

Taming and Functionalizing Volatile Alkanes by Using Organometallic Reagents

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Host: Titel Jurca

Catalytically converting natural resources such as methane and ethane, the main components of natural and shale gas, into more value-added materials under mild conditions, is one of the main objectives in my research program. I will start by presenting the reactivity of a transient titanium alkylidyne $(\text{PNP})\text{Ti}\equiv\text{C}^t\text{Bu}$ (pincer PNP = $\text{N}[2\text{-P}(\text{CHMe}_2)_2\text{-4-methylphenyl}]_2^-$), specifically how this species forms and engages in intermolecular C-H activation and dehydrogenation reactions. Such a system can dehydrogenate methane, and react with C2-C8 alkanes selectively by activating their alpha- and beta-positions. In the case of linear alkanes C4-C8, we only observe formation of the terminal olefin adduct. A new catalytic cycle for transfer dehydrogenation of alkanes will be also introduced in addition to unique platforms to form kinetically stable Ti^{II} reagents or $\text{Ti}=\text{CH}_2$ motifs, some of which are relevant to our proposed catalytic cycle. In the last component, I will introduce the use of well-defined Ir catalysts for the monoborylation of methane. Combining high-throughput screening and immobilization strategies have allowed for the discovery of some of the most active and recyclable catalysts known for controlled methane functionalization.