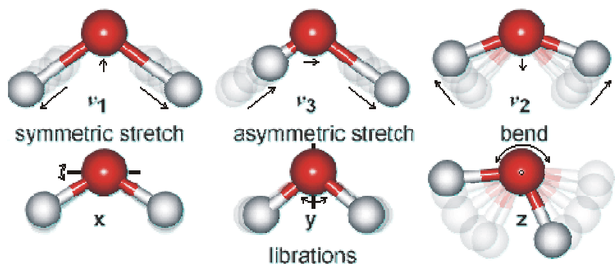
Modern Models of Motion **IR-Spectroscopy: Hooke's Law for Molecular Bonds**

Introduction:

Molecular bonds vibrate in a way that is similar to a spring undergoing simple harmonic motion. Each molecule will have several modes of vibration, each with its own natural frequency.



The frequency of vibration will depend on the bond strength and the atomic masses in the molecule. The bond strength can thus be determined from the frequency of vibration from the following expression derived from Hooke's law

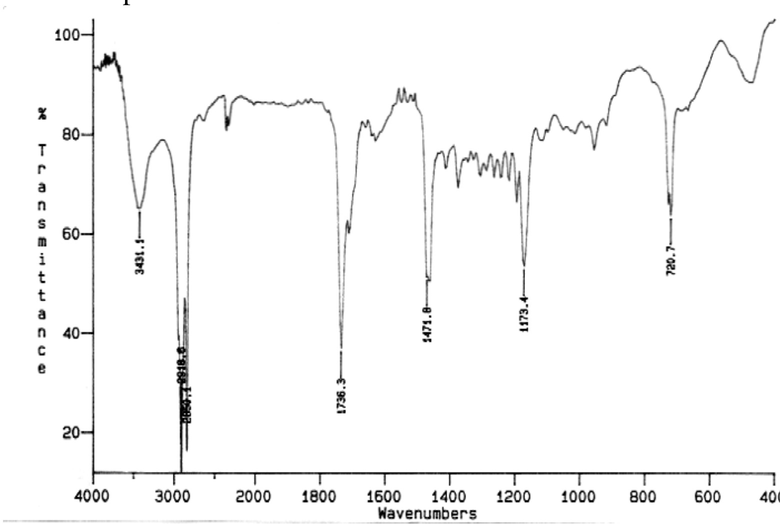
$$f = \frac{1}{2\pi}\sqrt{\frac{k}{\mu}}$$

where k is the spring constant, which is a measure of the bond strength, and μ is the effective or reduced mass, which takes into account that both masses are vibrating, rather than one.

$$\mu = \frac{m_1 m_2}{m_1 + m_2}$$

where m_1 and m_2 are the masses on each side of the bond.

The natural frequency of many molecular bonds is in the infra-red (IR) range, and it is possible to measure these frequencies precisely by making use of IR-spectroscopy. If the natural frequency of the molecular bond is in the infrared range and the vibration results in a change in the dipole moment of the molecule, then the molecule will absorb IR radiation at those frequencies, but allow other frequencies of IR radiation to pass through. The result is an IR spectrum for each vibration mode. An example is shown below:



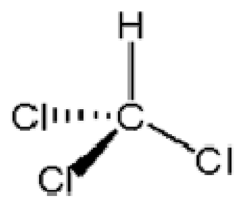
The IR spectrometer outputs the spectrum as wavenumbers,C in cm^{-1} instead of frequency in Hertz. In this case the wavenumber is simply the reciprocal of the wavelength $\upsilon' = \frac{1}{\lambda}$.

Given that $f = \frac{c}{\lambda}$ it follows that $\upsilon' = \frac{f}{c} = \frac{1}{2\pi\ c}\sqrt{\frac{k}{\mu}}$

Use this expression to solve for the spring constant *k* in terms of the wavenumber υ' and the reduced mass of the molecule μ.

Procedure:

In this lab you will measure the IR absorption spectrum for chloroform and chloroform-d. Chloroform has molecular formula $CHCl_3$ and chloroform-d or deuterated chloroform is $CDCl_3$,, Where hydrogen, H, has been replaced by deuterium, D, which is an isotope of hydrogen with twice the mass, but a similar bond strength with carbon). The molecular structure of chloroform is shown below:



The spectrum will show C-H stretching at about 3000 cm^{-1} , C-Cl symmetric and asymmetric stretching at about 670 and 760 cm^{-1}, and H-C-Cl bending at about 1200 cm^{-1}
We will be considering the C-H stretching.

1. Acquire the IR spectra for chloroform and chloroform-d using the FT-IR. (Someone with the license for the FT-IR spectrometer should run the machine).
2. Find C-H band and record its wavenumber in cm^{-1}.
3. Now use formula that you derived to find the spring constant. You should convert the wavenumber to m^{-1} , and make sure you calculate the reduced mass in kg, so that the spring constant is in N/m. Think carefully about what you should use for the two masses in the formula for the reduced mass. Is this a stiff spring or weak spring?
4. Now use your spring constant to predict what the wavenumber for the natural frequency for the C-D stretching in chloroform-d. Compare this value to the C-D band in the IR spectrum of chloroform-d
5. Calculate the period for the molecular vibrations of C-H and C-D.