

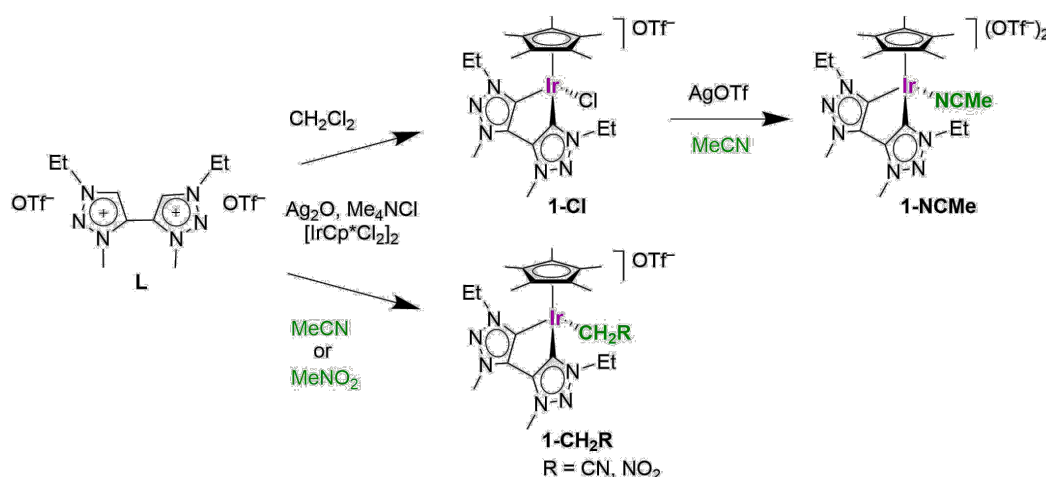
## Activation of $sp^3$ Carbon-Hydrogen Bonds Mediated by Bis(NHC) Iridium Complexes

Á. Vivancos<sup>1</sup>, P. Nyland<sup>1</sup>, M. Albrecht<sup>1\*</sup>

<sup>1</sup>Departement für Chemie und Biochemie, Universität Bern, Freiestrasse 3, CH-3012 Bern, Switzerland. E-mail: angela.vivancos@dcb.unibe.ch

The activation and functionalization of C-H bonds remains a significant challenge for organometallic chemistry, with wide implications for organic synthesis. Many transition-metal systems that initiate stoichiometric C-H activation are known, but complexes capable of both C-H activation and subsequent transformations of the substrate are relative rare,<sup>1</sup> especially for substrates with  $sp^3$  C-H bonds.<sup>2</sup> Considering the high activity of iridium complexes in mediating C-H bond activation, in particular when bound to triazolyldiene ligands,<sup>3</sup> we became interested in investigating a range of iridium complexes containing bis(carbene) ligands for facilitating alkyl C-H bond activation.<sup>4</sup>

Herein, we describe the C-H bond cleavage of acetonitrile and nitromethane by iridium(III) complexes bearing bis(triazolyldiene) ligands. Metal hydroxide species formed during the metalation step have been demonstrated to be responsible of the bond scission.<sup>5</sup> Moreover, we will discuss opportunities to couple this alkyl fragment to substrates, potentially providing a new method for alkyl functionalization.



[1] Olafs Daugulis, James Roane, Ly Dieu Tran, *Acc. Chem. Res.* **2015**, 48, 1053.

[2] Francisco Juliá-Hernández, Toni Moragas, Josep Cornella, Ruben Martin, *Nature* **2017**, 545, 84.

[3] a) Kate F. Donnelly, Ralte Lalrempuia, Helge Müller-Bunz, Eric Clot, Martin Albrecht, *Organometallics* **2015**, 34, 858. b) Ralte Lalrempuia, Helge Müller-Bunz, Martin Albrecht, *Angew. Chem. Int. Ed.* **2011**, 50, 9969.

[4] Ángela Vivancos, Martin Albrecht, *Organometallics* **2017**, 36, 1580.

[5] Byron J. Truscott, David J. Nelson, Cristina Lujan, Alexandra M. Z. Slawin, Steven P. Nolan, *Chem. Eur. J.* **2013**, 19, 7904.