Solvation shell spectroscopy

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It is the molecular interactions between a solute and solvent that brings a molecule into solution. These interactions in turn change the solvent in direct contact with the molecule. The affected water molecules define the solvation shell of a given molecule, which vary in size depending on the strength of the interaction between solute and solvent. For aqueous solutions, the interactions are captured by the spectrum of the OH stretch vibration. Here is vibrational frequency of a non-hydrogen-bonded OH is around 3700 cm-1, which shift to lower frequencies correlated with the strength of the hydrogen-bond to the OH. Hydrophobic regions of the solute cause a breaking of hydrogen-bonds of nearby water molecules in the solvation shell, which can be observed as a sharp peak around 3700 cm-1, whereas strongly hydrogen-bonded interactions can shift the OH stretch below 3000 cm-1.

Solvation shell spectroscopy is an experimental method based on ATR FTIR spectroscopy, where the spectrum of the solvation shell is extracted from the total solution spectrum. The solvation shell spectrum captures the distribution of hydrogen-bonded strengths reflected in the OH stretch of water in direct contact with the solute and is thus a direct measure of the solute-solvent interactions.

In this hands-on module, you will learn how to capture and analyze solvation shell spectra of a small alcohols in water. In order to do this, you will learn to obtain high quality vibrational spectra and how to analyze the vibrational features. You will learn how to extract the spectra of the solute and associated solvation shell from the total infrared spectra. Lastly, you will learn how to analyze and understand the spectra of the solvation shell.