Pharmaceutical applications of UV/Visible Spectroscopy

Supervised by:

Dr. Adel Magdy

Dr. Ahmed Hemdan

Presented by team:

Dr. Dev. Ibrahem Essam : 120 11 345

St. Mahmoud Hassan : 11910463

St. Mohamed Abd Elwahab : 120 10 445

St. Amr Hamdy : 11910507

St. Mohammed Abdelraheem Shabib : 120 11 678

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:

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

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:

$$HB <====> H^+ + B^-$$

$$K_a = [H^+][B^-] / [HB]$$

$$– \log Ka = – \log ([H^+]) – \log ([B^-] / [HB])$$

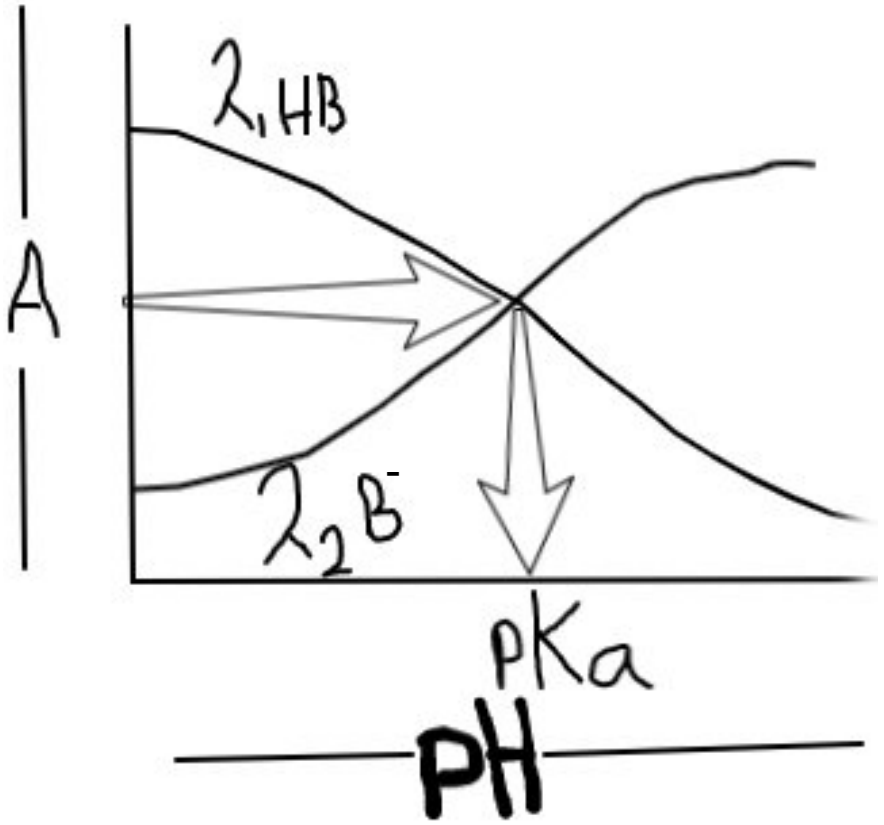
So, $\mathbf{pK_a = pH – \log ([B^-] / [HB])}$

From the above,

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

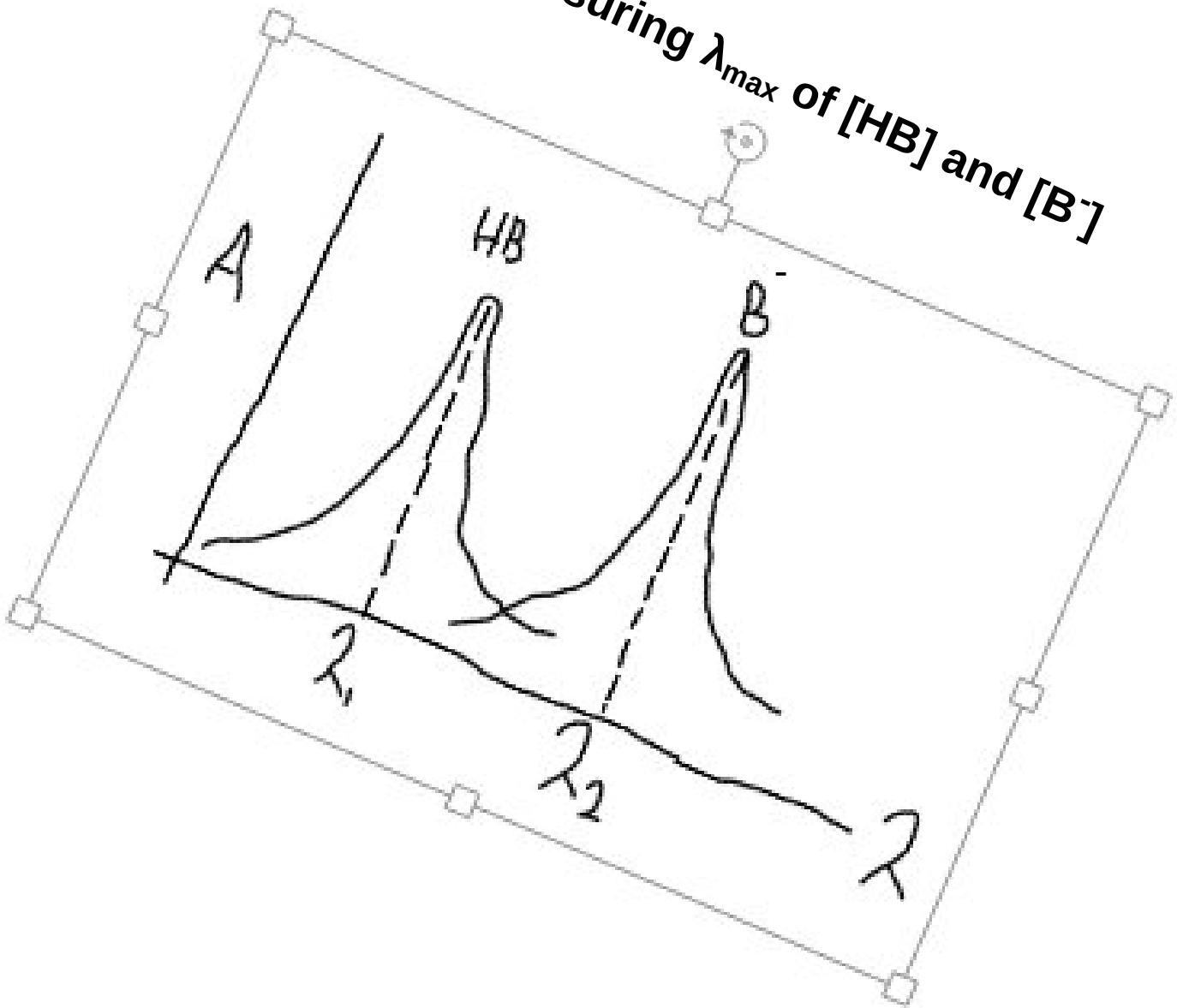
and $\mathbf{\log (1) = 0}$ .so, $\mathbf{pK_a = pH}$ at this point.

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**

Measuring λ_{max} of [HB] and [B^-]



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 spectrophpotometrically by preparing a suitable derivative of unknown compound.

- For example,
  if we want to determine the molecular weight of amine:
  - it is converted in to 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, $C = \frac{\log I_0 / I_t}{\varepsilon_{max} \times l}$
  the weight "w" of amine picrate is known.

- 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.**
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Thank
You!