

Dalton Discussion 4: Inorganic Reaction Mechanisms: Insights into Chemical Challenges

Kloster Banz, Germany

10-13 January 2002

PROGRAMME

Thursday 10 January

Session 1

Keynote 1

Applications of advanced experimental techniques: high pressure NMR

H Lothar, A Merbach*

University of Lausanne, Switzerland

In situ spectroscopic studies of the Friedel–Crafts acetylation of benzene in ionic liquids using AlCl_3 and FeCl_3

I Horvath,* S Csihony, Ö Farkas, H Mehdi, Z Homonnay, A Vertes, Eotvos

University, Hungary

Low temperature stopped-flow studies in inorganic chemistry

S Schindler,* M Weitzer

University of Erlangen-Nürnberg, Germany

Pulsed-accelerated-flow studies of the temperature dependence of fast reactions

R H Becker, W P Bartlett, E T Urbansky, D W Margerum*

Purdue University, USA

Early photochemical dynamics of organometallic compounds studied by ultrafast time-resolved spectroscopic techniques

A Vlček Jr.,* I R Farrell, D J Liard, P Matousek, M Towrie, A W Parker, D C Grills, M W George

Queen Mary and Westfield College, UK

Friday 11 January

Session 2

Keynote 2

Tools of the trade in modelling inorganic reactions. From balls and sticks to HOMO's and LUMO's

T Ziegler*

University of Calgary, Canada

Carbon–hydrogen bond activation in cyclopentadienyl dimethyl tungsten nitrosyl and carbonyl

Y Fan, M B Hall*

Texas A&M University, USA

The self-exchange of a nonbonding electron *via* the outer-sphere pathway: reorganizational energy and electronic coupling matrix element for the $\text{V}(\text{OH}_2)_6^{2+/3+}$, $\text{Ru}(\text{OH}_2)_6^{2+/3+}$, $\text{V}(\text{OH}_2)_6^{3+/4+}$, and $\text{Ru}(\text{OH}_2)_6^{3+/4+}$ couples

F P Rotzinger*

École Polytechnique Fédérale de Lausanne, Switzerland

Quantum mechanical modelling of alkene hydroformylation as catalyzed by xantphos-Rh complexes

C Landis,* J Uddin

University of Wisconsin, USA

Session 3

Keynote 3

Sterically hindered benzoates: a synthetic strategy for modeling dioxygen activation at metalloprotein active sites

W B Tolman,* L Que Jr.

University of Minnesota, USA

Activation of H₂ by halocarbonyl bis-phosphine and bis-arsine iridium(I) complexes. The use of parahydrogen induced polarisation to detect species present at low concentration and investigation of their reactivity

S K Hasnip, S A Colebrook, C J Sleigh, S B Duckett,* D R Taylor, G K Barlow, M J Taylor

University of York, UK

Mechanistic aspects of hydrogen addition during enantioselective rhodium-catalysed reduction of C=C double bonds with formic acid/triethylamine or molecular hydrogen

S Lange, W Leitner*

Max-Planck-Institut für Kohlenforschung, Germany

Catalytic ionic hydrogenations of ketones using molybdenum and tungsten complexes

M H Voges, R M Bullock*

Brookhaven National Laboratory, USA

Carbon monoxide activation in homogeneously catalysed reactions: the nature and roles of catalytic promoters

R Whyman*

University of Liverpool, UK

Saturday 12 January

Session 4

Keynote 4

Insights from protein film voltammetry into mechanisms of complex biological electron-transfer reactions

F Armstrong*

Oxford University, UK

Kinetics and mechanism of the oxidation of sulfur(IV) by iron(III) at metal ion excess

G Lente, I Fábián*

University of Debrecen, Hungary

Kinetics and mechanism of oxidation of thioglycolic acid by hexachloroiridate(IV)

J Sun, D M Stanbury*

Auburn University, USA

Electron-transfer kinetics and equilibria of copper(II/I) complexes with 1,4,7-trithiacyclononane. A square scheme mechanism involving ligand addition

A Kandegedara, K Krylova, T J Nelson, R R Schroeder, L A Ochrymowycz, D B Rorabacher*

Wayne State University, USA

Session 5

Keynote 5

Spin state tuning of non-heme iron-catalyzed hydrocarbon oxidations: participation of $\text{Fe}^{\text{III}}\text{-OOH}$ and $\text{Fe}^{\text{V}}=\text{O}$ intermediates

K Chen, M Costas, L Que Jr.*

University of Minnesota, USA

Reduction of short chain alkynes by a nitrogenase α -70^{Ala}-substituted MoFe protein

S M Mayer,* W G Niehaus, D R Dean

Virginia Polytechnic Institute and State University, USA

The reaction of ONOO^- with carbonyls: Estimation of the half-lives of ONOOC(O)O^- and $\text{O}_2\text{NOOC(O)O}^-$

S Goldstein,* J Lind, G Merényi

Hebrew University, Israel

Chemically modified mesoporous solids and their use in the polymerisation of hydrocarbon monomers

J H Clark,* K Shorrock, V Budarin, K Wilson

University of York, UK

Studies of copper(II)-binding to bacterioferritin and its effect on iron(II) oxidation

S Baaghil, A J Thomson, G R Moore, N E Le Brun*

University of East Anglia, UK