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Wednesday, January 16, 2013
Somerset-Bridgewater Hotel, Somerset, New Jersey
(Formerly Crowne Plaza Hotel)

Paul J. Chirik
Professor of Chemistry, Princeton University

Base Metal Catalysis

Transition metal catalyzed reactions have revolutionized the art of chemical synthesis. Applications range from the selective synthesis of single enantiomer drugs to the bulk production of high performance silicones. In most cases, these reactions rely on second and third row metals such as Pt, Pd, Rh, and Ir, which are expensive and toxic. My lecture will focus on replacing these metals with more environmentally benign and inexpensive iron and cobalt compounds. Our strategy has focused on so-called “redox-active ligands” – those that undergo reversible electron transfer with the metal. This concept is used to suppress the radical chemistry of the base metals and transmute the electronic structure of the first row ions into those more familiar with the heavy metals. Applications such as alkene hydrosilylation, asymmetric olefin hydrogenation and more unique cycloaddition chemistry will be presented. One illustrative example is the hydrosilylation of α -olefins. With iron catalysts, highly selective anti-Markovnikov additions are observed and have application in the industrial production of agrochemical compounds, tires and personal care ingredients. As will be highlighted, we have discovered that the base metals, likely by virtue of their unusual electronic structures, offer unique chemistry that has not been observed with their heavier congeners.

Brian M. Moreno
2012 Symposium Poster Winner
University of Delaware
Modeling Sorbitol Hydrodeoxygenation

Conversion of biomass into bio-oils is an important step in decreasing dependence on non-renewable energy sources. Fuels derived from bio-oils can be processed and distributed by the currently existing infrastructure used for petroleum-based fuels with only minor modifications. Fundamental kinetic studies of biomass conversion are

necessary to identify the novel oxygenated species found in bio-oils. Yet, such studies prove difficult because of its highly complex and variable composition. Thus, sorbitol is used as a surrogate molecule for biomass given its similarity to simple sugars like glucose and fructose. Like biomass, sorbitol must undergo hydrodeoxygenation to produce low-oxygen-content commodity chemicals such as fuels.

INGen, the Interactive Network Generator, automatically produced a sorbitol hydrodeoxygenation network that predicts all of the experimentally measured species. The reaction network was input to KME, the Kinetic Modeling Editor, for automatic generation and subsequent solution of kinetic rate law equations. Parity plots that compare predicted species composition to experimentally measured values demonstrate high model accuracy, indicating that the selection of reaction families and kinetic parameters captures the salient features of the experimental observations. This tuned kinetic model enables the prediction of product composition for varying feed composition and experimental conditions, determination of optimal conditions, as well as the potential to identify the most suitable feedstock compositions to obtain a desired product, all of which increase energy efficiency and reduce consumption of resources. Results will be used to direct further experimentation and utilization of sorbitol as a biomass surrogate molecule.

Dinner is a buffet, and includes <u>a choice of beef, chicken or fish</u>		Members	\$40
		Non-members	\$50
Social Hour (Cash Bar)	6:00 PM	Students	\$25 (Student Members = \$10)
Dinner	7:00 PM	Retired/Post-Doc/ Unemp.	\$40 (Members = \$30)
Presentation	7:45 PM	Annual Dues	\$35 (Student/Retired = \$15)

Deadline for dinner reservations is 2:00 p.m. Friday, January 11, 2013

Email Xiaoming Wang (xiaoming.wang@basf.com) for reservations. With the exception of extreme circumstances, anyone not canceling reservations by the above deadline will be billed for dinner regardless of attendance.

2012-2013 Officers: Simon Podkolzin (Chair), Lucas Dorazio (Chair-Elect), Marco Castaldi (Past Chair), Israel Wachs (Catalysis Society Rep), Xiaoming Wang (Secretary), John Brody (Treasurer), Robert McGuire (Webmaster), David Harris, Partha Nandi, John Byrne (Directors)