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Phase Diagram and Decomposition of 1,1-Diamino-2,2-Dinitroethene (FOX-7)[1] YUCHUAN TAO, ZBIGNIEW DREGER, YOGENDRA GUPTA, Washington State University — To understand the reactive behavior of 1,1-diamino-2,2-dinitroethene (FOX-7) at the thermo-mechanical conditions relevant to shock-wave initiation, Raman and FTIR measurements were performed at high-pressures (HP) and high-temperatures (HT). Experiments were performed on single crystals of FOX-7 in a diamond anvil cell to 10 GPa and 800 K to provide the phase diagram and to gain insight into the HP decomposition mechanisms. Previous studies have demonstrated that the ambient structure of FOX-7 (alpha) transforms to beta and gamma phases at higher temperatures, and phase I (2 GPa) and II (4.5 GPa) at higher pressures. In this work, we determined the boundaries between these phases and the decomposition/melting curve. In particular, we found that: (i) both beta and gamma phases exist in a limited P-T domain (>386 K and <1 GPa), (ii) the transition between phase-I and phase-II takes place along the isobar, (iii) the decomposition temperature increases significantly with pressure ($\sim$ 25 K / GPa), and (iv) pressure inhibits the decomposition. Using FTIR spectroscopy, we observed that CO_2 is the first dominating decomposition product, followed by N_2O, NO_2, HCN, and HNCO. Pressure effects on reaction kinetics will be presented along with the possible mechanisms of decomposition.

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