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De(Re)-hydrogenation Mechanisms of B-N-H Complexes at Elevated Pressure RAJA CHELLAPPA, MADDURY SOMAYAZULU, VIKTOR STRUZHKIN, RUSSELL HEMLEY, GL, CIW, THOMAS AUTREY, PNNL —

The goal of identifying a hydrogen storage material that possesses reversible hydrogen removal/addition characteristics with favorable thermodynamics and kinetics still remains elusive. In case of chemical & complex hydrides, it is increasingly realized that some “destabilization” is desired by altering the stoichiometry (dopants) or physical properties via mechanical preprocessing. In this study, a combined pressure-temperature approach (few GPa and 77-400 K) that has been used with great success for synthesizing novel hydrogen clathrates is extended to understand de(re)-hydrogenation mechanisms of B-N-H compounds. For example, Ammonia Borane (NH_3BH_3) has very high hydrogen content (19 wt.%) however its thermal polymeric residue does not re-uptake hydrogen. We will present some in situ Raman spectroscopy results from our attempts to create novel hydrogen complexes with this residue as well as with the parent compound. In general, the physics & chemistry of hydrogen interactions at high pressure with light element compounds containing hydrogen has been unexplored and this study is an attempt towards bridging that gap.

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