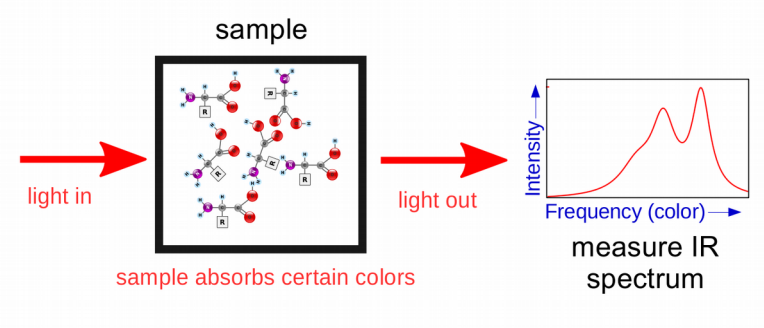
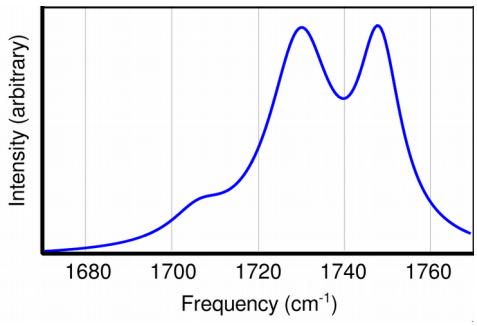
Exploring Solvation Environments with Infrared Spectroscopy and Molecular Dynamics

Chemists and physicists use infrared spectroscopy to learn about how atoms and molecules are arranged in many different compounds. A typical infrared spectroscopy setup is shown as a schematic below:



Since different molecules absorb different frequencies of light, it is possible to figure out what chemicals are in a sample simply by seeing what colors of light are absorbed. The most straightforward and widespread use of spectroscopy is simply to determine the presence or absence of chemicals of interest. Since spectroscopic tools are so convenient and effective for this task, their use is widespread in almost every technical discipline from biology to physics to the the oil and pharmaceutical industries.

It is also possible to use infrared spectroscopy to determine how molecules are arranged in a sample. That is, spectroscopy can tell us not just what molecules are present in a sample, but also how they are distributed and how they interact with one another. Take the infrared spectrum below for example:



This spectrum was taken of a solution of two liquids. Three peaks are clearly visible: two strong peaks around 1750 cm^{-1} and 1730cm^{-1} and a weaker peak around 1710 cm^{-1}. Given the molecules present in the sample, however, only one peak is expected in this area of the spectrum (the C=O stretching region). We observe multiple peaks because the molecules absorbing light are switching between three different environments!

To better understand what is going on, we can turn to molecular dynamics (MD) simulations. MD simulations are run on computers and generate 3D molecular movies of how we expect atoms and molecules to move around. We use spectroscopic measurements, such as the spectrum above, to check the predictions MD simulations make. If it seems like the MD movies are well explained by our real-world infrared spectra, it is reasonable to think that the simulation is close to reality.

Three snapshots from an MD movie for the solution we are working with are included in files named

0.pdb, 1.pdb, and 2.pdb. Your job is to analyze them and decide if they explain the IR spectrum shown above.

1. First, download SwissPDB viewer. You will need this program to open the MD snapshots. The program is available at http://spdbv.vital-it.ch/.
2. Try opening each of the .pdb files and viewing the MD snapshot.
3. Identify the different molecules present. What is the solvent? What is the solute?
4. Explain how you decided which molecule was the solute and which was the solvent.
5. Compare the three snapshots. How are they similar? How are they different? To help make your job easier, use some of the program's analysis tools to investigate properties of the molecules present. Try starting with “Tools > Compute H-bonds.” This utility will figure out how the molecules are hydrogen bonded and indicate the hydrogen bonds with dashed green lines.
6. Based on your investigation, does the MD simulation match the IR spectrum included? Why or why not?
7. Based on your investigation, does hydrogen bonding affect how molecules absorb infrared light? If it does, what is the effect?