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Neutron Diffraction of NaBD₄: Phase Transition, Rietveld Structure Refinements, and Equation of State
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BACKGROUND
NaBH₄ is a hydride with possible applications as a hydrogen storage material for future renewable energy technologies. Its dehydrogenation properties are enhanced with the mixture of particular catalysts through ball-milling techniques during which local pressures may exceed several GPa's. It is for this reason that understanding the behavior of pressure induced phase changes of its crystalline unit cell is an area of interest.

EXPERIMENTAL PROCEDURE & DATA ANALYSIS
This study makes use of neutron diffraction data collected from NaBD₄ up to about 12 GPa. The sample was held in a Paris-Edinburgh cell in non-hydrostatic pressure conditions. The program Topaz was used to perform Rietveld Refinement on the data, and external data on the structure and atom positions of Na and B was attained in order to determine the atom positions of hydrogen (in this case its isotope deuterium) within the unit cell. Volume vs. Pressure data was also collected in order to attain an appropriate equation of state and from it determine the compound’s bulk modulus.

RESULTS
Analysis of the neutron diffraction data using Rietveld Refinement showed a phase transition occurring into the orthorhombic phase between 6.3 and 7.9 GPa. However, this appeared to occur from the cubic phase, as the intermediate tetragonal structure of its crystalline unit cell is an area of interest.

CONCLUSIONS AND SUMMARY
When NaBD₄ is studied at high pressures up through 12.2 GPa, shifting of peaks to a higher 2θ in neutron diffraction patterns indicates a smaller d-spacing as the unit cell is compressed. The appearance of new peaks also indicates at least one phase transition to lower symmetry somewhere between 6.3 and 7.9 GPa, determined to be from a cubic Fm-3m space group to an orthorhombic Pnma one. The resulting pressure vs. volume data was used to fit a 3rd order Birch-Murnaghan equation of state to the cubic phase and a 2nd order one to the orthorhombic phase, with the determined values of B, B', and V₀ displayed in Fig. 2 (c).

REFERENCES

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