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PHYSICAL PHARMACEUTICS - I

UNIT 2

TOPIC :

- **Physicochemical properties of drug molecules :** Refractive index, optical rotation, dielectric constant, dipole moment, dissociation constant, determinations and applications

Physicochemical Properties of Drugs

- Physicochemical properties are the physical and chemical characteristics of a drug substance that influence its behavior in a biological system. These properties significantly affect the absorption, distribution, metabolism, and excretion (ADME) of drugs.
- Below are the important physicochemical properties of drugs:

1. Refractive Index

→ It is the ratio of the velocity of light in a vacuum to its velocity in the substance.
→ It helps in identifying and characterizing a compound.
→ Refractive index is influenced by temperature and wavelength of light.
→ It is also used in determining purity of the drug.

Formula:

$$\text{Refractive Index (n)} = \frac{\text{Velocity of light in vacuum (c)}}{\text{Velocity of light in substance (v)}}$$

Applications of Refractive Index:

- ✓ Used in identification of substances
- ✓ Helps in checking the purity of a compound
- ✓ Assists in determining the concentration of solutions
- ✓ Used indirectly for calculating dielectric constant of some substances

2. Optical Rotation

- Some drugs can rotate the plane of polarized light — such substances are called optically active compounds.
- The extent of rotation is measured using a polarimeter and expressed in degrees.
- Levorotatory (–): rotates light to the left
- Dextrorotatory (+): rotates light to the right
- Optical rotation is used to distinguish between enantiomers or chiral drugs.

Applications of Optical Rotation:

✓ To identify optically active compounds
✓ To differentiate between optical isomers (enantiomers)
✓ To determine purity of a substance (impurities may affect rotation)

3. Dielectric Constant

➢ It is the measure of a solvent's ability to reduce the electrostatic force between two charged particles.
➢ Affects the solubility of ionic drugs in different solvents.
➢ Solvents with high dielectric constants (like water) favor the dissolution of polar substances.
➢ Important in selecting appropriate solvent for drug formulation.

Applications of Dielectric Constant:

✓ Helps in determining the polarity of solvents
✓ Used for selection of appropriate solvents for reactions or formulations
✓ Important in calculating the dipole moment of molecules
✓ Assists in predicting drug solubility and stability

4. Dipole Moment

- Arises due to the separation of charge in a molecule.
- Indicates the polarity of a molecule.
- It affects solubility, binding with receptors, and biological activity.
- Molecules with higher dipole moments are usually more polar and more soluble in water.

Formula:

$$\mu = q \times d$$

Where:

- μ = dipole moment
- q = magnitude of charge
- d = distance between charges

Applications of Dipole Moment

- ✓ Helps to differentiate between polar and non-polar molecules
- ✓ Useful to predict the degree of polarity in compounds
- ✓ Assists in determining the shape or geometry of molecules (e.g., linear vs. bent)
- ✓ Important for understanding solubility and interactions of drugs with biological membranes

5. Dissociation Constant (pKa)

- It refers to the strength of an acid or base, showing its tendency to donate or accept protons.
- For drugs, pKa determines ionization in different pH environments.
- The degree of ionization affects absorption and solubility.
- Only the unionized form of a drug can easily cross biological membranes.

Relation with pH (Henderson-Hasselbalch equation):

For weak acid:

$$pH = pKa + \log\left(\frac{[A^-]}{[HA]}\right)$$

Applications of Dissociation Constant:

- ✓ Helps to determine the strength of acids and bases
- ✓ Useful in understanding ionization of drugs in biological fluids
- ✓ Plays a key role in Structure-Activity Relationship (SAR) studies
- ✓ Important in drug discovery and formulation
- ✓ Assists in buffer design for pharmaceutical preparations