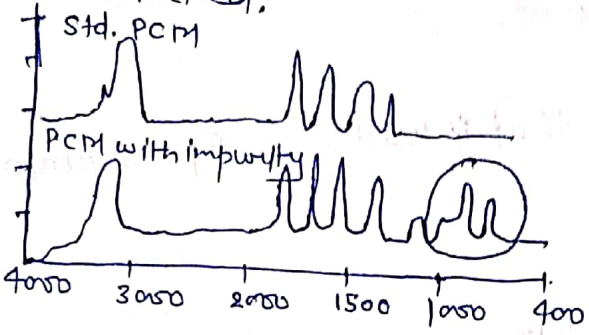
Application of Impurities U.V. and Visible spectroscopy

(1) Detection of Impurities -

UV absorption spectroscopy is one of the best methods for determination of impurities in organic molecules.
Additional peaks can be observed due to impurities in the sample and it can be compared with that of standard raw materials. By also measuring the absorbance at specific wavelength, the impurities can be detected.

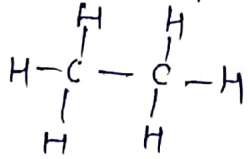


(2) Structure elucidation of organic compound -

UV spectroscopy is useful in the structure elucidation of organic molecules, the presence or absence of unsaturation, the presence of hetro atoms.

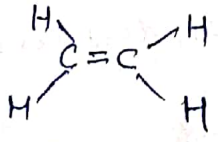
From the location of peaks and combination of peaks, it can be concluded that whether the compound is saturated or unsaturated, hetro atoms are present or not etc.

Saturated compounds only possess carbon-carbon single bonds.

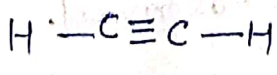


Ethane

Unsaturated compounds are organic chemical compounds where molecular structure contains one or more carbon-carbon double bonds or triple bonds. There can also be conjugated.



Ethene



Ethyene

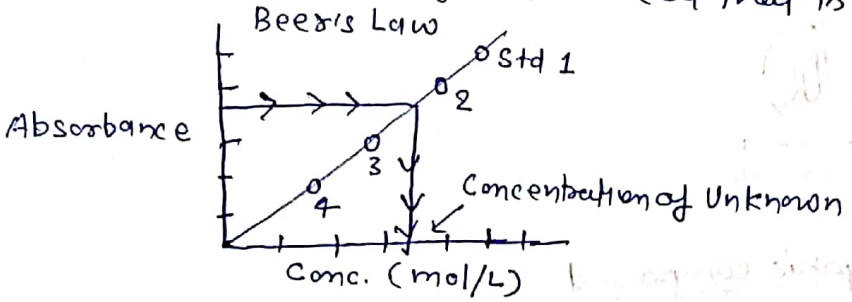
(3) Quantitative Analysis-

UV absorption spectroscopy can be used for the quantitative determination of compounds that absorb UV radiation. This determination is based on Beer's law which is as follows,

$$A = \log I_0/I_t = \log 1/T = -\log T = abc = \varepsilon bc$$

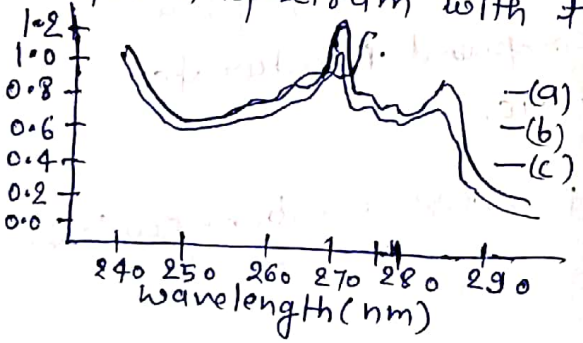
where,

ε = is extinction co-efficient.
c = is concentration, and
b = is the length of the cell that is used in UV Spectrophotometer.



(4) Qualitative Analysis -

UV absorption spectroscopy can characterize these types of compounds which absorb UV radiation. Identification is done by comparing the absorption spectrum with the spectra of known compounds.



U.V. Spectra of Ibuprofen

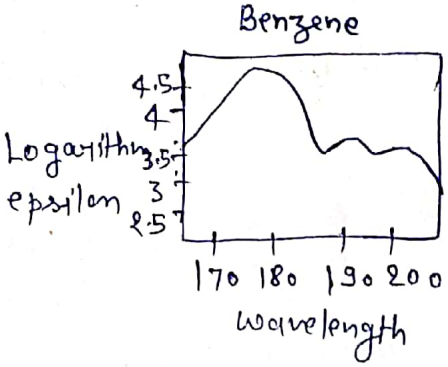
(5) Chemical kinetics-

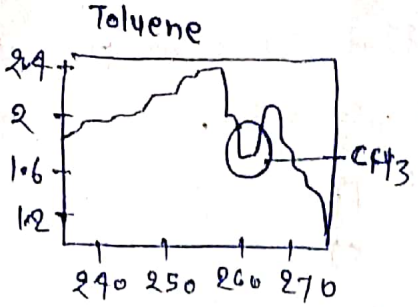
Kinetics of reaction can also be studied using UV spectroscopy. The UV radiation is passed through the reaction cell and the Absorbance changes can be observed.

(6) Detection of functional groups-

This technique is used to detect the presence or absence of functional group.

Absence of a band at particular wavelength regarded as an evidence for absence of particular group.





(7) Quantitative analysis of pharmaceutical substances -

Many drug are either in the form of raw material or in the form of formulation. They can be assayed by making a suitable solution of the drug in a solvent and measuring the absorbance at specific wavelength.

Diazepam tablet can be analyzed by 0.5% H_2SO_4 in methanol at the wavelength 284 nm.

(8) Examination of polynuclear hydrocarbons -

Benzene and polynuclear hydrocarbons have characteristic spectra in UV and visible region. Thus identification of Polynuclear hydrocarbons can be made by comparison with the spectra of known polynuclear compounds.

Polynuclear hydrocarbons are the hydrocarbon molecule with two or more closed ring; examples - are naphthalene, $C_{10}H_8$, with two benzene rings side by side, or diphenyl, $(C_6H_5)_2$, with two bond connected benzene ring. Also known as polycyclic hydrocarbon.

(9) Molecular weight determination -

Molecular weights of compands can be measured spectrophotometrically by preparing the suitable derivatives of these compounds.

for example, if we want to determine the molecular weight of amine then it is converted in to amine picrate. The known concentration of amine picrate is dissolved in a litre of solution and its optical density is measured at λ_{max} 380 nm

After the conc. of the salt in gm moles per litre can be calculated by using the following formula.

$$C = \frac{\log I_0/I_t}{\varepsilon_{max} \times l}$$

'C' can be calculated using above equation the weight "W" of amine picrate is known. From "C" and "W", molecular weight of amine picrate can be calculated. And the molecular weight of picrate can be calculated using the molecular weight of amine picrate.

(10) As HPLC Detector-

A UV/Vis spectrophotometer may be used as a detector for HPLC.