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

Abstract: The investigation of molecules capable of activating H₂, 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 H₂ with ease. Several different systems capable of this reactivity have been reported, and there have been extensive theoretical calculations into the mechanism of H₂ activation. Most studies point to a loosely associated “encounter complex” between the base and acid acting to split H₂. 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, tBu₃P and B(C₆F₅)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 [tBu₃PH][HB(C₆F₅)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.

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