

Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

A study of the eigenvectors of low frequency vibrational modes in crystalline cytidine via high pressure infrared absorption and molecular dynamics simulations. CARL STARKEY, University of Toledo, KRISTINA WOODS, Carnegie-Mellon University, SCOTT LEE, University of Toledo — High-pressure infrared absorption experiments and molecular dynamics simulations have been used to study the eigenvectors and eigenvalues of the vibrational modes of crystalline cytidine at 295 K by evaluating the logarithmic derivative of the vibrational frequency with respect to pressure: $\frac{1}{\omega} \frac{d\omega}{dP}$. Crystalline samples of molecular materials such as cytidine have vibrational modes that are localized within a molecular unit (“internal” modes) as well as modes in which the molecular units vibrate against each other (“external” modes). The value of the logarithmic derivative is a diagnostic probe of the nature of the eigenvector of the vibrational modes, making high pressure experiments a very useful probe for such studies. Internal stretching modes have low logarithmic derivatives while external as well as internal torsional and bending modes have higher logarithmic derivatives. Modes at about 503, 757, 795, 3093 and 3351 cm^{-1} are found to have negative logarithmic pressure derivatives, indicating a weakening of the effective force constants associated with those modes. The two modes above 3000 cm^{-1} are hydrogen-bond-stretching modes. The identity of all of these modes will be determined via molecular dynamical simulations.

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Date submitted: 05 Nov 2015

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