

High pressure phase transitions in Adamantane

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Angle dispersive x-ray powder diffraction measurements on Adamantane ($C_{10}H_{16}$) under pressure was carried out at the BL X 10 XU beam line of SPRING8 to characterize the phase changes revealed in our earlier Raman measurements¹ and the possible role of H---H bonds in inducing these changes

Measurements up to 26 GPa were carried out in a Mao-Bell type diamond anvil cell (DAC). Adamantane along with ruby pressure calibrant was loaded in a 100 μ m diameter hole of a stainless steel gasket. The diffracted x-rays from the sample were detected using a Rigaku image plate area detector.

Adamantane, though a poor scatterer, yielded good patterns because of the high beam intensity. The patterns from 0.6 GPa to 18.91 GPa can be indexed on a tetragonal cell. With pressure, the intensity of the (002) line decreases and by 12.49 GPa it disappears. At 12.49 GPa, the (112) and (201) lines merge and the width of the (202) line increases. Above 16 GPa, an increase in background and line broadening occur indicating disorder. Above 18.9 GPa, the pattern is not indexable on the tetragonal cell, possibly due to a multiphase region or a phase change.

From the simulated ADXRD patterns we conclude that the observed behaviour of (002), (112) and (201) lines is an indication of hydrogen

disorder under pressure. This along with the changes in the c/a shown in fig.1 and the P-V curve shown in fig.2 imply that the changes in the Raman spectra are due to a gradual

hydrogen bond disorder and a structural change above 19 GPa.

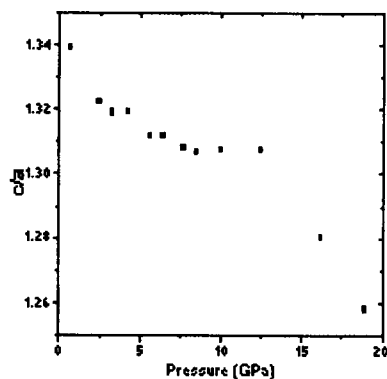


Fig. 1

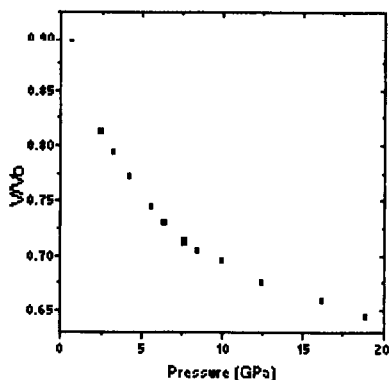


Fig.2

1] M. A.Rekha etal in Advances in High Pressure Science and Technology; proceedings of the IV NCHST, 1997, page 182, eds M. Yousuf , N. Subramanian, and K.Govinda Rajan, Universities press (India) Ltd.