COMPUTATIONAL FRAMEWORK FOR STUDYING H-BONDING IN THE OH STRETCH REGION OF VIBRATIONAL SPECTRA

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In many H-bonded complexes, there are two types of bands in the OH stretch region of the vibrational spectra; narrow peaks due to isolated OH stretches and a broadened feature reflecting hydrogen bonding. This second region can be as wide as several hundred wavenumbers and is shifted to the red of the narrow peaks. Furthermore, the extent of this broadening depends on system size and geometry. In this work we focus on $(CaOH)^{+}\cdot(H_2O)_n$ systems. For example, when n=4, the hydrogen bonding feature is several hundred wavenumbers. This is indicative of coupling between the OH stretches of the water molecules to the low frequency modes. To understand the broadening observed in the spectra, we have developed a computational framework in which we convolute the harmonic spectra of the OH stretches evaluated over the range of sampled intermolecular geometries. This framework will be discussed in context of several systems, including $(CaOH)^{+}\cdot(H_2O)_n$.