Spectroscopy
1– Electromagnetic Spectrum

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Introduction

Spectroscopic techniques are used to determine structure in organic chemistry.

They should destroy little or no sample, if possible.

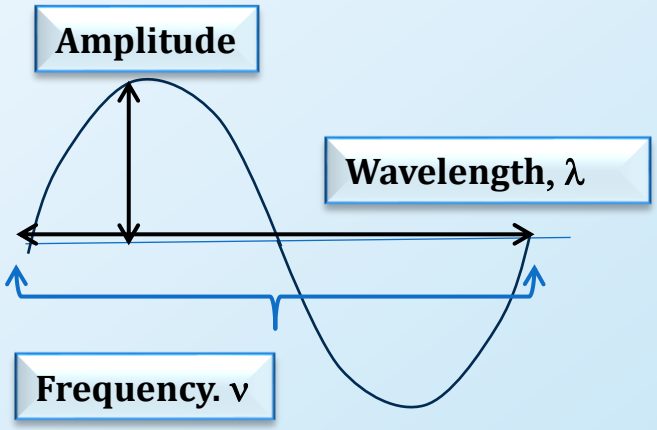
There are four main spectroscopy we will cover:

- Ultraviolet-Visible (UV-Vis) spectroscopy studies the electron transitions to determine bonding patterns.
- Infrared (IR) spectroscopy measures the bond vibration frequencies in a molecule and is used to determine the functional group.
- Mass spectrometry (MS) fragments the molecule and measures the masses and their relative abundance to determine the mass of the whole molecule and fragments.
- Nuclear magnetic resonance (NMR) spectroscopy detects signals from hydrogen and carbon atoms in presence of a magnetic field and can be used to determine the structure in great accuracy.

Wave Nature

All waves travel in a particular cycle of certain length which determines properties of that wave. The properties that determine the quality of the wave are:

- **Wavelength**: λ (*lambda*) distance between identical points on successive wave/peaks.
- **Frequency**:ν (*nu*) number of waves that pass a particular point in one second.
- **Amplitude**: the vertical distance from the midline of waves to the top of the peak.



Wave properties are mathematically related as:

$$c = \lambda\nu$$

Where,

- $c = 2.99792458 \times 10^8$ m/s (speed of light)

λ = wavelength (in meters, m)

ν = frequency (reciprocal seconds, s^{-1})

Electromagnetic Spectrum

Electromagnetic spectrum consists of various radiations divided by wavelength or frequency: X rays, microwaves, radio waves, visible light, IR, and UV.

- Frequency and wavelength are inversely proportional.
- $c = \lambda \nu$, where c is the speed of light.
- Frequency and energy are directly proportional.
- Energy per photon = $h \nu$, where h is Planck's constant, 6.62×10^{-37} kJ•sec.

Higher frequency
Shorter wavelength

Lower frequency
Higher wavelength

Wavelength, cm	Region	Energy, kJ/mol	Effect studied
10^{-9}	Gamma rays	10^{7}	
10^{-7}	Ultraviolet (UV)	10^{5}	
10^{-5}	Visible (Vis)	10^{3}	Electron transition
10^{-4}	Infrared (IR)	10	Molecular vibrations
10^{-1}	Microwave	10^{-2}	Rotational motion
10^{4}	Radio waves	10^{-4}	Nuclear spin transition

The Spectroscopy Regions

We will be studying the following aspects of the electromagnetic spectrum:

UV- Vis Spectroscopy

- Wavelength is measured in nm – 200-800 nm.

IR Spectroscopy

- Wavelengths usually 2.5-25 μm.
- More common units are wavenumbers, or cm^{-1}, the reciprocal of the wavelength in centimeters. 4000 – 400 cm^{-1}.

Nuclear Magnetic Resonance

- Uses radio frequency 60 - 1000 MHz.
- The common scale is ppm (parts per million).

Key Concepts

- Know the basics of electromagnetic spectrum.
- Relationship between wavelength and frequency and energy.