

Seminar on Applications of U.V. Spectroscopy



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INTRODUCTION:

- The word *spectroscopy* implies that we will use the electromagnetic *spectrum* to gain information about organic molecules. The modifier ultraviolet means that the information will come from a specific region of the electromagnetic spectrum called the ultraviolet region (**190 to 400 nm U.V. Region and 400 to 800 nm Visible Region**) .



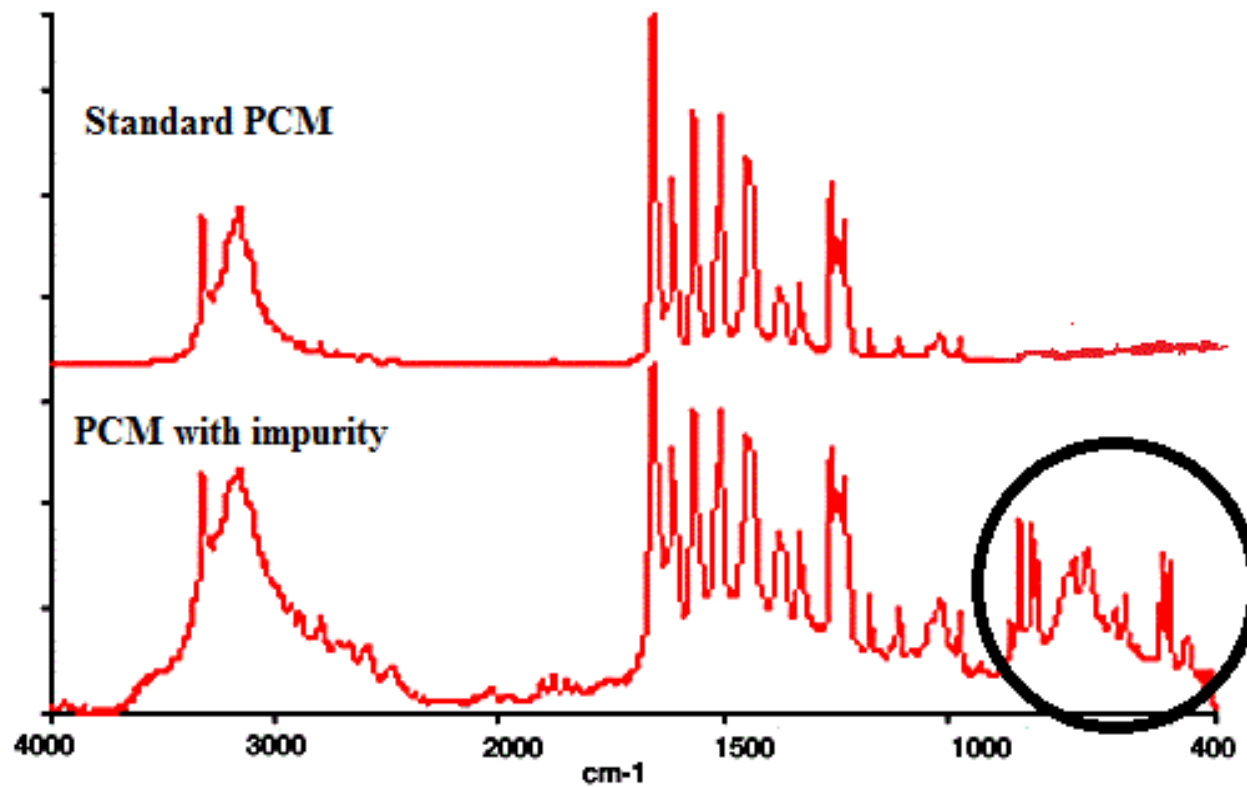
APPLICATIONS OF U.V. SPECTROSCOPY:

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 material. By also measuring the absorbance at specific wavelength, the impurities can be detected.



U.V. SPECTRA OF PARACETAMOL (PCM)



2. Structure elucidation of organic compounds.

- UV spectroscopy is useful in the structure elucidation of organic molecules, the presence or absence of unsaturation, the presence of hetero atoms.
- From the location of peaks and combination of peaks, it can be concluded that whether the compound is saturated or unsaturated, hetero atoms are present or not etc.



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.

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

Where :

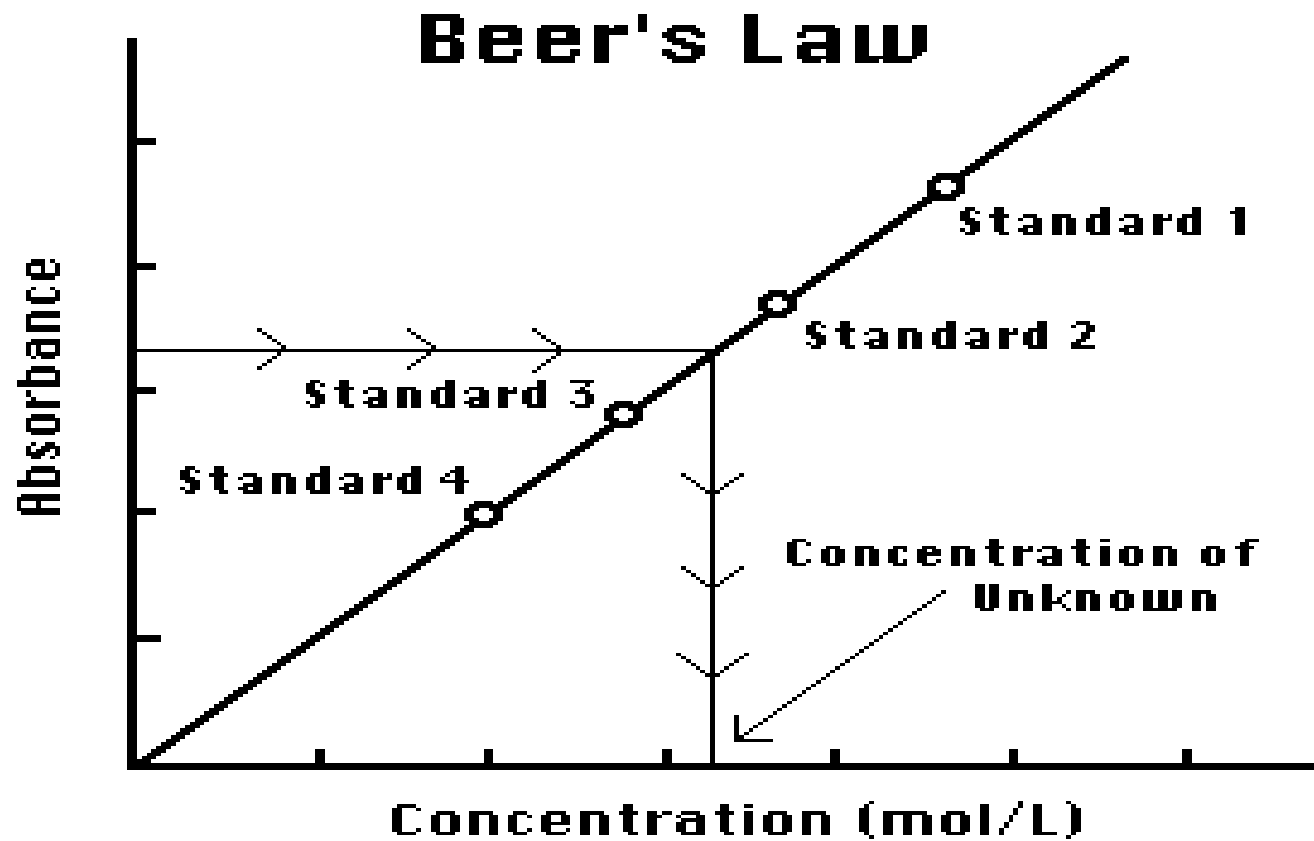
ϵ -is extinction co-efficient,

c- is concentration, and

b- is the length of the cell that is used in UV spectrophotometer.



BEER'S LAW

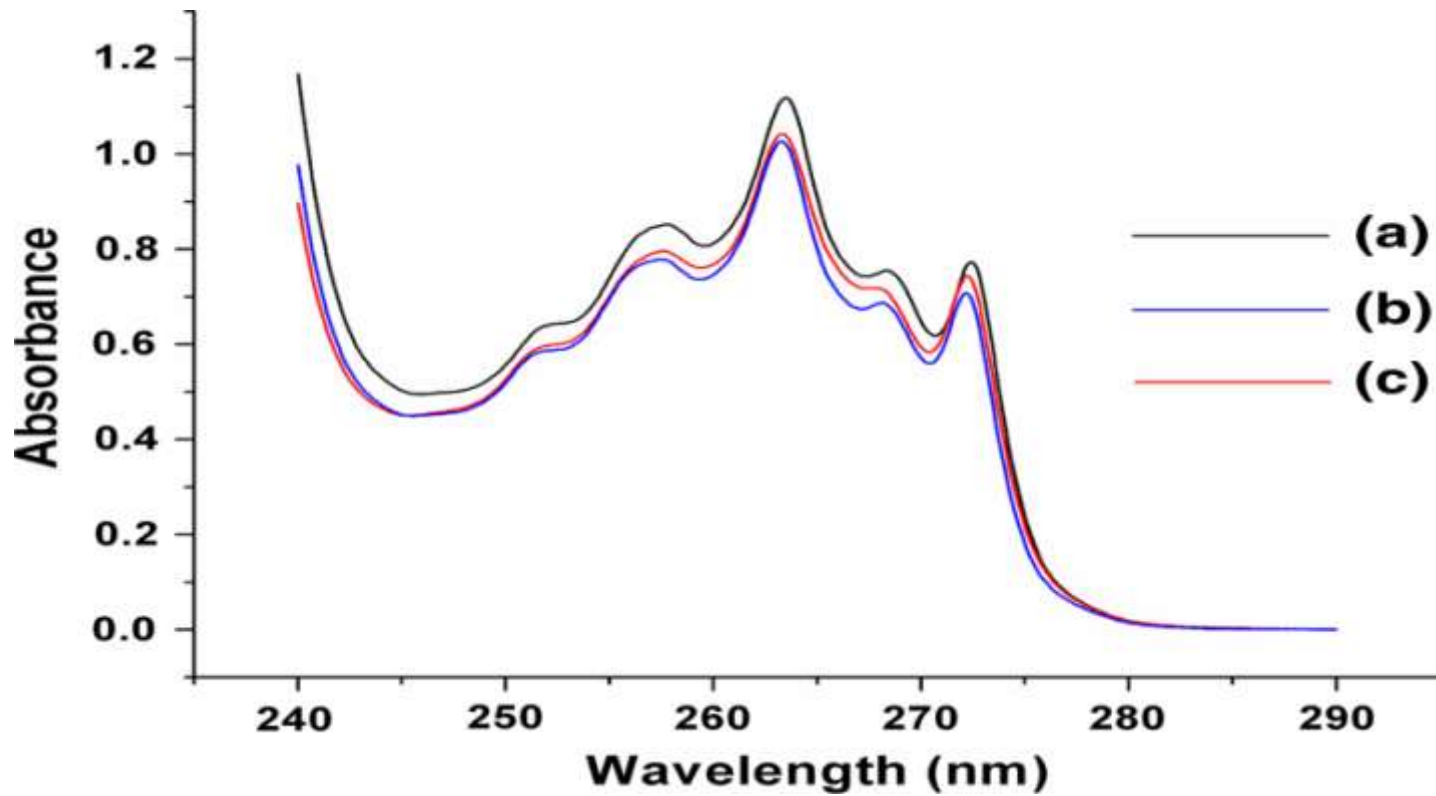


4. QUALITATIVE ANALYSIS

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



U.V. SPECTRA'S 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.



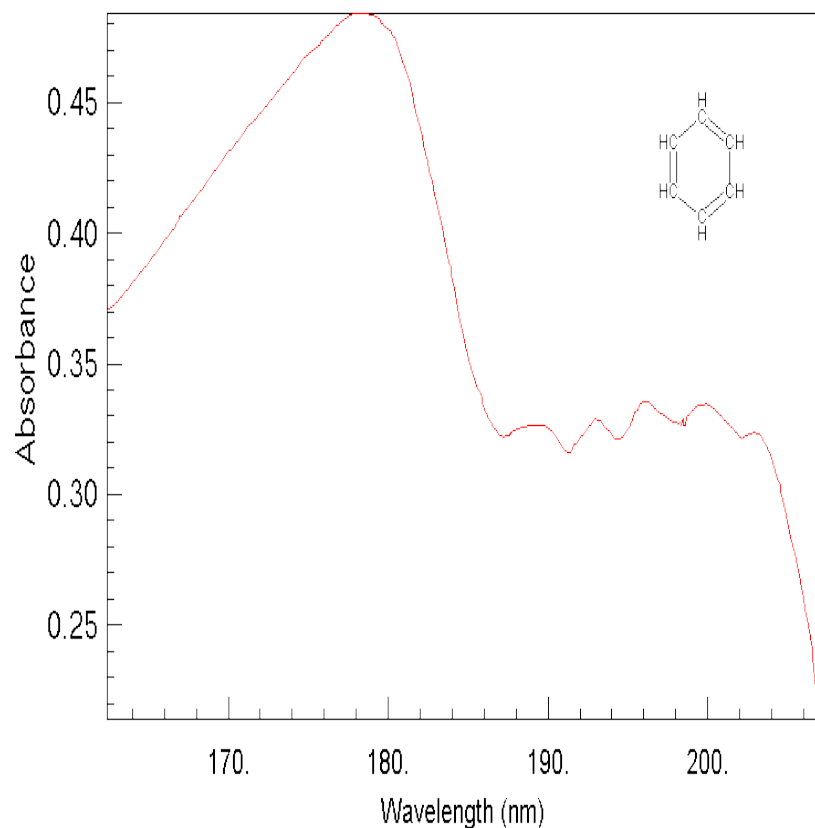
6. DETECTION OF FUNCTIONAL GROUPS

- This technique is used to detect the presence or absence of functional group in the compound
- Absence of a band at particular wavelength regarded as an evidence for absence of particular group



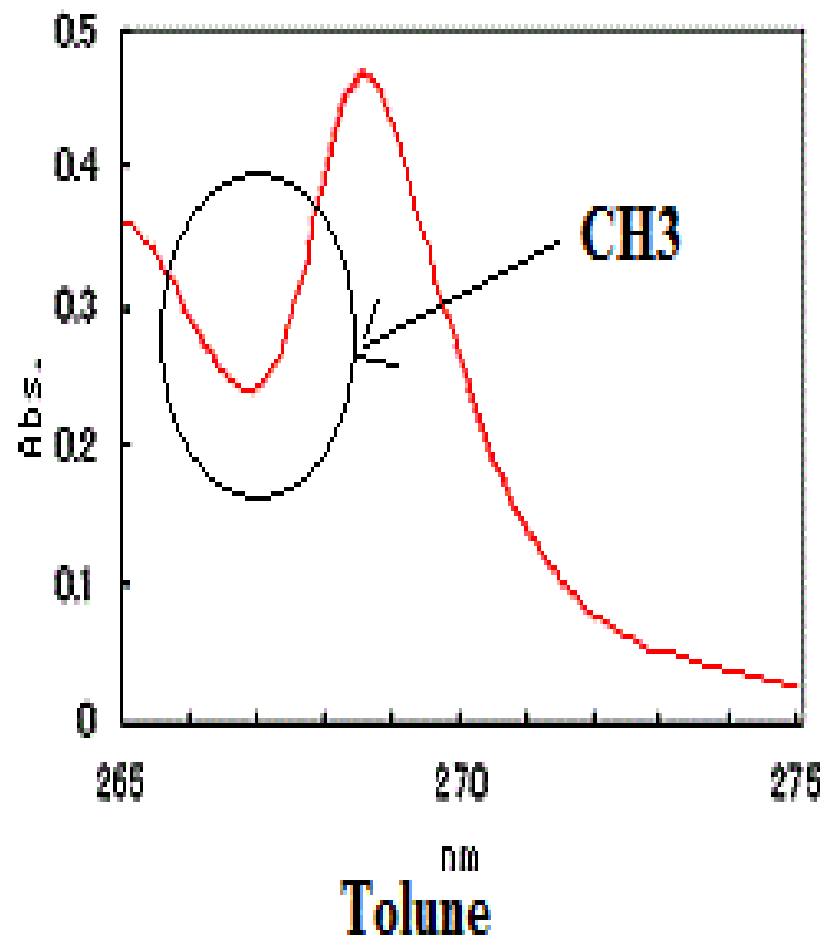
BENZENE

Benzene
UV/VIS SPECTRUM



NIST Chemistry WebBook (<http://webbook.nist.gov/chemistry>)

TOLUENE



nm
Toluene



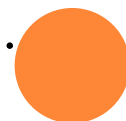
7. QUANTITATIVE ANALYSIS OF PHARMACEUTICAL SUBSTANCES

- Many drugs 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% H₂SO₄ in methanol at the wavelength 284 nm.



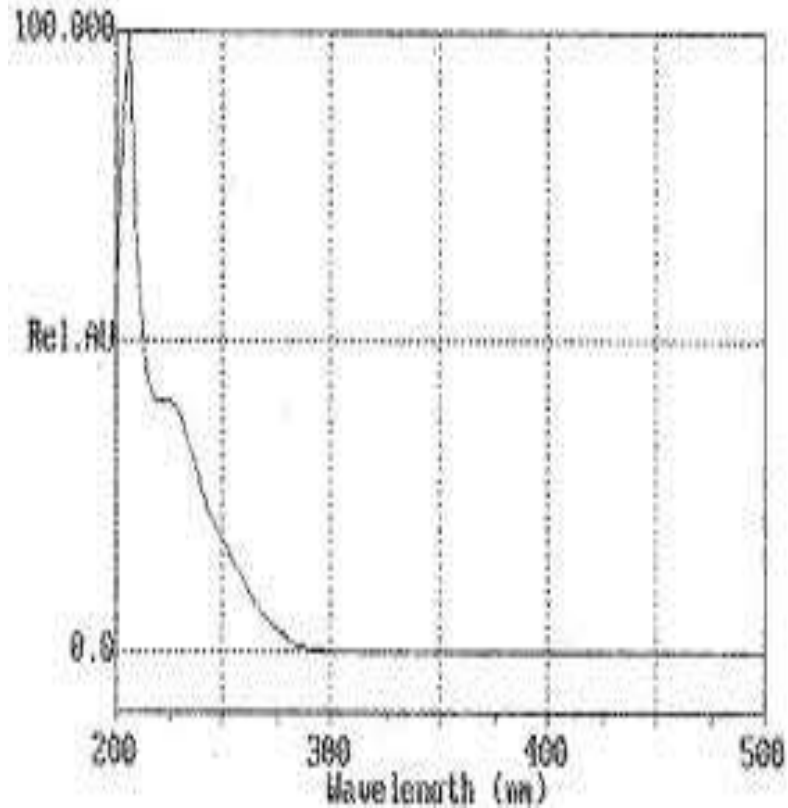
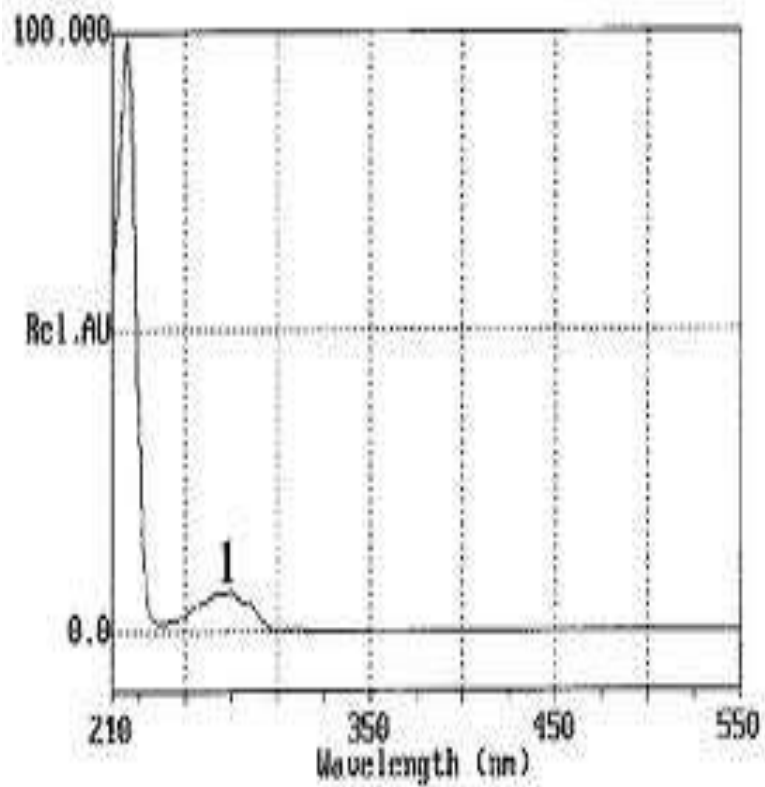
8. EXAMINATION OF POLYNUCLEAR HYDROCARBONS

- Benzene and Polynuclear hydrocarbons have characteristic spectra in ultraviolet 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 rings; 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 rings. Also known as *polycyclic hydrocarbon*.



NAPHTHALENE

DIPHENYL



9. MOLECULAR WEIGHT DETERMINATION

- Molecular weights of compounds 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 into *amine picrate*. Then known concentration of amine picrate is dissolved in a litre of solution and its optical density is measured at λ_{\max} 380 nm.



- ❖ After this the concentration of the solution in gm moles per litre can be calculated by using the following formula.

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

- ❖ "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.



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