

Abstract Submitted  
for the MAR06 Meeting of  
The American Physical Society

**High-Pressure Synchrotron Radiation X-Ray Diffraction and Vibrational Spectroscopic Studies of 3,3,7,7-tetrakis(difluoramino)octahydro-1,5-dinitro-1,5-diazocine (HNFx)<sup>1</sup>**

CEDRIC GOBIN, JERRALIE ORWIG, MALCOLM NICOL, High Pressure Science and Engineering Center, Department of Physics, University of Nevada Las Vegas, Las Vegas, NV 89154-4002, USA. — HNFx, 3,3,7,7-tetrakis(difluoramino)octahydro-1,5-dinitro-1,5-diazocine, belongs to a new class of compounds predicted to be potentially superior explosives or solid propellant oxidizers, the *gem*-bis(difluoramino)-substituted heterocyclic nitramines [1,2]. HNFx has been studied in diamond anvil cell up to 30 GPa by synchrotron radiation x-ray diffraction, Raman and infrared spectroscopy at ambient temperature. The pressure-induced alterations in the profiles of the peaks, including their positions, widths and intensities are presented. No phase transition was observed on this range of pressure. The bulk modulus and its pressure derivative were estimated by the third-order Birch-Murnaghan isothermal equation of state up to 6.6 GPa. To the best of our knowledge, this work presents the first high-pressure investigations of HNFx and more generally of a *gem*-bis(difluoramino)-substituted heterocyclic nitramine. [1] R. S. Miller; *Chemistry of Energetic Materials*; Ed. G. A. Olah and D. R. Squire; Chapt4; p77; (**1996**). [2] R. D. Chapman, R. D. Gilardi, M. F. Welker, C. B. Kreutzberger; *J. Org. Chem.*; 64; p960; (**1999**).

<sup>1</sup>Supported by ARO W911NF-05-1-0266

High Pressure Science and Engineering Center, Department of Physics, University of Nevada Las Vegas, Las Vegas, NV 89154-4002, USA

Date submitted: 29 Nov 2005

Electronic form version 1.4