

Abstract Submitted
for the SHOCK13 Meeting of
The American Physical Society

Boron and aluminum halides under pressure - polymerization and chemical transformations YANSUN YAO, University of Saskatchewan — High-pressure phase transitions of boron and aluminum halides have been theoretically studied. At low pressure, crystals of the familiar monomers (BX_3) and dimers (Al_2X_6) are the structures of choice. While the higher oligomers as well as three dimensional infinite polymers are unstable at ambient pressure, they are stabilized by application of external pressure, taking advantage of the extra orbitals made accessible by the increased coordination. Several new crystal structures of boron and aluminum halides have been predicted at high pressures. Calculated x-ray diffraction patterns and Raman spectra of these phases are in good agreement with available experimental data.

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Date submitted: 21 Feb 2013

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