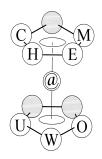


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THE PAUL de MAYO AWARD LECTURE Award Winner 2010 **Dr. Jason Laurence Dutton**

Experimental Mechanistic Investigations into the Activation of H₂ by Frustrated Lewis Pairs

Abstract: The investigation of molecules capable of activating H_2 , traditionally the domain of transition metals, has recently been extended into the main group. The focus has been on "frustrated Lewis pairs" (FLPs), the combination of a bulky Lewis base and Lewis acid. Amongst other remarkable reactivity, FLPs have been demonstrated to heterolytically cleave H_2 with ease. Several different systems capable of this reactivity have been reported, and there have been extensive theoretical calculations into the mechanism of H_2 activation. Most studies point to a loosely associated "encounter complex" between the base and acid acting to split H_2 . However, very little experimental mechanistic work has been performed in an effort to prove this.

In this context, we have performed a detailed mechanistic investigation on the quintessential FLP H₂ splitting system, Bu_3P and $B(C_6F_5)_3$, and found that the two species generate a small amount of catalyst (1) *in situ*. Compound 1 is found to be both chemically and kinetically competent as a catalyst in the formation of $[Bu_3PH][HB(C_6F_5)_3]$ from the Lewis pair and H₂. Overall, our studies show that FLP systems may not be as simple as generally thought and that additional investigations on other FLPs may reveal similar anomalies in the mechanism of their action.

 ${}^{t}Bu_{3}P: + B(C_{6}F_{5})_{3} \xrightarrow{H_{2}} [{}^{t}Bu_{3}PH][HB(C_{6}F_{5})_{3}]$ simple or complex mechanism? ${}^{t}Bu \xrightarrow{F} \xrightarrow{F} C_{6}F_{5}$ ${}^{t}Bu \xrightarrow{F} \xrightarrow{F} F \xrightarrow{F} C_{6}F_{5}$ 1

Monday, June 13, 2011 — 2:30 p.m. Room 0165, Biological & Geological Sciences Building

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