Abstract Submitted
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A study of the nature of the low frequency vibrational modes of crystalline nucleosides CRAIG KOONTZ, SCOTT LEE, University of Toledo — Raman spectroscopy was used to study the low-frequency ($\leq$ 200 cm^{-1}) vibrations in crystalline samples of six nucleosides: deoxythymidine (dT), deoxycytidine (dC), deoxyadenosine (dA), uridine (rU), cytidine (rC), and adenosine (rA). The modes in this frequency range can involve both external modes (in which two molecules of the unit cell "beat" against each other) and internal modes. These experiments were performed in order to test the predicted low-frequency vibrational modes of dT, dC and dA of Shishkin *et al.* (in "Theoretical analysis of low-lying vibrational modes of free canonical 2-deoxyribonucleosides," O.V. Shishkin, A. Pelmenschikov, D.M. Hovorun and J. Leszczynski, Chemical Physics, **260** (2000) 317-325). Our experiments support their theoretical result that the lowest frequency vibrational mode (near 30 cm^{-1}) in dA and dC is due to a rotational mode around the C(1')-N bond.

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