

**Dalton Discussion 6: Organometallic Chemistry and Catalysis**  
University of York, UK  
9 - 11 September 2003

**PROGRAMME**

**Session 1: New Chemistry of C-H and C-F Activation**

Keynote 1

**C-H activation, abnormal ligand binding and molecular recognition effects in carbene chemistry and catalysis**

Robert Crabtree

*Yale University, USA*

**C-F activation and derivatisation of fluorinated olefins at Rhodium**

Thomas Braun

*University of Bielefeld, Germany*

**Oxidative addition of RO-OH species at (diimine)PtMe<sub>2</sub> complexes. New Pt(IV) complexes that are relevant for alkane functionalisation chemistry**

Mats Tilset

*University of Oslo, Norway*

**Catalysed borylation of C-H bonds**

Todd Marder

*University of Durham, UK*

**C-H versus C-C agostic interactions in cycloalkyl niobium complexes: steric and electronic effects**

Michel Étienne

*Laboratoire de Chimie de Coordination du CNRS,  
Toulouse, France*

**Activation of carbon-fluorine bonds using Cp<sup>\*</sup><sub>2</sub>ZrH<sub>2</sub>: a diversity of mechanisms**

William D Jones

*University of Rochester, USA*

## **Session 2: Catalysis and Polymerisation**

Keynote 2

**Metal-catalysed synthesis of stereoregular polyketones, polyesters, and polycarbonates**

Kyoko Nozaki

*University of Tokyo, Japan*

**Orthopalladated phosphinite complexes as high-activity catalysts for the Suzuki reaction**

Robin Bedford

*University of Exeter, UK*

**Copper(I) mediated living radical polymerisation – mechanistic considerations**

David Haddleton

*University of Warwick, UK*

**Catalysing the formation of C-X bonds: mechanisms and development**

Barbara Messerle

*The University of New South Wales, Australia*

**Unprecedented copolymers from new early rare earth catalysts**

Marc Visseaux

*Université de Bourgogne, Dijon, France*

## **Session 3: Organometallic Materials**

Keynote 3

**Metal-catalysed routes to rings, chains and macromolecules based on inorganic elements**

Ian Manners

*University of Toronto, Canada*

**Stationary phases composed of sol-gel processed organometallic complexes functionalised with polyethylene glycol**

Hermann Mayer

*University of Tübingen, Germany*

**Mesoporous ta oxide reduced with bis(toluene) Ti: electronic properties and mechanistic considerations of nitrogen cleavage on the low-valent surface**

David Antonelli

*University of Windsor, Canada*

## **Session 4: Links to Enzymes and Biological Chemistry**

Keynote 4

**Life from hydrogen and carbon monoxide: structure/function relationships in hydrogenases and acetyl coenzyme A synthase**

Juan Fonticella-Camps

*Institut de Biologie Structurale, Grenoble, France*

**Targeting synthetic analogues of the metallo-sulfur active sites of nickel enzymes capable of important catalysis**

David Evans

*John Innes Centre, Norwich, UK*

**Hydrogenase on an electrode: a remarkable heterogeneous catalyst**

Fraser Armstrong

*University of Oxford, UK*

**Electrocatalysis of hydrogen production by active site analogues of the iron hydrogenase enzyme: structure/function relationships**

Marcetta Daresbourg

*Texas A & M University, USA*

## **Session 5: Organometallic Reactivity**

Keynote 5

**Generation and reactivity of sterically hindered iridium carbenes. Competitive *a* vs *b* hydrogen elimination**

Ernesto Carmona

*University of Seville, Spain*

**Cis to trans isomerisation of CpRe(CO)<sub>2</sub>(H)(ArF) (ArF = C<sub>6</sub>H<sub>n</sub>F<sub>5-n</sub>; n = 0-5) is the rate determining step in C-H activation of fluoroarenes : a DFT study**

Eric Clot

*CNRS, Montpellier, France*

**Nucleophilic addition of phosphines to rhenium allenylidenes. Unprecedented double P-H activation to give an *h*1-P-Phosphabutadienyl ligand**

Maurizio Peruzzini

*CNR, Florence, Italy*

**Redistribution at silicon by ruthenium complexes. Bonding mode of the bridging silanes in Ru<sub>2</sub>H<sub>4</sub>(*m*-h<sub>2</sub>:h<sub>2</sub>:h<sub>2</sub>:h<sub>2</sub>-SiH<sub>4</sub>)(PCy<sub>3</sub>)<sub>4</sub> and Ru<sub>2</sub>H<sub>2</sub>{*m*-h<sub>2</sub>:h<sub>2</sub>-H<sub>2</sub>Si(OMe)<sub>2</sub>}<sub>3</sub>(PCy<sub>3</sub>)<sub>2</sub>**

Sylviane Sabo-Etienne

*Laboratoire de Chimie de Coordination du CNRS,*

*Toulouse, France*

**Room temperature cyclometallation of amines, imines and oxazolines with [RuCl<sub>2</sub>(Arene)]<sub>2</sub> and [MCl<sub>2</sub>Cp\*]<sub>2</sub> (M = Rh, Ir)**

David L Davies

*University of Leicester, UK*

**Session 6: Mechanisms and Methods**

Keynote 6

**Using fast time-resolved infrared spectroscopy to probe excited states and reaction mechanisms**

Mike George

*University of Nottingham, UK*

**Marked influence of the bridging carbonyl ligands on the photo- and electrochemistry of the clusters [Ru<sub>3</sub>(CO)<sub>8</sub>(*m*-CO)<sub>2</sub>(L)] (L = 2,2'- bipyridine, 4,4'-dimethyl-2,2-bipyridine and 2,2'- bipirimidine)**

Frantisek Hartl

*University of Amsterdam, The Netherlands*

**High-pressure NMR studies on the alternating copolymerisation of styrene with carbon monoxide catalysed by a palladium(II)-(R,S)-BINAPHOS complex**

Jonathan Iggo

*University of Liverpool, UK*

**Computational study of the spin-forbidden H<sub>2</sub> oxidative addition to 16-electron Fe(0) complexes**

Rinaldo Poli

*Université de Bourgogne, Dijon, France*