



Pharmaceutical applications of UV/Visible Spectroscopy

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Ultraviolet/Visible Spectroscopy ?

- Ultraviolet/Visible (UV/Vis) light spectroscopy measures the absorbance of light by a sample in UV/Vis ranges to identify it.

Advantages:

- Easy to use: simple design of instrument.
- Fast results: quickly analyzes HPLC results [UV lamp].
- Maintains sample integrity: UV/Vis is a non-destructive technique compared to FTIR (Fourier-transform infrared spectroscopy).
- Highly sensitive in detecting organic compounds.

~: Applications :~

1. Structure inspection of organic compounds:

- Inspect organic molecules. From the location and combination of peaks, we find whether:
 - the compound is saturated or unsaturated.
 - hetero atoms are present or not....etc.

2. Detection of Impurities:

- Catalysts used in the reaction may still in the end product in small amounts as impurities.
- Additional peaks can be observed due to impurities in the sample compared with that of standard raw material.
- By also measuring the absorbance at λ_{max} of an impurity, the impurity can be detected.
- Ex: Benzene appears as a common impurity in cyclohexane. Its presence can be easily detected by its absorption at λ_{max} 255 nm.

3. Qualitative analysis:

- Used for compounds that absorb UV/Vis radiation.
- Identification is done by comparing the absorption spectrum with the spectra of known compounds.
- Ex:
 - used for characterizing:
 - aromatic compounds.
 - aromatic olefins.

4. *Quantitative analysis:*

- Used for compounds that absorb UV//Vis 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 molar absorptivity.

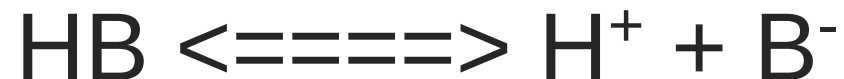
c is concentration.

b is the length of the cuvette used in UV spectrophotometer.

- Other methods for quantitative analysis are as follows:
 - I. difference spectrophotometric method. [variable length]
 - II. calibration curve method. [used in labs]

5. Dissociation constants of acids and bases:

Consider the weak acid HB during its dissociation:



$$K_a = [\text{H}^+][\text{B}^-] / [\text{HB}]$$

$$-\log K_a = -\log ([\text{H}^+]) - \log ([\text{B}^-] / [\text{HB}])$$

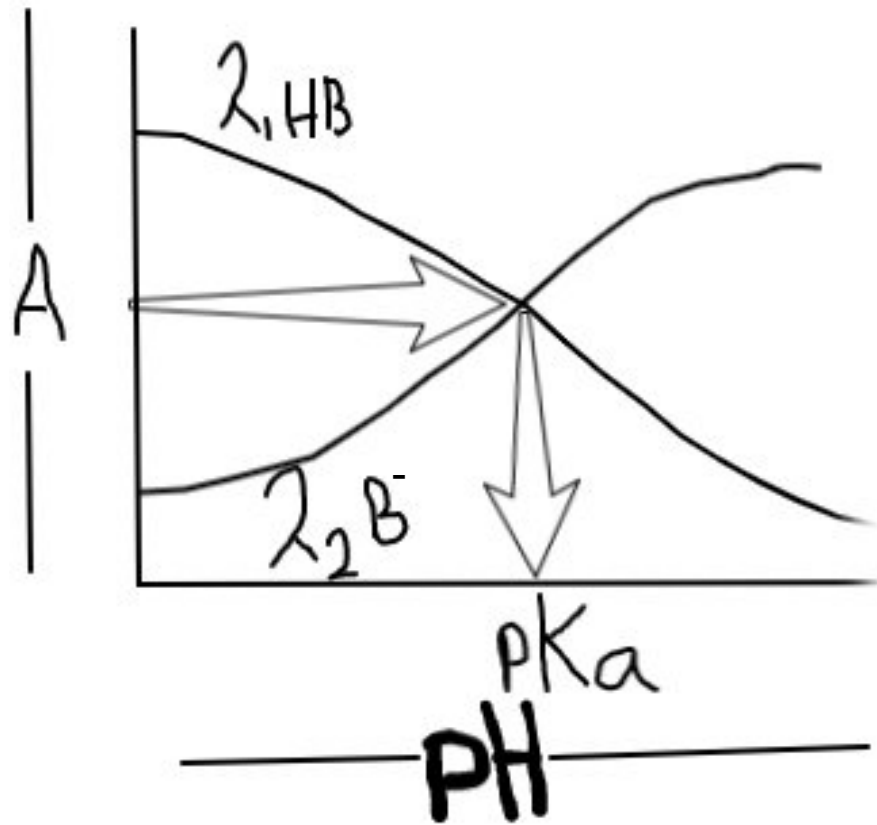
$$\text{So, } \mathbf{pK_a = pH - \log ([B^-] / [HB])}$$

From the above,

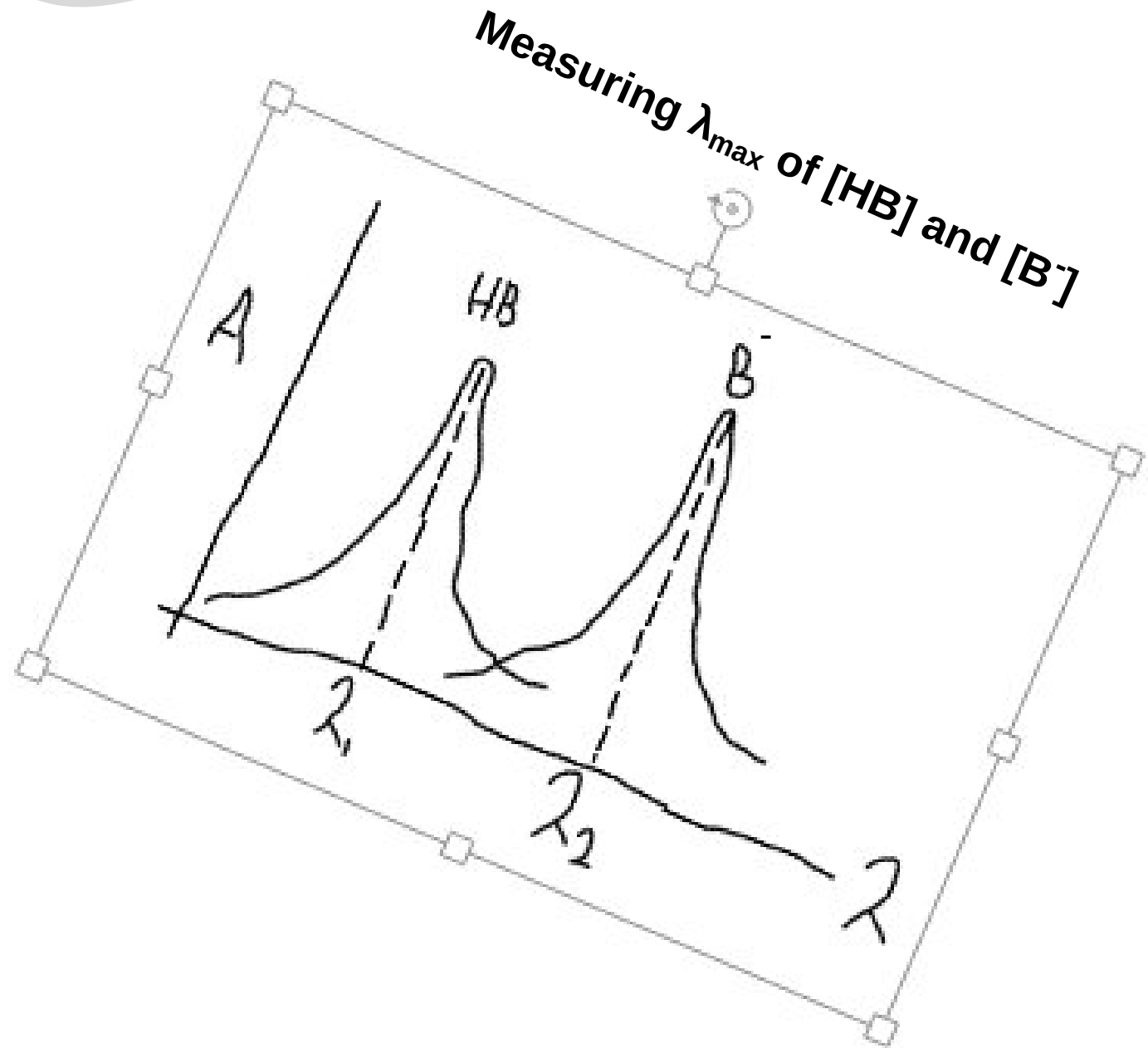
$$\text{when } [\text{B}^-] = [\text{HB}] , \mathbf{pK_a = pH - \log (1)}$$

and $\log (1) = 0$.so, $\mathbf{pK_a = pH}$ at this point.

Measuring real-time changes in Absorbance of $[HB]$ and $[B^-]$ at λ_{\max} of each one of them.



The **pH** at this point is **pK_a**



6. *Chemical kinetics:*

The UV radiation is passed through the reaction cell and the absorbance changes can be observed.

7. *As HPLC detector:*

- A UV/Vis spectrophotometer may be used as a detector for HPLC (high-performance liquid chromatography) (ie: UV lamp).
- The presence of an analyte gives a response which can be assumed to be proportional to the concentration.

8. Molecular weight determination:

- Molecular weights can be measured spectrophotometrically by preparing a suitable derivative of unknown compound.
- For example,
 - if we want to determine the molecular weight of amine:
 - it is converted into amine picrate.
 - known weight of amine picrate is dissolved in a litre of solution.
 - its optical density is measured at λ_{max} 380 nm.

After this, the concentration of the solution in moles per litre (Molar) can be calculated by using the following formula:

- "c" can be calculated using above equation, the weight "w" of amine picrate is known.

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

- From "c" and "w",
molecular weight of amine picrate can be calculated:
c = number of moles / volume in Liter
"c" is known, volume is 1 Liter. So, moles can be calculated.
And "w" represents these moles.
So, mol.wt of amine picrate
can be calculated by cross multiplication.
- And the molecular weight of amine can be calculated using the molecular weight of amine picrate.

~: References :~

- Dr. Adel's handout. [;]
- Dr. Ahmed's inspiration.
- <https://www.pharmatutor.org/pharma-analysis/analytical-aspects-of-uv-visible-spectroscopy/applications.html>
- https://www.researchgate.net/publication/322935261_Ultraviolet_spectroscopy_and_its_pharmaceutical_applications-_A_brief_review
- <https://www.laboratory-equipment.com/blog/absorption-spectroscopy-in-pharmaceutical-analysis/>

Thank
You!