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An investigation into the mechanism of transmetalation of primary and secondary alkylboron nucleophiles in palladium-catalyzed Suzuki reactions

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Through the past 40 years, carbon-carbon cross-coupling reactions have greatly enhanced the ability of chemists to synthesize C(sp2)-C(sp2) bonds and more recently C(sp2)-C(sp3) bonds. In particular, the Suzuki-Miyaura reaction has proven to be invaluable with its high yields, good functional group tolerance, and low toxicity of reagents. One of the component steps of the catalytic cycle of this reaction is transmetalation, in which the nucleophilic species transfers its organic component to the metal center (generally palladium). The mechanism of transfer from primary alkyl boron nucleophiles was studied in the 1990s via the use of deuterium-labeled probes and analysis by NMR, giving evidence to this being a stereo retentive SE2 mechanism. Subsequent work on secondary systems has highlighted the plausibility of both retentive and invertive mechanisms of transmetalation in Suzuki reactions. More recent research highlighted that the enantiospecific of such C(sp2)-C(sp3) reactions is not reliant solely upon the nucleophilic species. The selectivity is influenced by multiple factors including the ligand electronics, ligand steric, electrophile electronics, as well as the inclusion of exogenous additives. This poster will lay out the findings of the parameters that affect the transmetalation mechanism for primary and secondary trifluoroborate nucleophiles in cross-coupling reactions. The prominent use of NMR to decipher between gauche and anti-staggered vicinal protons on deuterium-labeled alkyl probes in order to determine mechanistic information of the transmetalation of primary alkyl boron nucleophiles will be demonstrated.

Biography

Benjamin Murray completed his master's in chemistry from the University of Glasgow (Scotland) in 2013. Additionally, as part of this degree, he worked for one year in the lab of Prof. Overkleeft at Leiden University (Netherlands). He has since been working towards his Ph.D. in the Biscoe Lab of City College of New York, where he is expecting to defend this Spring. His current research has focused on the transmetalation step in the Suzuki reaction and has recently had work published in the journal Science.

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