

# Thesis Defense in Chemistry



Friday, September 15, 2017 at 1:30pm  
Room 209 Havemeyer

## Using first-row transition metal hydrides as hydrogen atom donors

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Radical cyclizations are a mainstay of synthetic organic chemistry. Although these reactions are frequently used in small-scale synthetic applications, they are seldom used on industrial scale. This is due to a reliance on  $\text{Bu}_3\text{SnH}$ , which has historically been regarded as the best synthetic equivalent to a hydrogen atom. The toxicity and the poor atom-economy of the trialkyltin compounds demands that they be replaced; new hydrogen atom donors are needed. We have shown that transition metal complexes (e.g.  $\text{CpCr}(\text{CO})_3\text{H}$ ,  $\text{HV}(\text{CO})_4\text{dppe}$ , and  $\text{Co}(\text{dmgBF}_2)_2(\text{THF})_2$ ) can be used as hydrogen atom donors in radical reactions. Some of these hydrogen atom donors are regenerated from  $\text{H}_2$ , so the reactions using the transition-metal complexes are catalytic, and generate virtually no waste. In this talk, I will explain how we have used M–H bond thermochemistry to predict and control how a system processes a given organic substrate. I report on a new system,  $[\text{CpV}(\text{CO})_3\text{H}]^-$ , which catalyzes electron transfer from  $\text{H}_2$  (representing the interconversion of chemical energy and electrical energy). I have used this system to catalyze the radical cyclization of alkyl iodides.

