

Poster presentation

## Carbon-Hydrogen bond activation

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In early experimental studies of transition-metal activation of methane two alternative mechanisms were invoked: an exchange reaction via a sigma-bond metathesis route and the oxidative addition of methane to form a stable metal methyl hydride. Computational chemistry has provided considerable insight into details of the mechanisms operating in these bond activation reactions. For the low-temperature activation of alkanes by  $[\text{Cp}^*\text{Ir}(\text{PMe}_3)(\text{CH}_3)]^+$  density functional calculations predict an oxidative-addition pathway with a stable Ir(V) intermediate. Both of these mechanisms appear to be accessible for C-H activation by the reactive carbene intermediate  $\text{Cp}^*\text{W}(=\text{CRH})\text{L}$ ,  $\text{L} = \text{NO}, \text{CO}$ . Recently, in cases where the optimized transition states appear to resemble geometrically an oxidative-addition intermediate, various research groups have suggested alternative C-H activation mechanisms. A Bader analysis of these transition states is capable of resolving these alternatives and classifying them into a range of mechanisms. Recently, time resolved infrared spectroscopy and density functional calculations have revealed new details about the intermediates and transition states involved in the oxidative-addition reaction of alkanes by photochemically generated  $\text{TpRh}(\text{CO})$  and  $\text{CpRh}(\text{CO})$ .