

Abstract Submitted
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Study of the softening of infra-red active vibrational modes in crystalline cytidine as a function of pressure. CARL STARKEY, SCOTT LEE, University of Toledo, ANTHONY ANDERSON, University of Waterloo — DNA double helices are known to undergo conformational transitions when exposed to different conditions. The origins of these transitions are of great interest. It is possible that these transitions are driven by a weakening in the restoring forces associated with particular vibrational modes. We report the pressure dependences of the infrared-active vibrational modes of crystalline cytidine up to pressures above 4 GPa. Modes near 503, 758, 795, 3093, and 3351 cm^{-1} have negative pressure derivatives, indicating that the restoring forces of these modes are weakening with applied pressure. The two modes above 3000 cm^{-1} are hydrogen-bond stretching modes and their decrease in frequency with pressure shows the expected transfer of electrons from the molecular bond to the hydrogen bond as pressure is applied. The electronic wave function associated with the three modes below 800 cm^{-1} is changing in unexpected ways and indicates that the associated molecular components are losing electronic wave function.

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