

1835th Conference
GOICC 2018



24th Global Organic & Inorganic Chemistry Conference

July 18-19, 2018 | Atlanta, USA

Keynote Forum

Day 1

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Edward Lee-Ruff

York University, Canada

Preparation of novel nucleoside analogues from cyclobutane precursors as potential antiviral agents

Cyclobutanes represent strained compounds which exhibit chemical reactivity not encountered with unstrained ring systems. These properties have been exploited in their capacity as synthetic intermediates. Cyclobutane nucleosides as oxetanocin analogs have been shown to exhibit antiviral and other biological activities. Our interests in cyclobutanone chemistry has prompted investigations into the preparation of novel cyclobutane nucleoside analogs. We report in this paper the synthesis of novel cyclobutanols 2 and 3 from its precursor 1. The coupling of 6-chloropurine with 1 gives two regioisomers consisting of the N-9 and N-7 ketones with the latter formed as the major product.

Biography

Edward Lee-Ruff has received his B.Sc. and Ph.D. degree from McGill University. He was the NRC Post-Doctoral Fellow Columbia University under Professor Nick Turro. Since 1969 –present he is a full Professor at York University. He is also a fellow of Chemical Institute of Canada. His main research interest is in Photochemistry, Mechanisms and Organic Synthesis. He has over 120 publications and 2 patents. Also involved in outreach public presentations on brand name vs generic pharmaceutical products.

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P Gregory Van Patten

Middle Tennessee State University, USA

Developing cation exchange as a viable strategy for nanoparticle synthesis

Semiconductor quantum dots (QDs) are promising materials with interesting, size-dependent properties. Although a few model systems (CdSe, PbS, and some others) have been developed, optimized, and thoroughly studied over the past few decades, there remain several obstacles that prevent their adoption in a variety of applications. One principal challenge is the inability to access a diverse range of QD materials with excellent control over size, shape, crystallinity, and surface chemistry. Control over these QD characteristics is crucial for the production of high-quality materials. Since direct synthetic approaches that afford such control have been elusive, we have been exploring cation exchange (CE) as a route to QDs with new compositions. To make CE a viable approach, it must be scalable, must be widely applicable, and must proceed to completion. Additionally, it is desirable to be able to achieve partial exchanges to produce alloy or heterostructures. I will summarize our progress on these goals to date.

Biography

P Gregory Van Patten is Professor and Chair of Chemistry at Middle Tennessee State University specializing in the study of semiconductor quantum dots (QDs). His recent focus has been the study of cation exchange as a means to access new types of QDs that are challenging or impossible to synthesize by more direct routes. In the past, Van Patten has also studied QD self-assembly in solution, resonance energy transfer between QDs, and ultrafast photophysics of QDs. After earning his Ph.D. in Chemistry at the University of South Carolina, Van Patten served as a postdoctoral associate at the Los Alamos National Laboratory, studying the light harvesting properties of polymer films impregnated with metalloporphyrins and related dyes. His work has produced over 40 publications and 2 patents. In 2008, he was awarded a Research Fellowship by the Alexander von Humboldt Foundation.

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Yong-Li Zhong

Merck & Company Inc., USA

Practical asymmetric synthesis of a chronic hepatitis C virus nucleoside cyclic prodrug

Chronic hepatitis C virus (HCV) is a liver disease that has infected an estimated 130 to 150 million people worldwide as of 2016 and killed an estimated 500,000 people around the world annually. In spite of several medicine therapies for the treatment of HCV being available, treatment failure and resistance still remain a clinical challenge. For these reasons, the search for effective antiviral agents to combat HCV is an ongoing endeavor within the global medical/pharmaceutical community. As part of an ongoing drug discovery program in our laboratories, the title compound has been identified as one such selective and potent inhibitor of HCV NS5B nucleoside polymerase. This nucleoside cyclic prodrug is a complex, densely functionalized small molecule, which represents numerous challenges for chemical synthesis. Herein, we report a new asymmetric, practical synthetic route, which features several remarkably diastereoselective and high yielding transformations for the synthesis of the target starting from readily available starting materials.

Biography

Yong-Li Zhong has completed his PhD in 1998 from the Chinese University of Hong Kong and postdoctoral studies from The Scripps Research Institute in San Diego. He joined Process Research & Development, Merck & Company Inc., in 2001 and currently holds the position of principal scientist at Merck. He has published more than 85 papers in reputed journals and has 20 patents.

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Maged Henary

Georgia State University, USA

Microwave assisted synthesis of a library of near-infrared molecular probes for *in-vivo* imaging

A microwave-assisted method for the synthesis of a library of Near-Infrared (NIR) molecular probes such as symmetrical pentamethine cyanines and their corresponding precursors. This class of compounds is advantageous for *in vivo* imaging because of the low absorption of biological molecules in the NIR window. The microwave synthesis drastically reduced the reaction time for dye synthesis from days to min, as well as producing increased yields (89-98%) to the conventional heating method (18-64%). Also in this study, we demonstrate that it is possible to create tissue-specific (thyroid, salivary, and adrenal glands) near-infrared fluorophores using the inherent chemical structure. Thus, a single compact molecule performs both targeting and imaging.

Biography

In 1990, Maged Henary received his BSc. degree in chemistry from Alexandria University and in 2000 he received his Ph.D. degree in organic chemistry from Georgia State University (GSU) under the supervision of Professor Streckowski. Afterward, he joined Professor Fahnri's lab at Georgia Institute of Technology. Dr Henary developed sensors for imaging microscopy of labile zinc and copper pools in live cells. In 2005, he was appointed Lecturer at GSU instructing Undergraduate classes. In 2011, he accepted a position as Assistant Professor at GSU. His research focuses on the development of heterocyclic compounds, including NIR dyes for bioanalytical applications.

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Xin-Tao Wu

Chinese Academy of Sciences, China

Investigations of transition metal complexes with fluorescence or metal to metal charge transfer properties

Metal-organic framework materials with fluorescent, white light or gas-adsorption properties, and transition metal clusters with metal to metal charge transfer properties have become of much interest in fundamental research and modern material science. Recently, the following investigations have been made in my research group: (1) A series of neutral MOFs encapsulated various neutral and ionic guest dye molecules have been designed and synthesized, their luminescent properties have been investigated. The white light-emitting MOF materials could be designed and prepared when three red/green/blue-emitting dyes were introduced simultaneously into such MOF host. Interestingly, the white light is tunable by changing the content or type of the three dye guests, or the excitation wavelength. (2) A series of new luminescent zinc or lanthanide phosphonates and their luminescent properties have been investigated. Furthermore, some lanthanide phosphonates exhibit the remarkable capability to rapidly detect trace amounts of nitroaromatic explosives through luminescent quenching. The sensitivity, fast response, facile synthesis, low usage, cheapness, and good stability make it one of the most powerful nitroaromatic explosives sensors known. (3) A series of mixed valent cyanidometal bridged compounds have been designed, synthesized and characterized, their metal to metal charge transfer properties and the influence factors of electron transfer process have been investigated. In particular, an unusually delocalized mixed-valence state of a cyanidometal bridged compound induced by thermal electron transfer have been reported for the first time.

Biography

Xin-Tao Wu graduated from Xiamen University in 1960 and completed his Master Degree in Science from Fuzhou University in 1966. He is Professor of Chemistry, Director of the Academic Committee from 2000 to 2013, Fujian Institute of Research on the Structure of Matter, Chinese academy of Sciences, and has been a Member of the Chinese Academy of Sciences from 1999. He has published more than 300 papers in reputed international chemical journals.

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Yuichi Shimazaki

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Oxidation chemistry of group 10 metals-di(phenolate) complexes (Ni, Pd and Pt) with Schiff base ligands

Oxidation chemistry of redox-active transition metal complexes with pro-radical ligands and their detailed electronic structures have been actively pursued in recent years. Many efforts for determination of the experimental oxidation number have been close to the goal of the “truth oxidation state” in various oxidized metal complexes with non-innocent ligands. Depending on the relative energies of the redox-active orbitals, metal complexes with non-innocent ligands exist in two limiting descriptions, either a metal-ligand radical ($M^{n+}(L\cdot)$) or a high valent metal ($M^{(n+1)+}(L\cdot)$) complex. In order to understand what factors affect the oxidation locus of the oxidized metal(II)-salen-type complexes, we have investigated isolation and X-ray crystal structure determination of the one-electron oxidized metal(II)-salen-type complexes, and characterization of their electronic structures by various spectroscopic methods. Oxidized Ni^{II}-salen complexes, which have a diphenolate ligand with square planar geometry, are known to exist in either form, and the factors that control the locus of oxidation in these complexes are being pursued currently. One-electron oxidation of Ni-salen-type complexes forms the Ni^{II}-phenoxy radical species, while the addition of exogenous ligands to the Ni^{II}-phenoxy radical solution gives the metal-centered oxidation, Ni^{III}-phenolate species. On the other hand, Pd and Pt complexes show a different oxidation behavior and electronic structure. The one-electron oxidized Pt complex is preferable for the delocalization of the radical electron on the two phenolate moieties while the unpaired electron in the oxidized Pd complexes are more localized on the one-side of the phenolate moiety. In this presentation oxidation behavior of the Group 10 metal(II)-di(phenolate) complexes will be focused, especially detailed electronic structures of oxidized Group 10 metal(II)-di(phenolate) complexes.

Biography

Yuichi Shimazaki was born in 1970 in Toyama prefecture, Japan. He received his Doctor's degree in science from Nagoya University in 2000 under the supervision of Professor Osamu Yamauchi. He joined Professor Yoshinori Naruta's group at Kyushu University as Assistant Professor and worked on the redox behavior of various metal porphyrin complexes as models of the active site of metalloenzymes. In 2008 he was promoted to Associate Professor at the College of Science, Ibaraki University. His research interests include the oxidation chemistry of the complexes of various metal ions, model studies of metalloenzymes, bioorganometallic chemistry, and weak interactions in metal-organic molecule systems.

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Saad Alotaibi

Taif University, Kingdom of Saudi Arabia

Synthesis of magnesium aluminate composites reinforced with ceramic particulates for grinding applications

This project aimed at investigating the possibility to synthesize magnesium aluminate composite reinforced with ceramic particulates to be used as grinding materials. Generally, magnesium aluminate ($MgAl_2O_4$) is commonly used in the industries as refractories. Due to its high chemical stability, this project aims at broadening the industrial applications of magnesium aluminate to be used as grinding materials. Grinding materials are usually used in finishing the machining of metals parts to give it its final bright luster. This project is designed to increase the hardness of magnesium aluminate by incorporation of hard ceramic particulates such as borides or carbides. Titanium carbide (TiC) was chosen to be the reinforcement of magnesium aluminate matrix. This work targets at synthesizing $MgAl_2O_4$ -TiC composite in a high dense form. The target composite will be synthesized by self-propagating high-temperature synthesis (SHS). SHS is an *in-situ* process that can perform synthesis and sintering in one step. To the best of our knowledge this composite in its dense form does not prepare by SHS. Different factors controlling the physical and mechanical properties of the final object will be investigated. This factors include, grain sizes of the starting materials, pressing load, initial temperature of the reaction, amount of ceramic and metallic additions.

Biography

Saad Alotaibi has completed his PhD at the age of 28 years from Western Michigan University and postdoctoral studies from King Abdullah University School of Chemistry. He is the Dean of Turabah University College. He has published more than 8 papers in reputed journals and has been serving as an editorial board member of repute.

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Jun Yin

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Chemical tools to probe protein ubiquitination

Ubiquitin (UB) is transferred through an E1-E2-E3 enzymatic cascade to the substrate proteins to regulate their stability and biological functions in the cell. The human genome encodes 2 E1s, 45 E2s, and more than 600 E3s. Together they assemble a complex network of UB transfer for the modification of cellular proteins. Currently, key questions are unsolved on how to identify ubiquitination targets of important E3s to map them on the cell signaling networks, and how UB chains of specific linkages are assembled to encode unique signals in the cell. We have developed a method that we refer to as “orthogonal UB transfer” (OUT) to untangle the complexity of protein ubiquitination networks. The key to OUT is to engineer a cascade of engineered E1, E2 and E3 enzymes (xE1, xE2, and xE3) that exclusively transfers an engineered UB (xUB) to the substrates of a xE3. We express xUB and the OUT cascade in the cell, purify xUB-conjugated proteins, and reveal their identities by proteomics. The proteins from the OUT screen are the potential substrates of the E3 in the OUT cascade. We have developed OUT cascades with HECT E3 E6AP and U-box E3s E4B and CHIP and identified new cellular circuits regulated by these E3s. To investigate the mechanism of E2-catalyzed UB chain synthesis, we have generated linkage-specific di-UB conjugates by unnatural amino acid incorporation and expressed protein ligation. The di-UB conjugates mimic the binding modes of donor and acceptor UBs at the E2 active site for UB chain synthesis. By characterizing the structure of E2-diUB conjugates, we are to reveal how E2 regulates the synthesis of UB chains of different linkages.

Biography

Jun Yin has completed his PhD from University of California, Berkeley and postdoctoral studies from Harvard Medical School. He is an Associate Professor at the Department of Chemistry of the Georgia State University. His research focus is ubiquitin-mediate cell signaling processes and the catalytic mechanisms of protein ubiquitination enzymes.

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