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Analysis of spontaneous dehydrogenation reactions

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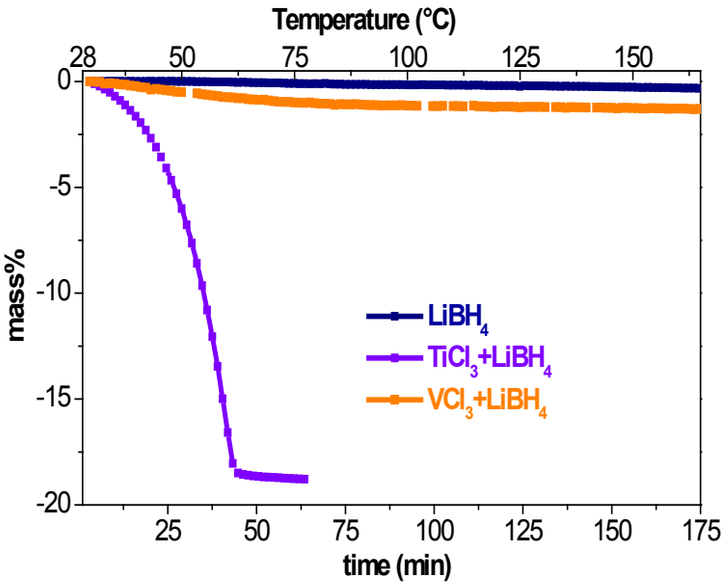
Introduction

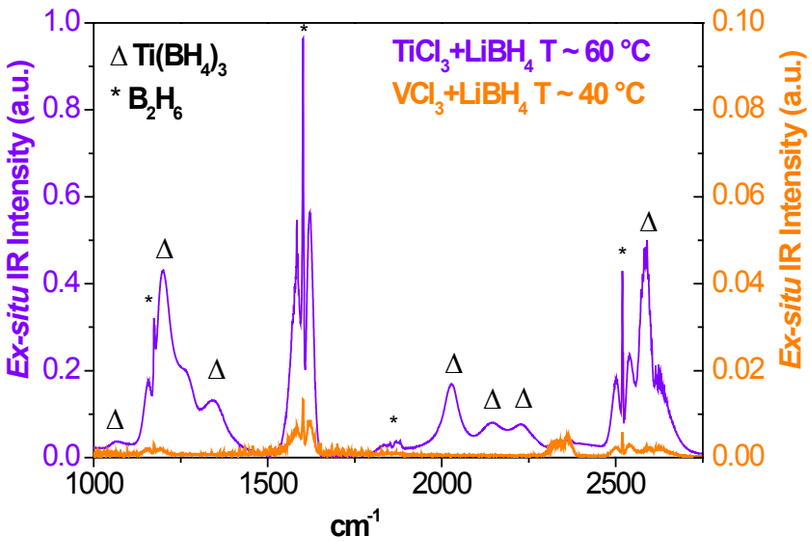
Metathesis and reactive milling are established methods to synthesize new compounds for energy storage materials. In many cases, intermediates and/or products formed are thermodynamically unstable. Their characterization and measurement as a function of time and temperature is a key problem for technologic transfer. We analyze the formation of intermediate species, studying the effect of different additives on the kinetics of $LiBH_4$, which does not emit diborane and releases hydrogen only above 300 °C, in 1 bar H_2 flow.

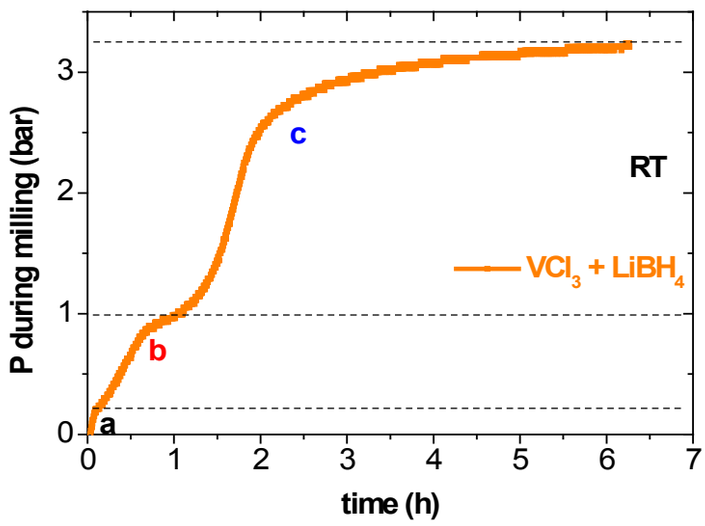
Analysis of spontaneous dehydrogenation reactions

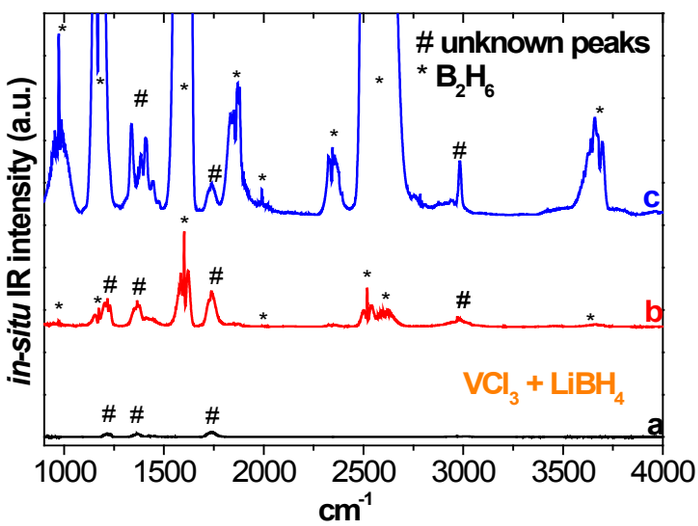
$3LiBH_4 + TiCl_3 \rightarrow Ti(BH_4)_3 + 3LiCl$



$3LiBH_4 + VCl_3 \rightarrow V(BH_4)_3 + 3LiCl$







Conclusions

Room temperature emission of diborane is the indirect proof that chlorides addition to $LiBH_4$ induces metathesis reactions. However, only the metathesis products which are thermodynamically stable are directly detectable. Here we presented two examples: $Ti(BH_4)_3$ is identified via *ex-situ* IR, while unknown peaks, maybe assignable to V-B complexes, were found only via *in-situ* IR, during the ball milling. Identification of species in progress.