## High pressure study of Pentaerythritol: a synchrotron infrared study

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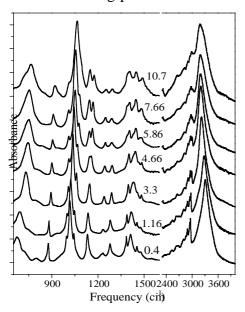
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Pentaerythritol (PET) is a simple molecule, which crystallizes as a solid in tetragonal I4 space group under ambient condition. The crystal has a layered structure with the PET molecules in the a-b plane connected by hydrogen bonding whereas the interlayer coupling is through weak Van der Waals force. Here we report a synchrotron radiation infrared high-pressure study upto a pressure of  $\approx 11$  GPa. The high-pressure experiments were carried out on 6% PET mixed with KBr powder in a membrane DAC with 450  $\mu$ m culet. The IR radiation from the Mirage beamline at LURE synchrotron was focused on a 100  $\mu$ m x 100  $\mu$ m spot in the DAC using a NicPlan IR microscope coupled to a FTIR spectrometer (Thermo Nicolet Magma 560). The figure shows the changes in the IR spectra with increasing pressure over the ranges 650 – 600 cm<sup>-1</sup> and 2300 – 4000 cm<sup>-1</sup> covering the internal modes of PET. The qualitative features of the spectra remain unchanged till  $\approx 4.7$  GPa beyond which the C-C skeletal stretch mode at 1131 cm<sup>-1</sup> and the O-H deformation mode at 1410 cm<sup>-1</sup> split into two modes. The changes in the frequencies of the bending, twist, deformation etc modes with increasing pressure shows that the modes at 662cm<sup>-1</sup>, 1375 cm<sup>-1</sup>, 1384 cm<sup>-1</sup> and



1410 cm<sup>-1</sup> modes exhibit sudden decrease in the slope beyond 4.7 GPa. The O-H mode at 3227 cm<sup>-1</sup> shows anomalous shift with the frequency decreasing at the rate of 27 cm<sup>-1</sup>/GPa till 4.7 GPa and then much more slowly with 3.7 cm<sup>-1</sup>/GPa. All these changes occurring at 4.7 GPa indicate that the crystal undergoes a phase transition beyond this pressure. On reducing the pressure, the spectrum changes to the ambient phase below  $\approx$  4.6 GPa showing that the transition is completely reversible. The transition pressure is close to the prediction made based on steric hindrance between the non-bonded hydrogen atoms.