

“Iron catalyzed deuteration reactions”

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The reduction of carbon-carbon double bonds remains a fundamentally important transformation in organic synthesis. Transfer hydrogenation (TH) offers a mild approach, alleviating the need for high pressures of hydrogen gas whilst improving chemo- and regioselectivity. We have developed a mild, iron-catalysed TH of alkenes using an alcohol/amine as the proton source and borane/silane as the hydride transfer agent. Using a D^+ or D^- source, complete selectivity for mono-deuteration of the resultant alkane product is achieved.

The ability to selectively mono-deuterate at the internal position of the C=C is thus far limited by the paucity of routes to prepare deuterated silanes. Although there are handful of catalytic methods for deuterating silanes, these mostly employ expensive precious metals and are limited to tertiary silanes: we sought to resolve this bottleneck in synthesis. Using the same iron pre-catalyst, under an atmosphere of deuterium gas, the substrate scope of our H/D exchange of silanes will be discussed.

Using both experimental and computational studies we have developed mechanistic understanding, unearthing the potential of our iron(II) β -diketiminato pre-catalyst in isotopic labelling chemistry.