

In the Lab

Rational Studies Towards Efficient, Scalable Catalytic Reactions

Johnson Matthey Technology Review features new laboratory research

Here we profile an upcoming researcher who has benefitted from Johnson Matthey's support in the past. David Nelson is a newly appointed Chancellor's Fellow and Lecturer at the University of Strathclyde, in Glasgow, UK. His research interests concern the development of useful transition metal catalysed processes for synthesis *via* a detailed understanding of mechanism, rate and selectivity in key steps.

About the Research

Transition metal complexes can perform an incredible range of chemical transformations, with new reactions, applications and processes being discovered and documented daily. However, many of these reactions are not well-developed enough for routine industrial application on a larger scale; while smaller-scale syntheses might employ these techniques, process chemists must often redesign synthetic routes to replace these reactions with more scalable or economical alternatives.

The aim of the group's research is to develop promising catalytic technologies to the stage that they can be deployed in an industrial setting on a large scale. The aim is to do this by conducting rational and quantitative studies of these catalytic reactions and key steps therein. The tools are those of synthetic organometallic and organic chemistry and of physical organic chemistry; including nuclear magnetic resonance (NMR), infrared (IR) and ultraviolet (UV)/visible spectroscopies, inductively coupled plasma mass spectrometry (ICP-MS), gas chromatography (GC), liquid chromatography (LC) and mass spectrometry (MS). Investigations into the rates and selectivities of key steps, how these depend

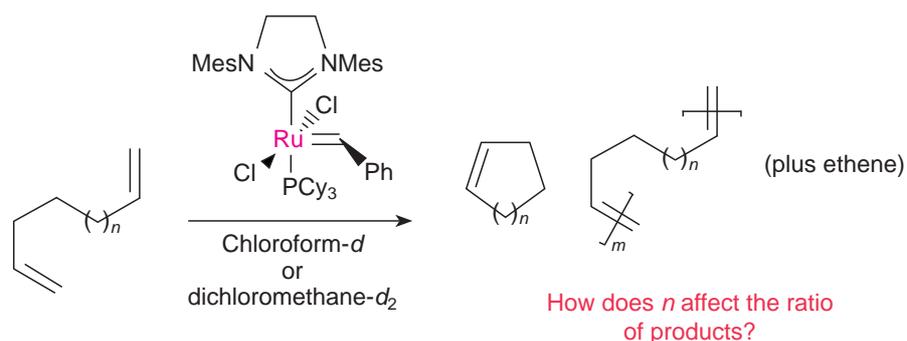
About the Researcher



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on catalyst structure and how these influence the overall performance of the reaction can provide useful information. Most importantly, this information can be used to inform the selection or design of catalysts and reaction conditions.

Dr David Nelson, group leader, has a background in the study of transition metal catalysed reactions, having held positions at the University of Strathclyde (PhD with Jonathan M. Percy) and the University of St Andrews, UK, (postdoctoral work with Steven P. Nolan FRSE). The work at Strathclyde looked at alkene metathesis reactions, predominantly using kinetic experiments. The effect of target ring size on the rate and selectivity



Scheme I. Partitioning between cycloalkene and oligomer in alkene metathesis (Mes = 2,4,6-trimethylphenyl)

of alkene metathesis, mediated by ruthenium carbene complexes, was probed (**Scheme I**); the latter study also showed that the selectivity for cycloalkene over oligomer (the effective molarity) could be predicted from density functional theory (DFT) calculations. Mechanistic understanding regarding the initiation event in Grubbs-Hoveyda type catalysts and deleterious isomerisation side reactions was also provided.

The work at St Andrews consisted of various studies of organometallic chemistry and catalysis, using late transition metals such as iridium, ruthenium, palladium

and gold. Highlights include: the preparation and study of *N*-heterocyclic carbene (NHC)-bearing iridium species, including $[\text{Ir}(\text{OH})(\text{COD})(\text{I}^i\text{Pr})]$ and $[\text{IrCl}(\text{COE})(\text{I}^i\text{Pr})_2]$ (see **Figure 1**) and derivatives and analogues thereof; the study of the decomposition processes that ruthenium metathesis catalysts undergo; and the application of these decomposition products in catalysis.

Current work in the Nelson group is focused on ruthenium-catalysed C–H activation and nickel-catalysed cross-coupling, aiming to bring together both organometallic and physical organic approaches in the research.

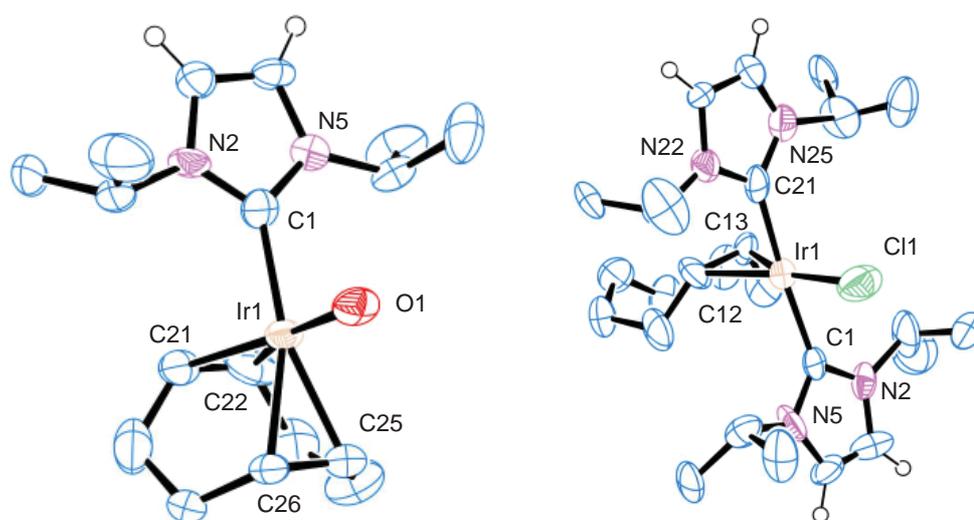


Fig. 1. Complexes $[\text{Ir}(\text{OH})(\text{COD})(\text{I}^i\text{Pr})]$ and $[\text{IrCl}(\text{COE})(\text{I}^i\text{Pr})_2]$

Selected Publications

S. Manzini, A. Poater, D. J. Nelson, L. Cavallo, A. M. Z. Slawin and S. P. Nolan, *Angew. Chem. Int. Ed.*, 2014, Accepted Manuscript

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B. J. Truscott, D. J. Nelson, C. Lujan, A. M. Z. Slawin and S. P. Nolan, *Chem. Eur. J.*, 2013, **19**, (24), 7904

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