لجان الدفعات

PHYSICAL PHARMACY

MORPHINE ACADEMY

تحديد الخواص الفيزيائية لجزيئات الدواء

DETERMINATION OF THE PHYSICAL PROPERTIES OF DRUG MOLECULES

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2026

Additive and constitutive properties

تعتمد على الجمع.

Additive properties

الخاصية الفيزيائية للمادة تعتمد بشكل عام على جمع مساهمات الذرات المكونة منها.

- Additive properties depend on the total contribution of the atoms in the molecules or on the sum of the properties of the constituents in a solution.

المجموع الكلي للذرات يختلف بشكل عام عن كتلة جزيئات الذرات مجتمعة.

- Example: Molecular weight (because it is the sum of the masses of the constituent atoms)
- The total mass of the solution is the sum of the masses of the individual components.

Additive.

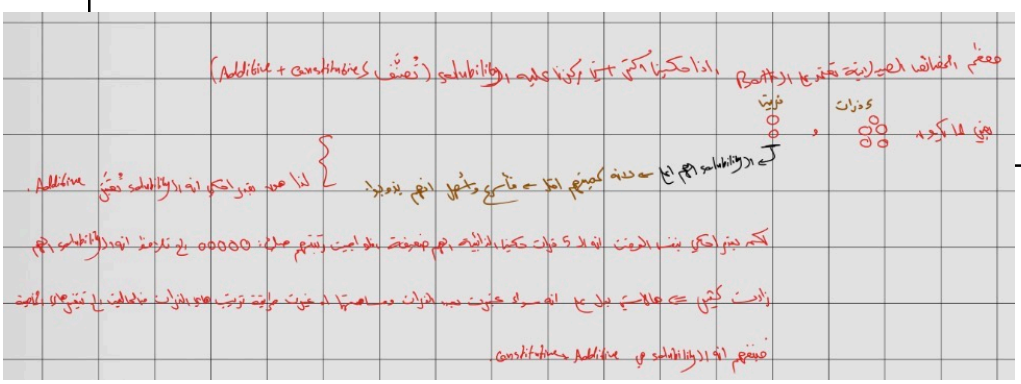
Additive and constitutive properties

Constitutive properties

- Constitutive properties depend on the arrangement and to a lesser extent on the number and kind of atoms within a molecule.
- These properties give clues to the constitution of individual compounds and groups of molecules in a system.

Additive and constitutive properties

- The refraction of light, electric properties, surface and interfacial characteristics, and the solubility of drugs are at least in part constitutive and in part additive properties.



Additive and constitutive properties

Refraction is the change of direction of propagation of any wave, such as an electromagnetic or sound wave, when it passes from one medium to another in which the wave velocity is different, or when there is a spatial variation in a medium's wave velocity.

TABLE 4–1
ATOMIC AND GROUP CONTRIBUTIONS TO MOLAR REFRACTION*

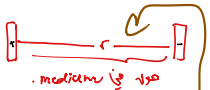
C— (single)	2.418
—C═ (double)	1.733
—C≡ (triple)	2.398
Phenyl (C_6H_5)	25.463
H	1.100
O (C═O)	2.211
O (O—H)	1.525
O (ether, ester, C—O)	1.643
Cl	5.967
Br	8.865
L	13.900

Additive and constitutive properties

- For the compound C2H5–CO–CH3 the molar refraction would be 19.998 while for the compound CH3–CH=CH–CH2–OH it will be 18.7.
- Thus, although these two compounds have the same number of carbon, hydrogen, and oxygen atoms, their molar refractions are not the same.
- The molar refractions of the atoms are additive, but the carbon and oxygen atoms are constitutive in refraction.
- A single-bonded carbon does not add equally as a double bonded carbon, and a carbonyl oxygen (C=O) is not the same as a hydroxyl oxygen; therefore the two compounds exhibit different molar refractions.

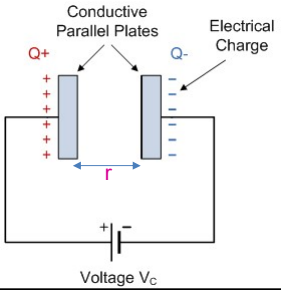
Dielectric constant

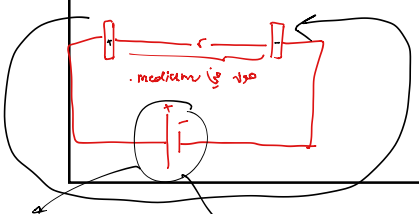
- To properly discuss dipoles and the effects of solvation, one must understand the concept of dielectric constant.
- Placing a molecule in an electric field is one way to induce a dipole.
- In a capacitor (condenser), there are two parallel conducting plates separated by a medium across a distance (r).



Dielectric constant

- Consider two parallel conducting plates, such as the plates of an electric condenser, which are separated by some medium across a distance *r* and apply a potential across the plates.
- Electricity will flow from the left plate to the right plate through the battery until the potential difference of the plates equals that of the battery supplying the initial potential difference.





Dielectric constant

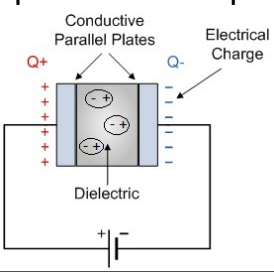
- The *capacitance, C* (in farads), is equal to the quantity of electric charge, *q* (in coulombs), stored on the plates, divided by the potential difference, *V* (in volts), between the plates:

$$C = q/V$$

- The capacitance of the condenser depends on the type of medium separating the plates as well as on the thickness *r.*
- When a vacuum fills the space between the plates, the capacitance is C_0.
- This value is used as a reference to compare capacitances when other substances fill the space.

Dielectric constant

- If water fills the space, the capacitance is increased, since the water molecule can orientate itself so that its negative end lies nearest the positive condenser plate and its positive end lies nearest the negative plate.
- This alignment provides additional movement of charge because of the increased ease with which electrons can flow between the plates.
- Thus, additional charge can be placed on the plates per unit of applied voltage.



H_2O is polar → molecules orient → dielectric polarization → more charge can be stored at same V → C↑

Dielectric constant

- A molecule can maintain a separation of electric charge either through induction by an external electric field or by a permanent charge separation within a polar molecule.
- Dielectric constant (relative permittivity) of a material is its (absolute) permittivity expressed as a ratio relative to the permittivity of vacuum.

$$\varepsilon = \frac{C_A}{C_0}$$

Dielectric constant

- The capacitance of the condenser filled with some material, C_x, divided by the reference standard C_0, is referred to as the *dielectric constant*, ε:

$$\varepsilon = C_x / C_0$$

- The dielectric constant ordinarily has no dimensions, since it is the ratio of two capacitances.

Vacuum	1.0 (by definition)
Metals	Infinite
Gases	1.00xx (at one atmosphere)
Water	87.9 (0°C) to 55.5 (100°C)
Hexane	1.8865 (20°C)
Cyclohexane	2.0243 (20°C)
Benzene	2.285 (20°C)
Hydrocarbon lubrication oils	2.1 to 2.4 (room temperature)

Table 1. Dielectric Constant of Common Materials

Polarity of molecules

- A dipole is a separation of two opposing charges over a distance r, and is generally described by a vector known as the dipole moment (μ).
- The dipole moment (μ) depends on the individual charge moments within the molecule and the distance of separation between charges. This magnitude is given by:

$$\mu = qr$$

- The unit of dipole moment is the debye, with one debye equals to 10^{-18} esu cm.
- The esu (electrostatic unit) is the measure of electrostatic charge in a vacuum that repels a like charge one centimeter away with a force of one dyne.

Polarity of molecules

- A molecule can maintain a separation of electric charge (i.e. get polarized) either:
  - By having a permanent charge separation within a polar molecule (permanent dipole moment).
  - Through induction by an external electric field or surrounding ions. Induced polarization can occur for both polar and nonpolar molecules (induced dipole moment).

Induced Polarization of nonpolar molecules

- When nonpolar molecules are exposed to an external electric field, their electron clouds become distorted, producing a temporary separation of charge.
- This phenomenon, known as **induced polarization**, causes the molecules to develop a transient dipole moment.
- Once the electric field is removed, the electron distribution returns to its original configuration, and the induced dipole disappears.
- The polarizability of a substance influences several important physical properties, including its refractive index, dielectric constant, and optical rotation.

Induced Polarization of nonpolar molecules

- The magnitude of the induced dipole moment is directly proportional to both the applied electric field (E) and the molecular polarizability (α_p):

$$\mu_{ind} = E \times \alpha_p$$

- Induced polarizability is defined as the ease with which an ion or molecule can be polarized by an external force.
- It is an intrinsic molecular property that depends on the size and electronic structure of the molecule.
- Polarizability is commonly expressed in units of $10^{-24}\ cm^3$ (or $Å^3$).

Induced Polarization of nonpolar molecules

- The induced molar polarization Pi represents the induced dipole moment per mole of nonpolar substance when the electric field strength of the condenser is 1 V/m.
- Pi ($cm^3\ mol^{-1}$) is defined by the Clausius-Mossotti equation as:

$$P_i = \frac{\varepsilon - 1}{\varepsilon + 2} \cdot \frac{M}{\rho}$$

- Where:
  - ε is the dielectric constant.
  - M is the molar mass (molecular weight) ($g\ mol^{-1}$).
  - ρ is the density ($g\ cm^{-3}$).

Induced Polarization of nonpolar molecules

EXAMPLE 4–1

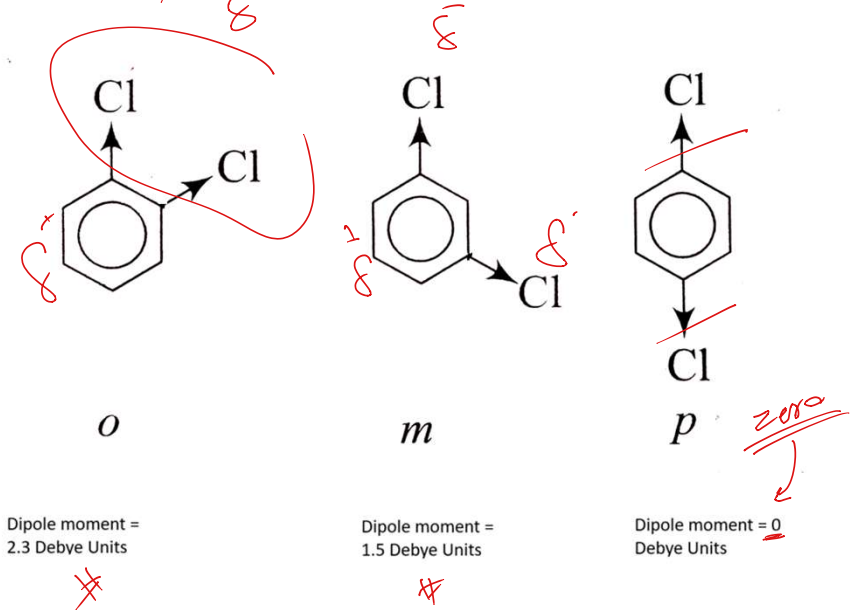
Polarizability of Chloroform

Chloroform has a molecular weight of 119 g/mole and a density of 1.43 g/cm^3 at 25°C. What is its induced molar polarizability? We have

$$P_i = \frac{(\varepsilon - 1)}{(\varepsilon + 2)} \times \frac{M}{\rho} = \frac{(4.8 - 1)}{(4.8 + 2)} \times \frac{119}{1.43} = 46.5\ \text{cm}^3/\text{mole}$$

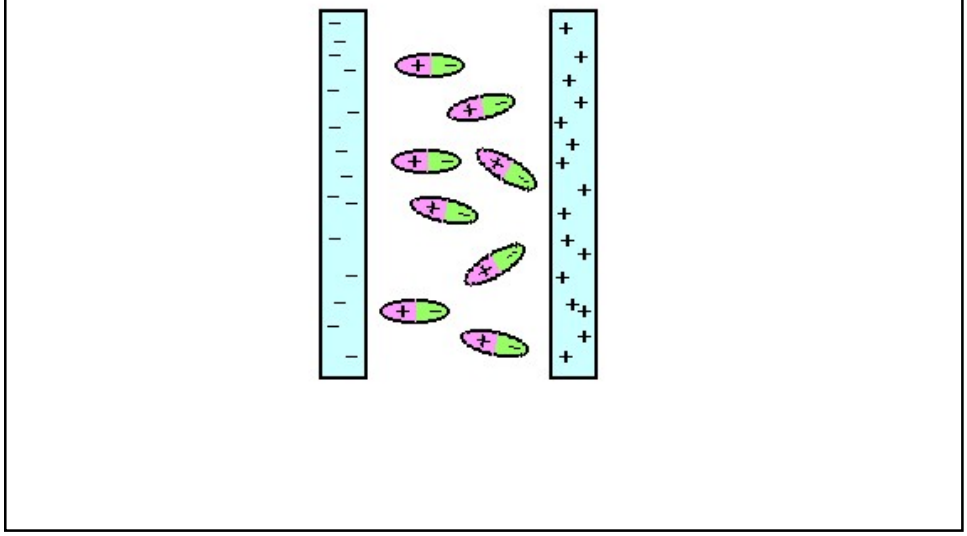
Permanent dipole moment

- In a polar molecule, the separation of positively and negatively charged regions can be permanent, and the molecule will possess a **permanent dipole moment**, μ.
- Dipoles therefore don't have a net charge, but this charge separation can often create charge-like interactions and influence several physical and chemical properties.
- The dipole moment is a vector property where the symmetry of the molecules affects generally its dipole moment. For example, carbon dioxide has no net dipole.
- Another example: Benzene and p-dichlorobenzene are symmetric planar molecules and have a dipole moment of zero. Meta (*m*-) and ortho (*o*-) dichlorobenzene are not symmetrical and have significant dipole moment.



Permanent dipole moment

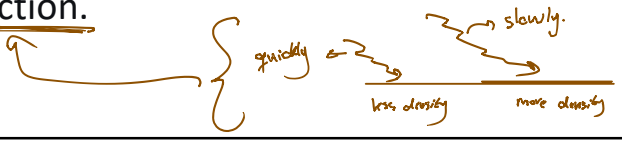
- When polar liquids are exposed to an external electric field, two types of polarization occur:
  - **Induced polarization**: Similar to nonpolar liquids, the electric field distorts the electron clouds, creating an induced dipole moment.
    - The magnitude of the induced polarization is proportional to the applied electric field strength and the molecular polarizability.
  - **Orientation polarization**: The electric field also aligns the permanent dipole moments of polar molecules along the field direction.
    - The overall polarization of a polar liquid is the combined result of induced polarization and orientation polarization.



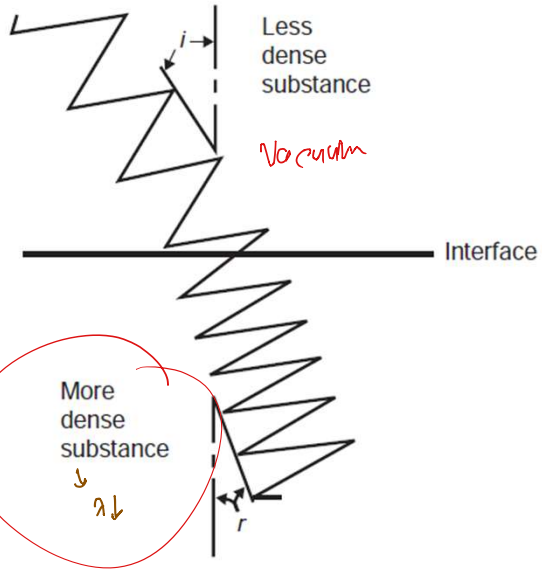
- The polarizability of a substance influences several important physical properties, including its refractive index, dielectric constant, and optical rotation.

Refractive Index

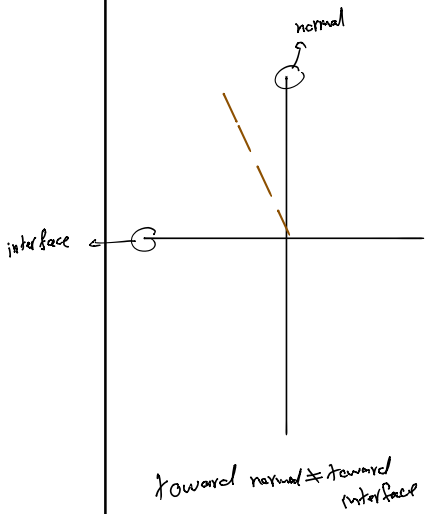
- Light passes more slowly through a substance than through a vacuum.
- As light enters a denser substance, the advancing waves at the interface are modified by being closer together owing to their slower speed and shorter wavelength.
- If the light enters a denser substance at an angle, one part of the wave slows down more quickly as it passes the interface, and this produces bending of the wave toward the interface. This phenomenon is called refraction.



Light enters more optically dense medium → speed↓ → λ↓ (f stays constant) → bends toward the interface → Refraction.



Waves of light passing an interface between two substances of different density.



toward normal ≠ toward interface

less dense → more dense = toward

more dense → less dense = away from

Refractive Index

- The relative value of refraction or bending of light between two substances is given by the **refractive index**, n:

$$n = \frac{\sin i}{\sin r}$$

$$n = \frac{\text{velocity of light in first substance}}{\text{velocity of light in second substance}}$$

- In which sin i is the sine of the angle of the incident ray of light and sin *r* is the sine of the angle of the refracted ray.
- Normally the numerator is taken as the velocity of light in air, and the denominator is the material being investigated.

Refractive Index

- Refraction varies with temperature and the wavelength of light; n_D^{20} is the refractive index using the D-line emission of sodium at 589 nm, at a temperature of 20°C.
- The refractive index can be used to identify a substance.
- Typically, a refractometer is used to determine refractive index.

Refractive Index

- Molar polarization, Pi, can be considered roughly equivalent to molar refraction, Rm, and can be written as follows:

$$\varepsilon = n^2{}_\infty$$

$$P_i = \left(\frac{n_\infty^2 - 1}{n_\infty^2 + 2}\right)\frac{M}{\rho} = \frac{4}{3}\pi N\alpha_p$$

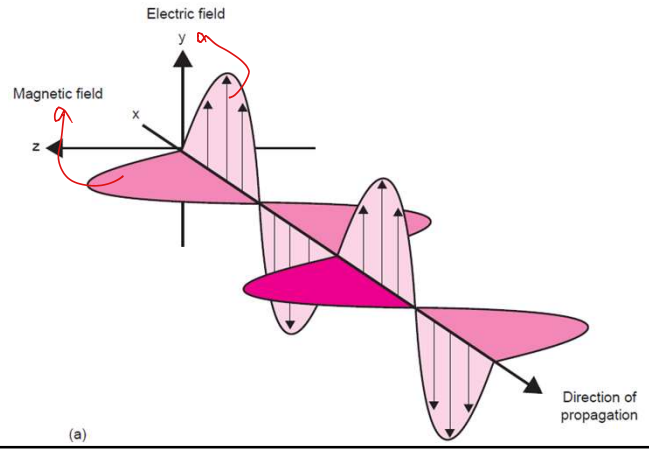
- n_∞ : refractive index for light of long wavelengths
- From this equation, the polarizability α_p of a nonpolar molecule may be obtained from a measurement of refractive index.

ELECTROMAGNETIC RADIATION

- Electromagnetic radiation is a form of energy that propagates through space as oscillating electric and magnetic fields atm right angles to each other and to the direction of the propagation.
- A form of energy that propagates through space.
- Travels as oscillating electric and magnetic fields.

ELECTROMAGNETIC RADIATION

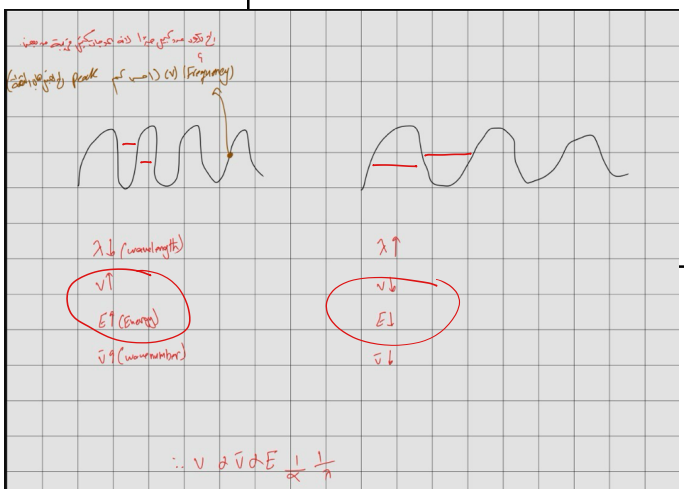
- Electric and magnetic fields are:
  - Perpendicular to each other.
  - Perpendicular to the direction of propagation.
- Both fields are described by **sinusoidal waves**.



ELECTROMAGNETIC RADIATION

Key Wave Parameters

- **Amplitude (A):** Height of the wave.
- **Frequency (ν):** Number of waves passing a fixed point each second (Hz).
- **Wavelength (λ):** Distance between two consecutive wave maxima.



ELECTROMAGNETIC RADIATION

- The velocity of electromagnetic radiation is given by:

$$v = u\lambda$$

where:

v = velocity of propagation
u = frequency
λ = wavelength

- In a vacuum:

$$c = 2.998 \times 10^8 \text{ m/s}$$

- Therefore,

$$u = c/\lambda$$

ELECTROMAGNETIC RADIATION

Important Points

- Frequency depends on the radiation source.
- Frequency remains constant when radiation enters another medium.
- Velocity and wavelength change depending on the medium.

ELECTROMAGNETIC RADIATION

Wave Number

- Wave number is defined as the reciprocal of wavelength:

$$\bar{\nu} = \frac{1}{\lambda}$$ Unit: **cm^{-1}**

- Represents the number of wavelengths per centimeter.
- Directly proportional to frequency and energy.

ELECTROMAGNETIC RADIATION

Photon Energy

- According to the Planck–Einstein equation:

$$E = h\nu$$

where:

- **E** = photon energy
- **h** = Planck's constant = **6.626×10^{-34} J·s**
- **ν** = frequency

- **Higher frequency (or wave number) → Higher energy**

ELECTROMAGNETIC SPECTRUM

- Classified according to **wavelength** or **wave number**.
- As wavelength decreases:
  - Frequency increases.
  - Photon energy increases.

Interaction of Electromagnetic Radiation with Matter

Importance in Spectroscopy

- Interaction of electromagnetic radiation with matter provides information about atomic and molecular structure.

Electric Field Component

Responsible for:

- Transmission
- Reflection
- Refraction
- Absorption
- Emission

❑ These phenomena form the basis of most **spectroscopic techniques**.

Magnetic Field Component

Responsible for:

- Electron Paramagnetic Resonance (EPR)
- Nuclear Magnetic Resonance (NMR)

❑ These techniques probe magnetic properties of electrons and nuclei.

UV–Visible Spectrophotometry

Principle

- UV–Visible spectroscopy measures the absorption of ultraviolet (UV) and visible (Vis) radiation by molecules and ions.
- The absorbed energy corresponds to electronic transitions between molecular energy levels.
- Electronic transitions depend on the electronic bonding within the molecule.
- Spectral region
  - UV: 200–400 nm
  - Visible: 400–700 nm

UV–Visible Spectrophotometry

Molecular Orbitals

- Covalent bonds are formed by overlapping atomic orbitals.
- Overlap produces molecular orbitals where bonding electrons are located.

Types of molecular orbitals

- **σ (sigma) orbital**
  - Associated with single covalent bonds.
- **π (pi) orbital**
  - Present in double bonds together with one σ bond.
- **n orbital**
  - Nonbonding electrons (e.g., lone pairs on oxygen or nitrogen).

UV–Visible Spectrophotometry

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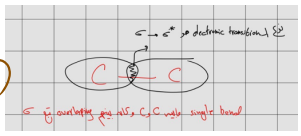
UV–Visible Spectrophotometry

Electronic Transitions in UV–Visible Spectroscopy

- When molecules absorb UV or visible light, electrons are promoted to higher-energy **antibonding orbitals (★).**
- Common transitions:
  - σ → σ*
  - n → σ*
  - π → π*
  - n → π*
- (* indicates an antibonding orbital.)



UV–Visible Spectrophotometry

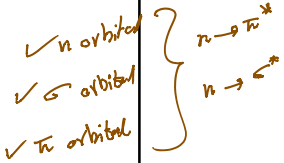
Relative Energies of Electronic Transitions in UV–Visible Spectroscopy

Transition	Relative Energy	Approximate Wavelength
σ → σ*	Highest	100–150 nm (vacuum UV)
n → σ*	High	~190 nm
n → π*	Lower	~280 nm
π → π*	Moderate	200–700 nm

UV–Visible Spectrophotometry

Relative Energies of Electronic Transitions in UV–Visible Spectroscopy – Example - Carbonyl Groups

- Carbonyl oxygen contains **nonbonding (n) electrons**, allowing:
  - n → π*
  - n → σ*
- Example: **Acetone**
  - n → π* : **280 nm**
  - n → σ* : **190 nm**
- For aldehydes and ketones:
  - Absorption around **270–290 nm** is characteristic of the carbonyl group.



UV–Visible Spectrophotometry

Relative Energies of Electronic Transitions in UV–Visible Spectroscopy

Chromophores

- A chromophore is the part of a molecule responsible for absorbing UV or visible light.
- Examples
  - Carbonyl (C=O)
  - Double bonds (C=C)
  - Aromatic rings
  - Conjugated systems
- Most UV applications involve transitions of
  - $n \rightarrow \pi^*$
  - $\pi \rightarrow \pi^*$
- because they occur in the convenient range of 200–700 nm.

UV–Visible Spectrophotometry

Beer–Lambert Law

$$A = -\log T = \log (I_0/I) = \varepsilon b c$$

where

A = absorbance

T = transmittance

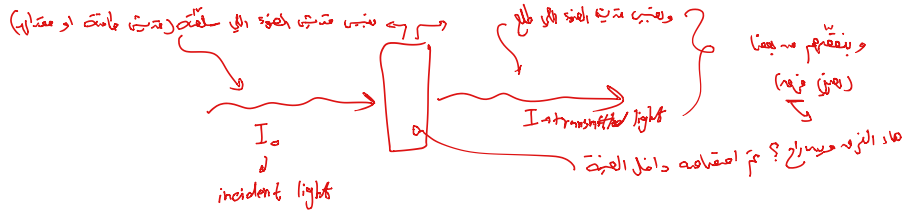
$\mathbf{I_o}$ = incident light intensity

I = transmitted light intensity

ε = molar absorptivity

b = path length (cm)

c = concentration (mol/L)



UV–Visible Spectrophotometry

Beer–Lambert Law

Molar Absorptivity (ε)

- Characteristic constant for each absorbing species.
- Depends on:
  - Molecule
  - Solvent
  - Temperature
  - Wavelength
- Large ε values indicate strong absorption.
- Highly conjugated molecules generally possess high molar absorptivity.
- Examples include
  - Aromatic compounds
  - Conjugated dienes
  - α,β-unsaturated carbonyl compounds

UV–Visible Spectrophotometry

Beer–Lambert Law

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Infrared (IR) Spectroscopy

- Infrared (IR) spectroscopy studies the interaction of infrared radiation with molecular vibrations and rotations.
- It analyzes the stretching and bending of chemical bonds within molecules.
- The resulting spectrum provides valuable information about molecular structure and functional groups.
- Commercial IR spectrometers typically operate in the:
  - Wavelength: 2.5–50 μm
  - Wavenumber: 4000–200 cm^{-1}
- The frequency of IR absorption depends on:
  - Atomic masses
  - Bond strength
  - Molecular symmetry

Infrared (IR) Spectroscopy

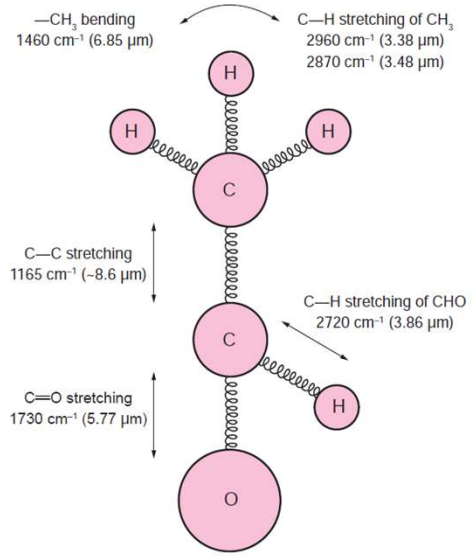
- Infrared absorption occurs only when a molecular vibration or rotation causes a change in the permanent dipole moment.
- Therefore:
  - Vibrations that change dipole moment → **IR active**
  - Vibrations that do not change dipole moment → **IR inactive**

Infrared (IR) Spectroscopy

Types of Molecular Vibrations

- **Stretching vibrations**
  - Symmetric stretching (IR inactive)
  - Asymmetric stretching (IR active)
- **Bending vibrations**
  - Scissoring
  - Rocking
  - Wagging
  - Twisting

➢ Different vibration modes absorb at characteristic infrared frequencies.



Bending and stretching frequencies for acetaldehyde.

Infrared (IR) Spectroscopy

- Infrared absorption frequencies correspond to specific molecular vibrations.

Example:

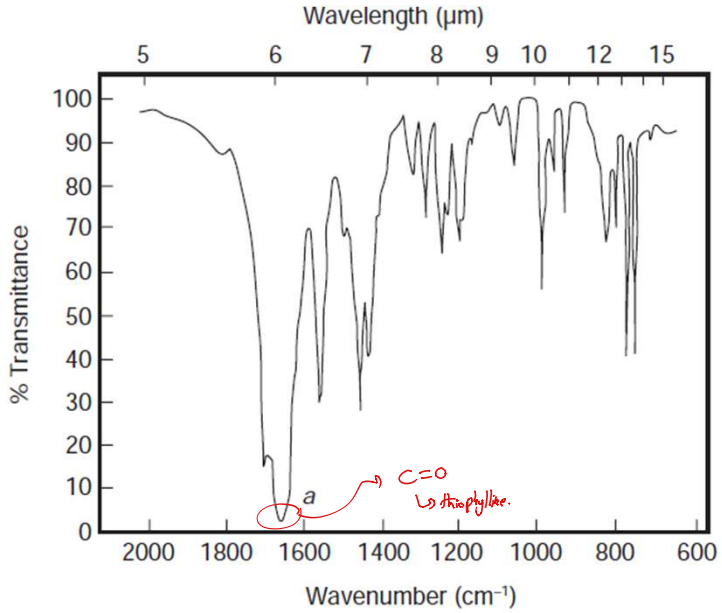
- Carbonyl (C=O) stretching
  - Approximately **1660 cm^{-1}** in theophylline

➢ Characteristic absorption bands allow identification of functional groups.

- Besides the fundamental absorption bands **overtone bands** may occur.
- Overtones appear at approximately **multiples of the fundamental frequency**.
- Example:
- Carbonyl stretching:
  - Fundamental = **1730 cm^{-1}**
  - Overtone ≈ **3460 cm^{-1}**

Infrared Fingerprint

- Vibrational frequencies are characteristic of specific bonds.
- The complete IR spectrum is unique for each compound.
- IR spectra therefore serve as molecular fingerprints.
- Applications:
  - Drug identification
  - Compound verification
  - Structural characterization



Infrared spectrum of theophylline

Factors Influencing Absorption Bands

Infrared spectra may vary with:

- Hydrogen bonding
- Concentration
- Steric effects
- Neighboring functional groups
- Phase changes (e.g. solid state changes)

Example:

- Alcohol O–H stretching
- Weak hydrogen bonding:
  - Around **3600 cm^{-1}**
- Increased hydrogen bonding:
  - Band position and shape change

Infrared (IR) Spectroscopy

Applications in Pharmacy

Infrared spectroscopy is widely used for:

- Drug identification
- Compound verification
- Qualitative analysis
- Quantitative analysis
- Characterization of pharmaceutical compounds

Near-Infrared Spectroscopy

- Near-infrared (**NIR**) spectroscopy is increasingly valuable for **pharmaceutical analysis**.
- NIR region:
- 10,000–4,000 cm^{-1} NIR spectra arise mainly from:
  - **Overtones**
  - **Combination bands**
- These originate primarily from stretching vibrations involving:
  - O–H
  - C–H
  - N–H bonds

NIR is therefore particularly useful for analyzing:
- Water
- Alcohols
- Amines

Near-Infrared Spectroscopy

- **Why Use NIR?**
- **Very rapid analysis**
- **Nondestructive** → العينة لا تتلف اثناء التحليل
- Little or **no sample preparation** → العينة متاح تحضير قليل
- Provides:
  - Qualitative information
  - Quantitative information
- Allows **multicomponent analysis**

Near-Infrared Spectroscopy

- **Applications of NIR**
- NIR spectroscopy can be used for:
  - Polymorph identification
  - Water content determination
  - Identification of active pharmaceutical ingredients (APIs)
  - Monitoring API content within:
    - Tablets
    - Other solid dosage forms

Near-Infrared Spectroscopy

Feature	Mid-IR	Near-IR
Region	~4000–400 cm^{-1}	10,000–4000 cm^{-1}
Main bands	Fundamental vibrations	Overtones & combinations
Band intensity	Stronger	Weaker
Sample preparation	May be required	Often minimal/none
Analysis	Qualitative & quantitative	Qualitative & quantitative
Process monitoring	Possible	Particularly advantageous

plane-polarized light كيف نحوّل الضوء العادي الى

OPTICAL ROTATION

Plane-Polarized Light

- Ordinary light contains waves with **randomly distributed orientations**.
- A **polarizing prism**, such as a Nicol prism, selectively transmits vibrations occurring in a **single plane**.
- **Result:**
- Ordinary light → Polarizer → **Plane-polarized light**

OPTICAL ROTATION

Plane-Polarized Light Interaction with Optically Active Substances

- Plane-polarized light can be rotated when it passes through an **optically active substance**.
- The interaction of polarized radiation with molecular electrons produces **electronic polarization**.
- This interaction alters the electric field and rotates the direction of vibration of the radiation.
- **Optical Activity**
  - **Chiral molecules** → optically active
  - **Achiral/symmetric molecules** → optically inactive

OPTICAL ROTATION

Direction of Optical Rotation

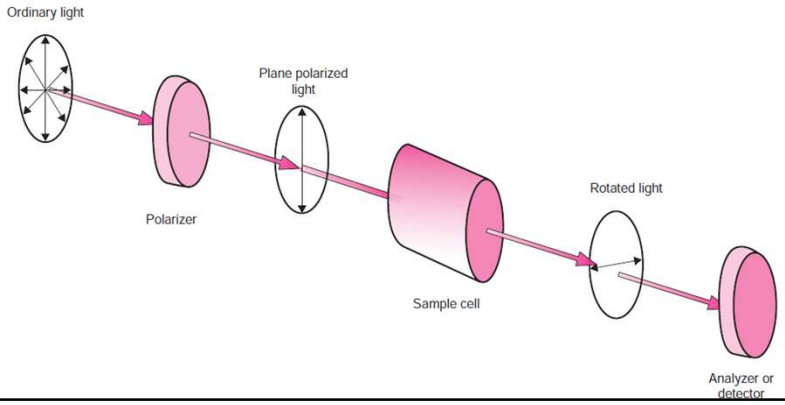
- **Dextrorotatory (+)**
- Rotates the plane of polarized light **clockwise**.
- Angle of rotation, **α**, is positive.
- **Levorotatory (–)**
- Rotates the plane of polarized light **counterclockwise**.
- Angle of rotation, **α**, is negative.
  - **Important:** The +/– designation describes the **direction of optical rotation** and does not by itself indicate the absolute configuration of a molecule.

OPTICAL ROTATION

Measuring Optical Rotation

Polarimeter

- A **polarimeter** is used to measure optical activity.
- The instrument measures the **angle of rotation (α)** produced by the sample.



α : observed rotation ∴ depends on directly:
① concentration.
② path length.

OPTICAL ROTATION

Dependence on Amount of Optically Active Substance

- Each molecule contributes a small amount to the total rotation.
- Therefore, optical rotation **α depends on the density/concentration** of the optically active substance.
- The observed rotation also depends on the **length of the optical path**.

Specific Rotation

- Specific rotation is a characteristic property of a pure optically active substance under specified conditions:

$$[\alpha]_{\lambda}^{t} = \frac{\alpha V}{lg}$$

α = observed optical rotation
V = volume of solution (mL)
l = path length (dm)
g = mass of optically active substance (g)
t = temperature
λ = wavelength

OPTICAL ROTATION

Reporting Specific Rotation

- Conditions Must Be Specified
- Specific rotation should be reported together with:
  - **Temperature**
  - **Wavelength**
  - **Concentration**
  - **Solvent**
- For example:
  - $[\alpha]_D^t$: The subscript **D** indicates measurement using the 589-nm sodium D line.

Why are conditions important?

- Specific rotation can vary with experimental conditions; therefore, values without temperature, concentration, or solvent information should be interpreted cautiously.

OPTICAL ROTATION

Pharmaceutical Applications of Optical Rotation

- Specific rotation can be used for:
  - Identification of optically active compounds
  - Confirmation of the identity of synthesized compounds
  - Assessment of purity
  - Characterization of:
    - Steroids
    - Carbohydrates
    - Amino acids
    - Other biologically important compounds

Key concept:

- Specific rotation provides information related to molecular structure.

* observed rotation α → الزاوية اللي بقيسها مباشرة بالـ polarimeter

↓

path length + concentration بتتأثر بـ

* specific rotation $[\alpha]$ → قيمة مميزة للمادة عند ظروف محددة بتحسبها

$$[\alpha]_{\lambda}^{t} = \frac{\alpha V}{l \rho}$$

↓

لما تكتبها لازم تفهم بـ :

- Temperature
- wavelength
- concentration
- solvent