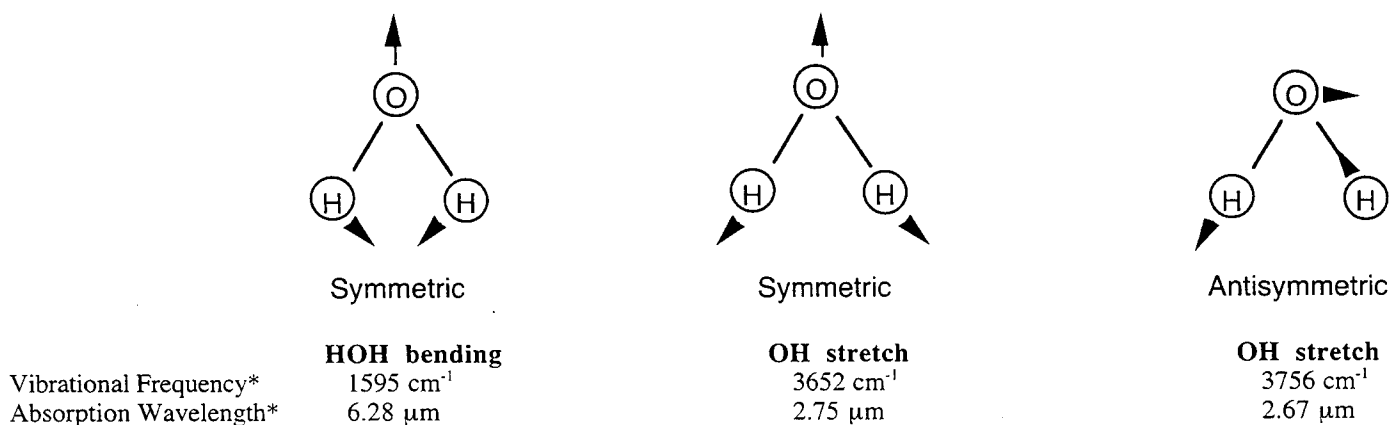


## (ii) Qualitative Identification of the Organic Acid Using Infrared Spectrometry

### Discussion

If we regard a polyatomic molecule as being comprised of mass points (atoms) joined together with springs (chemical bonds), then you can imagine that the addition of energy to such a system results in a complicated vibrational motion. It is easy to show, however, that this complex motion is the result of the combination of a relatively small number of what are termed normal vibrations or normal modes. If a molecule contains  $n$  atoms, then there are  $(3n - 6)$  distinct normal modes of vibration ( $3n - 5$  modes for a linear molecule). Associated with each vibrational mode is a set of energy levels. Electromagnetic radiation in the infrared region of the spectrum can induce transitions between these vibrational levels which is the physical basis for an important analytical technique called infrared spectroscopy.

For example, in the case of a bent triatomic molecule such as the water molecule, the following diagram pictures the three normal modes of vibration.



\*1595  $\text{cm}^{-1}$  means that there are 1595 waves per centimeter; 1  $\mu\text{m}$ , micrometer, is  $1.0 \times 10^{-6}$  meters or  $1.0 \times 10^{-4}$  cm. The frequency  $\tilde{\nu}$ , measured in  $\text{cm}^{-1}$ , is related to the wavelength,  $\lambda$ :  $\tilde{\nu} = 1/\lambda$ .

The use of vibrational (infrared) spectroscopy to solve problems of molecular structure (bond energies, molecular shapes, etc.) is important but somewhat more complex than we wish to tackle here. A more simple use of vibrational spectra consists in verifying the identity of a compound by matching its spectrum with that of known compounds. Infrared spectra of molecules containing a large number of atoms, while being complicated, show unique "fingerprint" patterns characteristic of each molecule. (You might see whether you can pick out of the spectra absorption peaks attributable to specific groups using a table of characteristic bond-stretching frequencies.)

Most transitions between vibrational levels in molecules occur in the wavelength range 2-15 microns. The Perkin-Elmer spectrophotometer you will use enables you to cover the important parts of this region of the spectrum, and thus by comparison with the spectra available in the laboratory you should be able to confirm the identity of your unknown acid.

## DETERMINATION OF INFRARED SPECTRUM

### Sample preparation

Transfer a very small sample (20-30 mg.) of the acid to the agate mortar and grind it into a very fine powder. Add 2 or 3 drops of Nujol and continue grinding until the mull is smooth and homogeneous. Select a pair of NaCl plates from the desiccator. Handle them with a piece of Kimwipe to protect them from the moisture from your fingers. To clean them, put 1 or 2 drops of Nujol on each side and wipe off with Kimwipe. Transfer a portion of the mull to one salt plate with the bottom of the pestle. Put the other plate on top and press the plates together to obtain an even film. After running the IR spectrum (get help from your TA), clean the salt plates with a little methylene chloride, and return them to the desiccator.

Compare your spectrum to those your instructor provides. Note that the height of the absorption peaks will depend on the thickness of the film of mull. The concentration of the mull will affect the relative size of the "nujol peaks" with respect to the peaks from your sample. The wavelength of each peak and the relative heights of your sample peaks will be independent of sample preparation. Use this information to match reference and unknown spectra.