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Metal-N-heterocyclic carbene complexes for catalytic applications

Ligand design is essential in the development of coordination and organometallic complexes, allowing their overall properties to be tuned and controlled in a precise manner, enabling new activities and reactivities to emerge. N-Heterocyclic carbenes (NHCs) have been studied widely as ancillary ligands for the preparation of metal-based catalysts, and have shown significant advantages over well studies and applied phosphine ligands (*e.g.* higher thermal stability, excess ligand not required in the reaction and greater tuneability). The steric and electronic versatility of NHCs is huge, through alteration of the nitrogen substituents and carbon backbone substituents (Figure 1. R^1-R^4), with more elaborate and versatile functional groups enabling finer tuning of the metal centre for more step-changing effects. We have previously shown that electrochemical methodology can be used for the synthesis of metal-NHCs (Figure 1).[1-2] Our route surpasses traditional synthetic routes as it negates the need for strong bases, strict inert conditions, the employment of stoichiometric silver salts, and is compatible with a wide range of ligand functionalities, including base sensitive substituents. This project will involve the electrochemical flow synthesis of a wide range of metal catalysts, and their application in processes of interest to industry (we currently work in collaboration with AstraZeneca). We envisage a complete flow process in which the catalyst is generated, the catalytic reaction proceeds and the metal is recovered and reused. Furthermore, we will work in collaboration with Dr Richard Bourne to fully optimise the process through using online analysis and feedback control systems.[3]

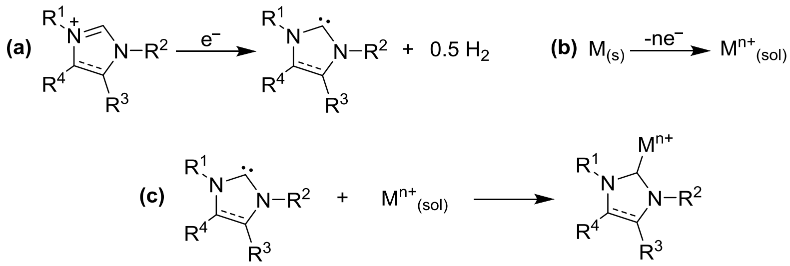

Figure 1. *Electrochemical synthesis of metal-NHC complexes; (a) reduction of imidazolium to NHC, (b) oxidation of metal, (c) combination of NHC and metal.*

The student working on this project will gain skills in synthetic organic and organometallic chemistry, catalysis, flow-chemistry and reaction engineering. In addition, a variety of analytical tools will be used including NMR and UV spectroscopy, mass spectrometry, LCMS, GC and X-ray crystallography. The industrial standard lab that is housed in the School of Chemistry at Leeds (iPRD) and the interdisciplinary research environment will provide a unique and relevant training environment for the student.

Please contact Dr. Charlotte Willans (c.e.willans@leeds.ac.uk) for further details about this opportunity.

References

1. B. R. M. Lake, E. K. Bullough, T. J. Williams, A. C. Whitwood, M. A. Little and C. E. Willans, *Chem. Commun.*, **2012**, *48*, 4887.
2. E. K. Bullough, M. A. Little and C. E. Willans, *Organometallics*, **2013**, *32*, 570.
3. R. A. Bourne, R. A. Skilton, A. J. Parrott, D. J. Irvine and M. Poliakoff, *Organic Process Research & Development*, **2011**, *15*, 932.