



The Chinese University of Hong Kong
Department of Chemistry
Faculty Distinguished Lecture Series

Speaker: Professor William D. Jones
Department of Chemistry
University of Rochester
U.S.A.

Title: Cleavage and Formation of Carbon-Carbon
Bonds at Transition Metal Centers: Elucidating
Factors that Control Selectivity

Date: May 3, 2019 (Friday)

Time: 4:30 p.m.

Venue: L1
Institute of Chinese Studies



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Contact Person:
Prof. Michael F.Y. Kwong

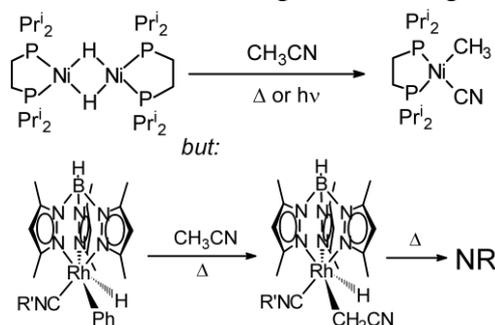
Cleavage and Formation of Carbon-Carbon Bonds at Transition Metal Centers: Elucidating Factors that Control Selectivity

William D. Jones

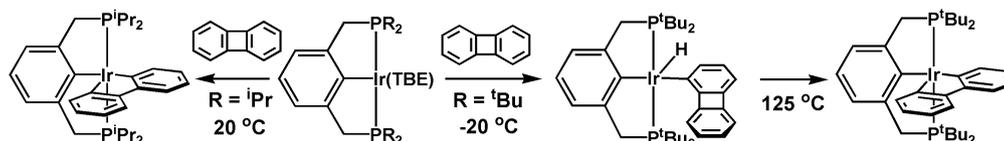
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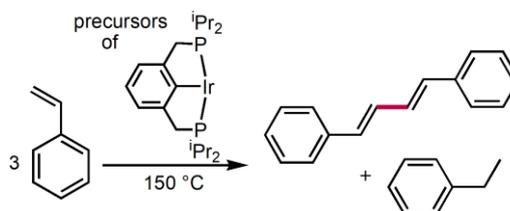
We have studied the cleavage of C-H and C-CN bonds by a variety of unsaturated metal fragments. We will compare and contrast the reactivities of the metal fragments [Ni(dippe)], [Pt(dippe)], [Tp'RhL], [Cp*RhL], and [Rh(dippe)]⁻ (L = PR₃ or CNR) with organic substrates. These studies allow direct comparison of Ni⁰ vs. Pt⁰ vs. Rh^I vs. Rh^{-I}, d⁸ vs. d¹⁰ systems, Cp* vs. Tp', and PR₃ vs. CNR. C-H, C-C, and C-S cleavage will be targeted to make these comparisons.



Pincer-ligated iridium complexes undergo oxidative addition of the strained C-C bond of biphenylene. The sterically crowded species (^tBuPCP)Ir (R^hPCP = κ³-1,3-C₆H₃(CH₂PR₂)₂) initially reacts with biphenylene to selectively add the C(1)-H bond. Upon heating at 125 °C for 24 h, full conversion to the C-C addition product, (^tBuPCP)Ir(2,2'-biphenyl), is observed. The much less crowded (ⁱPrPCP)Ir undergoes relatively rapid C-C addition at room temperature. Based on DFT calculations the large difference in the barriers to C-C addition can be explained in terms of a "tilted" transition state.



The pincer-iridium fragment (ⁱPrPCP)Ir has also been found to catalyze the dehydrogenative coupling of vinyl arenes to afford predominantly (*E,E*)-1,4-diaryl-1,3-butadienes. The eliminated hydrogen can undergo addition to another molecule of vinyl arene, resulting in an overall disproportionation reaction with one equivalent of ethyl arene formed for each equivalent of diarylbutadiene produced. Alternatively, sacrificial hydrogen acceptors (e.g. *t*-butylethylene) can be added to the solution for this purpose. Diarylbutadienes are isolated in moderate to good yields, up to ca. 90% based on the disproportionation reaction. The results of DFT calculations and experiments with substituted styrenes indicate that the coupling proceeds via an iridium(III) metalloindene intermediate, which then adds a β-vinyl C-H bond of a second styrene molecule before reductively eliminating product.





The Chinese University of Hong Kong
Department of Chemistry
Research Seminar Series

Speaker: Professor Xuhui Huang
Department of Chemistry
The Hong Kong University of Science and Technology

Title: Constructing Markov State Models to Elucidate the Functional Conformational Changes of Complex Biomolecules

< Abstract >

Simulating biologically relevant timescales at atomic resolution is a challenging task since typical atomistic simulations are at least two orders of magnitude shorter. Markov State Models (MSMs), a kinetic network model, built from molecular dynamics (MD) simulations provide one means of overcoming this gap without sacrificing atomic resolution by extracting long time dynamics from short MD simulations through the coarse graining on the phase space and time. In this talk, I will demonstrate the power of kinetic network models by applying it to simulate the complex conformational changes, that occurs at tens to hundreds of microsecond timescales for a large RNA Polymerase II complex containing nearly half million atoms. Furthermore, I will introduce a new efficient dynamic clustering algorithm for the automatic construction of MSMs for multi-body systems. We have successfully applied this new algorithm to model the protein-ligand recognition and self-assembly of co-polymers. Finally, I will introduce a new algorithm using the projection operator approach to identify optimal kinetic lumping and recover slowest conformational dynamics of complex systems.

Date: May 10, 2019 (Friday)

Time: 4:30 p.m.

Venue: LT1, Lady Shaw Building



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Contact Person:
Prof. Steve Y.L. Tse



The Chinese University of Hong Kong
Department of Chemistry
Research Seminar Series

Speaker: Professor Yoshiji Takemoto
Graduate School of Pharmaceutical Sciences
Kyoto University

Title: Organocatalyzed Reactions Directed Toward Natural Product Synthesis

<< Abstract >>

Strigolactones (SLs) constitute a new class of plant hormones of increasing importance in plant science. Avenaol, isolated from the allelopathic plant black oat, is the first C₂₀ germination stimulant related to SLs, and consists of a bicyclo[4.1.0]heptanone skeleton containing a cyclopropane ring bearing three main chains projecting in the same direction. We have completed the first total synthesis of (±)-avenaol using a robust strategy involving the formation of an all-cis-substituted cyclopropane via an Ir-catalysed stereoselective double-bond isomerization. We have also explored the enantioselective *O*-alkylation of enols with racemic chloro butenolide using chiral thiourea-ammonium salt hybrid catalyst. The application of this method to racemic synthetic intermediate successfully provides optically active avenaol via 2'-acetal. This study confirms the proposed structure of avenaol, including its unique all-cis-substituted cyclopropane moiety. In addition, I will discuss the catalytic *N*-glycosylation of glycosyl trichloroacetimidate and glycals with a wide range of amides and peptides using 2-halo-azolium salts.

Date: May 15, 2019 (Wednesday)

Time: 2:30 p.m.

Venue: Room 104, Y.C. Liang Hall



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Contact Person:
Prof. Y.Y. Yeung



*The Chinese University of Hong Kong
Department of Chemistry
Research Seminar Series*

Speaker: Professor Hidemitsu Uno
Executive Director and Vice President
Ehime University
Japan

Title: Preparation and properties of large
oligopyrrolic pi-systems

Date: May 16, 2019 (Thursday)

Time: 10:30 a.m.

Venue: Room 106
Y.C. Liang Hall





The Chinese University of Hong Kong
Department of Chemistry
Research Seminar Series

Speaker: Professor Yoshiji Takemoto
Graduate School of Pharmaceutical Sciences
Kyoto University

Title: Design of Bifunctional Thiourea Catalysts for
Asymmetric Reactions

<< Abstract >>

Hydrogen bonding is one of the fundamental intermolecular interactions and plays a crucial role in molecular assembly and recognition in biosynthesis and signal transduction. In the research area of synthetic organic chemistry, the hydrogen bonding interaction has been used for the promotion and stereocontrol of reactions. In order to develop a wide range of asymmetric reactions such as Michael addition, Mannich reaction, aldol reaction, and glycosylation, we have focused on chiral multifunctional thioureas as promising hydrogen-bond donor catalysts. In the lecture, I will discuss the catalyst design concept of our multifunctional thioureas for successful application to various types of reactions as well as the historical background of thiourea catalysis.

Date: May 17, 2019 (Friday)

Time: 2:30 p.m.

Venue: G18
Basic Medical Science Building



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Contact Person:
Prof. Y.Y. Yeung



The Chinese University of Hong Kong
Department of Chemistry
Research Seminar Series

Speaker: Professor Hua Zhang
Department of Chemistry
City University of Hong Kong

Title: Phase Engineering of Novel Nanomaterials

< Abstract >

In this talk, I will summarize the recent research on the phase engineering of nanomaterials in my group. It includes the first-time synthesis of hexagonal-close packed (*hcp*) Au nanosheets (AuSSs) on graphene oxide, the first-time synthesis of 4H hexagonal phase Au nanoribbons (NRBs), the synthesis of crystal-phase heterostructured 4H/*fcc* Au nanorods, the epitaxial growth of metals with novel phases on the aforementioned Au nanostructures, and the synthesis of amorphous/crystalline hetero-phase Pd nanosheets. In addition, the first-time synthesis of 1T'-MoS₂ and 1T'-MoSe₂ crystals have been achieved. Moreover, the phase transformation of transition metal dichalcogenide nanomaterials during our developed electrochemical Li-intercalation method will also be introduced. Interestingly, the lithiation-induced amorphization of Pd₃P₂S₈ is also achieved. Currently, my group focuses on the (crystal) phase-based properties and applications in catalysis, surface enhanced Raman scattering, waveguide, photothermal therapy, chemical and biosensing, clean energy etc., which we believe are quite unique and very important not only in fundamental studies, but also in practical applications. Importantly, the concepts of crystal-phase heterostructures and hetero-phase nanomaterials are proposed.

Keywords: Crystal Phase; Noble Metal Nanomaterials; Hexagonal-Close Packed; Face-Centered Cubic; Gold; Ultrathin Nanosheets; Transition Metal Dichalcogenides.

Date: May 24, 2019 (Friday)

Time: 2:30 p.m.

Venue: Room 103, Y.C. Liang Hall



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Contact Person:
Prof. Zuowei Xie