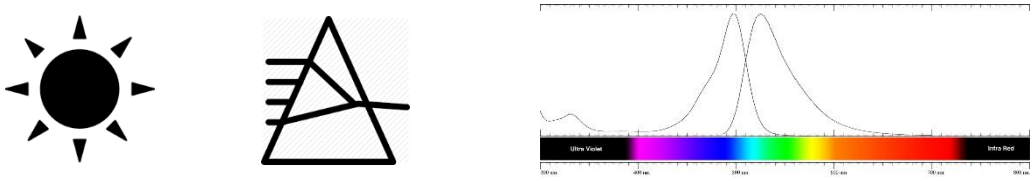
Spectroscope is...

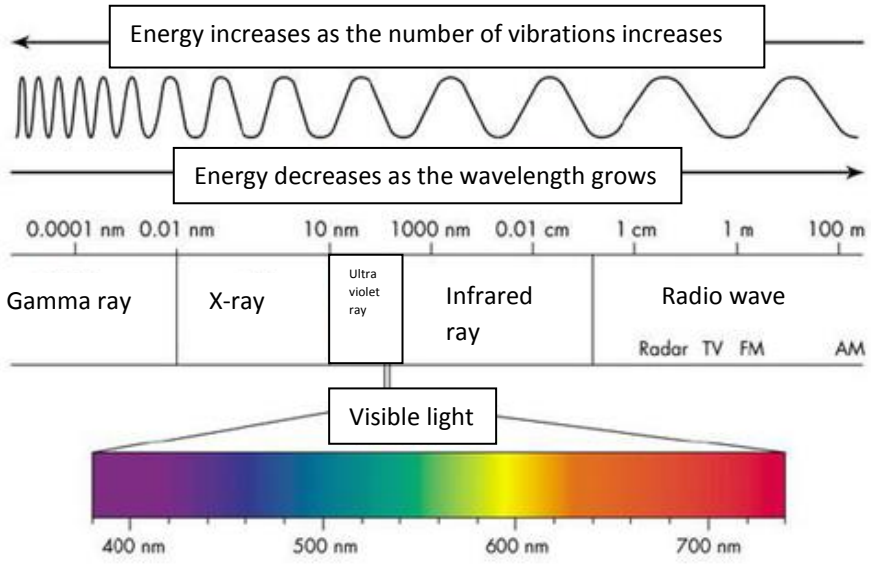
A spectroscope is an instrument which radiates light of a certain area of electromagnetic wave on the substance to be analyzed, and measures the light which has passed through the substance to be analyzed, and as the radiated light is absorbed or emitted according to the characteristics of the molecular structure of the substance, the device which measures this in the absorption intensity for the wavelength is called a spectrophotometer.

Light Sample Spectrum

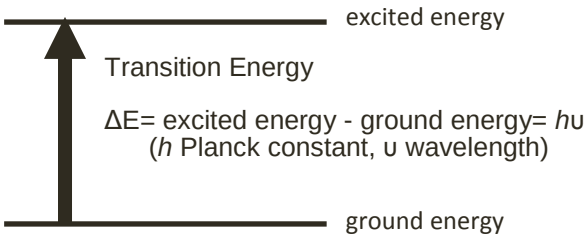


1. Light (Electromagnetic Wave)

The electromagnetic wave used in the spectroscope is called by the name of gamma ray, x-ray, ultraviolet ray, visible light, infrared ray, radio wave, and microwave according to the wavelength value. The electromagnetic spectrum per each wavelength area is as in the following figure.



When the substance to be analyzed receives the energy from each wavelength of the electromagnetic wave, transition occurs, and data can be obtained from the electromagnetic wave coming from specimens after the energy transition.



The spectroscope used per each wavelength area is as follows.

Electromagnetic wave area	Spectroscope	Energy transition form
γ-ray	Mossbauer spectroscope	Nuclear energy absorption
X-ray	X-ray spectroscope	Energy absorption of central electrons
Ultraviolet ray/visible light	UV/Vis spectroscope, atomic emission spectroscope	Energy absorption and emission of outermost electrons
Infrared ray	Infrared spectroscope, Raman spectroscope	Molecular vibration absorption energy
Microwave	Microwave spectroscope, ESR (Electron Spin Resonance) spectroscope	Molecular rotation electron spin energy absorption
Radio wave	NMR (Nuclear Magnetic Resonance)	Proton spin energy absorption
Ultraviolet ray / visible light	Atomic emission spectroscope	Atomic luminous energy
X-ray	Fluorescent spectroscope	
Infrared ray / visible light	Phosphorescent spectroscope, atomic fluorescent spectroscope	

2. Sample

The spectroscope that can measure the structure information of the sample to be verified is selected, and it is sampled according to each spectroscope for and measured. The specimen that can be measured with a spectroscope spans all states of solid, liquid, sol, and gel, and as for the liquid specimen, all substances that dissolve in the solvent such as organic, inorganic, ion, complex, etc. can be measured. As for the solid specimen, film, powder, fiber, glass shard, vinyl and such can be experimented.

3. Spectrum

A spectrum appears in wavelength and absorption intensity graphs. The molecular structure information of the specimen can be predicted from the maximum absorption wavelength of the sample peak, and the sample concentration can be found from the peak intensity.

UV/Vis Spectroscopy

Most organic compounds and functional groups transmits a part of the electromagnetic spectrum area between 190~800nm, which corresponds to the ultraviolet ray and visible ray area. The radiation of this area transfers the electron energy level of the substance, identifying the substance structural information and concentration, and the detailed information for structure can be valuably utilized for the compound structure estimation when the detailed information for infrared and nuclear magnetic resonance spectrum is provided

1. Characteristics of UV-VIS

1) It facilitates the specimen quantitative/qualitative analysis in the sample. According to the absorption peak, the concentration value can be estimated, and based on the relation between absorbance and sample concentration, the qualitative technology can be applied to the fields of water quality, food, beverage, pharmaceutical, chemical, and life science.

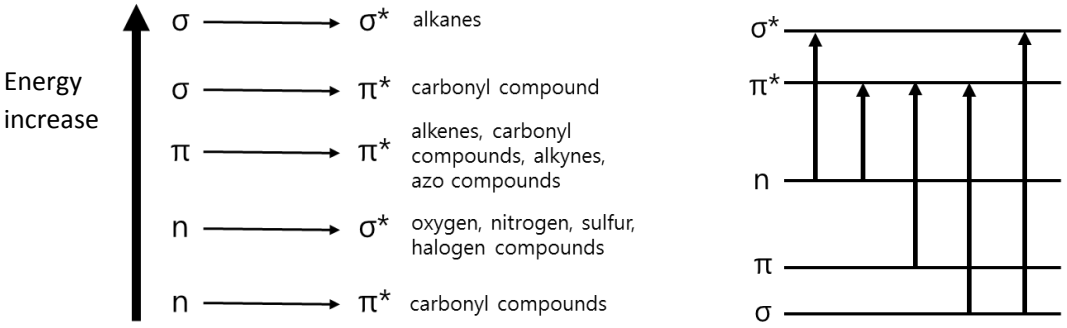
2) The data peak location provides information on the molecular structure of the sample. For example, the absorption wavelength is different for each of carbonyl, alkenes, and halogen group compounds, so the information of the functional group can be predicted by the location of the wavelength.

3) The spectrum shows the physical characteristics of the sample. The absorption coefficient has a value unique to the sample, and it can identify the melting point of DNA/RNA protein according to the temperature changes. Also, the observation of absorbance change according to time can determine the reaction kinetics of the substance.

4) The peak location and profile provide the information for the surrounding environment of the sample molecule. For example, the existence of foreign substances and other solvents influence the peak location and profile. In other words, the absorption wavelength can move due to the foreign substance or the peak may become flattened.

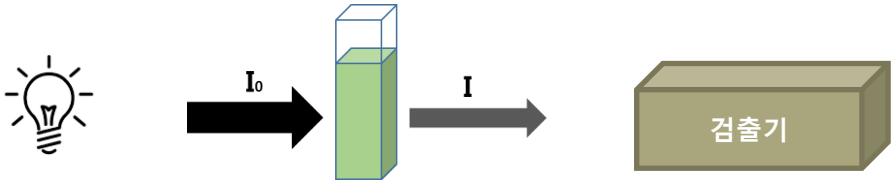
2. UV-VIS Absorption Principle

When a consecutive electromagnetic wave of 190nm~ 1100nm passes through the substance the energy state due to the electron transfer of the substance as much as the energy of that wavelength moves to the ground state and the excited state, and the wavelength is absorbed/emitted as much as the energy difference between the two states.



3. Transmittancy and Absorbance

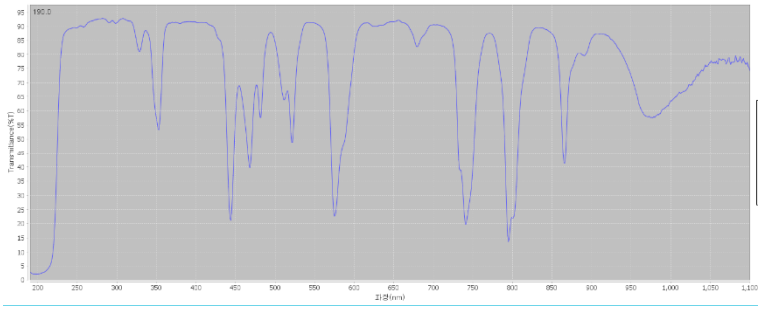
The amount of light absorbed by the specimen when the light passes through or reflects on the specimen is the difference between the incident radiation (I_0) and the transmitted radiation (I). The amount of the absorbed light is expressed in transmittancy or absorbance.



Transmittancy: the ratio of transmitted radiation to the incident radiation; it is expressed in the following equation.

$T = I/I_0$ or $\%T = (I / I_0) \times 100$

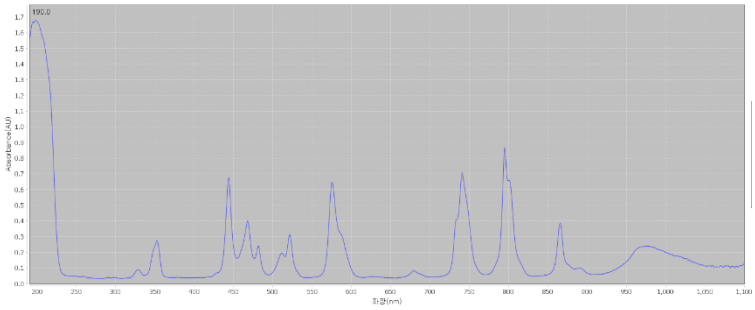
Transmittancy Spectrum



Absorbance: the intensity of the light absorbed by the sample. It has the negative log value of the transmittancy.

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

Absorbance Spectrum



4. Beer-Lambert Law

The more there are molecules that can absorb light at the given wavelength, the greater the light absorbance becomes. Therefore, the absorption intensity is proportional to the concentration of the specimen. Also, the absorbance intensity is proportional to the cuvette length.

This can be simply expressed in the following equation;

$$A = \varepsilon \cdot c \cdot d$$

A: absorbance

ε: molar extinction coefficient

c: specimen concentration

d: cuvette length