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High-Pressure Polymorphism of 1,1-Diamino-2,2-dinitroethene (FOX-7)[1] ZBIGNIEW DREGER, YUCHUAN TAO, YOGENDRA GUPTA, Washington State University — Understanding the polymorphic response of energetic crystals is important for understanding their initiation and reactive behavior. Here, we report on the high-pressure polymorphism of the energetic crystal FOX-7 [$C_2(NO_2)_2(NH_2)_2$]; the low sensitivity to initiation has attracted considerable research interest in this crystal. Micro-Raman spectroscopy and synchrotron x-ray diffraction measurements were used to gain insight into the mechanisms of polymorphic transformations, and their role in the high-pressure structural stability of FOX-7. Experiments were performed on single crystals compressed statically to 40 GPa (Raman) and to 12 GPa (x-ray). Two instances of spectral changes were detected at 2 and 4.5 GPa with Raman spectroscopy. Different experimental approaches, including isotope substitution (H/D), nonhydrostatic compression and laser radiation were used to understand the molecular processes associated with the observed spectral changes. The x-ray diffraction results demonstrated that the same space group, $P2_1/n$, is maintained to 4.5 GPa, the β angle reduces to almost 90^0, and the crystal shows anisotropic compression. Preliminary structure refinement results indicate that changes at 2 GPa can result from the amino groups twist out of the molecular plane. The structural changes at 4.5 GPa indicate the reconstructive character of the phase transition at this pressure.

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