Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Secondary decomposition reactions in nitramines[1]
IGOR SCHWEIGERT, U.S. Naval Research Laboratory — Thermal decomposition of nitramines is known to proceed via multiple, competing reaction branches [1], some of which are triggered by secondary reactions between initial decomposition products and unreacted nitramine molecules. Better mechanistic understanding of these secondary reactions is needed to enable extrapolations of measured rates to higher temperatures and pressures relevant to shock ignition. I will present density functional theory (DFT) based simulations of nitramines that aim to re-evaluate known elementary mechanisms [2,3] and seek alternative pathways in the gas and condensed phases. [1] S. Maharrey and R. Behrens, J. Phys. Chem. A, 109, 11236 (2005) [2] C. F. Melius and M. C. Piqueras, P. Combust. Inst., 29, 2863 (2002) [3] K. Irikura, J. Phys. Chem. A, 117, 2233 (2013)

[1]This work was supported by the Office of Naval Research, both directly and through the Naval Research Laboratory.

Igor Schweigert
U.S. Naval Research Laboratory

Date submitted: 05 Nov 2015 Electronic form version 1.4