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**The high pressure-temperature phase behavior of 2,4,6-trinitrotoluene (TNT)** PATRICK BOWDEN, RAJA CHELLAPPA, DANA DATTELBAUM, VIRGINIA MANNER, NATHAN MACK, Los Alamos National Laboratory, ZHENXIAN LIU, Brookhaven National Laboratory — 2,4,6-trinitrotoluene (TNT) is a widely used explosive that is relatively insensitive to initiation by shock loading. While the detonation properties of TNT have been extensively reported, the high pressure-temperature ( $P - T$ ) stability of TNT has not been investigated in detail. In addition, there are no studies that have determined the effects of pressure on the stability of the liquid phase. At ambient conditions, TNT crystallizes in a monoclinic lattice (space group  $P2_1/a$ ), and our previous x-ray diffraction (XRD) measurements at room temperature suggested a phase transition to orthorhombic (space group  $Pca2_1$ ) at  $\sim 20$  GPa. In this work, we have performed *in situ* synchrotron XRD and vibrational spectroscopy measurements at various  $P - T$  conditions along isothermal and isobaric pathways to confirm previously reported phase transitions, and investigate phase stabilities up to 30 GPa and 500°C. Using all the available data, we have established the first comprehensive high  $P - T$  phase diagram of TNT, including the melting line as a function of pressure. While our synchrotron IR and Raman spectroscopy measurements indicate spectral changes at  $\sim 2$  GPa, careful XRD measurements (hydrostatic, He medium and non-hydrostatic) reveal that the monoclinic phase is likely stable up to 20 GPa. We will present a self-consistent  $P - V - T$  equation of state derived from the reported structural and vibrational data.

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