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Determination of Equations of State for AlF_3 and AlI_3: Semi-empirical Modeling of Extreme Condition Halide Chemistry[1] JOSEPH ZAUG, Lawerence Livermore National Laboratory, ELISSAIOS STAVROU, Carnegie Institute of Washington, SORIN BASTEA, Lawerence Livermore National Laboratory, ALEXANDER GONCHAROV, Carnegie Institute of Washington, JONATHON CROWHURST, SARAH ROBERTS, JONATHAN PLAUE, Lawerence Livermore National Laboratory, JEFFREY CARTER, picarro.com, MICHAEL ARMSTRONG, Lawerence Livermore National Laboratory — Pressure dependent angle-dispersive x-ray powder diffraction measurements of alpha-phase aluminum trifluoride (alpha-AlF_3) and separately, aluminum triiodide (AlI_3) were conducted using a diamond-anvil cell. Results at 295 K extend to 50 GPa. The equations of state of AlF_3 and AlI_3 were determined through refinements of collected x-ray patterns. The respective bulk moduli and corresponding pressure derivatives using multiple orders of the Birch-Murngahan, Ff, and Gg EoS models will be discussed. Aluminum trifluoride exhibits no pressure induced structural phase transition while the triiodide data reveal a second-order iso-structural rearrangement: Applied stress transformed a monoclinicly distorted face centered cubic (FCC) structure into a perfect FCC structure. Results from semi-empirical thermochemical computations of energetic materials formulated with fluorine containing reactants will be presented.

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Joseph Zaug
Lawerence Livermore National Laboratory

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