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Tetragonal $I4_1/amd$ Crystal Structure of Li_3BN_2 from Dehydrogenated Li-B-N-H FREDERICK PINKERTON, JAN HERBST, General Motors Research and Development Center, Warren, MI — We have determined the crystal structure of Li_3BN_2 formed by dehydrogenation of $LiB_{0.33}N_{0.67}H_{2.67}$ from powder x-ray diffraction (XRD) data using the Rietveld method. XRD measurements indicate unambiguously that this Li_3BN_2 polymorph is distinct from any of the previously reported Li_3BN_2 phases. We find a body-centered tetragonal $I4_1/amd$ structure (space group No. 141 in the *International Tables for X-ray Crystallography*) with a = 6.60 Å and c = 10.35 Å. The structure features tightly coordinated, nearly linear N–B–N units with 1.3 - 1.4 Å B–N bond lengths suggesting covalently bonded $(BN_2)^{-3}$ anions. In situ temperature-dependent XRD showed that the body-centered tetragonal Li_3BN_2 phase was present both at elevated temperature during dehydrogenation and after cooling to room temperature. We also describe the results of first principles theoretical modeling of the body-centered tetragonal Li_3BN_2 polymorph as well as the tetragonal $P4_22_12$ and monoclinic $P2_1/c$ Li_3BN_2 structures previously reported. We obtained excellent agreement between the theoretically calculated $I4_1/amd$ Li_3BN_2 lattice constants and atomic positions and those obtained experimentally from XRD. The approximate enthalpy of formation of the $I4_1/amd$ Li_3BN_2 phase is $\Delta H = -495$ kJ/mole-formula unit.

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