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Identification of low frequency intramolecular vibrational modes in crystalline adenosine via high pressure Raman spectroscopy SCOTT LEE, University of Toledo, A. ANDERSON, University of Waterloo — DNA is predicted to have an internal vibrational mode, below about 100 cm^{-1} , involving stretching motions of the hydrogen bonds between the basepairs. This mode is potentially important for mediating strand separation, an integral part of transcription and replication. Experiments are performed on ordered fibers and films containing many DNA molecules, while theoretical calculations are performed on single molecules. In addition to internal vibrations, solid samples also have external vibrations in which molecules within the unit cell vibrate against each other, meaning that the measured vibrational spectra will have both internal and external vibrations. Since these external vibrations are not calculated in theoretical calculations, the comparison between observed and calculated spectra is difficult. However, the restoring forces associated with the external modes are due to the long-range interactions between the neighboring molecules. Such modes are strongly affected by the application of high pressure. Internal modes are associated with much shorter ranged restoring forces, and are not affected so strongly by high pressure. Thus, high pressure experiments can determine whether the observed modes are internal or external in character. Here we report our high-pressure Raman studies of crystalline adenosine to reveal the nature of all the low-frequency vibrational modes.

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