

Abstract Submitted
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High Pressure-Temperature Phase Diagram of 1,1-diamino-2,2-dinitroethylene¹ MATTHEW BISHOP, RAJA CHELLAPPA, Los Alamos National Laboratory, ZHENXIAN LIU, Geophysical Laboratory, Carnegie Institution of Washington, DANIEL PRESTON, MARY SANDSTROM, DANA DATTELBAUM, Los Alamos National Laboratory, YOGESH VOHRA, University of Alabama at Birmingham, NENAD VELISAVLJEVIC, Los Alamos National Laboratory — 1,1-diamino-2,2-dinitroethylene (FOX-7) is a less sensitive energetic material with performance comparable to commonly used secondary explosives such as RDX and HMX. At ambient pressure, FOX-7 exhibits complex polymorphism with at least three structurally distinct phases (α , β , and γ). In this study, we have investigated the high P-T stability of FOX-7 polymorphs using synchrotron mid-infrared (MIR) spectroscopy. At ambient pressure, our MIR spectra confirmed the known $\alpha \rightarrow \beta$ (110 °C) and $\beta \rightarrow \gamma$ (160 °C) phase transitions; as well as, indicated an additional phase transition, $\gamma \rightarrow \delta$ (210°C), with the δ phase being stable up to 250 °C prior to melt/decomposition. In situ MIR spectra obtained during isobaric heating at 0.9 GPa revealed that the $\alpha \rightarrow \beta$ transition occurs at 180°C, while $\beta \rightarrow \beta + \delta$ phase transition shifted to 300°C with suppression of γ phase. Decomposition was observed above 325°C. Based on multiple high P-T measurements, we have established the first high P-T phase diagram of FOX-7.

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