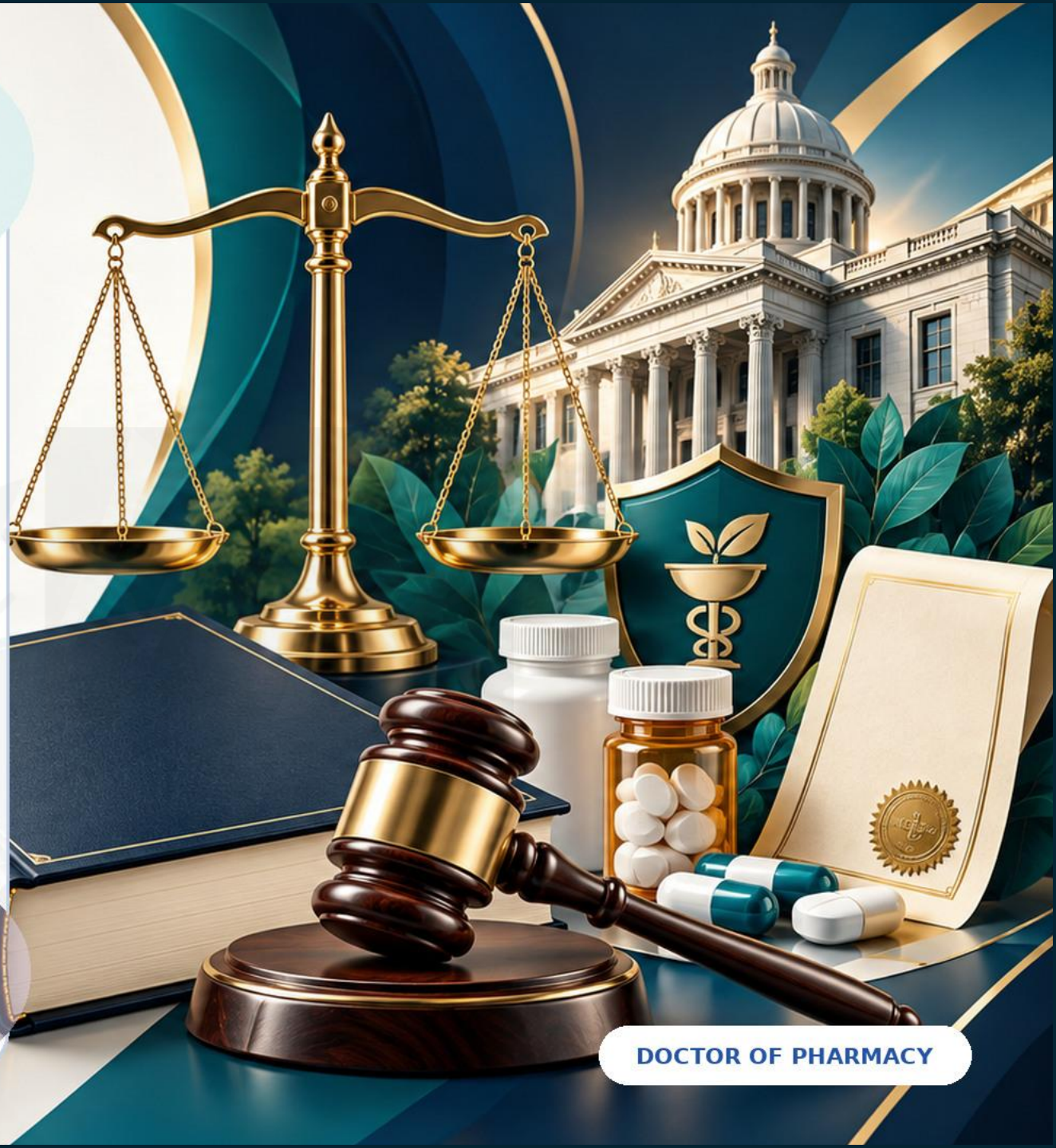
PHARM.D • YEAR 3

Pharmaceutical Analysis

CHAPTER 4.1

Absorption Spectroscopy (UV-Visible)

PPT CHAPTER COVER



DOCTOR OF PHARMACY

ATOMIC AND MOLECULAR ABSORPTION

Atomic absorption

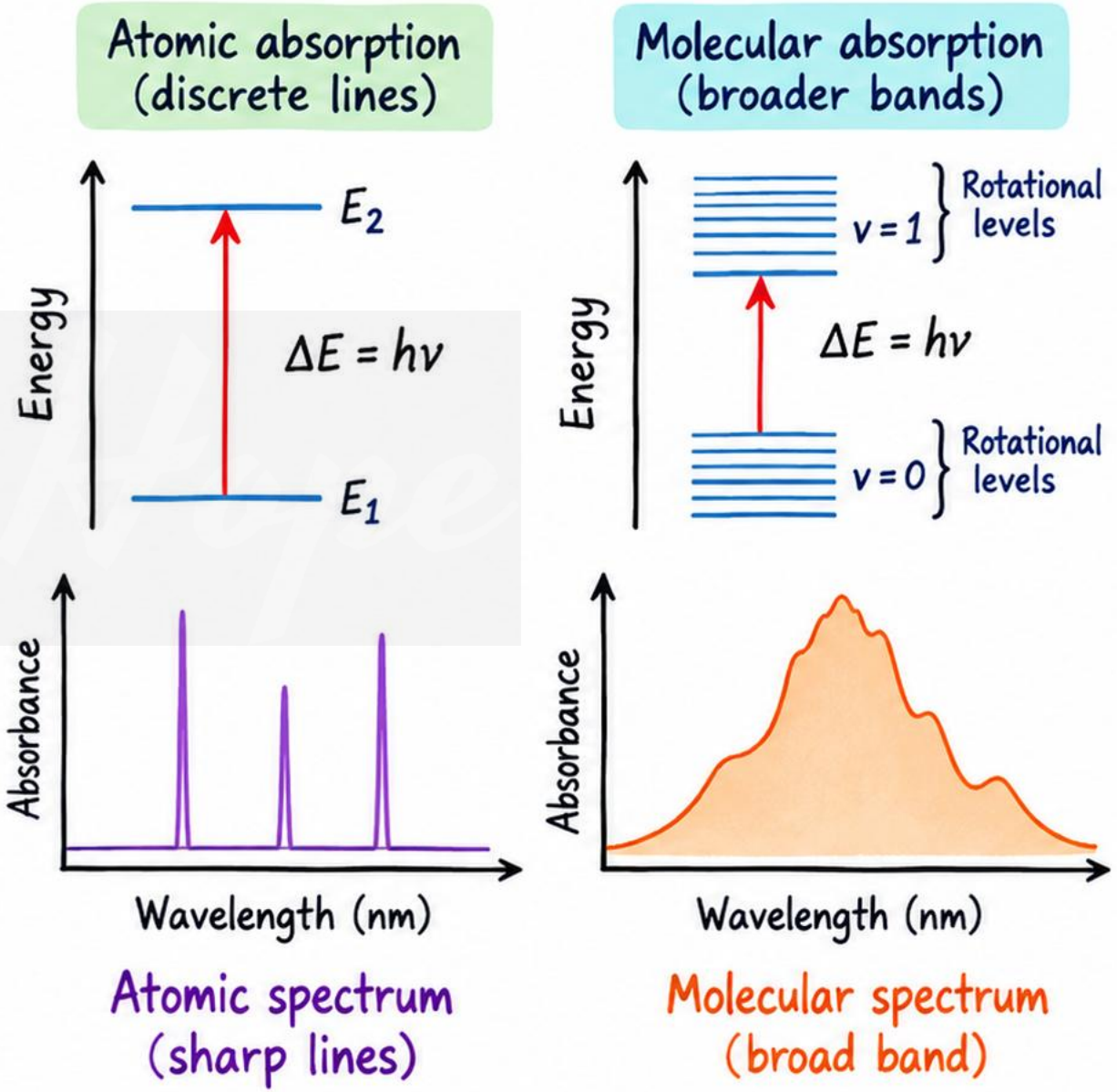
- Atoms have discrete electronic energy levels.
- Absorption promotes an electron when photon energy matches a permitted transition, giving characteristic atomic lines.

Molecular absorption

- Molecules also have vibrational and rotational levels within electronic states.
- Overlapping transitions commonly produce broader molecular bands.

Applications

- UV-visible molecular absorption is especially useful for compounds containing appropriate chromophores, including many conjugated systems.



ELECTRONIC TRANSITIONS AND PHOTON ENERGY

Photon energy

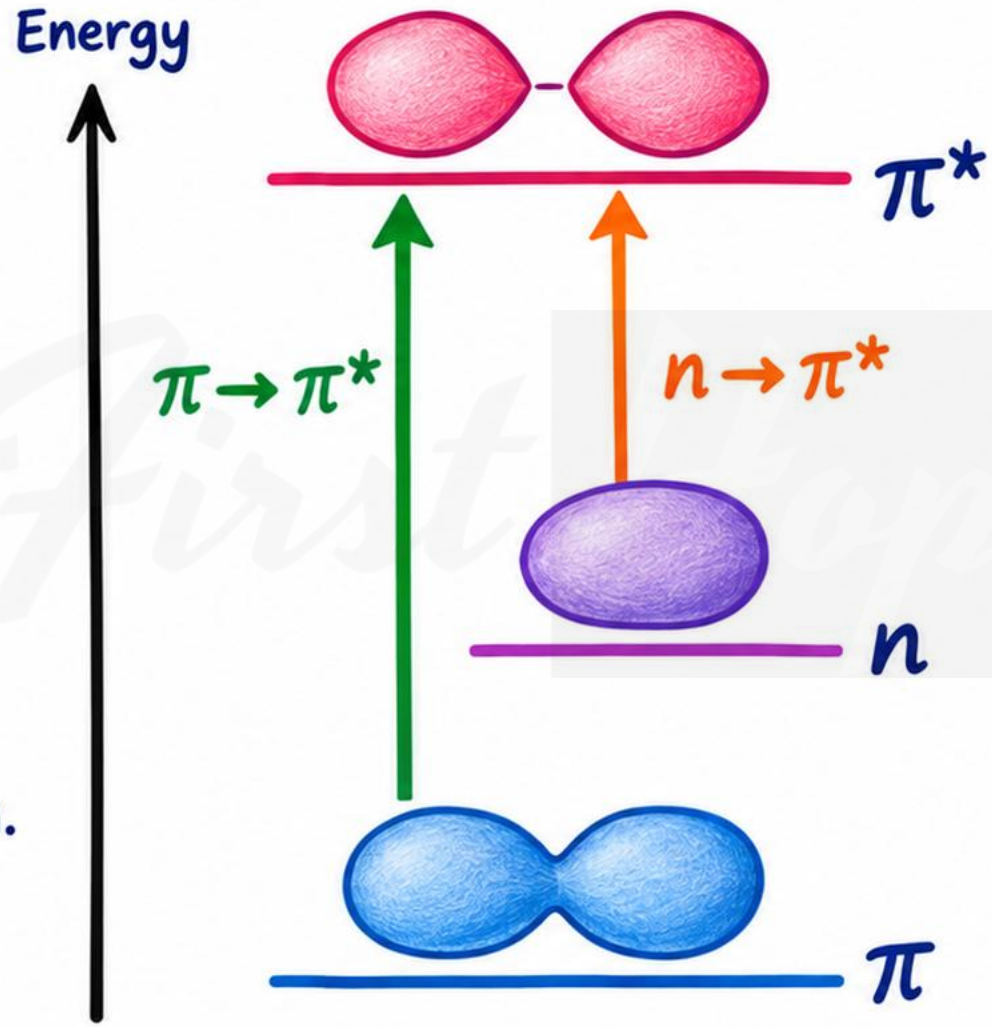
$$E = h\nu = \frac{hc}{\lambda}$$

A photon has energy $E = h\nu = hc/\lambda$.

Higher frequency means higher energy and shorter wavelength.

↑ ν ↑ → E ↑

↓ λ ↓ → E ↑



Molecular orbital energy levels

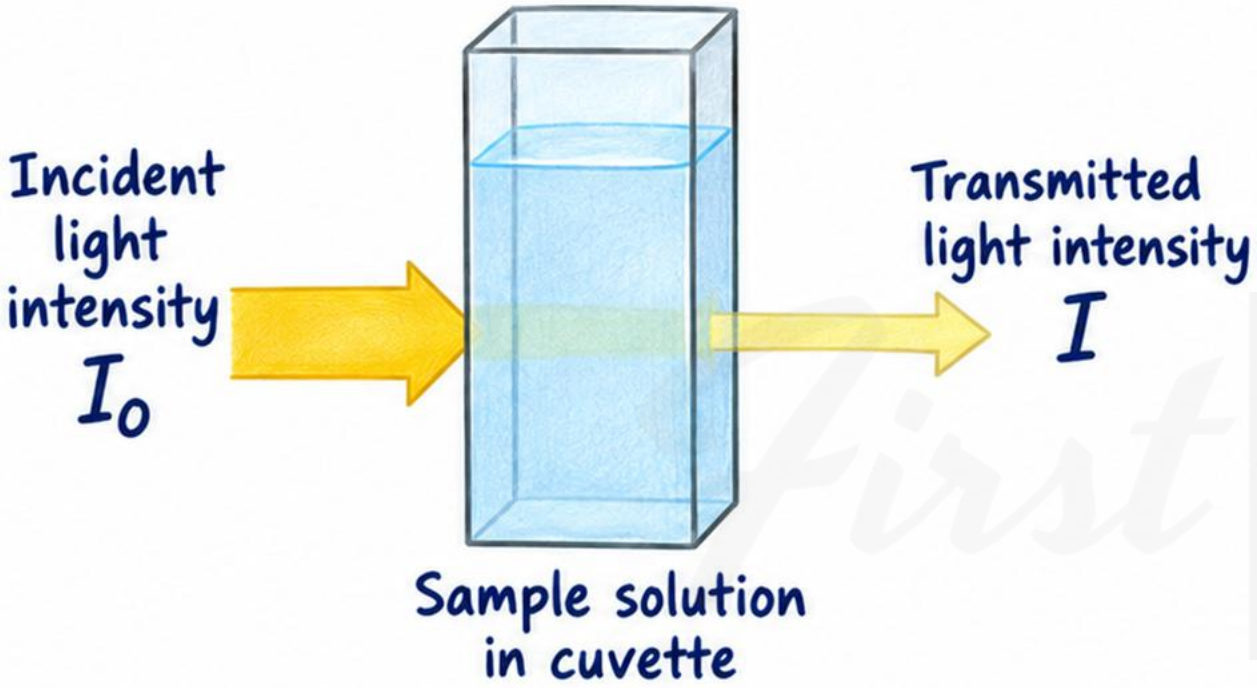
Common transitions

Molecular UV–visible absorption commonly involves transitions such as π to π* and n to π*. The asterisk denotes an antibonding orbital; n denotes nonbonding electrons.

Effect on spectrum

Transition energy and probability influence the position and intensity of absorption bands.

TRANSMITTANCE AND ABSORBANCE



Transmittance

T is transmitted intensity divided by incident intensity: $T = \frac{I}{I_0}$.

Absorbance

$$A = \log_{10}\left(\frac{I_0}{I}\right) = -\log_{10} T.$$

Absorbance is dimensionless.

Example

10% transmittance means $T = 0.10$ and $A = 1.00$.

Percent transmittance

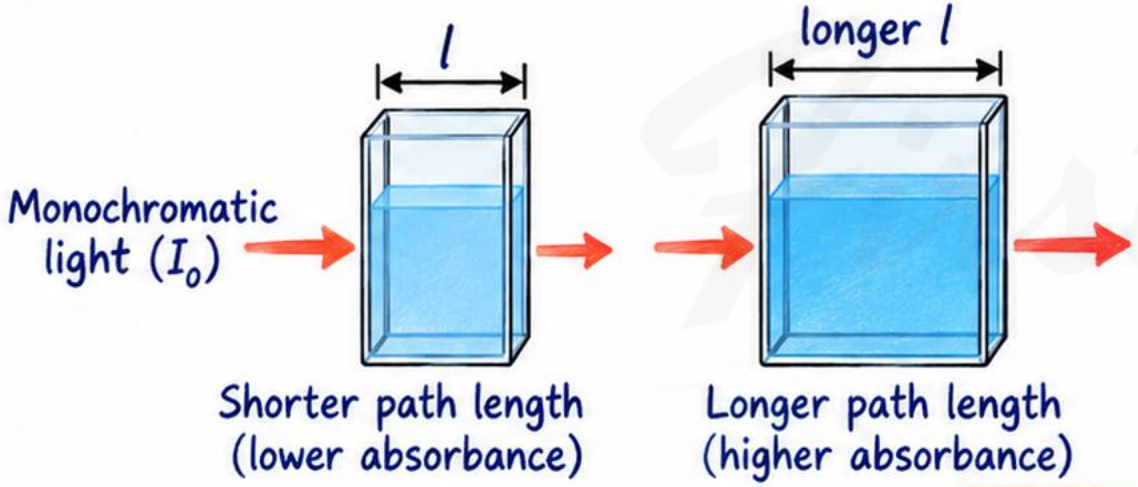
Percent transmittance is $100T$.

Use a suitable blank to account for the cell, solvent and other background contributions.

BEER AND LAMBERT RELATIONSHIPS

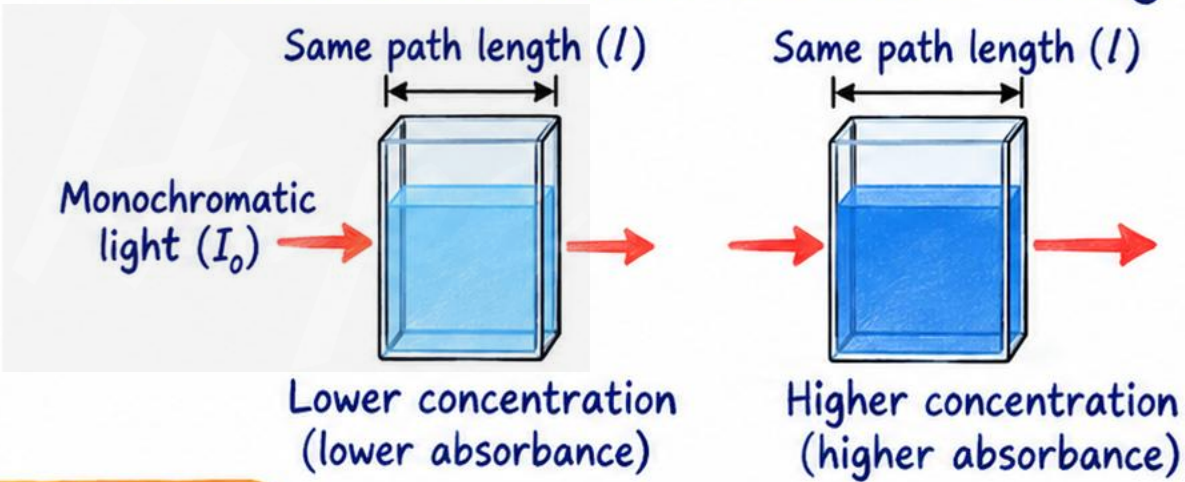
LAMBERT'S LAW

At fixed concentration and wavelength, absorbance increases with optical path length.



BEER'S LAW

At fixed path length and chemical conditions, absorbance increases with concentration within a suitable range.



$$A = \varepsilon c l$$

ε = molar absorptivity in $L \cdot mol^{-1} \cdot cm^{-1}$
c = concentration in mol/L
l = optical path length in cm

These units cancel to give dimensionless absorbance.

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