Ultraviolet-Visible Spectroscopy

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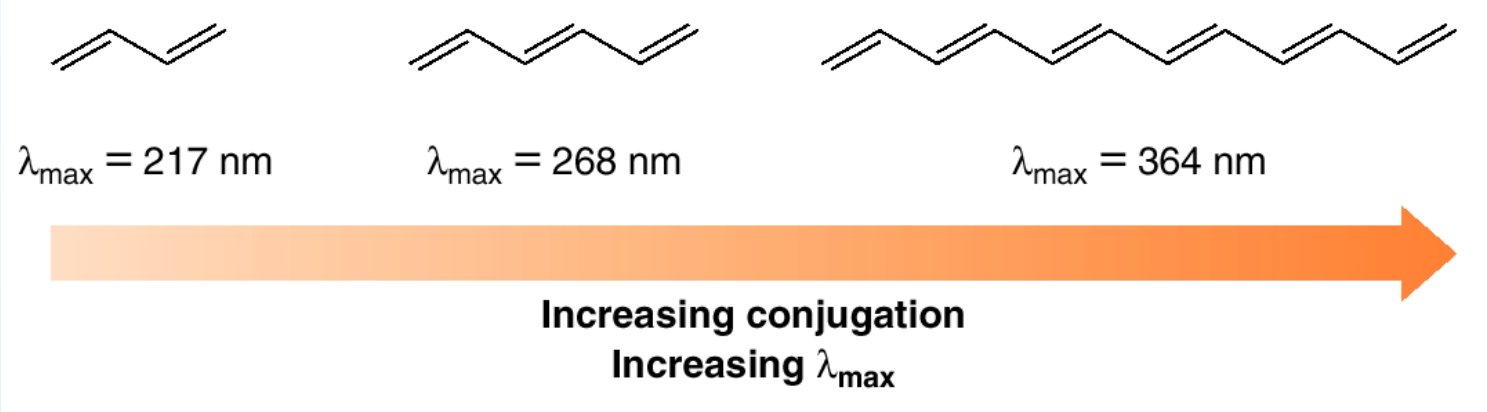
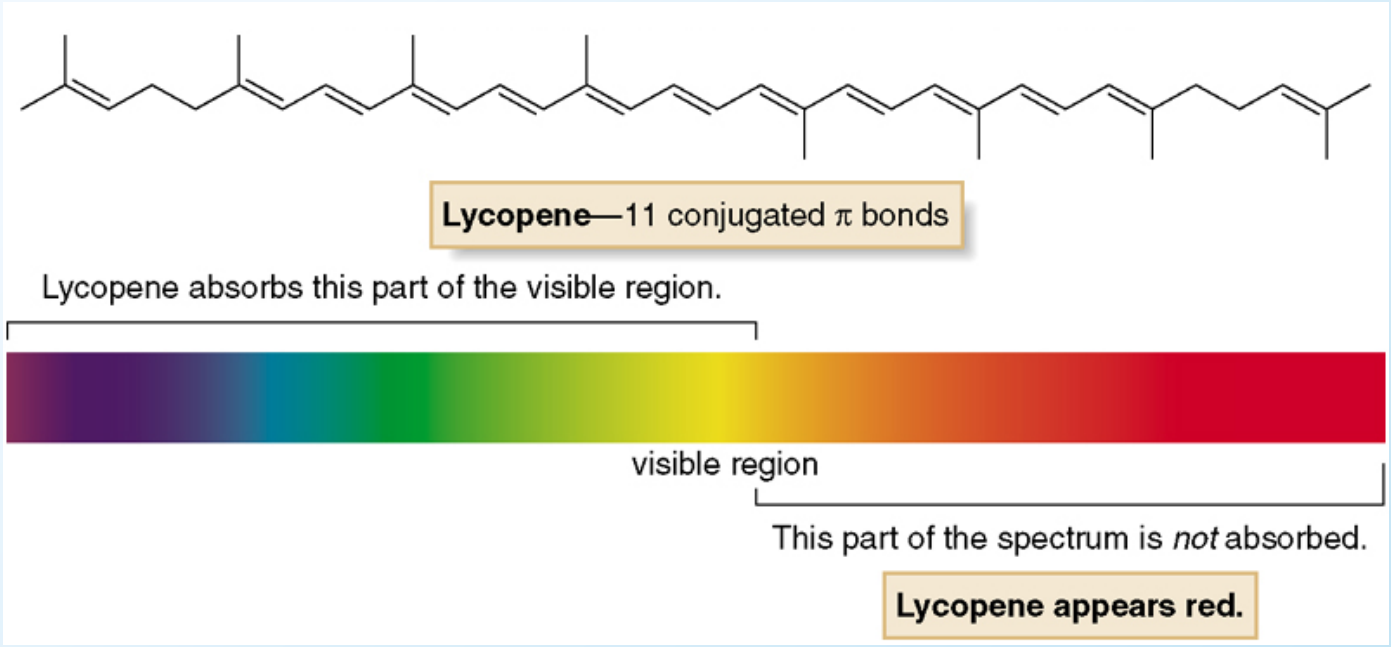
Ultraviolet-Visible Spectroscopy

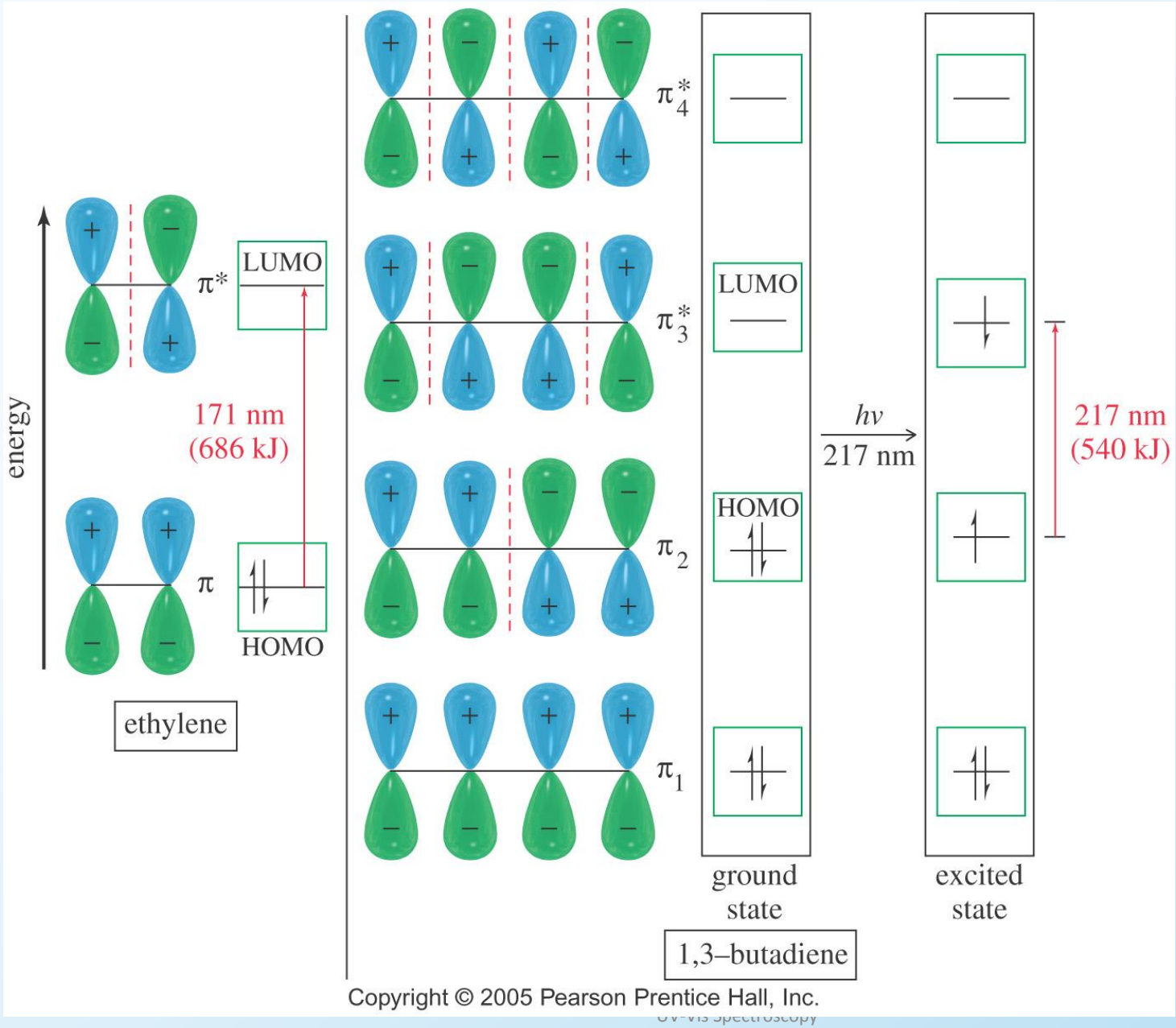
- In both UV (200-400 nm) and Visible regions (400-800 nm), photons excite electrons from a bonding orbitals to antibonding orbital i.e. electron transitions are occurring.
- Conjugated dienes have MO's that are closer in energy.
- A compound that has a longer chain of conjugated double bonds absorbs light at a longer wavelength.



Why Lycopene is Red

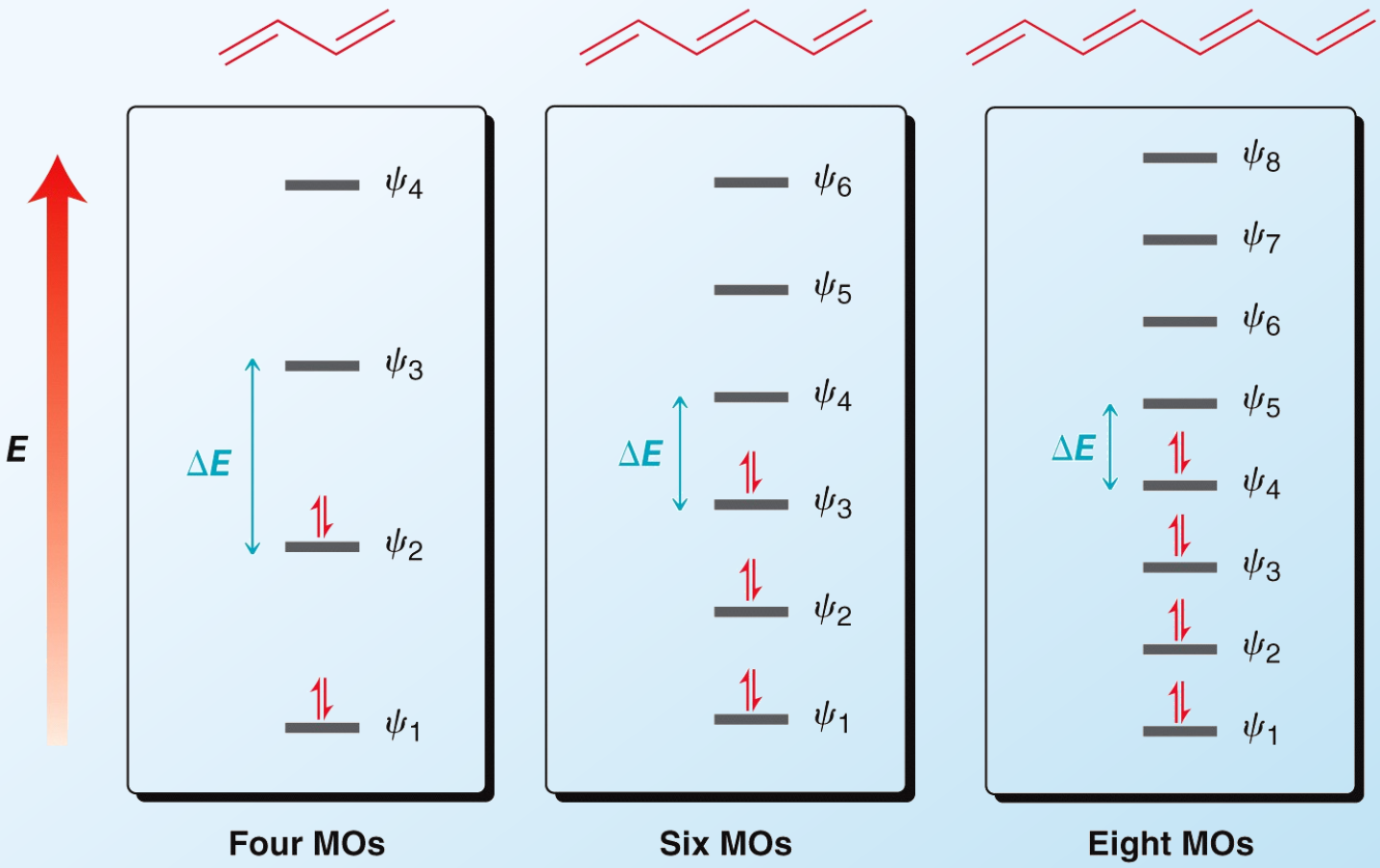
Lycopene absorbs visible light at λ_{max} = 470 nm, in the blue-green region of the visible spectrum. Because it does not absorb light in the red region, lycopene appears bright red.



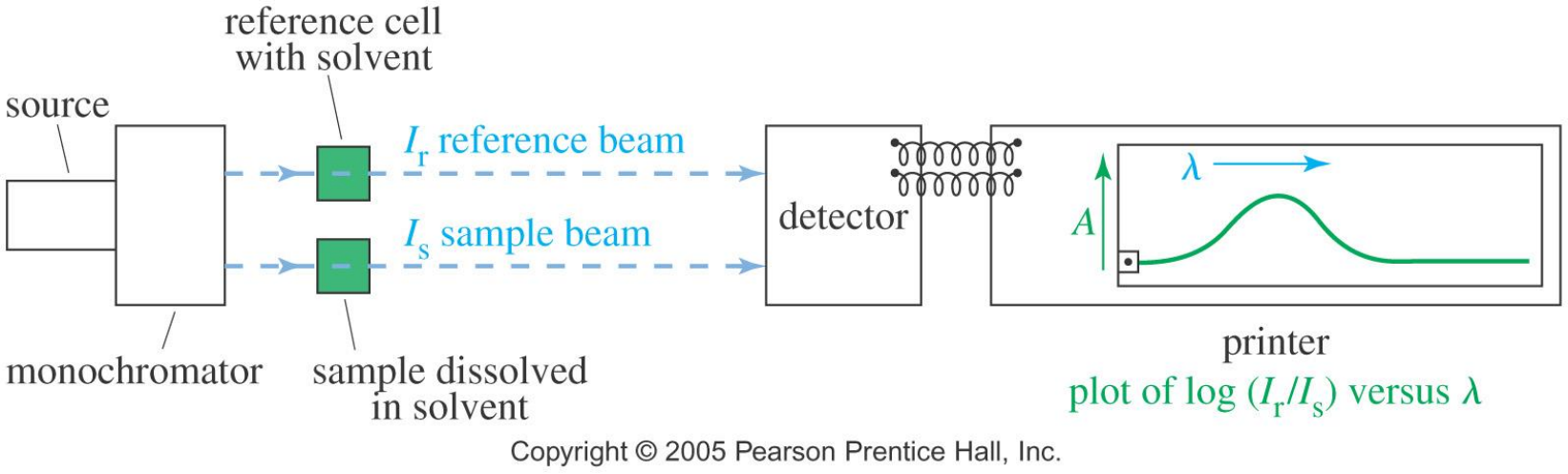


$\pi \rightarrow \pi^*$ for ethylene and butadiene

Conjugation and MOs



Obtaining a UV-Vis Spectrum



- The spectrometer measures the intensity of a reference beam through solvent only (***I***) and the intensity of a beam through a solution of the sample (***I_0***).
- Absorbance is the log of the ratio $A = \log \frac{I_0}{I}$

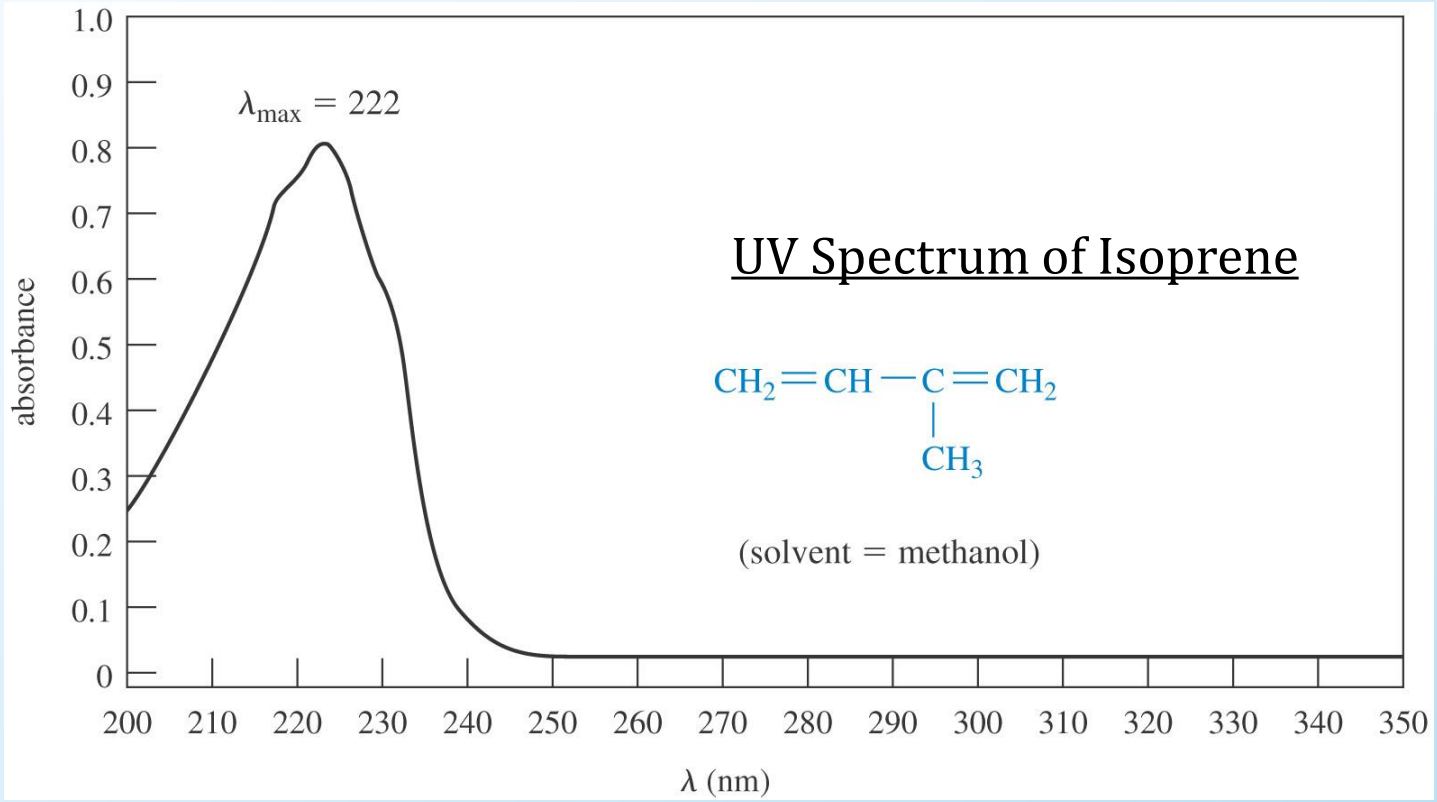
- Sample Preparation: dissolve the sample in a Vis range invisible solvent e.g. for most organic samples CH_2Cl_2 and MeOH. These solvents may not be good for UV region. Sample can be recovered after analysis.

The UV-Vis Spectrum

- Usually shows broad peaks.
- Read λ_{max} from the graph.
- Absorbance, A, follows Beer's Law:

$$A = \varepsilon cl$$

where ε is the molar absorptivity (extinction coefficient), *c* is the sample concentration in moles per liter, and *l* is the length of the light path in centimeters.



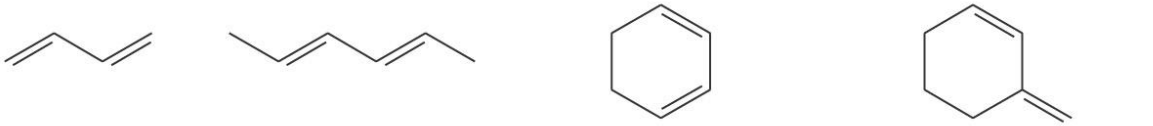
Sample UV-Vis Absorptions

TABLE 15-2 Ultraviolet Absorption Maxima of Some Representative Molecules

Isolated

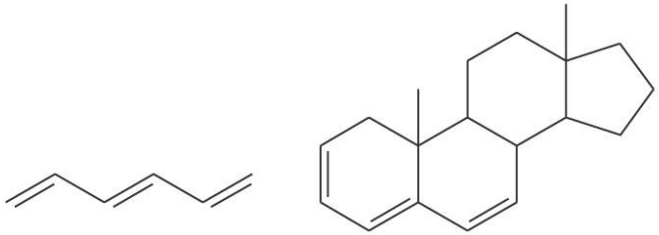
	ethylene	cyclohexene	1,4-hexadiene
λ_{max}:	171 nm	182 nm	180 nm

Conjugated dienes



	1,3-butadiene	2,4-hexadiene	1,3-cyclohexadiene	3-methylenecyclohexene
λ_{max}:	217 nm	227 nm	256 nm	232 nm

Conjugated trienes



	1,3,5-hexatriene	a steroid triene
λ_{max}:	258 nm	304 nm

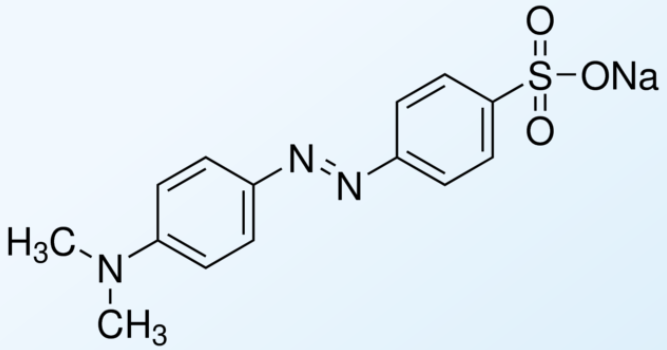
Conjugated tetraene

1,3,5,7-octatetraene
290 nm

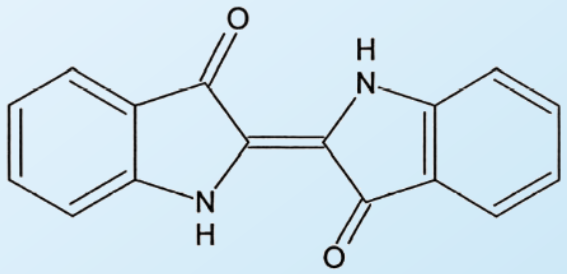
Visible Region Absorption of Dyes

Dyes absorb in the visible region because of conjugation.

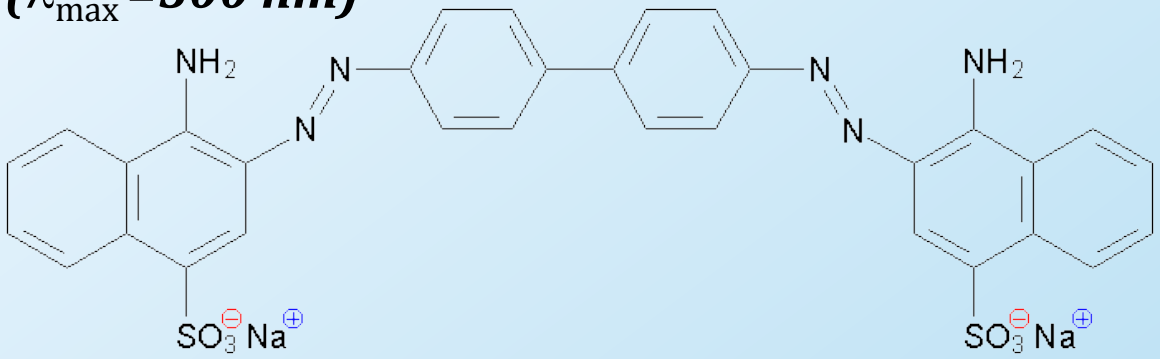
Methyl orange (λ_{max} =440 nm)



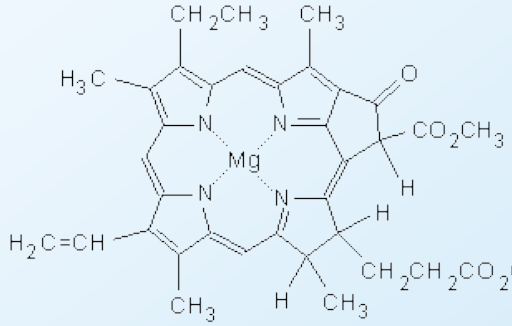
Indigo (λ_{max} =600 nm)



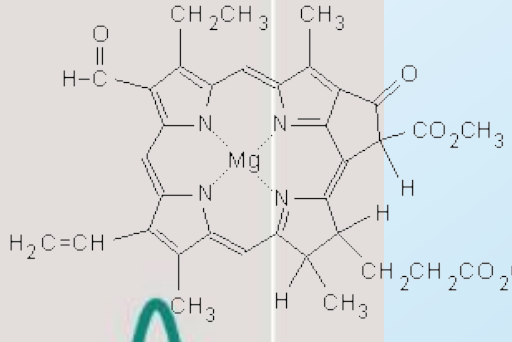
Congo Red (λ_{max} =500 nm)



Chlorophyll a and b UV-Vis



Chlorophyll a



Chlorophyll b

Key Concepts

- Recognize conjugation
- Predict which molecule will absorb in the red or violet region of UV-Vis.