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Structures and Bonding of Li-B-N-H Quaternary Hydrides HUI WU, 1. NIST Center for Neutron Research 2. University of Maryland, WEI ZHOU, TERRENCE UDOVIC, JOHN RUSH, TANER YILDIRIM, NIST Center for Neutron Research — Complex metal hydrides are of great interest for hydrogen-storage applications due to their potential high hydrogen capacity. Intense efforts has been made on the Li-B-N-H system, with the discovery of several novel quaternary phases. There have been prior studies investigating the structure of one of these new phases ($Li_4BN_3H_{10}$). However, all these studies were undertaken on hydrides without any isotope enrichment, thus resulted in diffraction data of limited quality and yielded structures with questionable bond lengths and uncharacteristically deformed anion groups. So far, no studies have been reported on the isotopically labeled samples, which are necessary to determine correct structures for these hydrides. We report for the first time the crystal structures of Li_2BNH_6 and $Li_4BN_3H_{10}$ derived from high-resolution neutron diffraction data on samples labeled with ^{7}Li, ^{11}B, and D. Our refined structures clarify the prevailing structural discrepancies. We also report corresponding neutron vibrational spectra combined with first-principles calculations to gain more insight between structure and bonding. The configurations of both BH_4^- and NH_2^- anions and the structural variations upon compositional changes will be discussed. Our study provides implications to the mechanisms of hydrogen absorption/desorption in these complex hydrides.

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