Chapter 12 – Infrared Spectroscopy

Lecture Notes

I. **Section 12.1 – Electromagnetic Radiation**

A. **Important Terms**

1. **Electromagnetic Radiation** – (EMR) - light and other forms of radiant energy.
2. **Wavelength** – (λ) distance between consecutive peeks on a wave.
3. **Frequency** – (ν) this is the number of full cycles of wave that pass a given point in a second. (Hertz or 1/s)

II. **Section 12.2 – Molecular Spectroscopy**

A. **What is spectroscopy?**

Spectro – ancient greek - light

Scopy - ancient greek - study of.

The general definition of spectroscopy: the study of the interaction of radiation (light) and matter (a ~~compound~~ Molecules) as a function of wavelength

B. **Molecular Spectroscopy** – the study of which frequencies of electromagnetic radiation are absorbed or emitted by a particular substance and the correlation of those frequencies with details of molecular structure.

C. The three types of spectroscopy that we're interested in:

Region of the Electromagnetic Spectrum	Frequency (hetz)	Type of Spectroscopy	Absorption of Electromagnetic Radiation Results in Transition Between
Radio frequency	3×10^{7}-9×10^{8}	Nuclear magnetic resonance	Nuclear spin states
Infrared	1×10^{13}-1×10^{14}	Infrared	Vibrational energy levels
Ultraviolet-visible	2.5×10^{14}-1.5×10^{15}	Ultraviolet-visible	Electronic energy levels

Table 12.3. Types of Energy Transitions from Absorption of Energy from Three Regions of the Electromagnetic Spectrum (pg. 458)

III. Section 12.3 – Infrared Spectroscopy

A. The Vibrational Infrared Spectrum

1. Range of IR spectra:

2. Unit of measurement:

3. Why do we use IR Spectroscopy??

a.

b. IR spectroscopy does this by probing the stretching and bending vibrations of organic molecules.

4. Sample spectrum – 3-methyl-2-butanone

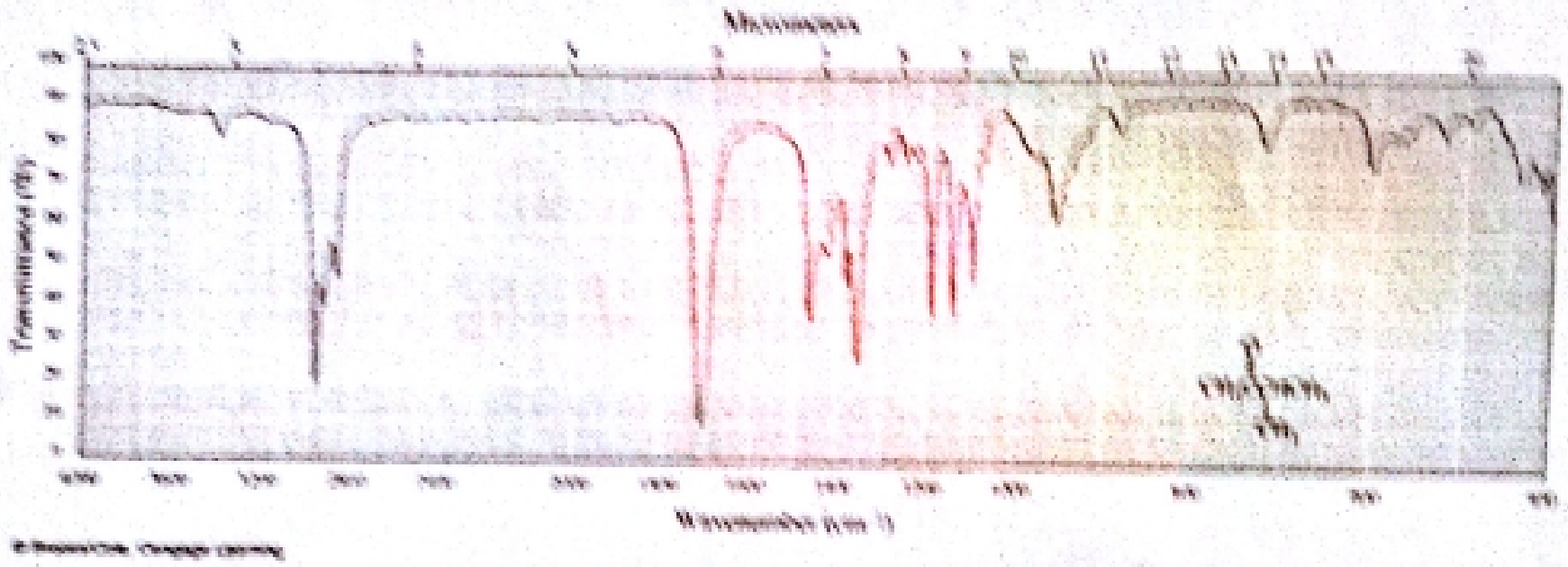

Figure 12.2. IR Spectra of 3-methyl-2-butanone (pg. 459)

a. Horizontal axis = frequency (wavenumbers)

b. Vertical axis = % Transmittance

i. Remember from the Spect-20s from Gen Chem lab: 100% Transmittance = 0 % Absorbance!

c. How do we prepare a sample for IR spectroscopy?

i. Liquid samples – place on KBr salt plates

ii Solid samples – dissolve in a solution that will have no effect on your spectra OR use Nujol Mull (an oil) and suspend your sample.

B. Molecular Vibrations

1. Atoms joined by covalent bonds undergo continual vibrations relative to each other.

2. The frequencies of these vibrations are quantized (this means that within a molecule, only specific vibrational energy levels are allowed).

3. The energies associated with transitions between vibrational energy levels correspond to frequencies in the IR region – between 4000 cm^{-1} and 400 cm^{-1}.

4. In order for a molecule to absorb IR radiation, two things must happen:
   a.

   b.

      I. A covalent bond which does not meet these criteria are said to be *IR inactive*.
         (a). Symmetrically substituted alkenes and alkynes are IR inactive. *Raman Spectroscopy studies these!*

5. For a non-linear molecule that contains *n* atoms, there are 3*n*-6 allowed fundamental vibrations.

   a. For even a very small molecule, there could be MANY different vibrational energy levels – which lead to complex spectra.

   b. The best vibrations that we see are stretching vibrations and bending vibrations. Figure 12.3 on pg. 460 show the principle absorption patterns in IR Spectroscopy.

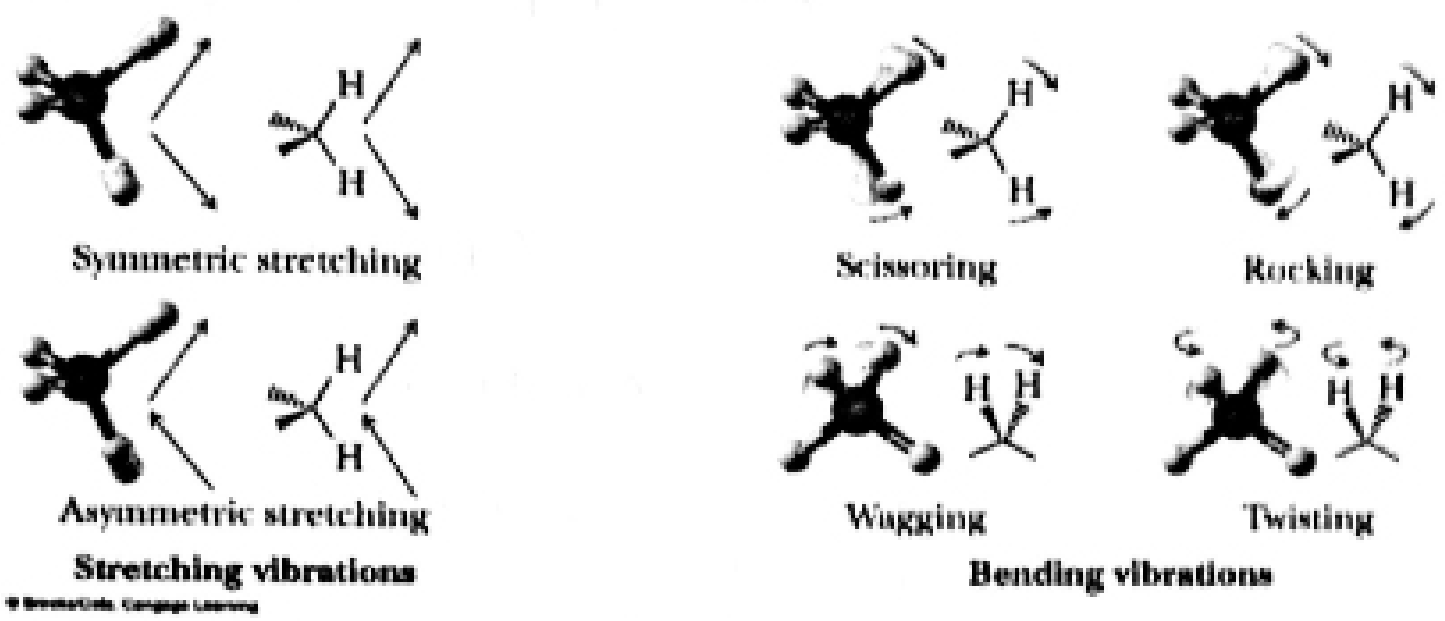

Figure 12.3. Fundamental stretching and bending vibrations for a methylene group (pg. 460)

C. Characteristic Absorption Patterns
   1. We can calculate where absorptions due to particular vibrational modes will appear in an IR spectrum. To do this, think of two atoms connected to each other on a spring.
      a. That means that the total energy...