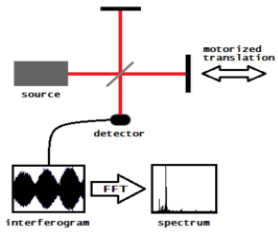
Name__Answer Key_____

Quiz 7 (10 pts)
CEM 434
Fall 2015

1. (2 pts). What happens in a molecule when IR light is absorbed? What is necessary for an IR transition to be allowed?

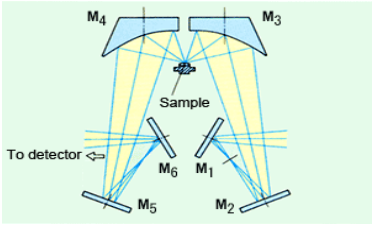
A molecule will absorb certain wavelengths of IR light that correspond to specific vibrational modes ($\Delta\nu$ = 1, ground state to an excited state). A bond in a molecule has a natural vibrational frequency which means the two atoms making up the bond are vibrating at this frequency. This frequency depends on the reduced mass (kg/atom) of each atom, what other atoms these two atoms are bonded to in the molecule and the force constant of the bond. If the optical energy matches this vibrational frequency, energy is absorbed and the amplitude of the vibration increases. A permanent dipole moment or an induced dipole moment (e.g., asymmetric stretch) is needed for a transition to be allowed.

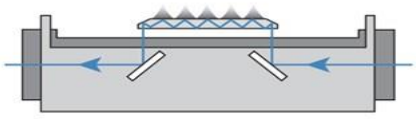
2. (3 pts). Sketch a detailed design (show optical path) of an FTIR spectrometer. How is the spectroscopy performed in comparison with a molecular UV/Vis absorption measurement?



Using an interferometer, all the optical frequencies from the source are modulated to produce a power-time spectrum (interferogram). This time domain spectrum contains all the optical frequency information (frequency domain). By recording time domain spectra with and without a sample, and then performing fourier transformation on the spectral information, one can create a typical frequency domain spectrum with the intensity at each wavenumber being related to whether or not there was any absorption by the sample. Many advantages of making the measurement in the time domaine: high optical throughput, high resolution, high speed and improved S/N due to the multiplex advantage.

3. (3 pts). Describe two modes of IR sampling other than the transmission measurement and show the designs of the sampling apparatus.





The left figure shows an attachment for a diffuse reflectance measurement. IR light intensity diffusely scattered from a powder sample is collected. The intensity at some of the wavenumbers is reduced due to absorption by the powder sample or molecules on the surface of the powders. The right figure shows an attenuated total reflectance attachment. IR light is directed down an optical waveguide with high refractive index at an appropriate incident angle. The light is totally contained within the waveguide but each time the packet of light reaches the interface, it escapes the waveguide by 1-2 μm before being bent back into the waveguide. During this time, a liquid or solid sample in direct contact with the waveguide can absorb certain energies. Multiple reflections (interactions with the sample) so improved S/N.

4. (2 pts). An IR measurement of a new compound with a pathlength of 0.5 cm revealed a transparency of 32% at 1650 cm^{-1} (C=O stretch) If the molar extinction coefficient was found to be 550 L/mol-cm then what is the concentration of the molecule present?

$$A = -\log T = -\log(0.32) = 0.495$$

$$A = \varepsilon bC = 0.495 = (550\ L\ mol^{-1}cm^{-1})(0.5\ cm)C$$

$$C = 1.80\ x\ 10^{-3}\ mol\ L^{-1}$$