Spectroscopy

Absorption - energy from electromagnetic radiation excites atoms or molecules from lower energy levels to higher energy levels

Emission - decay from a higher energy level to a lower level=electromagnetic radiation is emitted

Ultraviolet-Visible, Infrared, and Emission Spectroscopy-

Ultraviolet visible- measures the amount of a certain wavelength of light is absorbed by a sample. UV-vis can be used to determine relative energy levels of molecular excited statesIR

Infrared-An infrared beam can be passed through a sample and a spectrum can be produced from the wavelengths of infrared light the sample *absorbs.* It can be used to determine modes of intramolecular vibrations

Emission Spectroscopy looks at the spectrum of *emitted* electromagnetic radiation after atoms/molecules are excited to a higher temperature

Photochemical Spectroscopy

Absorption Spectroscopy- how molecules and atoms *absorb* light

Light is generated over a broad range of wavelengths and passed through the sample. A sensor is able to detect the intensity of the incident light, compare it to initial intensity, and produce a chart of Absorbance vs. Wavelength or Transmission vs. Wavelength

Atomic/Molecular Emission-How molecules and atoms emit light of different wavelengths and over time

A sample is excited by either high intensity light or electric potential. The light emitted from the sample is then filtered by wavelength, and sent to a detector

Mass Spectrometry- consist of three essential parts: ion source, a mass analyzer, and a detector

ion source-responsible for breaking up molecules into ionized fragments. fragments pass into the mass analyzer which applies magnetic and electric fields to the ions. Ions ofdifferent masses are deflected differently by the fields.

Mass analyzer- The mass analyzer separates the ions based on their charge/mass ratio by applying a combination of electric and magnetic fields.

From Lorentz force law we have: And Newton's second law:

$$F = q[E + (v \times B)] \qquad F=ma$$

We can derive the expression-shows the dependence of a particles trajectory on mass:charge

$$(m/Q)a=E + v \times B$$

Dectors in an Array

A particle is deflected by magnetic and electric fields differently based on its mass to charge ratio so will strike the detector at a different location. Sensitivity is increased and multiple ions can be detected at the same time

NMR Spectroscopy- the study of how the nuclei of atoms interact with electromagnetic radiation while exposed to a constant magnetic field.

Particle Spin and Magnetic Moment- the spin state for nuclei is *m.* . Both protons and neutrons have a magnetic moment w/o an external magnetic field, these energy levels of the two spin states are degenerate. In an external magnetic field the magnetic moments of the nuclei will align with the field. Because nuclei have a positive charge, the nuclei with magnetic moments that are parallel to the magnetic field will have a lower energy and thus be more stable. We can only study nuclei which have either an odd number of protons and or an odd number of neutrons.

Zeeman Effect-the energy of the *i*th spin state is directly proportional to the value of m_i and the strength of the constant magnetic field

From NMR to MRI-MRI machines are developed out of NMR machines

Non-invasive and does not depend on radiation. The body contains large quantities of hydrogen. The patient is inserted inside a 2T field. A radiofrequency magnetic field is then turned on, causing the hydrogen to line up with the B-field. When this RF magnetic field is turned off, the nuclei emit radiofrequency, which can be detected. Diseased tissue emit energy at a different rate.