

Internal Seminar

Mechanistic insights into small molecule ($R_2HN\cdot BH_3$, H_2 , CH_4 , $HCOOH$, CO_2) activation using electrophilic Ru(II)-complexes

Rahul Kumar

Indian Institute of Sciences, Bangalore

Though amine-boranes ($R_2HN\cdot BH_3$), hydrogen (H_2), methane (CH_4), formic acid ($HCOOH$) and carbon dioxide (CO_2) are small molecules, they have huge impacts on chemical industries (energy sector and pharmaceuticals) and environment [CO_2 and CH_4 are potent greenhouse gases] as well. However, they are relatively inert molecules, especially CH_4 and CO_2 , and impose very tough challenges to activate and functionalize them into useful products under ambient conditions. The partial oxidation of the strong C-H bond in CH_4 for its transformation into methanol under relatively mild condition using an organometallic catalyst is considered as a holy grail in the field of catalysis. More importantly, to develop better and highly efficient homogeneous catalytic systems for the activation of these molecules, it is imperative to understand the mechanistic pathways using well defined homogeneous metal complexes. Thus, an understanding of the interaction of these inert molecules with metal centre is obligatory. In this context, discovery of σ -complex of H_2 by Kubas and co-workers gave remarkable insights into H-H bond activation pathways and its implications in catalytic hydrogenation reactions. Subsequently, σ -borane complexes of amine-boranes were discovered and found to be relatively more stable because of stronger M-H-B interaction and hence act as good models to study the M-H-C interaction of elusive σ -methane complex. On the other hand, $HCOOH$, a promising hydrogen storage material and its efficient catalytic dehydrogenation/decarboxylation and CO_2 hydrogenation back to $HCOOH$ using well defined homogeneous catalysts could lead to a sustainable energy cycle. Keeping the above facts in view, we have investigated the mechanistic pathways for the activation of these small molecules using electrophilic Ru(II)-complexes by NMR spectroscopy which will be presented in this talk.

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2:00 PM (Tea/Coffee at 1:45 PM)

Seminar Hall, TCIS