

Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Preferential condensation of β RDX on In metal surfaces TERRENCE JACH, NIST, Gaithersburg, MD, ILANA G. GOLDBERG, Transportation Security Laboratory, Atlantic City, NJ, FERNANDO D. VILA, Dept. of Physics, U. of Washington, Seattle, WA — The energetic compound cyclotrimethylenetrinitramine (RDX) normally crystallizes out of solution at standard temperature and pressure in the α form. This consists of two nitro groups in pseudoaxial positions in relation to the C-N ring, and one nitro group in a pseudoequatorial position in an orthorhombic lattice. A metastable phase, labeled the β phase, is difficult to create and rarely observed. It consists of all three nitro groups in pseudoaxial positions, occupying a trigonal lattice. We have observed by means of Raman spectroscopy that RDX crystallized from solution on In metal foil preferentially adopts the β phase. We discuss a possible mechanism for this behavior in the context of recently published DFT calculations for RDX on a metal cluster.

Terrence Jach
NIST, Gaithersburg, MD

Date submitted: 07 Nov 2012

Electronic form version 1.4