Pressure induced structural transitions in the potential hydrogen storage compound NH₃BH₃

RAVHI KUMAR, HiPSEC, University of Nevada Las Vegas, JIANZHONG ZHANG, MONIKA HARTL, ZHIJUN LIN, SVEN VOGEL, LUKE DAEMEN, LANSCE, ANDREW CORNELIUS, MALCOLM NICOL, HiPSEC, University of Nevada Las Vegas, YUSHEN ZHAO, LANSCE — Ammonia borane has received much attention in recent years as it is reported to have up to 19.6 wt % of hydrogen [1-2]. Hydrogen is released in a three step process when heated above 100°C. To understand the structural stability of this compound under compression, we have performed high pressure angle dispersive x-ray diffraction experiments up to 27 GPa using synchrotron x-rays at HPCAT, Advanced Photon Source. Two successive pressure induced structural phase transitions were observed. The ambient tetragonal structure transforms to an orthorhombic structure around 1.2 GPa and then to another high pressure phase above 8 GPa. Complementary neutron diffraction experiments performed up to 5 GPa at LANSCE are in good agreement with the x-ray results. The structural details of the high pressure phases will be presented.


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