

## INSIGHTS INTO HYDROGEN BONDING FROM VIBRATIONAL SPECTRA

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The vibrational frequencies of water molecules that are incorporated into water clusters encode an abundance of information about the strength of inter- and intramolecular interactions, and how these interactions are affected by the hydrogen-bonding environment. The addition of intensity information provides insights on how the electronic structure changes with molecular vibrations. In this talk, we will focus on the spectra of water and water clusters, and will explore how the strength and types of hydrogen bonds are encoded in these spectra. We start by considering the 1-0 transitions of the OH oscillators in the 3000 – 3500  $\text{cm}^{-1}$  region. A challenge with this spectral region comes from the fact that with increased hydrogen bond strength, the OH stretch frequency becomes more red-shifted, the intensity increases, and the transitions become more spread out. This makes it difficult to use the shape of spectral envelope in this region to enumerate the number of water molecules that sample a specific hydrogen bonding environment. In contrast, the sensitivity of the intensity to the hydrogen bonding environment is much weaker for transitions to states with one quantum of excitation in both the OH stretching and the HOH bending vibrations in the same water molecule. We will explore the origins of the differences in the sensitivity of the intensities of these two types of transitions to the hydrogen bonding environment, and how we can use the shape of the spectral envelope in the 5200  $\text{cm}^{-1}$  region to enumerate of the hydrogen bonding environments sampled by individual water molecules.