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Characterization of Lithium Borohydride using Neutron Scattering Techniques MICHAEL HARTMAN, JACK RUSH, TERRY UDOVIC, National Institute of Standards and Technology — Lithium borohydride, $LiBH_4$, is a complex metal hydride that shows great promise as a hydrogen storage medium with a volumetric hydrogen density of 122 kg H/m^3 and a gravimetric hydrogen density of 18.5 wt. %. While numerous NMR, Raman, and infrared investigations have been reported in the literature, neutron scattering investigations of $LiBH_4$ have been limited due to the large neutron absorption cross-section of naturally occurring lithium and boron. We have recently synthesized an isotopically-enriched lithium borohydride, containing ^{7}Li and ^{11}B, which eliminates the large neutron absorption cross-section that arises from the presence of ^{6}Li and ^{10}B. The results of powder neutron diffraction, inelastic neutron scattering, and quasi-elastic neutron scattering investigations on the $^7Li^{11}BH_4$ material are presented. These measurements provide a fundamental understanding of the behavior of hydrogen within lithium borohydride, and they provide a basis to understand changes concomitant with the introduction of catalytic or destabilizing compounds.

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