ORIGINS OF THE INTENSITY OF THE STRETCH-BEND COMBINATION TRANSITION IN WATER CLUSTERS AND IMPLICATIONS FOR CHARACTERIZING HYDROGEN BONDING

RACHEL M. HUCHMALA, ANNE B McCOY, *Department of Chemistry, University of Washington, Seattle, WA, USA*.

Water and hydrogen bonding have been actively studied for many years. The unique features of hydrogen bonding lead to processes such as proton transport which is essential to a variety of chemical, biochemical, and electrochemical processes. Despite the long-standing interest, many questions still remain surrounding the intricacies of hydrogen bonding. One goal of this study is to understand how the strength and other properties of hydrogen bonding can be extracted from the spectral signatures near 5000 cm^{-1}, which corresponds to combination transitions involving the HOH bend and the OH stretch. This region is of interest because, like the bend region, the intensities are relatively insensitive to the hydrogen bonding environment. At the same time, unlike the bend fundamental region, the frequencies of the transitions reflect the hydrogen bond strength as they follow the trends for the ν=1 levels of the OH stretches. This makes interpretation easier and introduces an interesting question, what are the origins of the intensities of the bend and the combination transitions? In order to investigate this question, we use various structures of water clusters, and dissect the intensity of the combination transition into mechanical and electrical contributions. Through this process, we are able to gain insights into the origin of the intensities. Further for the electrical contributions, we explore how the bending vibration is tuning the transition moment for the OH stretch.