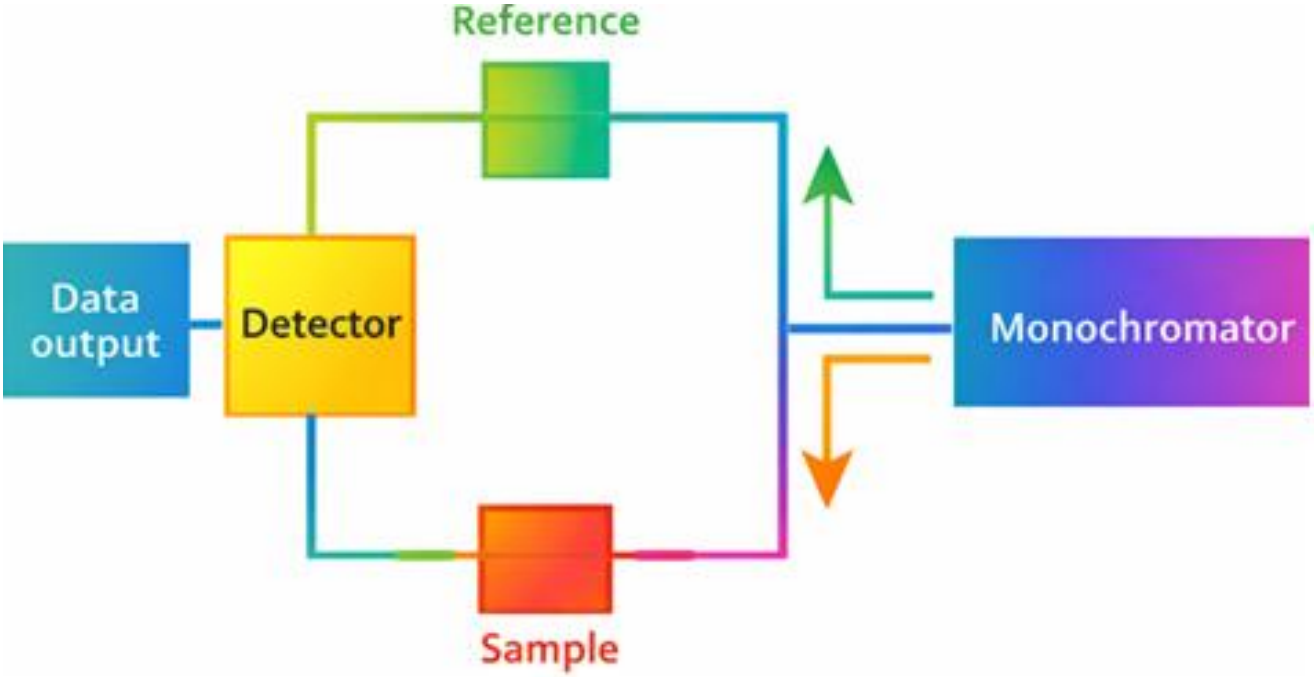
UV Visible spectroscopy

UV-Visible Spectroscopy

Overview

- UV-Visible spectroscopy is a technique used to measure the absorption of light in the ultraviolet (200-400 nm) and visible (400-700 nm) regions of the electromagnetic spectrum by a sample.
- This method provides valuable information about the electronic structure of molecules, particularly the presence of chromophores and their environment.
- **It is widely utilized in:**
    - Quantitative analysis
    - Identifying compounds
    - Studying reaction kinetics
    - Determining molecular concentrations



Basic Principle

- When a molecule absorbs light, its electrons are excited from a lower energy orbital to a higher energy orbital.
- The energy difference between these orbitals corresponds to the energy of the absorbed photon, which is inversely proportional to its wavelength.
- By measuring the absorbance at specific wavelengths, various properties of the sample can be inferred.

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Electronic transitions

Definition

- Electronic transitions refer to the movement of electrons between different energy levels within a molecule upon absorption of light.
- In UV-Visible spectroscopy, these transitions typically include:

1. π → π*:

- Electrons in pi bonds (π bonds) are excited to anti-bonding pi-star (π*) orbitals.

2. n → π*:

- Non-bonding electrons (n electrons), often lone pairs on heteroatoms like oxygen or nitrogen, are excited to anti-bonding pi-star (π*) orbitals.

3. σ → σ*:

- Electrons in sigma bonds (σ bonds) are excited to anti-bonding sigma-star (σ*) orbitals.
- These transitions generally require higher energies (shorter wavelengths) compared to π → π* or n → π* transitions.

Energy Levels

1. Ground State:

- The lower energy state of the molecule, where electrons are in their stable, unexcited state.

2. Excited State:

- The higher energy state reached after electrons absorb energy and move to higher orbitals.

Selection Rules

- Not all electronic transitions are permitted.
- **The likelihood of a transition depends on certain selection rules:**

1. Allowed Transitions:

- Transitions that typically involve a change in dipole moment, e.g., π → π* and n → π*.

2. Forbidden Transitions:

- Transitions that do not involve a change in dipole moment; for example, those occurring between orbitals of the same symmetry.
- These transitions are less likely or weaker in intensity.

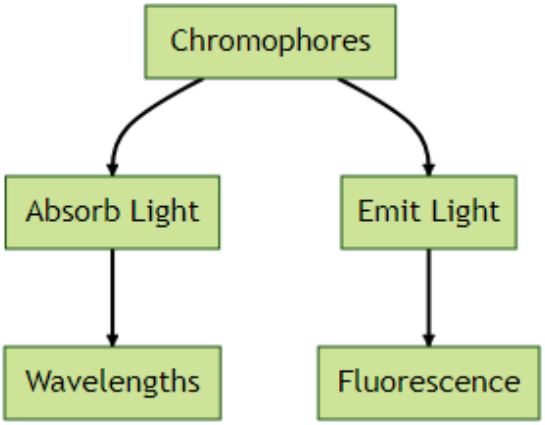
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Chromophores

Definition:

- Parts of a molecule responsible for its color.
- Chromophores contain conjugated systems (alternating single and double bonds) that allow delocalization of electrons, facilitating electronic transitions that absorb light.



Key Features:

- **Conjugation**: More conjugation lowers the energy required for transitions, often shifting absorption into the visible region.
- **Functional Groups**: Common chromophores include carbonyl (C=O), azo (-N=N-), nitro (-NO_2), and aromatic rings.

Examples:

- **Beta-Carotene**: A long conjugated system, giving it an orange color.
- **Hemoglobin**: Porphyrin rings act as chromophores, responsible for blood's red color.

Auxochromes

Definition

- An **auxochrome** is a functional group that, when attached to a chromophore:
  - Modifies the position (λ_{max}) and/or intensity (ε) of the chromophore's absorption.
  - Does not strongly absorb visible or UV light by itself.
  - Often causes bathochromic shift (red shift) and/or hyperchromic effect (increased intensity).

Mechanism of Actions

- Acts through resonance or inductive effects.
- Alters energy levels of π or non-bonding orbitals.

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