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A study of the eigenvectors of low frequency vibrational modes in crystalline cytidine via high pressure Raman spectroscopy SCOTT A. LEE, University of Toledo — High-pressure Raman spectroscopy has been used to study the eigenvectors and eigenvalues of the low-frequency 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. All of the Raman modes below 200 cm⁻¹ in cytidine are found to have high logarithmic derivatives, consistent with being either external modes or internal torsional or bending modes.

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