Green Chemistry Seminar (CCVC) (Open to public)

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Title: Transition-Metal Catalyzed Deoxygenation of Biomass to Petrochemicals and Fuels - Strategies, Challenges and Some Successes

Tuesday, October 5, 1:00PM

Location: Otto Maass Chemistry Building (McGill University), RM 10

Biomass is characterized by a high oxygen content (typically ≥ 40 % w/w). Its conversion into feedstocks that can be used in existing petrochemical feed streams will therefore require an efficient and selective deoxygenation chemistry. Economically attractive and ecologically justifiable examples of such processes are the conversion of sugars and sugar alcohols $HOCH_2(CHOH)_nCH_2OH$ (n = 1-4) to high-value added C3 to C6 building blocks or the upgrading of pyrolysis bio-oil obtained from ligno-cellulosic agri/silvicultural waste to engine fuel.

Regardless of the biomass source used the chemical transformations required can be reduced to only five reactions leading to net oxygen content reduction: 1) alcohol dehydration, 2) alkene hydrogenation, 3) ether hydrogenolysis, 4) ester hydrogenolysis and 5) acid ketonization. In order to achieve an efficient deoxygenation these reactions should ideally take place in the same reaction vessel via an iterative reaction cascade of acid-catalyzed dehydrations and metal-catalyzed hydrogenations generating water and possibly CO_2 as the reaction byproducts. By definition any catalyst used must therefore be acid- and water-stable and also be able to withstand the temperatures (> 175 °C) required to overcome the activation barrier for the dehydration of the polyalcohol functionalities found in the biomass substrates.

Homogeneous ionic hydrogenation/hydrogenolysis catalysts may be uniquely suitable for these reactions. The design, synthesis and structure of a series of catalysts based on ruthenium and chelating nitrogen-donor ligands and their activity and limitations in the fundamental reactions using model and actual biomass substrates will be discussed. Also presented will be some surprising discoveries about the catalytic activity of 316SS under acidic aqueous conditions and the use of Red Mud as a sacrificial non-toxic bio-oil upgrading catalyst.

a) Schlaf, M. (**2006**). *Journal of the Chemical Society, Dalton Transactions* (*39*): 4645-4653.
b) Taher, D., M. E. Thibault, et al. (**2009**). *Chemistry- A European Journal*: 10132-10143.
c) Karimi, E., A. Gomez, et al. (**2010**). *Energy & Fuels 24*: 2747-2757.