory T. Papanikos

THE ATHENS INSTITUTE FOR EDUCATION AND RESEARCH





2<sup>nd</sup> Annual International  
Conference on Chemistry  
21-24 July 2014, Athens,  
Greece

Edited by Gregory T. Papanikos

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# Preface

This abstract book includes all the abstracts of the papers presented at the *2<sup>nd</sup> Annual International Conference on Chemistry, 21-24 July 2014*, organized by the Athens Institute for Education and Research. In total there were 23 papers and presenters, coming from 16 different countries (Brazil, Bulgaria, Chile, China, Germany, India, Iran, Israel, Italy, Korea, Mexico, Palestine, Taiwan, Turkey, UK, USA). The conference was organized into six sessions that included areas such as Organic Chemistry, Electrochemistry, Biotechnology, Medicinal Chemistry and Health Issues, Green Chemistry and Environmental Issues, Materials and Energy and other related fields. As it is the publication policy of the Institute, the papers presented in this conference will be considered for publication in one of the books of ATINER.

The Institute was established in 1995 as an independent academic organization with the mission to become a forum where academics and researchers from all over the world could meet in Athens and exchange ideas on their research and consider the future developments of their fields of study. Our mission is to make ATHENS a place where academics and researchers from all over the world meet to discuss the developments of their discipline and present their work. To serve this purpose, conferences are organized along the lines of well established and well defined scientific disciplines. In addition, interdisciplinary conferences are also organized because they serve the mission statement of the Institute. Since 1995, ATINER has organized more than 150 international conferences and has published over 100 books. Academically, the Institute is organized into six research divisions and twenty-seven research units. Each research unit organizes at least one annual conference and undertakes various small and large research projects.

I would like to thank all the participants, the members of the organizing and academic committee and most importantly the administration staff of ATINER for putting this conference together.

**Gregory T. Papanikos**  
**President**





**FINAL CONFERENCE PROGRAM**  
**2<sup>nd</sup> Annual International Conference on Chemistry, 21-24 July 2014,**  
**Athens, Greece**

**PROGRAM**

**Conference Venue:** Titania Hotel (52 Panepistimiou Avenue)

**ORGANIZING AND SCIENTIFIC COMMITTEE**

1. Dr. Gregory T. Papanikos, President, ATINER.
2. Dr. Chris Sakellariou, Vice President of Finance, ATINER & Associate Professor of Economics, Nanyang Technological University, Singapore.
3. Dr. George Poulos, Vice-President of Research, ATINER & Emeritus Professor, University of South Africa, South Africa.
4. Dr. Nicholas Pappas, Vice-President of Academic Affairs, ATINER & Professor, Sam Houston University, USA.
5. Dr. Panagiotis Petratos Vice President of ICT, ATINER & Associate Professor of Computer Information Systems, California State University, Stanislaus, USA.
6. Dr. Ethel Petrou, Professor and Chair, Department of Physics, Erie Community College-South, State University of New York, USA & Academic Member, ATINER.
7. Dr. Andreas Toupadakis, Lecturer, University of California, Davis, USA.
8. Dr. Nicolas Abatzoglou, Head, Environment Research Unit, ATINER & Professor, Department of Chemical & Biotechnological Engineering, University of Sherbrooke, Canada, Chair Pfizer, PAT in Pharmaceutical Engineering, Director GREEN-TPV and GRTP-C & Pwelcomes.
9. Dr. Bruce Lloyd, Professor, London South Bank University, U.K.
10. Dr. Andy Stergachis, Professor, University of Washington, USA.
11. Dr. Hudu Mikail Garba, Ph.D. Candidate, Department of Pharmacology, School of Medicine, UOA, Greece.
12. Dr. Xiaodong Zhang, Postdoctoral Fellow, University of Texas at Austin, USA.

**Administration**

Fani Balaska, Stavroula Kiritsi, Eirini Lentzou, Konstantinos Manolidis, Katerina Maraki, Celia Sakka, Konstantinos Spiropoulos & Ioanna Trafali

**C O N F E R E N C E P R O G R A M**  
(The time for each session includes at least 10 minutes coffee break)

**Monday 21 July 2014**

**09:00-09:30 Registration**

**09:30-10:00 Welcome and Opening Remarks**

- Dr. Gregory T. Papanikos, President, ATINER.
- Dr. George Poulos, Vice-President of Research, ATINER & Emeritus Professor, University of South Africa, South Africa.

**10:00-11:30 Session I: Advancements, Science and Education**

**Chair:** Olga Gkounta, Researcher, ATINER.

1. Bernd Wrackmeyer, Professor, University of Bayreuth, Germany, Elena. V. Klimkina, Researcher, University of Bayreuth, Germany & Wolfgang Milius, Researcher, University of Bayreuth, Germany. Novel 1,3-Dichalcogeno-2-Phospholanes with an Annelated 1,2-Dicarba-Closo-Dodecaborane(12) Unit.
2. Hyun-Kyung Kim, Researcher, Korea Institute for Curriculum and Evaluation, Korea. An Analysis of Science Academic Achievement of Multiple-cultural and North Korean Migrant Students in Korea.
3. Latif Abuhijleh, Professor, Birzeit University, Palestine. Oxidation and Superoxide Dismutase Activities of Mononuclear Copper (II) Acetate with Imidazoles as Models for Copper Containing Enzymes.
4. Ok-Sang Jung, Professor, Pusan National University, Korea. Synthesis and Applications of Palladium(II) Coordination Cages.

**11:30-13:00 Session II: Materials, Energy and Technology**

**Chair:** Bernd Wrackmeyer, Professor, University of Bayreuth, Germany

1. Dimitris Argyropoulos, Professor, North Carolina State University, USA. Toward Carbon Fibers & Thermoplastic Lignin Polymers; Chain Extension Chemistry via Propargylation, Oxidative Coupling & Claisen Rearrangement. (Monday 21 July 2014, morning session).
2. Claudia Crestini, Tor Vergata University, Italy. Lignin Nanocapsules: Sustainable, Innovative Systems for Actives Storage and Delivery. (Monday 21 of July, morning session).
3. Hilal Kivrak, Assistant Professor, Yuzuncu Yil University, Turkey, Ozlem Sahin, Research Assistant, Selcuk University, Turkey. Methanol Electro-Oxidation Study on Cnt Supported Pt-Ru Direct Methanol Fuel Cells Anode Catalyst.
4. Pedro Antonio Marquez Aguilar, Research Professor, Autonomous University of Morelos, Mexico, Marina Vlasova, Research Professor, Autonomous University of Morelos, Mexico, Abigail Parra Parra, Student, Autonomous University of Morelos, Mexico & Mykola Kakazey, Research Professor, Autonomous University of Morelos, Mexico. Adsorptive Properties of Carbonized Foam-Glass.

**13:00-14:00 Lunch**

**14:00-15:30 Session III: Green Chemistry and Environmental Issues**

**Chair:** Dr. George Poulos, Vice-President of Research, ATINER & Emeritus Professor, University of South Africa, South Africa.

1. Wen-Zhen Wang, Professor, Xi'an Shiyou University, China. Rare Earth Complex Catalysts Transferring CO<sub>2</sub> to Cyclic Carbonate at Mild Conditions.

**21:00-23:00 Greek Night and Dinner (Details during registration)**

**Tuesday 22 July 2014**

**08:30-10:00 Session V: Medicinal Chemistry and Health Issues**

**Chair:** Lital Alfonta, Professor, Ben-Gurion University, Israel.

1. Bras Oliveira, Professor, Parana University, Brazil & Keylla Mischiatti, Ph.D. Student, Parana University, Brazil. Preparation of 2- Phenylquinoline Derivative by Biotransformation and Determination of Anti- Leishmania Activity in Vitro.
2. Pranab Jyoti Das, Professor, Gauhati University, India & Jupitara Das, Post Doctoral Fellow, Indian Institute of Technology, India. A Facile Synthesis of Xanthenes And Benzoxanthenes Promoted by Combined Use of Microwave and Simple Ionic Liquids.
3. Devendra Pratap Rao, Assistant Professor, D.A-V. (P.G.) College, Kanpur, India. Cis-Dioxomolybdenum(VI) Complexes with Symmetrical Tetradentate Schiff Bases and their Antibacterial Activity.
4. Lorena Andrea Gerli Candia, Academic, Catolica University of Santissima Concepcion, Chile. Theoretical Study of 1, 3- Dichlorobenzene.

**10:00-11:30 Session VI: Electrochemistry and Biotechnology**

**Chair:** Bras Oliveira, Professor, Parana University, Brazil

1. \*Lital Alfonta, Professor, Ben-Gurion University, Israel. Site Specific Wiring of Surface Displayed Redox Enzymes to Electrodes.
2. \*Michael M. Meijler, Professor, Ben-Gurion University, Israel, Aviad Mandabi, Ben-Gurion University, Israel, Niva Levy, Ben-Gurion University, Israel, Rachel Gregor, Ben-Gurion University, Israel & Josep Rayo, Ben-Gurion University, Israel. Chemical Signaling within and between Species.
3. Rafaela Vasiliadou, Ph.D. Student, University of Hull, UK & Kevin Welham, Lecturer, University of Hull, UK. Electrochemical Synthesis of Quinone-Glutathione Adducts.
4. Ozlem Sahin, Research Assistant, Selcuk University, Turkey & Hilal Kivrak, Assistant Professor, Yuzuncu Yil University, Turkey. Detection of Hydrogen Peroxide by Platinum based Bimetallic Catalysts.
5. Ivaylo Parushev, Ph.D. Student, Shumen University, Bulgaria, Darina Bachvarova, Post Doc, Shumen University, Bulgaria. Urbach's Rule Region of  $A^{13+}$  and  $P^{5+}$  in the Single and Double Doped  $Bi_{12}TiO_{20}$ .

**11:30-13:00 Session VII: Organic Chemistry**

**Chair:** \*Michael M. Meijler, Professor, Ben-Gurion University, Israel

1. Alejandro Cruz, Profesor, National Polytechnic Institute -UPIBI, Mexico, Itzia-Irene Padilla-Martinez, Professor, National Polytechnic Institute -UPIBI, Mexico & Efen-Venancio Garcia Baez, Profesor, National Polytechnic Institute -UPIBI, Mexico. Chiral 2-Guanidinebenzothiazols from Aminoacids.
2. Arif Kivrak, Associate Professor, Yuzuncu Yil University, Turkey & Richard C. Larock, Distinguished Professor Emeritus, Iowa State University, USA. Synthesis of Dihydrobenzoxazole Derivatives and Their Coupling Reactions.
3. \*Nader Noroozi Pesyan, Faculty Member, Urmia University, Iran, Behzad Zeinizadeh, Faculty Member, Urmia University, Iran & Michael Alinejad, M. Sc. Student, Urmia University, Iran. New Mono - and Bis-Cyclopropane Tetramethanamines as a Bis-Tetradentate Ligand.
4. Fabio Costa, Professor, Federal University of Goias Campus Jatai, Brazil, Fernanda Costa, Professor, Federal University of Rio de Janeiro IPPN, Brazil, Gilda Leitao, Professor, Federal University of Rio de Janeiro IPPN, Brazil & Mauro De Amorim, Professor, Federal University of Rio de Janeiro IPPN, Brazil. Bathysa Australis Vanillic Acid Isolation by Countercurrent Chromatographic and Characterization by NMR 1H and 13C Experimental and Theoretical GIAO-B3PW91/cc-pVDZ//B3PW91/cc-pVDZ Chemical Shifts.
5. Kuang-Hway Yih, Professor, Hungkuang University, Taiwan. Synthesis and Crystal Structures of the Organometallic Molybdenum(II) Complexes With the Diselenophosphinate Containing Ligand.

**13:00-14:00 Lunch**

**17:30-20:30 Urban Walk (Details during registration)**

**21:00-22:00 Dinner (Details during registration)**

**Wednesday 23 July 2014**

Cruise: (Details during registration)

**Thursday 24 July 2014**

Delphi Visit: (Details during registration)

**Latif Abuhijleh**

Professor, Birzeit University, Palestine

## **Oxidation and Superoxide Dismutase Activities of Mononuclear Copper(II) Acetate with Imidazoles as Models for Copper Containing Enzymes**

Copper plays an important role in a variety of enzyme-catalyzed reactions. Copper containing enzymes have mononuclear and binuclear structures. Over the years we have prepared and studied several mono-nuclear and binuclear Cu(II) carboxylate complexes with several nitrogen based ligands as biomimetics for copper containing enzymes. The mononuclear complexes have the formula,  $\text{Cu(II)(L}_{2-6}\text{)(RCOO)}_2$ , where L= imidazole type ligand. Most of imidazoles interact with copper(II)acetate or with other copper(II) carboxylates to produce mono-nuclear structures. Previously, we prepared and determined the molecular structures of copper acetate with imidazoles. While the interaction of copper acetate with imidazole produced trans- bis-adduct and tetrakis-adduct, the interaction with 2-methylimidazole and with 1,2-dimethylimidazole produced cis-bis-adducts. In the imidazole tetrakis-adduct (1) the four imidazole rings occupies coplanar positions with respect to Cu(II) and the two acetate anions coordinate axially through one of the acetate oxygen atoms to form tetragonally elongated  $\text{CuN}_4+\text{O}_2$  chromophore. In bis-adducts the copper ion is coordinated to two 2-methylimidazole (2) or 1,2-dimethylimidazole (3) nitrogen atoms in cis-configuration and two carboxylate oxygen atoms from each acetate ligands. The second carboxylate oxygen atoms interact weakly in the axial positions to form cis-  $\text{CuN}_2\text{O}_2 +\text{O}_2$  chromophore.

The biomimetic catalytic activities of these complexes as models for copper containing enzymes are reported. The superoxide dismutase (SOD) mimetic activities of the complexes are determined using the indirect xanthine-xanthine oxidase -nitroblue tetrazolium method and compared to those for other Cu(II) carboxylate complexes. The results indicated that these complexes are potent SOD mimics, especially the tetrakis-imidazole adduct (1). The polyphenol oxidase activities of these complexes are studied and found to catalyze the oxidation of 3,5-di-tert-butylcatechol to the corresponding o-quinone and the oxidative dealkylation of 2,4,6-tri-tert-butylphenol to 2,6-di-tert-butyl-1,4-benzoquinone and 4,6-di-tert-butyl-1,2-benzoquinone as the main products. The catalytic oxidative coupling of two molecules of aromatic amines o-aminophenol to 2-aminophenoxazin-3-one and o-phenylenediamine to 2,3-diaminophenazine by these complexes will be also presented. These reactions are relevant to the action of type 2

copper-containing oxidase phenoxazinone synthase enzyme. Phenoxazinone chromophore is the final step in the biosynthesis of actinomycin D which is used clinically for the treatment of certain types of cancer. The formation of copper ion semiquinone species in the above oxidative reactions, which may be the catalytic intermediate that reacts with oxygen which leads to the formation of the respective product, will be discussed and is demonstrated spectrophotometrically.

**Lital Alfonta**

Professor, Ben-Gurion University, Israel

## **Site Specific Wiring of Surface Displayed Redox Enzymes to Electrodes**

Bacterial systems are being extensively studied and modified for energy, sensors, and industrial chemistry; yet, their molecular scale structure and activity are poorly understood. Designing efficient bio-engineered bacteria requires cellular understanding of enzyme expression and activity. Bacteria were engineered such that alcohol dehydrogenase II (ADHII) was surface displayed. A quinone, an electron transfer mediator, was covalently attached site specifically to the displayed ADHII. An AFM probe was used to lift a single bacterium off the surface as well as a working electrode for electrochemical analysis in a redox-free buffer. An Electrochemical comparison between two quinone-containing mutants with different distances from the NAD<sup>+</sup> binding site in alcohol dehydrogenase II was performed. Electron transfer in redox active proteins showed increased efficiency when mediators are present closer to the NAD<sup>+</sup> binding site. This study demonstrates that an integrated AFM-electrochemical approach to single cell analysis allows for detailed understanding of enzyme activity integral to creating efficiently engineered biosensors and biofuel cells.

**Dimitris Argyropoulos**

Professor, North Carolina State University, USA

## **Toward Carbon Fibers & Thermoplastic Lignin Polymers; Chain Extension Chemistry via Propargylation, Oxidative Coupling & Claisen Rearrangement**

Despite its aromatic and polymeric nature, the heterogenous, stochastic and reactive characteristics of softwood kraft lignin seriously limits its potential for thermoplastic & carbon fiber applications. Our continuing efforts toward creating thermoplastic lignin polymers & carbon fibers are now focused at exploring propargylation derivatization chemistry and its potential as a versatile novel route for the eventual utilization of technical lignins with a significant amount of molecular control. To do this we initially report the systematic propargylation of softwood kraft lignin and demonstrate the selectivity of the reaction toward the phenolic -OHs while leaving the aliphatic -OHs unaffected. The synthesised derivatives were extensively characterized with thermal methods (DSC, TGA), proton, carbon and <sup>31</sup>P NMR and IR spectroscopies as well as size exclusion chromatography. Further on in our work we demonstrate the versatile nature of the lignin pendant propargyl groups by demonstrating two distinct chain extension chemistries; the solution based, copper mediated oxidative coupling and the thermally induced solid state Claisen rearrangement polymerization chemistries. In this paper we demonstrate that it is possible to modulate the reactivity of softwood kraft lignin via a combination of methylation and chain extension providing a rational means for the creation of thermoplastic materials with the desired control of structure-property relations.



**Fabio Costa**

Professor, Federal University of Goiás, Brazil

**Fernanda Costa**

Professor, Federal University of Rio de Janeiro IPPN, Brazil

**Gilda Leitao**

Professor, Federal University of Rio de Janeiro IPPN, Brazil

&

**Mauro De Amorim**

Professor, Federal University of Rio de Janeiro IPPN, Brazil

## **Bathysa Australis Vanillic Acid Isolation by Countercurrent Chromatographic and Characterization by NMR <sup>1</sup>H and <sup>13</sup>C Experimental and Theoretical GIAO-B3PW91/cc- pVDZ//B3PW91/cc-pVDZ Chemical Shifts**

In this work, we report the first time isolation of vanillic acid from *Bathysa australis* (Rubiaceae) using Countercurrent Chromatography (CCC) and its structural assignment by <sup>1</sup>H and <sup>13</sup>C NMR GIAO-B3PW91-cc-pVDZ and experimental data. We will also present a comparative study with González-Baro protocol in determining the chemical shifts of the vanillic acid (VA). Although González-Baro VA chemical shifts ( $\delta$ s) calculations were carried out at the GIAO-B3LYP/6-311++G(d,p)//B3LYP/6-311++G(d,p) and the solvent effects were taking into account using PCM model. A randomized conformational search of the VA molecule using the Monte Carlo (MC) method with a search limit of 200 structures, and employing the Merck molecular force field (MMFF) was performed. Population-averaged  $\delta$ s for the selected conformers were computed assuming Boltzmann statistics, based on B3PW91/cc-pVDZ free energies:

$$\langle \delta \rangle = \sum_i \frac{\delta_i e^{-\Delta E_i/kT}}{\sum_i e^{-\Delta E_i/kT}}$$

So, the <sup>1</sup>H and <sup>13</sup>C NMR  $\delta$ s were calculated. Our protocol GIAO-B3PW91-cc-pVDZ presented lower MAD and RMS errors despite its lower computational efforts demanding. In conclusion, GIAO-B3PW91/cc-pVDZ//B3PW91/cc-pVDZ scaling factor is a very attractive tool as an alternative to more computationally demanding approaches, which are usually applied in order to achieve <sup>1</sup>H and <sup>13</sup>C NMR chemical shift calculation.

**Claudia Crestini**

Assistant Professor, Tor Vergata University, Italy

## **Lignin Nanocapsules: Sustainable, Innovative Systems for Actives Storage and Delivery**

Oil-filled microcapsules of kraft lignin were synthesized by first creating an oil in water emulsion followed by a high intensity ultrasound assisted cross-linking of lignin at the water/oil interface. The rationale behind our approach is based on promoting documented lignin hydrophobic interactions within the oil phase, followed by locking the resulting spherical microsystems by covalent crosslinking using a high intensity ultrasound treatment. Confocal and optical microscopies confirmed the resulting uniformly spherical morphology of the created lignin microparticles offering further evidence in support of our rationale. The precise elucidation of the cross-linking processes was carried out using GPC and quantitative <sup>31</sup>P-NMR analyses. The ability of lignin microcapsules to incorporate and release Coumarin 6 was evaluated in detail. In vitro studies aimed to follow the way the synthesized capsules were incorporated within Chinese hamster ovary, CHO, cells were supplemented with confocal laser microscopic analyses. This part of our work demonstrated that the lignin microcapsules are not cytotoxic and readily incorporated in the CHO cells.

**Alejandro Cruz**

Profesor, National Polytechnic Institute -UPIBI, Mexico

**Itzia-Irene Padilla-Martinez**

Professor, National Polytechnic Institute -UPIBI, Mexico

&amp;

**Efren-Venancio Garcia Baez**

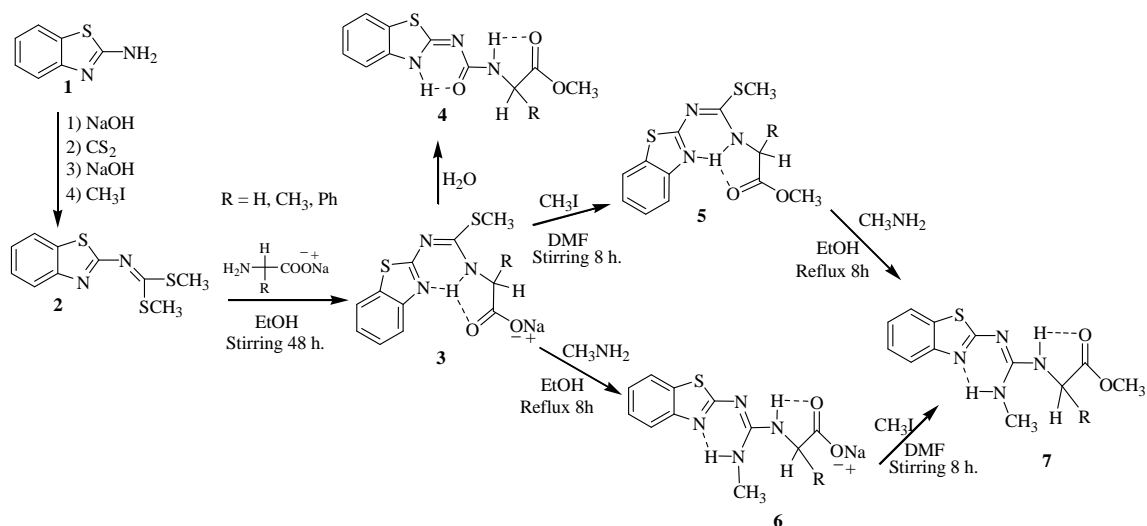
Profesor, National Polytechnic Institute -UPIBI, Mexico

**Chiral 2-Guanidinebenzothiazols from Aminoacids**

A continuous interest in the transformation of amines to corresponding guanidine compounds has been shown, because guanidine group significantly increases the potency and/or selectivity of biologically active compounds. As a consequence, guanidine synthesis from amines has been intensively investigated.

On this base, we recently synthesized symmetric and nonsymmetric guanidinebenzothiazoles from the reaction of ammonia, aliphatic and aromatic amines with dithiomethylcarboimidatebenzothiazole **2** derived from 2-aminebenzothiazole **1**.

In this work, we report the reaction of **2** with one molar equivalent of the corresponding aminoacid to give the respective S-methylbenzothiazolylisothiurea sodium carboxylates **3**, which are methylated with methyl iodide to afford S-methylbenzothiazolylisothiurea methylcarboxylates **5**. Isothiureas **3** and **5** are used to react with alkylamines to get the respective guanidines **6** and **7**. All compounds were characterized by <sup>1</sup>H, <sup>13</sup>C NMR spectroscopy and compounds **5** by X-ray diffraction analysis.



**Pranab Jyoti Das**

Professor, Gauhati University, India

&

**Jupitara Das**

Post Doctoral Fellow, Indian Institute of Technology, India

## **A Facile Synthesis of Xanthenes and Benzoxanthenes Promoted by Combined Use of Microwave and Simple Ionic Liquids**

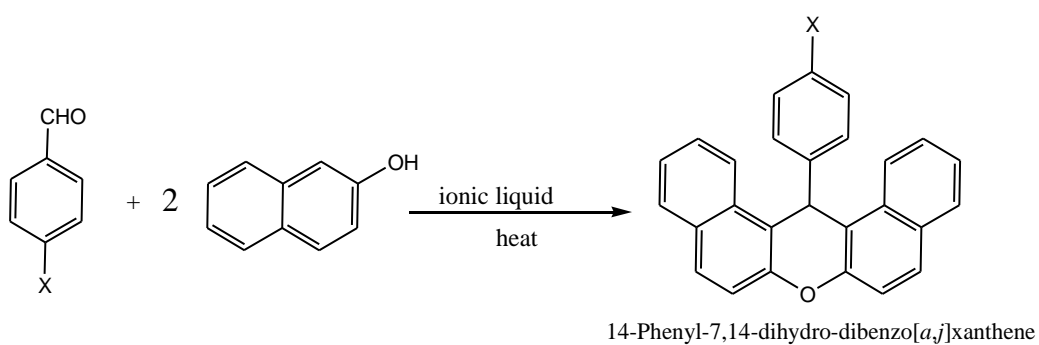
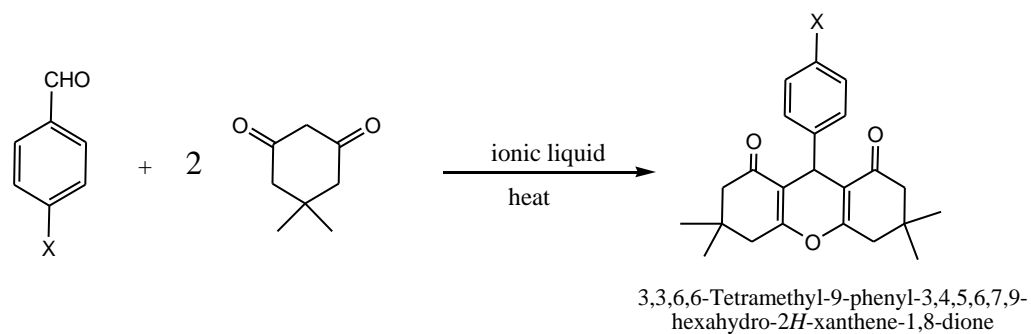
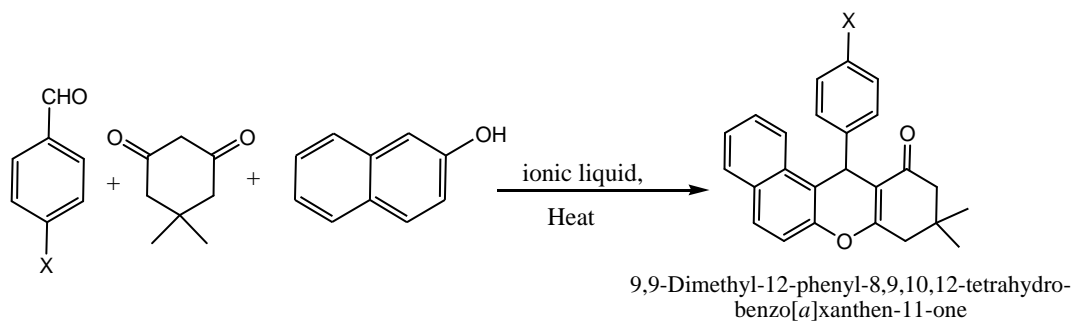
The revolutions of green chemistry play an important role in synthetic Organic chemistry. One of such revolutionary process includes Multi Component Reactions (MCRs) which are continuously increasing their importance in organic, medicinal and natural product chemistry. Apart from this, organic syntheses using ionic liquids as promoters have been investigated due to stringent environment and economic regulations

The synthesis of xanthenes, especially benzo xanthenes has attracted great interest in recent years due to their wide range of biological and pharmaceutical properties such as antiviral, antibacterial, and anti-inflammatory activities as well as sensitizers in photodynamic therapy. Furthermore, these compounds can be used as leuco-dyes, pH-sensitive fluorescent materials for visualization of biomolecules and utilized in Laser Technologies. In the drug discovery process multi component reaction strategies offer significant advantages over conventional linear type syntheses

A facile, efficient and environment-friendly protocol for the synthesis of 9,9-Dimethyl-12-phenyl-8,9,10,12-tetrahydrobenzo[a]xanthen-11-one, 3,3,6,6-Tetramethyl-9-phenyl-3,4,5,6,7,9-hexahydro-2H-xanthene-1,8-dione and 14-Phenyl-

14H-dibenzo[a,j]xanthene by a one-pot condensation of 2-Naphthol, 5, 5- dimethyl-1,3-cyclohexadione and aromatic aldehydes promoted by ionic liquid under solvent-free conditions is reported. The synthetic approach offer the advantages of clean reaction, simple methodology, short reaction time, high yield, easy purification, and easy preparation of the catalysts. The synthesis carried out is shown in Scheme 1. Experimental details will be presented.

Scheme 1



**Lorena Andrea Gerli Candia**

Academic, Catholic University of the Most Holy Conception, Chile

## **Theoretical Study of 1,3- Dichlorobenzene**

In the last 40 years society has become aware of the threats of the increasing release of synthetic chemicals, produced by industrial activity, on human health and ecosystems. Efforts have focused on a class of substances called Persistent Organic Pollutants (POPs), which correspond to toxic chemicals, that are hydrophobic and resistant to photolytic and biological degradation, and, have residence times in the atmosphere that exceed decades.

Among these compounds are chlorobenzenes, which are mainly used as intermediates in the synthesis of pesticides and other chemicals. These are released directly into the environment due to their use as vectors for pesticides, deodorants, fumigants, degreasers, insecticides and herbicides. 1,3- Dichlorobenzene belongs to the group of halogenated organic compounds (1,3 -DCB), which is used as a fungicide, insecticide, solvent, chemical intermediate for the manufacturing of dyes, agrochemicals and pharmaceutical products.

For this reason, computational studies were performed using the AB- initio methodology, in the program Gaussian 09, which uses density functional methods.

For calculations of the molecular structure and properties of the system under study, we used the functional density of B3LYP, PBE0, M06, M06L, M06-2X, M06-HF, CAM-B3LYP, wB97XD and LC-M06L, which provide satisfactory results of structural and thermodynamic properties. The theoretical values found that optimized link lengths differed at most by 0.03 Å from the values reported experimentally.

A series of chemical descriptors of the molecule under study, and the extracted HOMO and LUMO were obtained. These correspond to: chemical potential, electronegativity, hardness and electrophilicity. We did not observe significant difference between the values of these descriptors using the different methodologies.

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## Synthesis and Applications of Palladium(II) Coordination Cages

Diverse poly-pyridyl N-donor ligands that can coordinate two or more remote metal centers were used to construct desirable molecular structures. Unique cage complexes  $[[(\text{Me}_4\text{en})\text{Pd}]_3(\text{L}_1)_2](\text{X})_6$  ( $\text{L}_1 = 1,3,5$ -tris(isonicotinoyloxyethyl)cyanurate;  $\text{X}^- = \text{BF}_4^-$  and  $\text{ClO}_4^-$ ) were constructed. A single water molecule in a skeletal cage was reversibly associated and dissociated via a combination of the adequate space, polar environment, and conformational flexibility of the cage. In Suzuki-Miyaura C-C cross-coupling reactions, the cage complex showed significant catalytic activity along with the effects of the isolated single water molecule. On the other hand, I will lecture the synthesis and operation of a nano-dimension  $24 \times 24 \times 15 \text{ \AA}^3$  "ball-joint-type host-guest system" consisting of unprecedented conglomerate of two distinct helical metallacyclophanes, chiral isomer (P)- $[\text{Pd}_3\text{X}_6(\text{L}_2)_2]@(\text{M})-[\text{Pd}_3\text{X}_6(\text{L}_2)(\text{L}_3)]$  and its enantiomer (M)- $[\text{Pd}_3\text{X}_6(\text{L}_2)_2]@(\text{P})-[\text{Pd}_3\text{X}_6(\text{L}_2)(\text{L}_3)]$ , via the reaction of racemic helical metallacyclophanes, (P,M)- $[\text{Pd}_3\text{X}_6(\text{L}_2)_2]$  with tridentate  $\text{L}_3$ , or direct reaction of 10 small components (six palladium(II), three  $\text{L}_2$ , and one  $\text{L}_3$ ,  $\text{L}_2 = \text{N,N',N''}$ -tris(2-pyridinylethyl)-1,3,5-benzenetricarboxamide;  $\text{L}_3 = \text{N,N',N''}$ -tris(3-pyridinylpropyl)-1,3,5-benzenetricarboxylate;  $\text{X}^- = \text{Cl}^-$  and  $\text{Br}^-$ ). The host-guest aggregation can be ascribed to one  $\pi \cdots \pi$  interaction and three  $-\text{NH} \cdots \text{O}=\text{C}-$  hydrogen-bonds along with the combined helicity. The host-guest system shows a reversible equilibrium between the aggregate and its dissociated species in solution. Such equilibrium control of the host-guest system is reminiscent of "left and right ball-and-socket joint" behavior.

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## **An Analysis of Science Academic Achievement of Multi-cultural and North Korean Migrant Students in Korea**

The National Assessment of Educational Achievement (NAEA) of Korea is a large-scale assessment for monitoring the quality of education at the national level and the appropriateness of national curriculum. In this study, we analyzed, both quantitatively and qualitatively, the characteristics of science academic achievement of multiple-cultural and North Korean migrant students, percentage of correct answer per items and per groups, item discrimination per items and per groups, and content domains in the NAEA. The results revealed that the degree of science academic achievement of the students from multiple culture and North Korean migrant was much lower than that of the general students, and that the science academic achievement of the students from multiple culture and North Korean migrant was found to be different from that of the general students. Especially, science academic achievement of the immigrant students and the North Korean migrant students was lowest. The analysis of items with a big difference in the percentage of correct answer showed that students from multiple culture and North Korean migrant were equally deficient in all content domains, whereas students from international marriage family were weak in some areas. Based on the findings, the appropriate the teaching and learning methods and the educational supports for these students were suggested.



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&amp;

**Richard C. Larock**

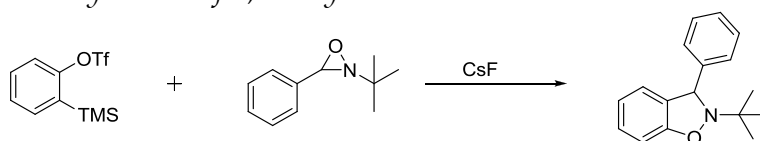
Distinguished Professor Emeritus, Iowa State University, USA

## Synthesis of Dihydrobenzoxazole Derivatives and Their Coupling Reactions

For decades, an intense research effort has been devoted to the synthesis of biologically and pharmaceutically important heterocyclic compounds. Although, dihydrobenzoxazoles appear to have considerable pharmaceutical promise, there are relatively few methods to synthesize dihydrobenzoxazole derivatives.

In this study, we synthesized a variety of five-membered bicyclic 2,3-dihydrobenzoxazoles by the [3+2] cycloaddition of oxaziridines and arynes via C-O bond cleavage (Figure 1). Then, the resulting halogen-substituted dihydrobenzoxazoles are readily elaborated to more complex products using palladium-catalyzed crossing-coupling processes. The scope, limitations, mechanism of these reactions and results will be discussed.

**Figure 1.** *Synthesis of 2,3-dihydrobenzoxazole derivatives*



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**Ozlem Sahin**

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## **Methanol Electro-Oxidation Study on Cnt Supported Pt-Ru Direct Methanol Fuel Cells Anode Catalyst**

Direct Methanol Fuel Cells (DMFCs) are promising power sources for portable electronic devices because methanol is readily available, relatively easy to store, transport, handle. Platinum (Pt) nanocatalyst is employed at the anode and cathode of (Proton exchange membrane fuel cells) PEMFCs because it has a high catalytic activity for the methanol oxidation reaction (MOR) and oxygen reduction reaction (ORR). Nevertheless, carbon monoxide (CO) is strongly adsorbed on the Pt active sites and poisons the Pt surface. Hence, the performance of DMFC decreases severely at the low operating temperatures of DMFCs. By virtue of compensation this CO inverse effect on Pt, other metal/metals can be added in to the Pt cubo-octahedral structure to form Pt binary/ternary catalysts (Kiraly et al., 2007; Kivrak et al., 2009). Conventional carbon supported Pt-Ru bimetallic anode catalysts for methanol electro-oxidation is an effective way to solve the catalyst poisoning problems. The use of multiwalled carbon nanotubes (MWCNTs) as a platinum support for proton exchange membrane fuel cells has been investigated as a way to reduce the cost of fuel cells through an increased utilization of platinum. MWCNTs were produced by chemical vapor deposition method. Furthermore, Pt and Ru metals were deposited in these carbon nanotubes and characterized by electrochemical methods as cyclic voltammetry, chronoamperometry, electrochemical impedance spectroscopy. These measurements were carried out on these MWCNT supported Pt-Ru electrodes in a solution of 1 M CH<sub>3</sub>OH and 0.5 M H<sub>2</sub>SO<sub>4</sub> at 25 °C. Results showed that The MOR catalytic activity of the Pt-Ru/CNT catalyst was higher than that of Pt-Ru/C catalyst. Furthermore, the MOR on the different CNT supported Pt-Ru catalysts at various potentials showed different impedance behaviors. The details of this kinetic study will be presented.

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**Marina Vlasova**

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## **Adsorptive Properties of Carbonized Foam-Glass**

In this investigation the solution of two important environmental problems was considered: 1) the use of technogenic waste for synthesis of new materials, and 2) synthesis of porous glass / ceramic material for purification of water from dissolved pollutants (dyes).

To implement the objective 1) the cullet, which is one of the most representative types of waste, was selected. In the basis of resolving the problem 2) the method of burning out additives for formation of porous body was chosen. As such additive was proposed to use bio-waste from water treatment plants.

The experiments showed that at various dispersity of glass powders, different content of components (glass / biomass) and at sintering under different regimes (temperature and time) it is possible to obtain a wide range of products from foam glass, which can be used as a construction material and as filter from solid and dissolved impurities in water. In the case of use as filter, the temperature regime of sintering must not be accompanied by a complete burn out of organic waste but also their partial carbonization, i.e. the transition of the part of bio-waste into the carbon nano-powder, which is a set of different-sized two-dimensional carbon fragments.

Feature of the preparation of such adsorbents from carbonized foam glass is the formation of the specific structure of the work item, which includes a porous shell of glass and an inner core consisting of a mixture of glass and carbon nano-particles.

Conducted experiments on water purification from dissolved dyes have shown that by using glass particles  $d_v < 90 \mu\text{m}$ , sintering at 650 – 750 °C during 30 minutes, the water solution of methylene blue with concentration 25 ppm. cleared completely from the dye for 3 days at a ratio solid/liquid = 3gr. / 20ml.

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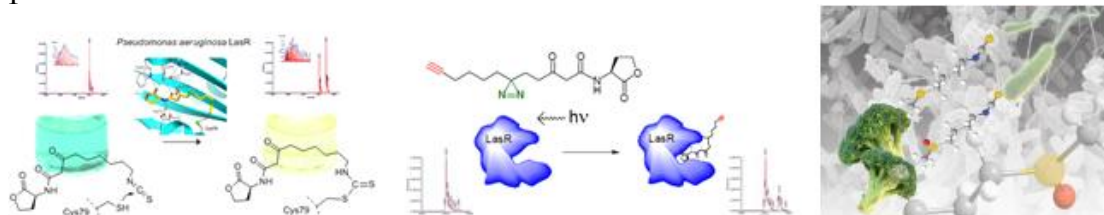
**Josep Rayo**

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## Chemical Signaling within and between Species

Quorum sensing enables unicellular organisms to coordinate their behavior and function in such a way that they can adapt to changing environments and compete, as well as coexist, with multicellular organisms. *Pseudomonas aeruginosa* is an opportunistic pathogen that causes disease in immunocompromised patients. Quorum sensing in this pathogen is mediated by binding of the transcriptional activator, LasR, to its ligand 3-oxo-C<sub>12</sub>-HSL, leading to biofilm formation and secretion of virulence factors. We are targeting QS in *P. aeruginosa* and other bacteria with various chemical tools, such as a set of electrophilic probes that are designed to bind LasR covalently, leading to inhibition of QS regulated gene expression. These probes can be used as molecular tools to obtain new insights into the mechanisms of activation and deactivation of bacterial quorum sensing.

Furthermore, we recently found that certain QS molecules and other natural products can also directly affect the behavior of other bacterial species as well as that of eukaryotes. Diverse eukaryotes have been found to react strongly to the presence of these compounds (often initiating counter-warfare to jam bacterial communication), however, to date no eukaryotic protein has been identified that binds bacterial QS molecules. We have synthesized and evaluated a set of 'tag-free' probes to isolate and identify such receptors, in order to unravel mechanisms that govern these important interkingdom signaling events. We have also discovered several previously unknown signaling molecules from plants that interfere with bacterial communication.



**Bras Oliveira**

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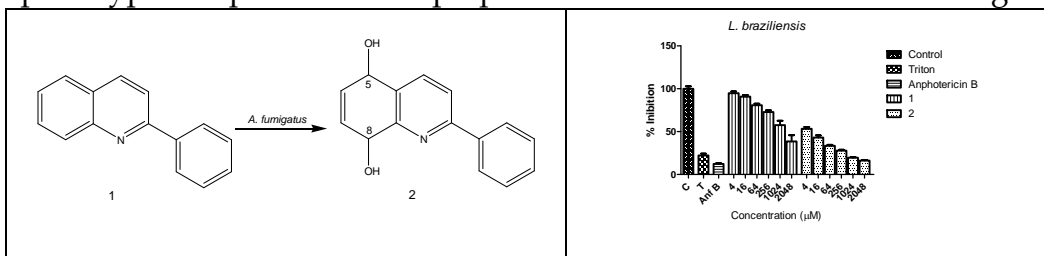
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## Preparation of 2- Phenylquinoline Derivative by Biotransformation and Determination of Anti-*Leishmania* Activity in Vitro

Leishmaniasis is a worldwide disease caused by parasites of the *Leishmania* genus. Its treatment is difficult due to many factors including the toxicity of the drugs currently in use, and also by the development of resistance by the parasite. New drugs are therefore needed. Quinoline alkaloids are one class of natural compounds which has attracted attention, and various derivatives have been obtained and tested. One of them is 2-phenylquinoline (**1**) which has been found in many plant species, and has weak activity against the parasite. Our objective was to prepare derivatives of 2-phenylquinoline using biotransformation by microorganisms. This procedure has many advantages when compared with chemical synthesis due to the characteristics of enzymatic catalysis such as selectivity and mild reaction conditions. Initial screening experiments showed that the fungus *Aspergillus fumigatus* was able to metabolize the compound. Preparative experiments were then carried out and a compound was isolated by column chromatography from the crude extract. The solid obtained, 5,8-dihydro-2-phenylquinoline-5,8-diol (**2**), was characterized by spectroscopic methods, specially 2D NMR. The derivative was tested *in vitro* against the promastigote form of *Leishmania* species using anphotericin B as positive control. The results showed that the derivative was more active than the parent compound in a dose dependent manner (figure below). The increased activity of the dihydroxy derivative may be related, among other factors, to its increased hydrophilicity. 2-Phenylquinoline, therefore, is a promising prototype compound for the preparation of new anti-leishmania drugs.



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## **Urbach's Rule Region of Al<sup>3+</sup> and P<sup>5+</sup> in the Single and Double Doped Bi<sub>12</sub>TiO<sub>20</sub>**

The absorption coefficient of Bi<sub>12</sub>TiO<sub>20</sub>:Al, Bi<sub>12</sub>TiO<sub>20</sub>:P and Bi<sub>12</sub>TiO<sub>20</sub>:Al+P single crystals is measured in the spectral region 2,25 – 3,1 eV at room temperature. The validity of the Urbach's rule has been verified. The constant of the electron-phonon interaction and the value of the dynamic disorder in the crystal lattice are calculated in the cases of doping with Al, P and Al+P. Urbach's energy and the cross-section of the impurity absorption are presented as function of the energy of photons  $h\nu$ .

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**Michael Alinejad**

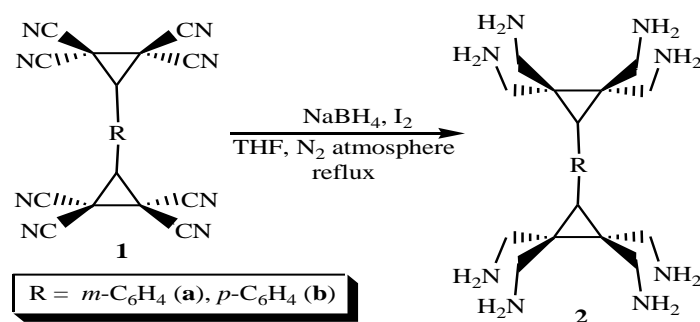
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## New Mono - and Bis-cyclopropane Tetramethanamines as a Bis-tetradentate Ligand

Many of natural basic compounds consisting of one or more nitrogen atoms such as alkaloids have amine nature. On the other hand, many of compounds consist of amine function, are known as pharmaceutical effects. Moreover natural and synthetic cyclopropanes bearing simple functionalities are endowed with a large spectrum of biological properties ranging from enzyme inhibitions to antibiotic, antiviral, antitumor and neurochemical properties [1-4]. Recently, the compounds **1** as a starting material, is reported via a versatile route in excellent yields in very short reaction time (5 seconds) [5].

This article describes the conversion of 3,3'-(1,3- (1a) and 3,3'-(1,4-phenylene)bis(cyclopropane-1,1,2,2-tetracarbonitrile) (**1b**) to (3-(3- (2a) and (3-(4-(2,2,3,3-tetrakis(aminomethyl)cyclopropyl)phenyl)-1,2,2-tris(aminomethyl)cyclopropyl)methanamines (**2b**), respectively, in NaBH<sub>4</sub>-I<sub>2</sub> system in THF under reflux at inert atmosphere (N<sub>2</sub>) in excellent yield (Scheme 1).

**Scheme 1.**



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## **Cis-dioxomolybdenum(VI) Complexes with Symmetrical Tetradentate Schiff Bases and Their Antibacterial Activity**

Five new dioxomolybdenum(VI) complexes,  $[\text{MoO}_2(\text{L})](\text{acac})_2$ ,  $[\text{MoO}_2(\text{mac}^1)](\text{acac})_2$ ,  $[\text{MoO}_2(\text{mac}^2)](\text{acac})_2$ ,  $[\text{MoO}_2(\text{mac}^3)](\text{acac})_2$  and  $[\text{MoO}_2(\text{mac}^4)](\text{acac})_2$ , (where  $\text{mac}^1$ ,  $\text{mac}^2$ ,  $\text{mac}^3$  and  $\text{mac}^4$  are ligands derived from condensation of thenil with 2,3 - diamino - 5 - bromopyridine and their cyclization with  $\beta$ -diketones) have been synthesized. The complexes have been characterized by elemental analyses, molar conductance data, UV - Vis, IR spectra and thermal studies. The probable coordination number of molybdenum is six. Molybdenum has octahedral geometry in each complex. Almost all the synthesized complexes showed low to moderate activity against *S. aureus* and *S. typhi*, the enhancement in the antibacterial activity being explained on the basis of chelation theory.



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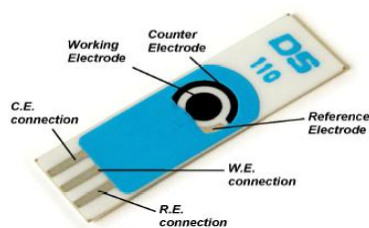
## **Detection of Hydrogen Peroxide by Platinum Based Bimetallic Catalysts**

The detection of hydrogen peroxide ( $H_2O_2$ ) is investigated as a reaction intermediate or product in many reactions (Rosenzweig et al. 1996, Zhang et al., 2010). Several analytical techniques (such as chromatography, chemiluminescence and electrochemistry) have been reported for the determination of  $H_2O_2$ . Among them, electrochemical techniques for detection of  $H_2O_2$  based on noble metals, metal oxides, and graphene have received considerable interest due to their rapid response, high sensitivity, and good selectivity. The studies on this area focused on the use of enzymes to accelerate the electron transfer between the electrodes and  $H_2O_2$ . However, the use of enzymes for biosensor is limited due to ease of denaturation, leakage, time-consuming, costly preparation and purification process of enzymes. To minimize these limitations, chemically modified electrodes have been used to detect  $H_2O_2$  as rapid and accurate routes, due to their low expense and simple fabrication. It is well known platinum based alloy systems have frequently been used to improve the catalytic activity for  $H_2O_2$  (Janyasupab et al., 2013). The addition of second metal to platinum forms alloy structure, resulting in the variations in chemical and physical properties so improves the catalytic activity and selectivity. In this study, carbon supported platinum-ruthenium (Pt-Ru/C) bimetallic nanocatalysts at different atomic ratios were prepared by ethylene glycol reduction method. Electrochemical methods (cyclic voltammetry and amperometry) were used to evaluate the electrocatalytic activities of the catalysts towards  $H_2O_2$  oxidation. Both the cyclic voltammograms and the amperometric responses indicated that Pt-Ru/C possesses a higher oxidation current than either Pt/C or Ru/C.

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&  
**Kevin Welham**  
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## Electrochemical Synthesis of Quinone-Glutathione Adducts

Screen printed electrodes (SPE) are low cost disposable sensors, widely used in the field of electroanalytical chemistry. An attractive choice since all of the electrodes (working, reference and auxiliary) are gathered in a single device, low volumes are required (up to 200  $\mu$ l) and tedious polishing methods are avoided [1]. SPE have applications in environmental studies, pharmaceuticals, food analysis and forensics [1, 2, 3, 4]. Herein, we report the application of SPE for the electrochemical synthesis of reactive and short lived quinone metabolites. Cyclic voltammetry, provided a valuable tool for identifying the reaction mechanism in terms of electron and proton transfer. In particular the effect of various pHs was investigated in order to identify the participation of protons. Additionally, varying scan rates were conducted for two main reasons, firstly for the determination of the mode of mass transport within the electrolyte -electrode interface and secondly for studying the electron transfer kinetics. Quinone intermediates have an electrophilic character, which allows their conjugation with soft nucleophiles such as glutathione. The quinone-glutathione adducts are well known as phase II metabolites formed via Michael addition [5]. Cyclic voltammetry, in the presence of excess glutathione was investigated at a constant scan rate for the electrochemical conjugation of quinone with glutathione. A comparison between the voltammograms of quinone in the presence and without the presence of excess glutathione showed significant changes in terms of electron transfer. However, the quantities of quinone -glutathione adducts formed via cyclic voltammetry were very low for detection. For this reason, constant potential microelectrolysis was performed for 0.5 min and subsequently the generated quinone-glutathione adducts were identified off line in terms of positive electrospray- mass spectrometry.



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## **Rare Earth Complex Catalysts Transferring CO<sub>2</sub> to Cyclic Carbonate at Mild Conditions**

The development of environmentally friendly processes based on carbon dioxide has attracted considerable attention in recent years. The chemical fixation of carbon dioxide into valuable chemicals, such as cyclic carbonate, dimethyl carbonate, methanol, dimethyl ether, and so on, is generally regarded as an excellent solution both from an environmental protection and resource utilization standpoint. Although the synthesis of propylene carbonate (PC) from carbon dioxide and propylene oxide has been applied in industrial scales, the process requires high temperature and pressure. Therefore, great efforts are still being made to develop novel and efficient catalyst system to catalyze cycloaddition reaction of carbon dioxide under mild reaction conditions.

The catalysts of this transformation include heterogeneous catalysts and homogeneous catalysts. The inherent problems, however, are their low activity, high pressure, high temperature conditions and they also need the use of co-solvents. In many cases, salen complexes are moisture sensitive, and low-valent metal complexes are oxygen sensitive.<sup>21</sup> Metal porphyrin and phthalocyanine complexes agglomerate with each other and need to be used in large quantities and require co-solvents to achieve excellent activity.

Up to now, reports on rare earth complex catalysts on the cycloaddition of carbon dioxide to propylene oxide for the synthesis of PC remain extremely scarce, and the catalytic function of heterocyclic amine ligand complexes for this series has been rarely explored. Considering that rare earth metal ions have high charges, high coordination numbers and incompact room compared with common transition metal ions, it is our interest to investigate the novel and efficient rare earth metal catalyst system for synthesizing PC under relatively mild reaction conditions. Here we report our recent research results using various rare earth metal compound catalyst systems to catalyze the reaction of carbon dioxide with propylene oxide to generate PC. An efficient rare earth metal complex-catalyzed cycloaddition reaction of CO<sub>2</sub> with propylene oxide using *N*-donor heterocyclic ligand has been accomplished in good to excellent yields with high selectivity. The effects of different rare earth metal salts, ligands and reaction conditions were examined. Catalytic reaction tests demonstrated that the incorporation of LnCl<sub>3</sub> (Ln = rare earth metal) and *N*-donor heterocyclic ligand can significantly catalyze the

cycloaddition reaction of CO<sub>2</sub> and propylene oxide towards PC under mild conditions without any co-solvent

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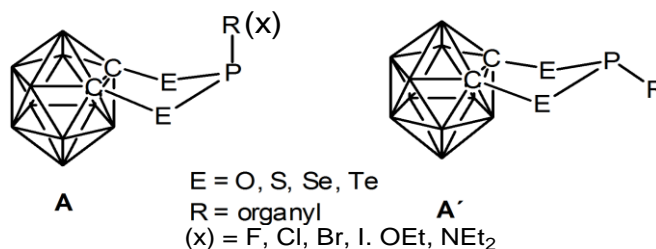
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## Novel 1,3-Dichalcogeno-2-Phospholanes with an Annelated 1,2-Dicarba-Closo-Dodecaborane(12) Unit

1,3-Dichalcogeno-2-phospholanes are well known for E = O, less well studied for E = S, hardly known for E = Se, and virtually unknown for E = Te. We have prepared such compounds for the whole series of E with the annelated 1,2-dicarba-*closo*-dodecaborane(12) unit. This enables to demonstrate structure/reactivity principles resulting from steric and kinetic effects. Thus, for E = O, we observe fast dimerization of derivatives with organyl substituents on phosphorus, because the inherent strain of the five-membered ring is further enhanced by steric interactions between the group R (or the lone pair of electrons) and the rigid three-dimensional carborane skeleton. For E = S, and Se, dimerization also takes place, however, less fast, and for E = Se, this process is readily reversible in most cases. By contrast, no dimers were observed for E = Te.



In principle, these compounds can adopt the structures A or A'. The "normal" structure is A, with its envelope conformation, the phosphorus atom in the flap and the substituent in axial position, leaving room for the lone pair of electrons in the equatorial position. We show for the solid state (X-ray analysis) and in solution (multinuclear NMR spectroscopy accompanied by DFT calculations) that, depending on R or X, both conformations may be present. Clearly, the lone pair of electrons in the axial position presents a sort of a bad compromise. The extensive NMR studies of the novel compounds have revealed useful and new information, among them secondary isotope

effects such as isotope-induced chemical shifts  ${}^n\Delta^{12}{}^{13}\text{C}(^{31}\text{P})$ . For  $n = 2$ , these effects are unusually large, exerted by the carborane carbon atoms, and appear to be a special property of the five-membered rings.

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## Synthesis and Crystal Structures of the Organometallic Molybdenum(II) Complexes with the Diselenophosphinate Containing Ligand

Reaction of the allyl-molybdenum complex  $[\text{Mo}(\eta^3\text{-C}_3\text{H}_5)(\text{CO})_2(\text{CH}_3\text{CN})_2\text{Br}]$  **1**, and ammonium diselenophosphinate,  $\text{NH}_4\text{Se}_2\text{PPh}_2$  in methanol at room temperature yielded the first  $\eta^2$ -diselenophosphinate coordinated allyl-molybdenum complex  $[\text{Mo}(\eta^3\text{-C}_3\text{H}_5)(\text{CO})_2(\eta^2\text{-Se}_2\text{PPh}_2)(\text{CH}_3\text{CN})]$  **2**. Reactions of **2** and bidentate ligands bipy, phen, tridentate ligand potassium tris(pyrazoyl-1-yl)borate and  $\text{PhCCPh}$  in dichloromethane yielded  $\eta^1$ -diselenophosphinate coordinated molybdenum complexes  $[\text{Mo}(\eta^3\text{-C}_3\text{H}_5)(\text{CO})_2(\eta^1\text{-Se}_2\text{PPh}_2)(\text{Bipy})]$  **3**,  $[\text{Mo}(\eta^3\text{-C}_3\text{H}_5)(\text{CO})_2(\eta^1\text{-Se}_2\text{PPh}_2)(\text{Phen})]$  **4**,  $\eta^2$ -diselenophosphinate complex  $[\text{Mo}(\eta^3\text{-Tp})(\text{CO})(\eta^2\text{-Se}_2\text{PPh}_2)]$  **5**, and bis- $\eta^2$ -diselenophosphinate complex  $[\text{Mo}(\eta^3\text{-PhCCPh})_2(\eta^2\text{-Se}_2\text{PPh}_2)_2]$  **6**, respectively. The single crystal structures of complex **2** and **3** have been determined by X-ray diffraction analyses. Crystal data for **2**: space group, *Pbca* with  $a = 15.3764(8) \text{ \AA}$ ,  $b = 13.8041(8) \text{ \AA}$ ,  $c = 19.4922(11) \text{ \AA}$ ,  $V = 4137.4(4) \text{ \AA}^3$ ,  $Z = 8$ . The structure was refined to  $R = 0.0392$  and  $R_w = 0.0828$ . Treatment of **2** with piperidine results in the formation of complex  $[\text{Mo}(\eta^3\text{-C}_3\text{H}_5)(\text{CO})_2\{\eta^2\text{-Se}_2\text{PPh}_2\}(\text{C}_5\text{H}_{10}\text{NH})]$  **7**, in which the labile  $\text{CH}_3\text{CN}$  ligand was substituted by  $\text{C}_5\text{H}_{10}\text{NH}$ . The rotational behaviors of complex **2** and **7** in solution state were detected by variable-temperature  $^1\text{H}$  NMR spectroscopy. The mechanism can be described as a trigonal twist, in which the rotation of the triangular face formed by the nitrogen ligand and the two selenium atoms relative to the face formed by the allyl and the two carbonyl groups.