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New Quaternary Hydride Li₃BN₂H₈ with >10 wt% Hydrogen: I. Material Synthesis and Structural Characterization GREGORY P. MEISNER, FREDERICK E. PINKERTON, MARTIN S. MEYER, MICHAEL P. BALOGH, General Motors Research and Development Center, MATTHEW KUN-DRAT, Aerotek Corp. — We report a new quaternary hydride Li₃BN₂H₈ synthesized from mixed LiNH₂ and LiBH₄ powders in a 2:1 molar ratio by ball milling. X-ray diffraction (XRD) results show that as milling time increases, the LiNH₂ and LiBH₄ diffraction peaks weaken and a new set of peaks emerges. At 40 min, the sample is substantially converted to the new phase, with only a small remnant of LiNH₂ in the XRD pattern. After 300 min the conversion is complete, and continued milling up to 960 min produces no further change. The final XRD pattern appears to be single phase, except for a small amount of Li₂O impurity, and has a background intensity that is essentially unchanged with milling time, implying that ball milling does not produce an amorphous phase. All of the observed XRD peaks can be indexed as a single BCC quaternary phase with a =10.76 Å. Our in-situ XRD data show that Li₃BN₂H₈ forms when mixed LiNH₂ and LiBH₄ powders are heated to above ~95°C without ball milling, then melts at ~190°C, and finally forms a mixture of solid Li₃BN₂ polymorphs upon H₂ gas release above $\sim 250^{\circ}$ C.

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