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Electronic requirements for C-H activation in half-sandwich complexes**Ashoka G Samuelson and Murugesan Thenraj**
Indian Institute of Science, India

Activation of C-H bonds continues to attract significant attention. The interaction of C-H bonds plays an important role in several reactions besides being the key step for activating alkanes. We have carried out computational study of the interaction half-sandwich metal fragments (metal=Re/W/Ru, electron count= d^6/d^8), containing linear nitrosyl (NO^+), carbon monoxide (CO), trifluorophosphine (PF_3), N-heterocyclic carbene (NHC) ligands with alkanes using density functional theory employing the hybrid meta-GGA functional (M06). With d_6 metal complexes, electron deficiency on the metal improves the formation of stable alkane complexes in the order $\text{NHC} < \text{CO} < \text{PF}_3 < \text{NO}^+$, which corresponds to the electron withdrawing capacity of the ligand. Thus NO^+ leads to more stable alkane complexes than NHC, a strong electron donor. Stabilization is primarily due to an orbital interaction involving the sigma bond electron density from the alkane flowing to the empty acceptor orbital on the metal. Reactions and C-H activation of the alkane fragment are best facilitated by strong electron donor ligands. These results match most of the experimental results known for CO and PF_3 complexes. Our work suggests a new way of C-H activation, which emphasizes the importance of back donation to the alkane in metal complexes rather than electron donation to the metal.

Biography

Ashoka G Samuelson had his early education in Tiruchirapalli, India. After obtaining a Master's degree in Chemistry from the Indian Institute of Technology, Madras at Chennai he finished his Doctoral studies at Cornell University, Ithaca. He has been working in the Department of Inorganic and Physical Chemistry at the Indian Institute of Science, Bangalore since then. His research interests are organometallic and coordination chemistry of transition metals. Their goal is to utilize the reactivity of organometallic compounds to devise new catalysts or anticancer active molecules. His research group often employs computational tools to supplement and complement their experimental findings.

ashoka@ipc.iisc.ernet.in

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