X-RAY DIFFRACTION AND HIGH PRESSURE STUDIES ON ORGANIC THERMAL ENERGY STORAGE MATERIALS – TRIS(HYDROXYMETHYL) AMINOMETHANE (TRIS)

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Organic thermal energy storage materials, or Orientationally disordered crystals (ODIC), such as polyalcohols and amines are useful for thermal energy storage due to the presence of the solid state phase transitions where the latent heat can be utilized to store energy. The effects of temperature and pressure on the X-ray diffraction patterns and Raman spectra of tris(hydroxymethyl) aminomethane ($C(CH_2OH)_3NH$, TRIS) were measured. X-ray diffraction and DSC results show that the $\alpha \rightarrow \gamma$ solid state phase transition of TRIS occurs at 133.7°C and the crystal structure change from orthorhombic (α-phase) to BCC (γ-phase) at ambient pressure (1 atm). The volume thermal expansion equations of α and γ phases were calculated as $V_\alpha = 0.01789 \times T(K) + 146.73$ (298-403 K) and $V_\gamma = 0.07901 \times T(K) + 128.62$ (403-418 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 ~1 GPa. A new high pressure β-phase were observed at a pressure range from ~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.