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Pressure-induced phase transitions in energetic materials revealed by single-crystal diffraction studies[1] SAMANTHA CLARKE, BRAD STEELE, MATTHEW KROONBLAWD, JOSEPH ZAUG, I-FENG KUO, SORIN BASTEA, PHILIP PAGORIA, LAURENCE FRIED, ELISSAIOS STAVROU, Lawrence Livermore Natl Lab, JESSE SMITH, Argonne National Laboratory, DONGZHOU ZHANG, University of Chicago, OLIVER TSCHAUNER, University of Nevada, Las Vegas, DYLAN SMITH, BRIAN LITTLE, U. S. Air Force Research Laboratory — Understanding the high-pressure structure of energetic materials is essential for the realistic modeling of shock initiation and improvement of code. Pressure-induced structural phase transitions where the symmetry and structure are altered can be exceptionally difficult or impossible to unravel using conventional high-pressure powder X-ray diffraction (XRD). To address this problem, we performed single crystal (SC) XRD studies. In the case of TATB, an insensitive energetic material, our SCXRD results reveal a structural phase transition, reported for the first time, towards a monoclinic structure above 4-5GPa. These experimental results are further supported by calculations that suggest alteration of the stacking of the layers of the TATB molecules. We also investigate Al(IO3)3(HIO3)2(H2O)6, a promising energetic salt, and find through SCXRD a hexagonal to monoclinic phase change at ˜6 GPa. These systems highlight the use of SCXRD in characterizing complex, high pressure phase changes.

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