Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Hydrogen Bonding at Extreme Conditions[1] RIAD MANAA, Lawrence Livermore National Laboratory — Triamino-trinitro-benzene (TATB) exhibits unusually strong intramolecular hydrogen bonding as evidenced by the high rotational energy barrier of the nitro and amino groups. In the condensed phase, competing intermolecular hydrogen bonding becomes pronounced at high-pressure. In this talk, I will present the results of recent first-principal computational studies concerning the effect of isotropic high-pressure on the atomistic structure of TATB up to 250 GPa. Along a specific crystal lattice direction, there exists a pressure regime beyond which both the inter and intra-molecular hydrogen bonding become equivalent. In the lower pressure regime of up to 50 GPa, the prediction of theory will be compared with on going experimental high-pressure X-ray diffraction studies. Possible mechanisms of phase transitions in the lower pressure regime will be discussed.

[1]This work was performed under the auspices of the U.S. Department of Energy by the Lawrence Livermore National Laboratory under contract number W-7405-Eng-48.

Riad Manaa
Lawrence Livermore National Laboratory

Date submitted: 18 Nov 2004 Electronic form version 1.4