

Abstract Submitted
for the SHOCK05 Meeting of
The American Physical Society

Pressure-Induced Phase Transitions in Pentaerythritol (PE) Crystals ZBIGNIEW A. DREGER, YOGENDRA M. GUPTA, Washington State University, CHOONG-SHIK YOO, HYUNCHAE CYNN, Lawrence Livermore National Laboratory — Pentaerythritol [C(CH₂OH)₄] is a simple solid polyalcohol with a crystal structure determined by balance between weak van der Waals interactions and relatively strong hydrogen bonds. To determine the stability of this structure under compression we have examined the response of PE at high pressures using Raman spectroscopy and synchrotron x-ray diffraction. It is shown that PE can exist in three different phases at pressures up to 10 GPa. Analyses of Raman spectra and x-ray diffraction data indicate onset of phase transitions at ~ 4.8 GPa and ~ 7.2 GPa. The phase I \rightarrow II transition at ~ 4.8 GPa, transforms the ambient tetragonal structure into an orthorhombic structure (*Pnn2* space group) with PE molecules occupying C₂ symmetry sites. Furthermore, we propose that the phase I \rightarrow II transition involves changes in the hydrogen bonding network (from quadrilateral to quasi one-dimensional). The proposed structure in phase II is consistent with available experimental data. Finally, we suggest that the crystal structure of phase III is a conformational variant of phase II, based on the similarity in their x-ray diffraction patterns. Work supported by DOE.

Zbigniew Dreger
Washington State University

Date submitted: 06 Apr 2005

Electronic form version 1.4