Composition dependence of hydrogen and ammonia release in the lithium-boron-nitrogen-hydrogen quaternary system

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— The new quaternary hydride in the lithium-boron-nitrogen-hydrogen (Li-B-N-H) quaternary phase diagram forms by the reaction of lithium amide (LiNH$_2$) and lithium borohydride (LiBH$_4$) near the approximate composition LiB$_{0.33}$N$_{0.67}$H$_{2.67}$. When heated, the quaternary hydride first melts and then releases greater than 10 wt% hydrogen and a small amount of ammonia (2-3 mole% of the generated gas). We studied hydrogen and ammonia release from the series of reactant mixtures (LiNH$_2$)$_x$(LiBH$_4$)$_{1-x}$ as a function of composition using volumetric, gravimetric, mass spectrometer, and in situ x-ray diffraction measurements. We found that maximum hydrogen and minimum ammonia release do occur for $x = 0.67$. We observe that this composition corresponds to the ternary decomposition end product Li$_3$BN$_2$ rather than to the true single phase composition of the quaternary hydride as determined from our single crystal x-ray diffraction measurements.