

Department of Chemistry and Molecular Biology Seminar

October 4, 2007

3:45 pm in Dunbar 152

“Effects of hydrogen bonding on the ring breathing modes of pyridine and pyridinium”

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Abstract

We use a variation of coherent anti-Stokes Raman scattering to study the effects of hydrogen bonding on the ring stretching dynamics of pyridine and pyridinium. Hydrogen bonding blue-shifts the ring breathing mode of pyridine while leaving the “triangle” ring stretching mode relatively unperturbed. The blue-shifting of the ring breathing mode allows it to be used as a probe for gaining an understanding of the hydrogen bond dynamics in pyridine/hydrogen bond donor mixtures. A very simple model for the electronic behavior in pyridine that is based on electrostatics and molecular orbital theory seems to capture the essential features of the experimental data obtained for these mixtures.