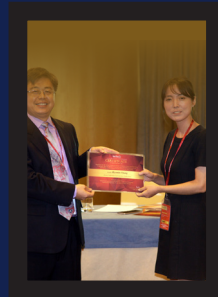
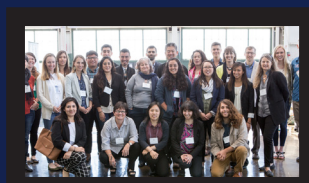


DAY 1

Scientific Tracks
& Abstracts



2nd Edition of EuroSciCon Conference on

CHEMISTRY

February 19-20, 2019 | Prague, Czech Republic

DAY 1

February 19, 2019

Sessions

Organic Chemistry | Chemical Engineering |
Material Science and Chemistry | Electrochemistry
| Environmental Chemistry | Nano-Chemistry and
Technologies | Inorganic Chemistry

Session Chair

Dieter Herlach

Ruhr-Universität Bochum, Germany

Session Co-Chair

Won-Chun Oh

Hanseo University, South Korea

Session Introduction

Title: Gold-catalyzed one-pot synthesis of substituted oxazoles from 3-trimethylsilyl propargylic alcohols and amides

Nobuyoshi Morita, Showa Pharmaceutical University, Japan

Title: Cross-sections, transport coefficients and dissociation rate constants of rare gas dimer ions in collision with their parent gas for cold plasma modelling

Malika Benhenni, Université de Toulouse III Paul Sabatier, France

Title: Can innovative chemical technologies improve radical chemistry?

Estelle Banaszak-Léonard, TIMR UTC/ESCOM Compiègne, France

Title: Synthesis of silacyclic compounds induced by addition of in-situ generated silyl cations to multiple bonds

Takayuki Kawashima, Gunma University, Japan

Title: Effect of reagent chemistry on flotation of mixed copper ore

Silpa Sweta Jena, IIT (ISM) Dhanbad, India

Title: Application of chemistry for the advancement of froth flotation process: an overview and visionary approach

Abhyarthana Pattanaik, Indian Institute of Technology (Indian School of Mines), India

Title: The optimisation of complex industrial processes

Robert Meier, DSM Materials Science Center, The Netherlands

GOLD-CATALYZED ONE-POT SYNTHESIS OF SUBSTITUTED OXAZOLES FROM 3-TRIMETHYLSILYL PROPARGYLIC ALCOHOLS AND AMIDES

Nobuyoshi Morita

Showa Pharmaceutical University, Japan

Oxazole is a structural motif in huge number of natural products and biologically active compounds. Among the numerous procedures reported for the synthesis of substituted oxazoles, cycloisomerization of propargylic amides to substituted oxazoles has attracted much attention. On the other hand, the one-pot synthesis of substituted oxazoles directly from propargylic alcohols and amides *via* propargylic amides as intermediates remains a challenging task, although both propargylic substitution and subsequent cycloisomerization might proceed effectively under the same reaction conditions. Herein, we present the one-pot synthesis of substituted oxazoles by gold-catalyzed propargylic substitution followed by cycloisomerization promoted by β -cation-stabilizing effect of the silicon atom of 3-trimethylsilyl propargylic alcohols.

Biography

Nobuyoshi Morita was born in Iruma, Saitama, Japan in 1973. He received his B.S. degree from Meiji Pharmaceutical University (Prof. Dr. Masanori Sakamoto) in 1997 and his Ph. D. degree from Osaka University (Prof. Dr. Yasuyuki Kita) in 2003. After three years (2003-2006) postdoctoral work at Dortmund University of Technology in Germany (Prof. Dr. Norbert Krause), he was then recruited as Assistant Professor of organic chemistry in Showa Pharmaceutical University (Prof. Dr. Osamu Tamura) in 2006 and became an Associate Professor of organic chemistry in Showa Pharmaceutical University in 2016.

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Benhenni Malika et al., J Org Inorg Chem 2019, Volume: 5
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CROSS-SECTIONS, TRANSPORT COEFFICIENTS AND DISSOCIATION RATE CONSTANTS OF RARE GAS DIMER IONS IN COLLISION WITH THEIR PARENT GAS FOR COLD PLASMA MODELLING

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Transport coefficients and dissociation rate constants of positive rare gas ions are needed input data in chemical electro-hydrodynamic plasma models for a better understanding and optimization of plasma reactors used in applications such as biomedicine or spacecraft. A dynamical hybrid method has been used to calculate momentum transfer for the non-dissociative ion scattering and collision induced dissociation. The hybrid method uses a classical formalism for nuclei and quantum treatment for electrons where the electronic Hamiltonian is calculated *via* a diatomics-in-molecules (DIM) semi-empirical model. Effects of dimer rare gas ion rovibronic excitations are also included in the hybrid dynamical method to improve the agreement between calculated and experimental dimer ion mobility. Moreover, for comparison, momentum-transfer cross-sections have also been derived from an inverse method (based on JWKB approximation and an empirical potential) which fits experimental data available on a limited reduced field range and extends it to a wider range. These collision cross-sections are then used in an optimized Monte Carlo code that simulates the ion trajectory to calculate transport coefficients (mobility and diffusion) and dissociation rate constant of He²⁺, Ne²⁺, Ar²⁺, Kr²⁺ and Xe²⁺ dimer ions in collision with their parent gas over a wide range of reduced field.

Biography

Benhenni Malika has obtained her PhD in 1990 from University of North Carolina at Chapel Hill, USA, in Atomic Physics and concerns the electron capture and excitation processes by Auger electron spectroscopy for hot plasma applications. She was a Research Assistant in 1991 in Laboratoire Grenoblois des Ions, Plasmas et Physique Atomique. She is an Associate Professor at University of Toulouse III-Paul Sabatier in France. Her current research is carried out in Laboratoire Plasmas et Conversion d'Énergie and focuses on modelling of basic data for cold plasma applications such as biomedicine, flue gas pollution control, etc. She is Referee in several international journals.

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CAN INNOVATIVE CHEMICAL TECHNOLOGIES IMPROVE RADICAL CHEMISTRY?

Estelle Banaszak Léonard, C Imbs and V Jeux

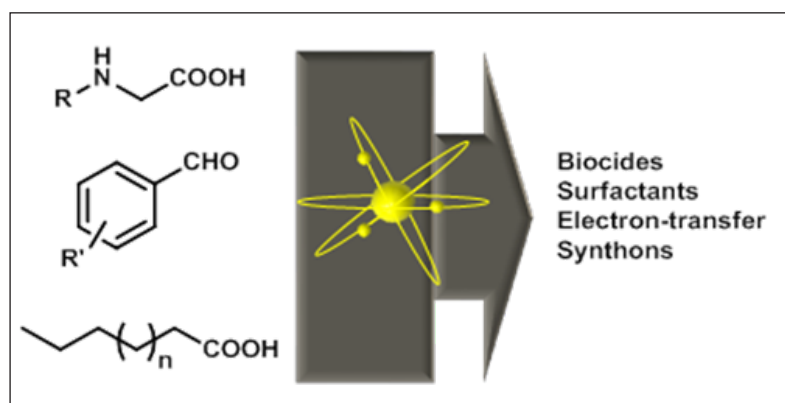
ESCOM-UTC, France

Radical chemistry is of great interest in many chemical areas, such as medicinal chemistry, material chemistry or polymers, or even formulation, in order to understand and prevent radical disorders. However, despite the lasting interest in performing radical syntheses, the use of innovative techniques for a more eco-friendly approach remains occasional. We will focus on examples showing how natural products can undergo radical transformations under innovative techniques. It will be shown that the combination of uncommon energetic devices with greener solvent can shorten reaction times, or even promote the envisioned reaction. By using aromatic aldehydes, (un)modified amino acids or fatty acids, the molecules from such radical processes can be used in a wide range of applications. Biocides, surfactants, electron-transfer materials or even synthons are real options for molecules valorization.

Biography

Estelle Banaszak-Léonard has received her PhD from Lorraine University in Polar Organometallic Field. Then, she moved to Birmingham (UK) University for her first Postdoctoral position, followed by a second one in Le Mans University, where she began to study azobenzenes for the CNRS Center. Since 2008, she is serving as an Assistant Professor in ESCOM/TIMR in Compiègne and in charge of the Organic Team from 2017.

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SYNTHESIS OF SILACYCLIC COMPOUNDS INDUCED BY ADDITION OF IN-SITU GENERATED SILYL CATIONS TO MULTIPLE BONDS

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A silyl cation is well known to be one of the highly reactive Lewis acids, and is available for activation of unsaturated compounds. We developed a sila-Friedel-Crafts reaction, in which the addition of silyl cation to the aromatic moiety followed by deprotonation induces Si-C bond formation and applied it to synthesize various dibenzosiloles such as trisilasumanene and so on. We thought an intermediary silyl cation or its arene complex can add to multiple bonds to form σ -silyl cations, which undergo Friedel-Crafts reaction with an aromatic ring existed in a molecule to give the corresponding silacyclic compounds. We have investigated the reactions using dialkylbenzylhydrosilanes and dialkylhydro-1-naphthylsilanes as precursors of silyl cations, alkynes, alkenes, allenes, carbon dioxide, and aldehydes as multiply bonded compounds, trityl tetrakis(pentafluorophenyl)borate (TPFPB) as a hydride-abstracting reagent, and 2,6-di-tert-butyl-4-methylpyridine as a base. Interestingly, we have found that cyclization occurred only at the 8-position of the naphthalene ring in the reactions using dialkyl-1-naphthylsilanes and alkenes. We also studied on intramolecular version of the reactions using alkynes. Namely, we prepared aromatic compounds bearing trimethylsilyl-ethynyl and dialkylhydrosilyl groups at the neighboring position and treated them with a small amount of TFPBP to give the corresponding aromatic ring-fused siloles and disiloles via single and double intramolecular chain hydrosilylation reactions with silyl cations as chain carriers, respectively. In these reactions, σ -silyl cations are considered to have undergone hydride abstraction from the starting hydrosilanes instead of Friedel-Crafts reactions in the former reactions. In this presentation, we wish to report on the details of these reactions.

Biography

Takayuki Kawashima has received his DSci degree in 1974 from the University of Tokyo under the supervision of Professor Naoki Inamoto. He became a Professor of Department of Chemistry, Graduate School of Science, The University of Tokyo in 1998 via a Research Associate, a Lecturer, and an Associate Professor. From 1976 to 1978, he did Postdoctoral research with Professor J G Verkade at Iowa State University and with Professor W G Bentrude at University of Utah. In 2010, he retired and became Professor Emeritus at the University of Tokyo. He is now a Visiting Professor of Graduate School of Science and Technology, Gunma University after that of Gakushuin University. He received 2013 The Society of Silicon Chemistry, Japan Award. He has 263 original papers. He is a Member of Editorial Board of *Heteroatom Chemistry* from 2003 and International Board on International Conference on Phosphorus Chemistry from 2006.

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EFFECT OF REAGENT CHEMISTRY ON FLOTATION OF MIXED COPPER ORE

Silpa Sweta Jena, N R Mandre and R Venugopal

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Reagent chemistry plays a vital role in numerous unit processes of mineral processing for separation of valuable minerals from gangue. For selective separation, proper choice of reagent is obligatory. Flotation is the most adoptable unit process for copper beneficiation. The process of flotation is extremely challenging due to interdependence of various operating parameters. Current study focused on the selection of reagent system based on the complex mineralogy of Malanjkhand copper-molybdenite deposit. The Malanjkhand porphyry copper deposit is of mixed type (both copper sulphide and copper oxide minerals) and lean grade ore. After continuous mining, the deposits are now left with low grade ores which contain copper sulphide as the major valuable mineral along with higher quantity of silica. In this case, flotation becomes tougher due to mixed mineralic system. From past reviews, the recovery of copper from sulphide mineral using xanthate and pine oil is relatively easy, but mixed oxide-sulphide minerals do not respond to traditional sulphide collector. There is no common reagent to recover copper from both oxide and sulphide mineral, which is a great challenge in flotation of both the minerals simultaneously. Therefore, a comparative flotation study was carried out using traditional sulphide collector (sodium iso propyl xanthate-SIPX), hydroxamate (benzo hydroxamic) collector and mixed (SIPX + benzo hydroxamic) collector system to understand how the reagent chemistry influence the selectivity in the flotation of mixed copper ore.

Biography

Silpa Sweta Jena is a Research Scholar pursuing PhD from Department of Fuel and Mineral Engineering, IIT (Indian School of Mines) Dhanbad, Jharkhand, India. She has completed B Tech in Mineral Engineering from Government College of Engineering, Keonjhar, Odisha, India. She is working on beneficiation of copper ore. She has published more than six papers in reputed international journals and international conferences.

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APPLICATION OF CHEMISTRY FOR THE ADVANCEMENT OF FROTH FLOTATION PROCESS: AN OVERVIEW AND VISIONARY APPROACH

Abhyarthana Pattanaik and Venugopal Rayasam

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Depletion of high grade resources has necessitated the use of low grade fines, which contain good amount of mineral values and liberate in finer sizes. Froth-flotation, a physico-chemical surface based process, is the most established solution, both technologically and economically compared to other alternatives for fines beneficiation. For successful and effective flotation performance, an understanding of the mineral surface specific adsorption mechanism and proper selection of the reagents regimes along with their molecular chemistry is mandated. This study focuses on the complexity of the flotation process along with adsorption and interaction mechanism of different surfactants in accordance to mineral surface characteristics and their dependency on many micro events. Chemistry lays the foundation and plays a major role in advancement of flotation process. In flotation, many branches of chemistries are involved i.e. study of mineral is related to inorganic and crystal chemistry, interaction between slurry solution and mineral surface is associated with physical chemistry, surfactants used in flotation are related to organic chemistry, structural chemistry, polymer chemistry, electro chemistry and finally product examination are related to analytical chemistry. To further strengthen mineral flotation chemistry, research gears at investigating new surfactants, as it is hard to imagine flotation without chemistry. The selection of reagents with appropriate chemical composition and their administration are of critical importance in view of varied mineralogy, chemical complexity and size consist of feed material. Future investigative research should be towards development of selective and cost effective flotation reagents by insertion of new functional groups, molecular modelling of reagents for more environmental friendly nature, modifying the structure of other chelating agents and novel green chemicals from renewable resources, adding aliphatic alcohol and carboxylic acid to bio-based collectors, adding chaotropic anions to alkyl and aryl surfactants, organic and inorganic salts having strong orientation with more proton donor and acceptor, another cationic group to known surfactants, can be tried for enhanced flotation performance. The study also provides a glimpse on the effect of other parameters like pH, composition of pulp, zeta potential, electrostatic potential etc.

Biography

Abhyarthana Pattanaik currently works as Research Scholar (PhD) in the Department of Fuel and Mineral Engineering, Indian Institute of Technology (ISM) Dhanbad. She currently works on the area of Flotation of iron ore fines and slimes, a potentially commercializable process for fines processing. She has done extensive survey of the process, has put a lot of research efforts so far, attempted new reagent regimes, the fundamentals of reagent-mineral surface interaction chemistry etc. Besides the exhaustive physical, chemical and mineralogical characterization of the iron ore sample, she has carried out flotation experiments (both direct and reverse flotation). She has published five international journal papers in reputed journals and has published more than six papers in international and national conferences and has won two awards for research during her PhD career.

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THE OPTIMISATION OF COMPLEX INDUSTRIAL PROCESSES

Robert J Meier

DSM Materials Science Center, The Netherlands

To achieve the Paris climate goals on the one hand, and on the other, ensure the European industry to stay competitive, production processes need to be optimized. Operation costs need to be reduced and an optimal performance of the processes should allow the reduction of energy consumption and raw materials, the number of defects/rejects, reduce waste and increase productivity. The EU Horizon 2020 project COCOP (Coordinating Optimisation of Complex Industrial Processes, <https://www.cocop-spire.eu/content/home>) has the objective to define, design and implement a concept that integrates existing industrial control systems with efficient data management and optimisation methods and provides means to monitor and control (large) industrial production processes. This should lead to a tool that assists the operators in a plant to optimize production continuously, using real-time monitoring and real-time advice given by the control system. The final objective of COCOP is to demonstrate prototype implementation and user acceptance. Within the project, there are two large industrial case studies, one using legacy (existing physical) models; the other one will involve a neural network based model. The advantages of neural network based modelling will be illustrated using a case from the chemical field, but these methodologies are truly field independent. Finally, unique in this context, is the social innovation part in which operators and plant staff are considered crucial stakeholders in the process of developing as well as accepting new ways of working.

Biography

Robert J Meier has completed MSc chemistry at University of Amsterdam, cum laude in 1974-1979; Charles Coulson (Advanced) Summer School in Theoretical Chemistry, Oxford in 1978 & 1980; PhD in experimental physics, University of Amsterdam in 1984. He served different positions such as group-leader ESR, Raman spectroscopy and Theoretical Chemistry at DSM (1985-1993); Research Fellow 'Modelling and Spectroscopy' within DSM (1993-2001); Corporate Scientist in the DSM Research organization (2001-2010); Programme manager Corporate R&D programme Industrial Chemicals (50%) and Corporate Scientist (50%) DSM (2002-2009); Visiting Scientist Research Center Juelich, Germany (part-time, 2002-2014); Principal Scientist In Silico Experimentation (2010-2018) and Senior Grants Manager DSM Materials Sciences (2014-till date). He was appointed as Visiting Fellow Chemistry Department of the University of York (1994-1997) and Honorary Visiting Professor University of York (1997-2016). He (Co-) Authored 134 peer reviewed publications, book on polymer analysis, several worlds' first break-throughs.

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