High pressure study of Pentaerythritol: a synchrotron infrared study

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Pentaerythritol (PET) is a simple molecule, which crystallizes as a solid in tetragonal $I\bar{4}$ 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 ≈ 11 GPa . The high-pressure experiments were carried out on 6% PET mixed with KBr powder in a membrane DAC with 450 μm culet. The IR radiation from the Mirage beamline at LURE synchrotron was focused on a 100 μm x 100 μm 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^{-1} and 2300 – 4000 cm^{-1} covering the internal modes of PET. The qualitative features of the spectra remain unchanged till ≈ 4.7 GPa beyond which the C-C skeletal stretch mode at 1131 cm^{-1} and the O-H deformation mode at 1410 cm^{-1} 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^{-1}, 1375 cm^{-1}, 1384 cm^{-1} and 1410 cm^{-1} modes exhibit sudden decrease in the slope beyond 4.7 GPa. The O-H mode at 3227 cm^{-1} shows anomalous shift with the frequency decreasing at the rate of 27 cm^{-1}/GPa till 4.7 GPa and then much more slowly with 3.7 cm^{-1}/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 ≈ 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.