

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

List of Posters

Only the affiliation of the poster presenter (underlined) is given in this listing.

- P.1 The Catalytic Synthesis of Phosphine Ligands. Applications in Catalysis**
Colin Baillie and J Xiao *University of Liverpool*
- P.2 Ligand Dependence of White Phosphorus Activation**
In $[\text{NiL}_2\text{P}_4]^q (q=0,2) (\text{L}=\text{bipy}, \text{phen})$
Ivan Ogurtzov and V Mirzac, Yu H Budnikova *Academy of Sciences of Moldova*
- P.3 Random Copolymerization of Norbornene with Styrene with $\text{Ni}(\text{tropolonate})_2/\text{MAO}$ System**
Hajime Yasuda and H Suzuki, S Matsumura *Hiroshima University*
- P.4 Computational Modelling of Hydride Protonation and Dihydrogen Deprotonation in Solution**
Agustí Lledós and M Besora, F Maseras *Universitat Autònoma de Barcelona*
- P.5 Binap: An Industrial Approach to Manufacture**
Garreth Aspinall and G F Docherty *Rhodia PPD Ltd*
- P.6 Synthesis of New Pd and Ni Complexes Bearing Ferrocene-based Bidentate (P,S) and Tridentate (S,P,S) Ligands**
German Ferrando-Miguel and I Krummenacher, A Togni *ETH Hönggerberg*
- P.7 Synthesis and Reactivity of Ni(II)-Complexes with PPP/PSP-Ligands for the Asymmetric Hydroamination of Activated Olefins**
Luca Fadini and P Eisenberger, A Togni *ETH Hönggerberg*
- P.8 Electrophilic Fluorination Catalyzed by Rh and Ir Complexes**
Isabelle Haller and D Broggini, A Togni *Swiss Hönggerberg*
- P.9 Synthesis of New Electron-deficient PNNP Ruthenium Complexes for the Asymmetric Cyclopropanation of Olefins**
Cristina Bonaccorsi and F Santoro, S Bachmann, A Mezzetti *Hönggerberg*
- P.10 New Organometallic Materials with Heteroaromatic Proton "Sponges"**
William Kaska and H U Wüestefeld, F Schüth *University of California Santa Barbara*
- P.11 Ligand Effects on Oxidative Addition and Migratory Insertion on Rhodium**
John Wilson and J A Gaunt, S K Spitzmesser, V C Gibson, A Haynes *University of Sheffield*
- P.12 Synthesis of Di-phenol and Di-naphtho Crown Ether Compounds with 14-18 membered Macrocycles via Ring Closing Metathesis**
Haider Behbehani *Kuwait University, Faculty of Science*
- P.13 Characterization Reaction of Benzoyl Methylene Triphenylphosphorane and Benzoyl Methylene Tri-n-butylphosphorane with Rhodium (III) and Ruthenium (III) Chloride, A Multinuclear NMR Study**
Seyyed Javad Sabounchei and K Karami *Bu-Ali-Sina University*

- P.14 Transition Metals Thiolate , CO and CN Chemistry**
Fabio Lorenzini and F Marchetti, A C Marr *The Queen's University Belfast*
- P.15 Synthesis and Characterization of the New Water Soluble Ruthenium Complex**
 $[\text{Ru}(\mu\text{-PCH}_2\text{OH})\{(\mu\text{-P,O-P}(\text{CH}_2\text{O})(\text{CH}_2\text{O})_2)\text{Cl}_2\}_2]$
Antonio Romerosa and T Campos-Malpartida, M Serrano-Ruiz, M Peruzzini *Universidad de Almería*
- P.16 Imine Complexes as Ethene Oligomerisation Catalyst Precursors**
Burgert Blom and M J Overett, J R Moss *University of Cape Town*
- P.17 Activation of White Phosphorus in Coordination Sphere of Nickel Complexes with σ -donor Ligands**
Yulia Budnikova and D I Tazeev, A G Kafiatullina, D G Yakhvarov, O G Sinyashin *Kazan Scientific Center of Russian Academy of Sciences*
- P.18 Fluoride as Bridging Ligand for Ruthenium**
Claus Becker and IKielsch, D Brogini, A Mezzetti *Hönggerberg*
- P.19 Iron Complexes with one Bulky Alkylcyclopentadienyl Ligand**
Helmut Sitzmann and M Wallasch, G Vollmer *Fachbereich Chemie de Universität*
- P.20 Preparation and Transformation of Chiral 1,2-disubstituted Ferrocenes: A Chiral Ferrocene with a Better Arm**
Shin-ichi Fukuzawa and S Itoh *Institute of Science and Engineering, Chuo University*
- P.21 Theoretical Study on the Origin of the Enantioselectivity in the Vanadium-Catalyzed Oxidation of Bis (Tert-Butil) Disulphide**
David Balcells and F Maseras, A Lledós *Universitat Autònoma de Barcelona*
- P.22 σ -borane and Dihydroborate Complexes of Ruthenium**
Sébastien Lachaize and V Montiel, B Chaudret, S Sabo-Etienne, K Essalah, J-C Barthelat *Laboratoire de Chimie de Coordination du CNRS*
- P.23 Metallabenzene: A DFT Investigation into their Intriguing Reactivity and Optical Properties**
Mark Iron and A Karton, M E van de Boom, J M L Martin *Weizmann Institute of Science*
- P.24 Dialkylaminoethyl-Substituted *ansa*-Zirconenes: Switchable Precatalysts for Olefin Polymerisation**
T Hagemester and P Jutzi, C Müller, T Braun *University of Bielefeld*
- P.25 Fluorinated Organic Derivates by Nickel Mediated C-F Activation of Heteroaromatics**
M I Sladek and T Braun *University of Bielefeld*
- P.26 DFT Studies on $\text{M}(\text{C}_5\text{R}_5)\text{L}(\text{C}_2\text{H}_5)^+$ [$\text{M}=\text{Co},\text{Rh}$, $\text{L}=\text{PMe}_3$, C_2H_4 , $\text{R}=\text{H},\text{Me}$] investigating the Electronic Effects which influence Hydrogen Transfers**
Ben Herbert and W Tomlinson, J C Green *University of Oxford*
- P.27 Counterion Effect on the Heterolytic Splitting of a Dihydrogen: deprotonation of $\text{trans-}[\text{FeH}(\eta^2\text{-H}_2(\text{dppe})_2)]^+$ with NEt_3**
Agustí Lledós and M Besora, F Maseras *Universitat Autònoma de Barcelona*
- P.28 Electronic and Steric Effects in the QM/MM Modeling of Organometallic Complexes**
Olivier Maresca and F Maseras, A Lledós *Universitat Autònoma de Barcelona*
- P.29 The Role of Alkali Metal and Alkaline Earth Promoters in Iridium and Ruthenium Catalyzed 1-hexene Hydroformylation**
M A Moreno and S Jääskeläinen, T A Pakkanen, M Haukka *University of Joensuu*

- P.30 Mechanism of Olefin Epoxidation Promoted by Mo(VI) Complexes in the Presence of TBHP**
Maria José Calhorda and L F Veiros, F E Kühn *Universidade de Lisboa*
- P.31 Diphosphinocetenimines as Precursors of Highly Functionalized Diphosphines**
Marta Gonzalez-Mosquera and G García, F Marquínez, V Riera, J Ruiz *Universidad de Oviedo*
- P.32 Elucidation of Palladium Carbomethoxy Catlytic Cycle in the Pd-Catalysed CO/Ethylene Reaction**
Jianke Liu and J A Iggo, B T Heaton, R Whyman *University of Liverpool*
- P.33 A Study of the Electronic Spectroscopy and Redox Properties of Novel Heterobimetallic Complexes Containing Carbene and W(CO)₅ Acceptor Units**
Denise Rooney and K O Doyle, C T O'Brien, M T Pryce *NUI*
- P.34 An Investigation of Palladium-(2-pyridyldiphenylphosphine) Complexes as Possible Precursors in Alkyne Carbonylation**
Kelly Sheridan and B T Heaton, J A Iggo, C Jacob, R Whymann *University of Liverpool*
- P.35 Discovery of New Lanthanide Catalysts Using High Throughput Methods**
Charlotte Willans and F Kerton *University of York*
- P.36 Synthesis of Novel Nitrogen and Phosphorus Containing Bridging Ligands**
Iman Khazal and F Kerton *University of York*
- P.37 Ligand Design for Metal Catalyzed Reactions in Supercritical Carbon Dioxide**
Shohreh Saffarzadeh-Martin and F Kerton, C Rayner *University of York*
- P.38 Synthesis of N-Heterocyclic Carbene-Amine Hybrid Ligands and their Transition Metal Complexes**
Jennifer Houghton and R E Douthwaite *University of York*
- P.39 Synthesis and Catalytic Application of New Chiral N-Heterocyclic Carbene Metal Complexes**
Richard Hodgson and R E Douthwaite *University of York*
- P.40 In situ Photolysis of Organometallic Complexes**
Kirsten Ampt and P Callaghan, S B Duckett, R N Perutz *University of York*
- P.41 Yttrium Chelating Diamide Complexes; Synthesis, Characterisation and Polymerisation Studies**
Benjamin Elvidge and F G N Cloke, P B Hitchcock *University of Sussex*
- P.42 Efficient preparation of C2-symmetrical Chiral Ferrocenyldiols by Catalytic Enantioselective Reduction of Diacylferrocens**
Hirohide Sato *Chuo University*
- P.43 Photochemistry of Novel Thienylporphyrins**
Jonathan Rochford and M T Pryce, A D Rooney *Dublin City University*
- P.44 Spectroscopic Studies on Catalytic Intermediates Involved in the Pd-Catalysed Methoxycarbonylation of Ethylene**
Alexandre Pépin and D G Eastham, B T Heaton, J A Iggo, R Whyman *University of Liverpool*
- P.45 Insertion of Phosphinoalkyne into Pt-C and Pd-C Bonds**
Kien-Wee Tan and P-H Leung *National University of Singapore*

- P.46 Asymmetric Hydrophosphination and Diels-Alder Reactions of Phosphinoalkenes Assisted by Palladium(II) and Platinum (II) Complexes**
Sumod Pullarkat and P-H Leung *National University of Singapore*
- P.47 Novel Water Soluble Ru-PTA Complexes: Recent Advances in Catalytic and Biological Applications**
Andrew Phillips and L Gonsalvi, A Romerosa, F Vizza, M Peruzzini *Istituto di Chimica dei Compositi Organometallici*
- P.48 C-F Activation of Fluoropyridines by Platinum (0)**
Naseralla Jasim and R Perutz *University of York*
- P.49 Unprecedented Ruthenium(II)-carbene Complexes from bis(iminophosphorano)methanediides**
José Gimeno and V Cardiero, J Díez, J García-Alvarez *Universidad de Oviedo*
- P.50 Selective Oxidation of Aniline to Nitroso-benzene with Aqueous Hydrogen Peroxide Catalyzed by Some Different Heteropolyoxometalates**
Reza Tayebee *Sabzevar University*
- P.51 An NMR and DFT Study of H₂ Addition to [Ir(CO)₂I₂]**
Charlotte Elkington and S B Duckett and J E McGrady *University of York*
- P.52 Insertion Reactions of Rh(III) Methyl and Acetyl Complexes**
Kevin Bonnington and C E Haslam, L Parish, T B Marder, A Haynes *University of Sheffield*
- P.53 Isolation, Structure and Reactivity of an Iridium Acetyl Intermediate in the BP Cativa Process**
Paul Elliott and A Haynes *University of Sheffield*
- P.54 A Comparison of the Photochemistry of [(L-L)Re(CO)₃(pyridine)][Co(CO)₄] Contact Ion Pairs with their PF₆⁻ Analogues**
Ciara O'Brien and R N Perutz, P Callaghan, P Anders Gabrielsson, A Vlcek *NUI Maynooth*
- P.55 Fluxionality and Isomerism in Complexes Ru(CO)₂(H)₂L₂: Evidence for the Involvement of η²-H₂ Species**
Danièle Schott and S B Duckett, R J Mawby *University of York*
- P.56 Photochemical Generation and Reactivity Study of the Carbene Complexes Rh(Cl)(PPh₃)₂(=CR₂)**
Daniele Schott and R N Perutz, S B Duckett *University of York*
- P.57 Synthesis and Reactivity of Pt(0) and Pt(II) Complexes Towards Mercury Compounds**
Maria Gálvez López and J Vicente, A Arcas, P G Jones *Universidad de Murcia*
- P.58 Platinum-Catalysed Cascade Reactions and Their Application in the Synthesis of Taxol-Like Compounds**
Gabriele Wagner and A Mahamoodally, R Herrmann *University of Surrey*
- P.59 Thermal and Microwave-Assisted Cycloaddition of Nitrones to Free and Coordinated Cinnamitrile**
Gabriele Wagner and B Desai, T N Danks *University of Surrey*
- P.60 Synthesis and Reactivity of Iridium Allyl Complex. Detection of Novel Reaction Intermediates using ParaHydrogen Induced Polarisation**
S B Duckett, Cyril Godard and, C Henry, S Polas *University of York*

- P.61 Photochemical Synthesis of Novel Rhodium Pyridyl Complexes**
Cyril Godard and S B Duckett, R N Perutz, S Parsons *University of York*
- P.62 A Comparative Quantum Chemical Study of White Phosphorus Activation in the $[M(\text{bipy})\text{P}_4]^q$ ($M=\text{Ni, Cu, Fe}$; $q=0, 2$)**
Ivan Ogurtsov and V Mirzac *Academy of Sciences of Moldova*
- P.63 Catalytic Hydrogenation and Hydroformylation Reactions by Ruthenium(0) Complexes: A Parahydrogen Investigation**
John Dunne and S B Duckett, D Blazina *University of York*
- P.64 Utilising Parahydrogen to prepare Pure Initial States for Nuclear Magnetic Resonance Quantum Computing**
D Blazina and M S Anwar, S B Duckett, J A Jones, H Carteret, T K Halstead, C M Kozak, R J K Taylor *University of York*
- P.65 Oxidative Addition of HB(pinacolate) at Ruthenium and Rhodium Phosphine Centres**
Sebastien Lachaize and E Rivalta, R Fernandez-Pacheco, R N Perutz *University of York*
- P.66 Synthesis and NMR Characterisation of Hexene / Acrylamide Copolymers/ Oligomers using a α -diimine Nickel Catalyst**
Susete Fernandes and J R Ascenso, S I Costa, P T Gomes, A R Dias, J C W Chien, M M Marues *Instituto Superior Técnico*
- P.67 Synthesis of Functionalized Helicene Scaffold in a Nonracemic Form**
Petr Sehnal and I G Strará, F Teplý, Z Alexandrová, I Starý, D Šaman, P Fiedler *Institute of Organic Chemistry and Biochemistry*
- P.68 Arene-ruthenium(II) complexes containing phosphino-benzaldehyde or phosphino-alcohol ligands: synthesis and involvement in C-C and C-heteroatom coupling processes**
José Gimeno and P Crochet, M A Fernández-Zumel, A E Díaz-Álvarez *Universidade de Oviedo*
- P.69 The Stille Reaction: A Mechanistic Study of a Model System and New Catalytic Applications**
Ola Wendt and P Nilsson, D Olsson, F Plamper, M El Masnaouy *Lund University*
- P.70 Detection of a Ru(IV) Tetrahydride Complex via the Formation of a BH_3 Adduct by Parahydrogen Induced Polarisation**
J A Brannigan and S B Duckett, J Lowe, R J Mawby, C J Sleigh, N J Wood *University of York*
- P.71 Metal Alkoxides as Transesterification Catalysts**
James Hobson and R N Perutz, B Stengel, P H Walton *University of York*
- P.72 Phosphorus Ligands in Polyolefin Catalysis**
Cassandra McCann and P G Pringle *University of Bristol*
- P.73 Phosphacycles in Hydroformylation**
Annie Middleton and P G Pringle *University of Bristol*
- P.74 Chiral Phospholane Ligands for Asymmetric Catalysis**
Karl von der Luehe and P G Pringle *University of Bristol*
- P.75 Reactivity of Square Planar Nickel Fluoropyridyl Fluoride Complexes: Steps towards new Fluoropyridines**
Richard Lindup and S Burling, P Elliott, J McKenna, R N Perutz *University of York*