These notes can be obtained at: http://www.ndsu.nodak.edu/instruct/grcook/chem342/notes.shtml

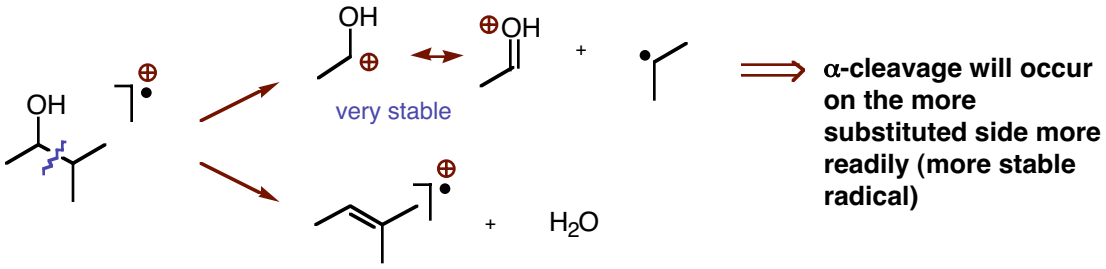
## Chapter 12: Mass Spectrometry and Infrared Spectroscopy

### Mass Spectrometry

Alcohols fragment by alpha cleavage (next to the alcohol)

Dehydration of alcohols is common

Can be difficult to see the $M^+$ (intact molecule)




### Infrared Spectroscopy

The electromagnetic spectrum encompasses frequencies from $10^{20}$ Hz (gamma rays, high energy) or wavelengths from $10^{-10}$ cm to $10^{8}$ Hz (radio waves) or <1 cm. The region from wavelengths of $3.8 \times 10^{-5}$ cm to $7.8 \times 10^{-5}$ is the narrow band of visible light. The infrared region lies just below from $10^{-4}$ cm to $10^{-2}$ cm.

We can relate the wave properties of electromagnetic radiation with the following equations

Wavelength x frequency = speed of light ($\lambda \times \nu = c$). This can be rewritten in terms of wavelength or frequency: ($\lambda = c/\nu$) or ($\nu = c/\lambda$). Wavelength and frequency are inversely proportional.

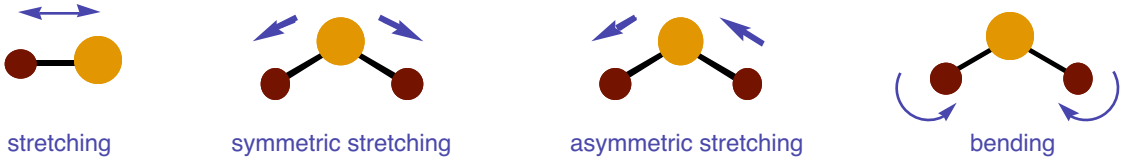
The energy of one photon = Planck's constant x frequency ($\varepsilon = h\nu$) or ($\varepsilon = hc/\lambda$). Thus energy is directly proportional to frequency and inversely proportional to wavelength.

Infrared Spectroscopy affords information about functional groups present in a molecule due to the absorbance of infrared radiation. When infrared light is passed through a molecule, the frequencies (or wavelengths) that correspond to the types of bonds present will be absorbed. These absorbances are characteristic for different functional groups.

The IR scale is often reported in units of Wavenumbers ($cm^{-1}$) which is simply the reciprocal of the wavelength ($1/\lambda$). The range in the IR spectrum of most organic molecules is 4000 $cm^{-1}$ to 400 $cm^{-1}$.

The y axis of the IR spectrum usually is in units of percent transmittance - that is if none of the light is absorbed at a specific wavenumber, all of it would be transmitted through the sample, and this is defined as 100% transmittance. As the radiation is absorbed, less of the light passes through and there is less than 100% transmittance.

The energy of the IR range of the EM spectrum corresponds to the energies associated with the vibrations of molecular bonds.




Different types of bonds will vibrate at different frequencies, so functional groups can be identified by what frequency the molecule absorbs IR radiation.