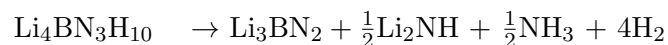


Abstract Submitted  
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**Electronic Structure and Energetics of the Quaternary Hydride  $\text{Li}_4\text{BN}_3\text{H}_{10}$**  JAN HERBST, LOUIS HECTOR JR., GM Research and Development Center, Warren, MI 48090-9055 —  $\text{Li}_4\text{BN}_3\text{H}_{10}$  has been synthesized recently from  $\text{LiNH}_2/\text{LiBH}_4$  mixtures and its crystal structure determined. We have calculated the electronic structure of this complex hydride and investigated its thermodynamic stability and decomposition energetics. We find that its enthalpy of formation is  $-708$  kJ/mole with respect to the elemental constituents and  $-6$  kJ/mole relative to a 3:1 molar  $\text{LiNH}_2/\text{LiBH}_4$  mixture, in qualitative agreement with experiment. Reaction enthalpies computed for several decomposition pathways suggest



as the likely dehydriding route.

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