

## Programme

### Dalton Discussion 12: Catalytic C-H and C-X Bond Activation 13 – 15 September 2010 Durham University, UK

#### Monday 13 September

13:45	<b>Welcome and Introductions</b> Professor Graham Sandford and Dr Phil Dyer, <i>Durham University, UK</i>
<b>Session 1</b>	Professor Todd Marder, <i>Durham University, UK</i>
14:00	Introduction to session Hans de Vries
14:10 <b>I1</b>	<b>The mechanism of the modified Ullmann reaction</b> Hans de Vries <i>DSM Pharmaceutical Products, The Netherlands</i>
14:20 <b>C3</b>	<b>Highly efficient manganese catalyzed C-H activation with H<sub>2</sub>O<sub>2</sub> – design rules for ligands</b> Dirk Pijper, Pattama Saisaha, Lea Buettner, Christian Smit, Johannes W de Boer, Ronald Hage, Paul L Alsters, Ruben van Summeren, Ben L Feringa and Wesley R Browne* <i>University of Groningen, The Netherlands</i>
14:25	Discussion
15:00	<b>Afternoon Tea</b>
<b>Session 2</b>	Dr Warren Cross, <i>University of Leicester, UK</i>
15:30 <b>K1</b>	<b>Arylation of unactivated arenes</b> Aiwen Lei* <i>Wuhan University, Peoples' Republic of China</i>
16:15 <b>C1</b>	<b>A versatile gold synthon for acetylene C-H bond activation</b> Steven P Nolan and George Fortman* <i>University of St Andrews, UK</i>
16:20 <b>C2</b>	<b>Pd-catalysed regioselective C-H functionalisation of 2-pyrones</b> Michael J Burns, Robert J Thatcher, Richard J K Taylor and Ian J S Fairlamb* <i>University of York, UK</i>
16:25	Discussion
17:15	<b>Close of Session</b>
18:00 – 19:00	Dinner at Collingwood College
19:15	<b>Poster Session and Wine Reception (ES228/229)</b>

## Tuesday 14 September

<b>Session 3</b>	Dr Ian Fairlamb, <i>University of York, UK - Dedication to Keith Fagnou</i>
09:00 <b>K2</b>	<b>Cross coupling reactions of polyfluoroarenes</b> Jennifer Love* <i>University of British Columbia, Canada</i>
09:45 <b>C5</b>	<b>Studies in catalytic C-H amination involving nitrene C-H insertion</b> Florence Collet, Camille Lescot, Chungen Liang and Philippe Dauban* <i>Institut de Chimie des Substances Naturelles, CNRS Gif-sur-Yvette, France</i>
09:50	Discussion
10:40	<b>Morning Coffee</b>
<b>Session 4</b>	Professor Sue Gibson, <i>Imperial College London, UK</i>
11:20	Introduction to session John M Brown
11:30 <b>I2</b>	<b>Anilide activation of adjacent C-H bonds in the palladium-catalysed Fujiwara-Moritani Reaction</b> John M Brown* <i>University of Oxford, UK</i>
11:40 <b>C7</b>	<b>Catalytic C-H functionalization of iminophosphoranes</b> <b>Regioselective C-H bond activation and C-C, C-O and C-X bond formation</b> David Aguilar, Rafael Navarro, Tatiana Soler and Esteban P Urriolabeitia* <i>University of Zaragoza, Spain</i>
11:45 <b>C8</b>	<b>Ruthenium vinylidene complexes as catalysts for C-O bond formation: the role of carboxylate ligands</b> Nicholas C Hiett, David G Johnson, Jason M Lynam*, John M Slattery, Adrian C Whitwood and Christine E Welby <i>University of York, UK</i>
11:50	Discussion
12:40	<b>Lunch/Posters</b>

<b>Session 5</b>	Dr Tony Haynes, <i>University of Sheffield, UK</i>
14:15 <b>K3</b>	<b>LiCl-Promoted Pd(II)-Catalyzed ortho Carbonylation of N,N-Dimethylbenzylamines</b> Zhang-jie Shi* <i>Peking University, Peoples' Republic of China</i>
15:00 <b>C9</b>	<b>Alkyne insertion into cyclometallated pyrazole and imine complexes of iridium, rhodium and ruthenium; relevance to catalytic formation of carbo- and heterocycles</b> Y Boutadla, D L Davies*, O Al-Duaij, J Fawcett, R Jones and K Singh <i>University of Leicester, UK</i>
15:05 <b>C10</b>	<b>Molecular mechanism of acid-triggered aryl-halide cross-coupling reaction via reductive elimination in well-defined aryl-Cu(III)-halide species</b> Alicia Casitas, Albert Poater, Miquel Solà, Shannon S Stahl, Miquel Costas and Xavi Ribas* <i>University of Girona, Spain</i>
15:10	Discussion
16:00	<b>Afternoon Tea</b>
<b>Session 6</b>	Professor Peter Scott, <i>University of Warwick, UK</i>
16:35	Introduction to session Robin Bedford
16:45 <b>I3</b>	<b>Solvent-free aromatic C-H functionalisation/halogenation reactions</b> Robin Bedford* <i>University of Bristol, UK</i>
16:55 <b>C12</b>	<b>Evidence for surface catalysed Suzuki-Miyaura cross-coupling over Pd nanoparticles: an operando XAS study</b> Peter J Ellis, Ian J S Fairlamb, Simon F J Hackett, Karen Wilson and Adam F Lee* <i>Cardiff University, UK</i>
17:00 <b>C13</b>	<b>Alkylation and alkenylation of C–H bonds by nickel catalysis</b> Yoshiaki Nakao* <i>Kyoto University, Japan</i>
17:05	Discussion
17:45	<b>Close of Session</b>
19:30	<b>Pre-dinner drinks</b>
20:00	<b>Conference dinner</b>

## Wednesday 15 September

<b>Session 7</b>	Dr Jason Lynam, <i>University of York, UK</i>
09:00 <b>K4</b>	<b>The ortho fluorine effect through M-C/H-C bond energy correlations of fluorinated aromatic hydrocarbons</b> Taro Tanabe, Meagan E Evans and William D Jones* <i>University of Rochester, US</i>
09:45 <b>C13</b>	<b>Implications for catalytic C-C bond formation of stronger metal-aryl bonds with ortho-fluorine substituents</b> Robin N Perutz*, Eric Clot, Odile Eisenstein and Julie Guihaumé <i>University of York, UK</i>
09:50	Discussion
10:25	<b>Morning Coffee</b>
<b>Session 8</b>	Professor Odile Eisenstein, <i>Université Montpellier II, France</i>
11:00	Introduction to session Stuart Macgregor
11:10 <b>I4</b>	<b>Computational Study of Ethene Hydroarylation at [Ir(<math>\kappa^2</math>-OAc)(PMe<sub>3</sub>)Cp]<sup>+</sup></b> David L Davies, Stuart A Macgregor*, and Amalia Poblador-Bahamonde <i>Heriot-Watt University, Edinburgh, UK</i>
11:20 <b>C15</b>	<b>DFT study of the mechanism of benzocyclobutene formation by palladium-catalyzed C(sp<sup>3</sup>)-H activation: role of the nature of the base and the phosphine</b> Christos Kefalidis, Olivier Baudoin and Eric Clot* <i>Université Montpellier 2, France</i>
11:25 <b>C16</b>	<b>Combined experimental and theoretical investigation into C-H activation of cyclic alkanes by Cp'Rh(CO)<sub>2</sub> (Cp'=h<sup>5</sup>-C<sub>5</sub>Me<sub>5</sub> or h<sup>5</sup>-C<sub>5</sub>H<sub>5</sub>)</b> Mike George* <i>University of Nottingham, UK</i>
11:30	Discussion
12:20	Acknowledgements
12:25	<b>Close of Meeting</b>
	<b>Lunch is not available – delegates to make own arrangements.</b>