

## X-RAY AND RAMAN SPECTRA STUDIES ON THERMAL ENERGY STORAGE MATERIALS - TRIS(HYDROXYMETHYL)AMINOMETHANE

<sup>1</sup>Wen-Ming Chien, <sup>1</sup>Vamsi K. Kamiseti, <sup>1</sup>Juan C. Fallas, <sup>1</sup>Dhanesh Chandra, <sup>2</sup>Erik D. Emmons, <sup>3</sup>Aarron M. Covington, <sup>4</sup>Raja S. Chellappa, and <sup>5</sup>Simon Clark

<sup>1</sup> Metallurgical and Materials Engineering /MS388, University of Nevada, Reno, Reno, NV 89557

<sup>2</sup> U.S. Army Edgewood Chemical Biological Center, AMSRD-ECB-RT-DL/BLDG E5560, 5183 Blackhawk Road, Aberdeen Proving Ground, MD 21010-5424

<sup>3</sup> Department of Physics /MS220, University of Nevada, Reno, Reno, NV 89557

<sup>4</sup> Carnegie/DOE Alliance Center, Geophysical Laboratory, Carnegie Institution of Washington, Washington, DC 20015

<sup>5</sup> Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA 94720

### Abstract

Organic thermal energy storage materials are useful for thermal energy storage due to the presence of solid-state phase transition where the latent heat can store energy. The effects of temperature and pressure on the X-ray diffraction patterns and Raman spectra of tris(hydroxymethyl)aminomethane (TRIS,  $C(CH_2OH)_3NH_2$ ,  $C_5H_{13}NO_3$ ) were measured. X-ray diffraction and DSC results show that the solid state phase transition ( $\alpha$ -orthorhombic to  $\gamma$ -BCC) of TRIS occurs at 133.7°C at ambient pressure (1 atm). The volume thermal expansion equations of  $\alpha$  and  $\gamma$  phases were calculated as:  $Vol_\alpha = 0.01789 \times T + 146.73$  (298 K - 403 K) and  $Vol_\gamma = 0.07901 \times T + 128.62$  (403 K - 418 K). At room temperature, the high pressure synchrotron X-ray diffraction patterns and Raman spectra by using Diamond Anvil Cell (DAC) show that TRIS undergoes a phase transition ( $\alpha \rightarrow \beta$ ) starting at  $\sim 1$  GPa. A new high pressure  $\beta$ -phase were observed at a pressure range from  $\sim 1$  GPa to 9.3 GPa. The effects of hydrogen bonding on the broad OH and sharp NH stretching modes will be discussed. Detail results of temperature dependent effects on high pressure Raman spectra and Pressure-Temperature (P-T) phase diagram of TRIS will be presented.