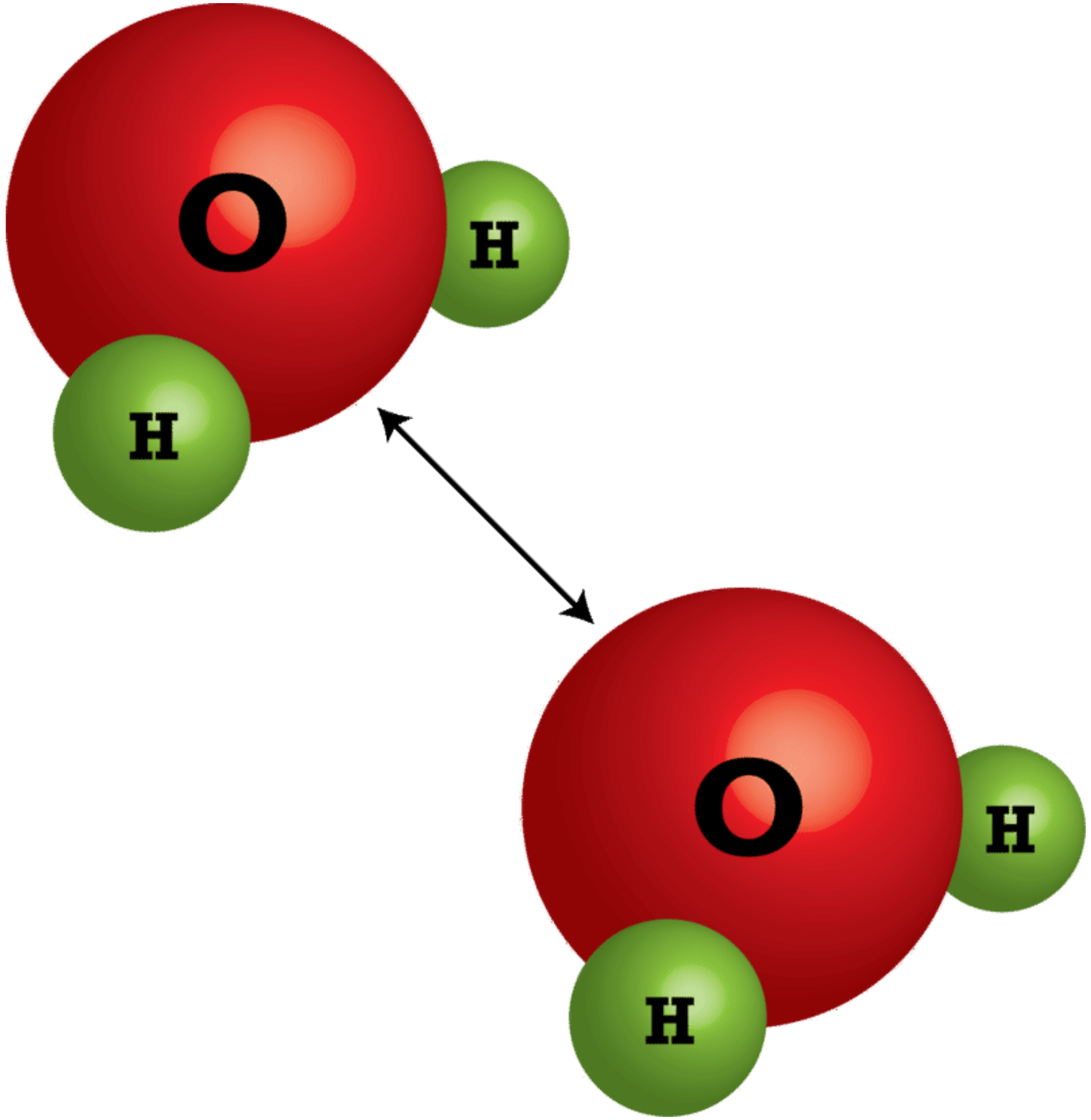
Unit 3

Intermolecular Forces

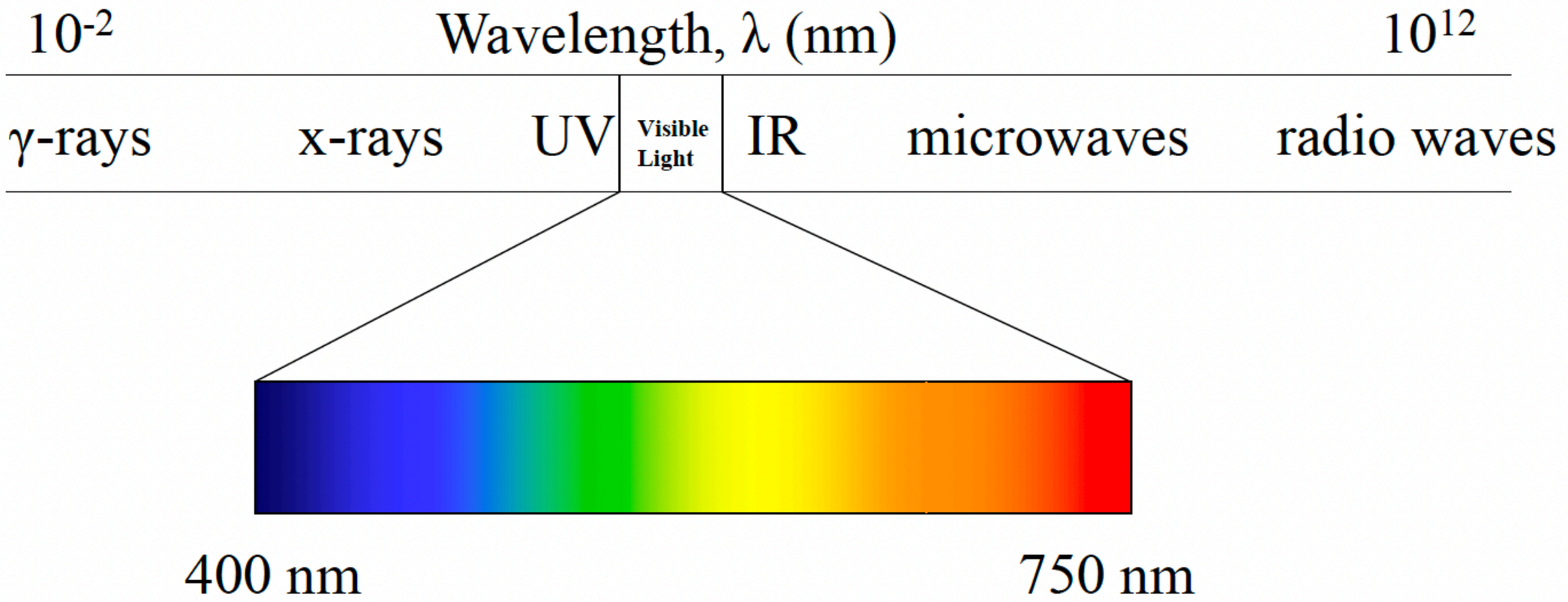


3.11 Spectroscopy
3.13 Beer-Lambert Law

- Electromagnetic Spectrum
- UV/Vis Spectroscopy
- IR Spectroscopy
- Microwave Spectroscopy

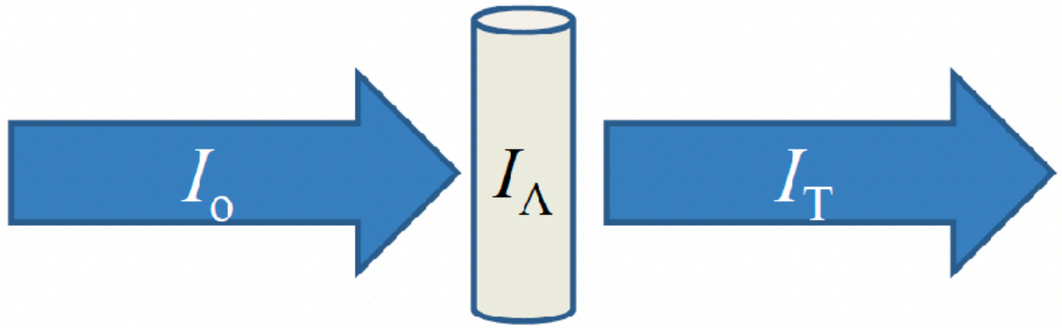
The Electromagnetic Spectrum

- Every wavelength of light is represented in the continuous spectrum.



Spectroscopy

- Method of analysis which is based upon the absorbance of electromagnetic (EM) radiation by matter.
- Used to gather data pertaining to the structure of a molecule or the concentration of a species.



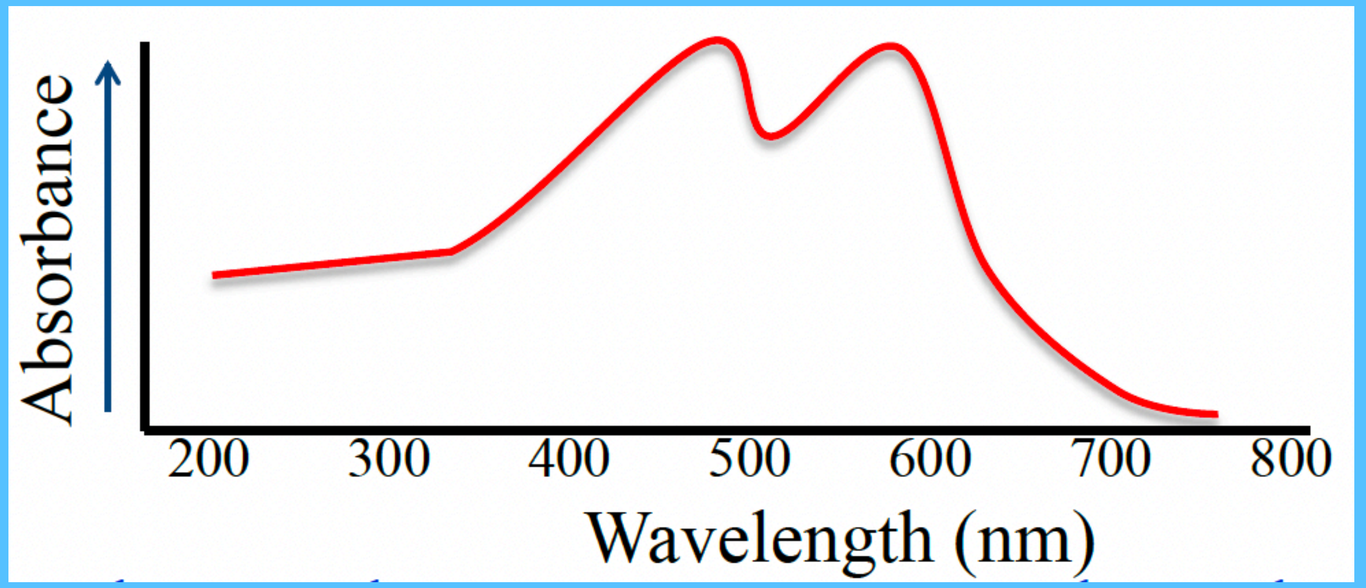
$$I_o = I_T + I_A$$

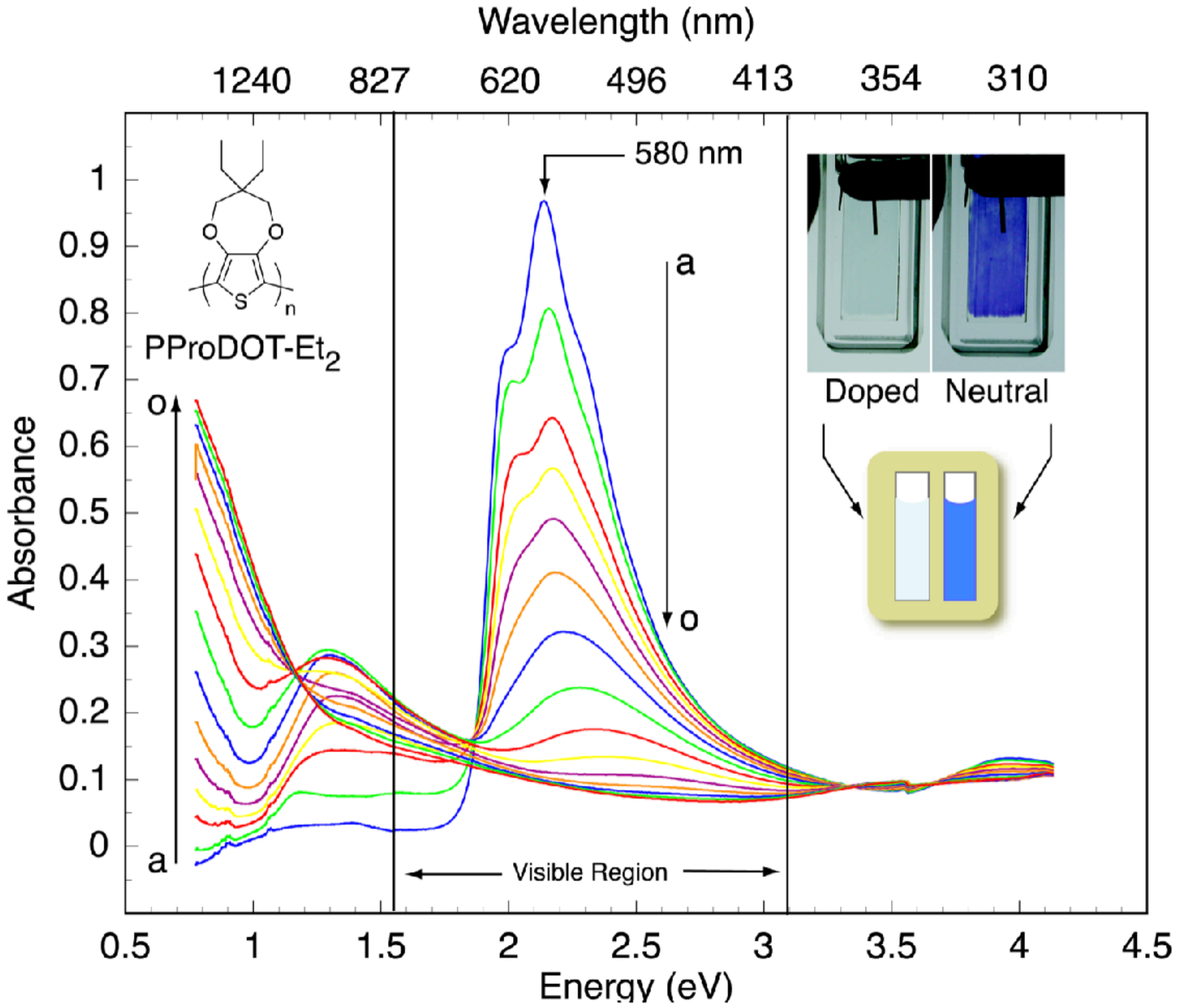
- I_o = intensity of the EM radiation striking sample.
- I_T = intensity of EM radiation exiting sample.
- I_A = intensity of EM radiation absorbed by sample.

Spectroscopy

Ultraviolet / visual (UV/Vis)

- Transitions in electronic energy levels.
- Used to probe the electronic structure of certain compounds.
- Used to determine concentrations of solution that contain certain compounds.
- 400-800 nm





Gaupp, C. L.; Welsh, D. M.; Reynolds, J. R. *Rapid Macromol. Commun.* 2002.

Beer-Lambert Law

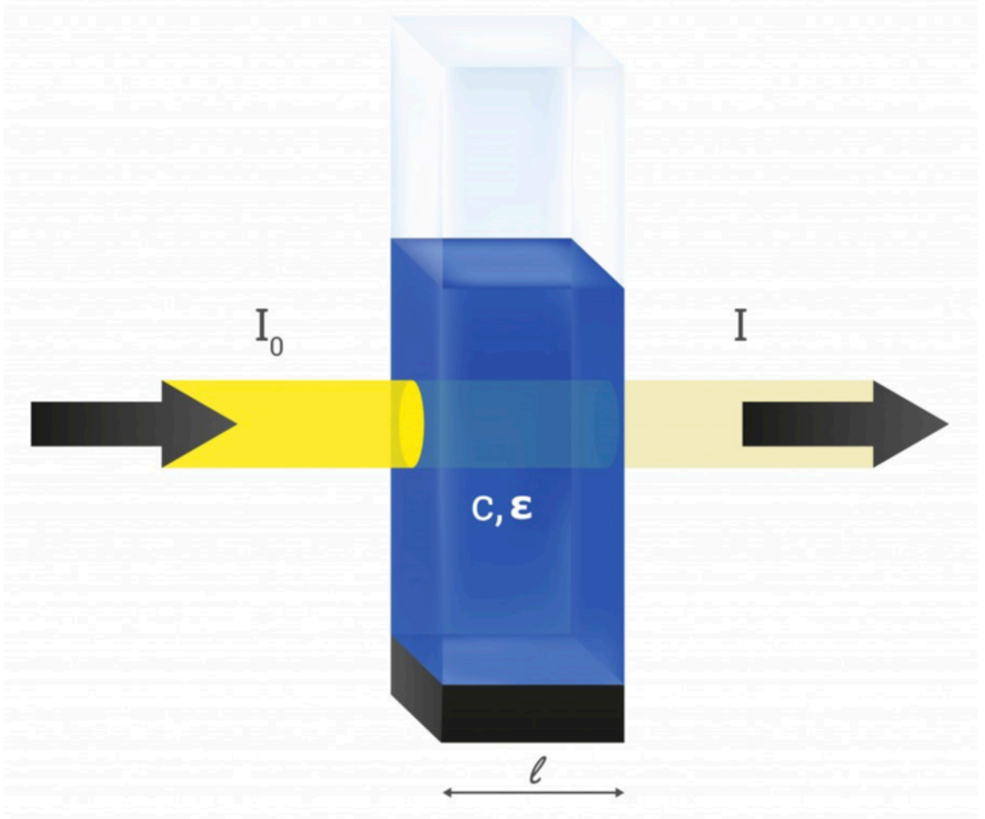
$$A = \varepsilon bc$$

A = absorbance

ε = molar absorptivity ($M^{-1}cm^{-1}$)

b = path length of sample cell (cm)

c = concentration (M)



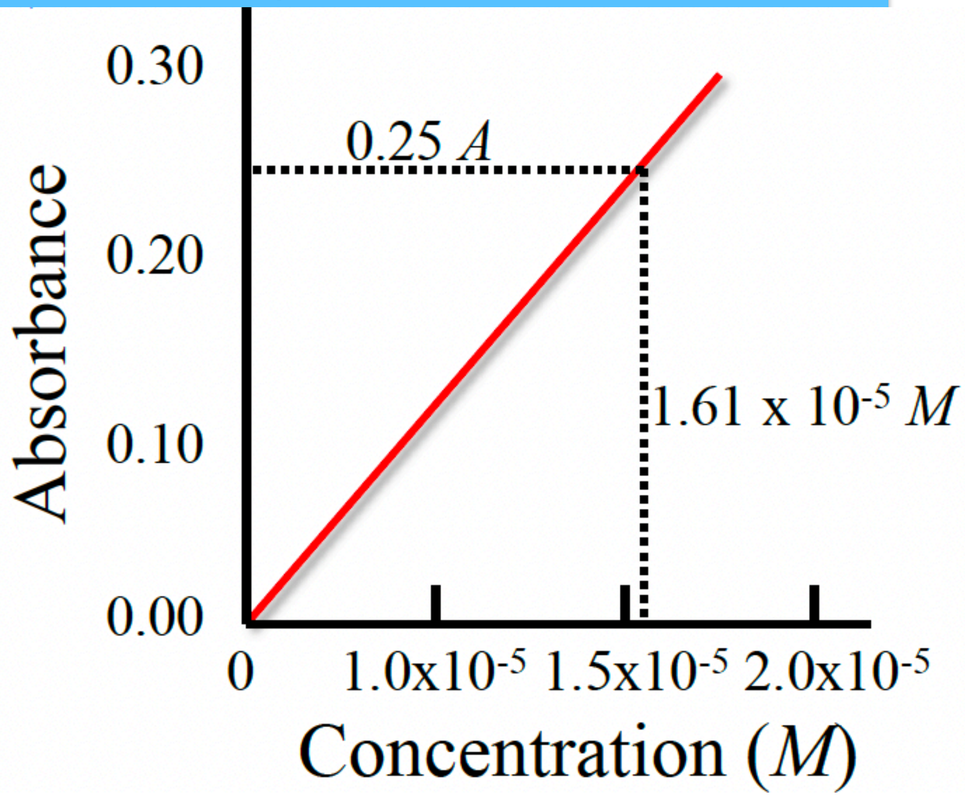
- ε describes how intensely a sample absorbs light at a specific wavelength.
- In most experiments, *b* and λ are constant, so ε also remains constant.
- *A* is only proportional to *c*.

Ex: UV/Vis Spec Experiments

A spectrophotometer with a 1.00 cm path length cuvette (cubic glass tube) was used to measure the absorbance of a hemoglobin solution. At 576 nm the absorbance was measured to be 0.25 *A*.

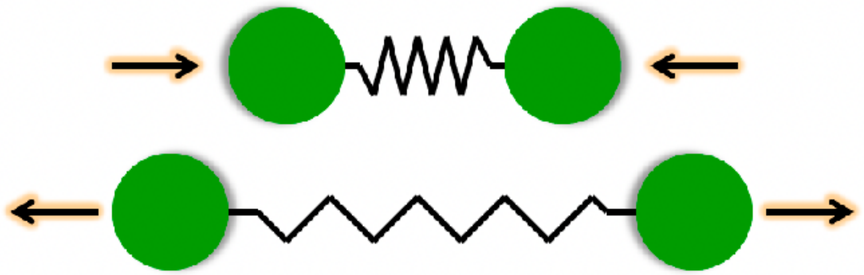
(a) Use the Beer's Law plot for hemoglobin to find the molar absorptivity (ε) of the solution.

(b) Find the concentration if the absorbance is 0.46 *A*.



Infrared (IR) Spectroscopy

Examines transitions in molecular vibrations
Used to detect the presence of different types of bonds and to identify molecules (via comparison)



- All covalent bonds in molecules are vibrating.
- Bond length is the average distance between nuclei.
- Covalent bonds have a vibrational frequency that is in the IR region of the EM spectrum.
- IR radiation of exactly the same frequency will be absorbed by the molecule.

Infrared (IR) Spectroscopy

Vibrational frequencies depend on the mass of the atoms and strength of the bonds.

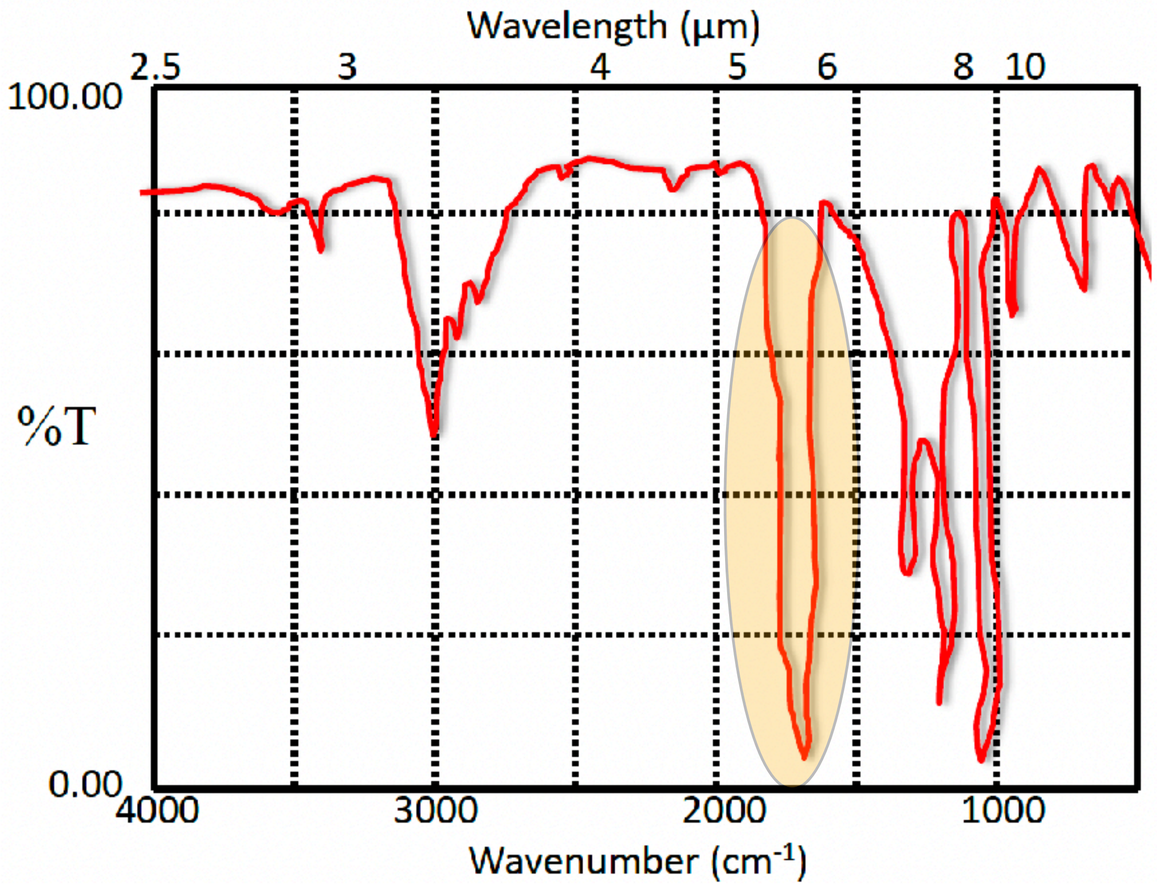
Frequency is related to wavelength: $c = \lambda \cdot \nu$

IR Wavelengths and Wavenumbers of Absorption

Bond Type	Range of Wavelengths (μm)	Range of Wavenumbers $(cm)^{-1}$
-C-H	3.38 – 3.51	2960 – 2850
=C-H	3.23 – 3.33	3100 – 3000
C=C	5.95 – 6.17	1680 – 1620
O-H	2.74 – 4.00	3650 – 2500
N-H	2.94 – 3.13	3400 – 3200
C-O	7.69 – 10.00	1300 – 1000
C=O	5.56 – 6.13	1800 – 1630

Ex: IR Spectrum - Acetone

Use the table of IR wavelengths and wavenumbers of absorption to identify the peak associated with the C=O bond.



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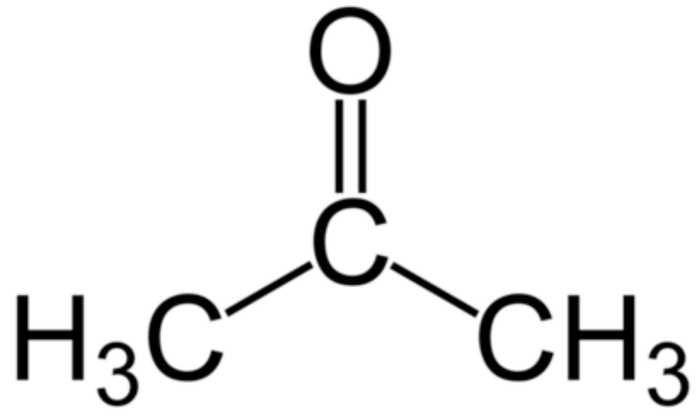

Microwave Spectroscopy

- Microwaves cause polar molecules to rotate.
- Each type of polar molecule has specific rotational frequencies that it can exhibit.
- The peaks below correlate with the different rotational frequencies for a specific polar molecule.
- Data from MW spectra can be used to calculate bond length of diatomic polar molecules and to determine the shapes of polar molecules.