ICDC
INORGANOMETALLIC CATALYST DESIGN CENTER

Agenda
Reaction Mechanisms Workshop

Part I - Tuesday, August 16, 2016

1:00pm - 3:00pm

Back to Basics:

- Electron counting in metal complexes
- Covalent bond classification of ligands
- Classifying a ligand: a case study of Zeise's Salt

Group Breakout #1: Electron Counting

Elementary Inorganic & Organometallic Reaction Mechanisms:

- Metal requirements for elementary steps
- Predicting stability and relative reactivity

Group Breakout #2: Classifying reactions, electron counts, etc.

3:00pm - 3:20pm: ***Refreshment Break***

3:20 pm - 5:00pm

Tools of the Trade Part 1:

- How do we determine mechanism when we can't see TSes?
- Indirect Methods: Product analysis, isotope labels, crossover experiments, and the principle of microscopic reversibility
    - *Case Study #1: Insertions into Mn carbonyls*
    - *Case Study #2: How does oxidative addition occur?*

Group Breakout #3: Mechanism of alkene trimerization

Part II - Wednesday, August 17, 2016

8:30am - 10:30am

Tools of the Trade Part 2:

- Kinetics: an indirect method of "observing" TSes.
- Kinetic Isotope Effects and Linear Free Energy Releationships (LFERs)
- Reaction Progress Analysis: Kinetic modeling using COPASI & least squares analysis
    - *Case Study #1: Ligand Substitution*
    - *Case Study #2: Hydroformylation, Hydrogenation & "Halpern's Rule"*

Group Breakout #4: Determining mechanism from kinetic data

10:30am - 10:50 am: ***Refreshment Break***

10:50 am - 12:30pm

ICDC-Relevant Transformations & Concluding Remarks

- C-H activation and H-atom transfers
- Homogeneous mechanisms *vs* heterogeneous mechanisms
- Concluding remarks on deducing mechanism