

UV- visible spectroscopy

2/1/08 - 1

Highest occupied M.O. (HOMO)
Lowest unoccupied M.O. (LUMO)

UV	180-400 nm) electronic transitions
vis	400-780 nm	

an e^- is promoted from HOMO \rightarrow LUMO

groundstate \rightarrow excited state

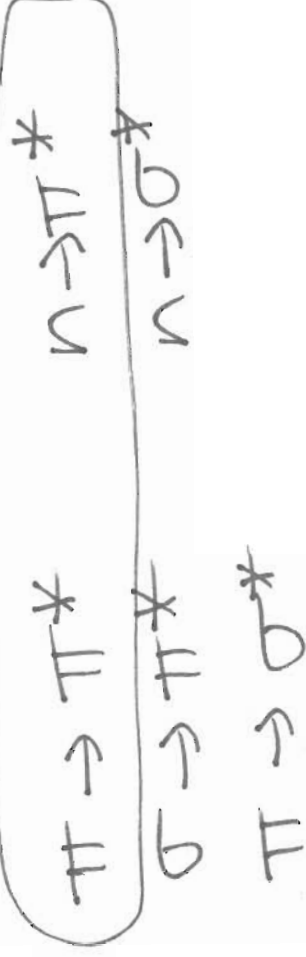
possible HOMOs: π bonds (orbitals)

σ bonds (orbitals)

nonbonding orbitals (n)

possible LUMOs: π^* σ^* antibonding orbitals

transitions:



Therefore: only organic molecules containing π systems will show absorption in the UV-vis spectrum.

UV-vis detects conjugation.

We say it identifies the presence of chromophores

Recall: Beer's Law (aka Beer-Lambert)

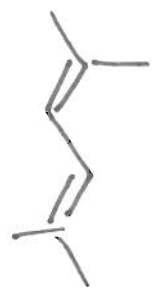
$$A = \epsilon b C$$

\uparrow absorbance
 \leftarrow conc. mol/L
 \nwarrow path length = 1 cm
 \nearrow molar absorptivity refers to how strongly the chromophore absorbs UV-Vis light.

examples.



$\lambda_{max} = 224 \text{ nm}$

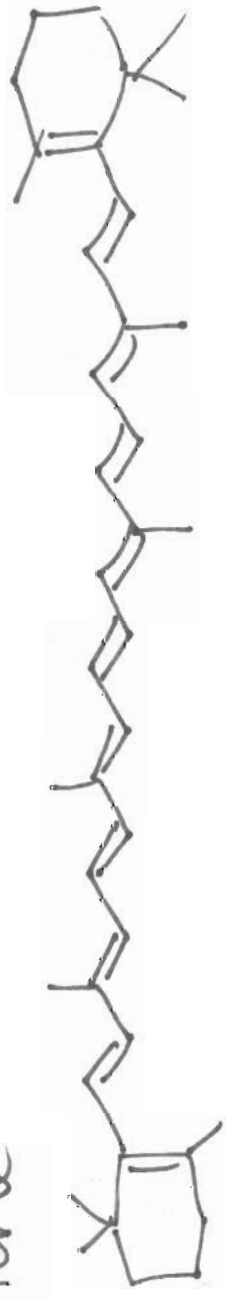


$\lambda_{max} = 248 \text{ nm}$

auxochromes - substituents on the chromophore that alter the observed λ_{max}

e' donors \rightarrow larger numbers
 e' withdrawer \rightarrow smaller numbers

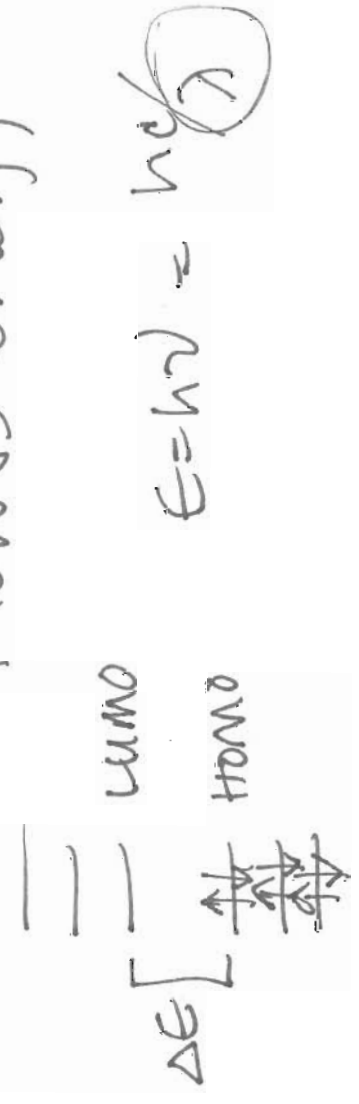
β -carotene



$$\lambda_{max} = 425, 450, 477$$

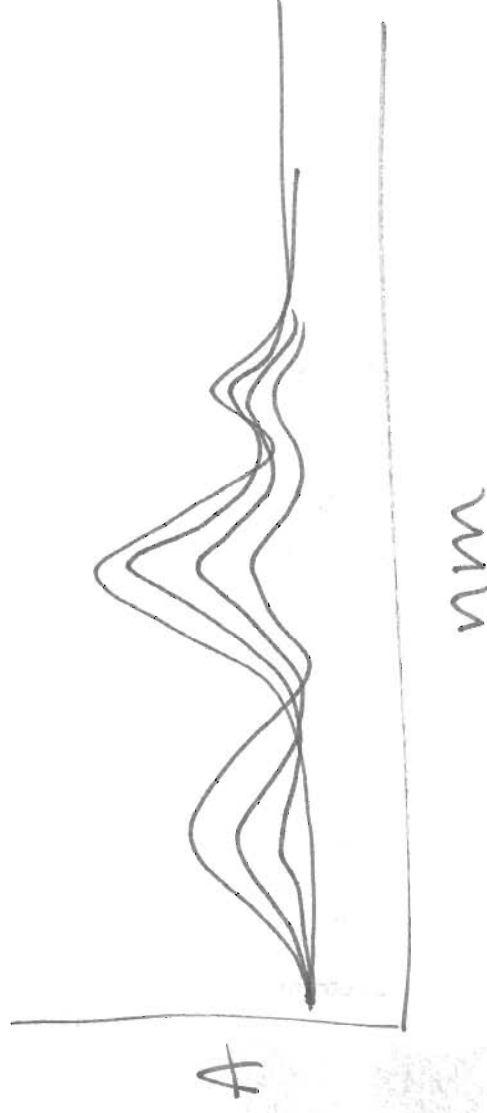
extended conjugation \Rightarrow larger wavelength max.

Why? conjugation raises energy of HOMO + lowers energy of LUMO.



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What do we do with UV-vis?

1. structure determination - detect presence of conjugation.
2. monitor rxn rate



3. various biochemical applications

mass Spectrometry - does not use e⁻ mag.
radiation

uses a beam of high energy e⁻s to
fragment your molecule. Goal: determine
molecular mass +, ideally, molecular formula.

Chapter 12

Mass Spec...

"Very Condensed"

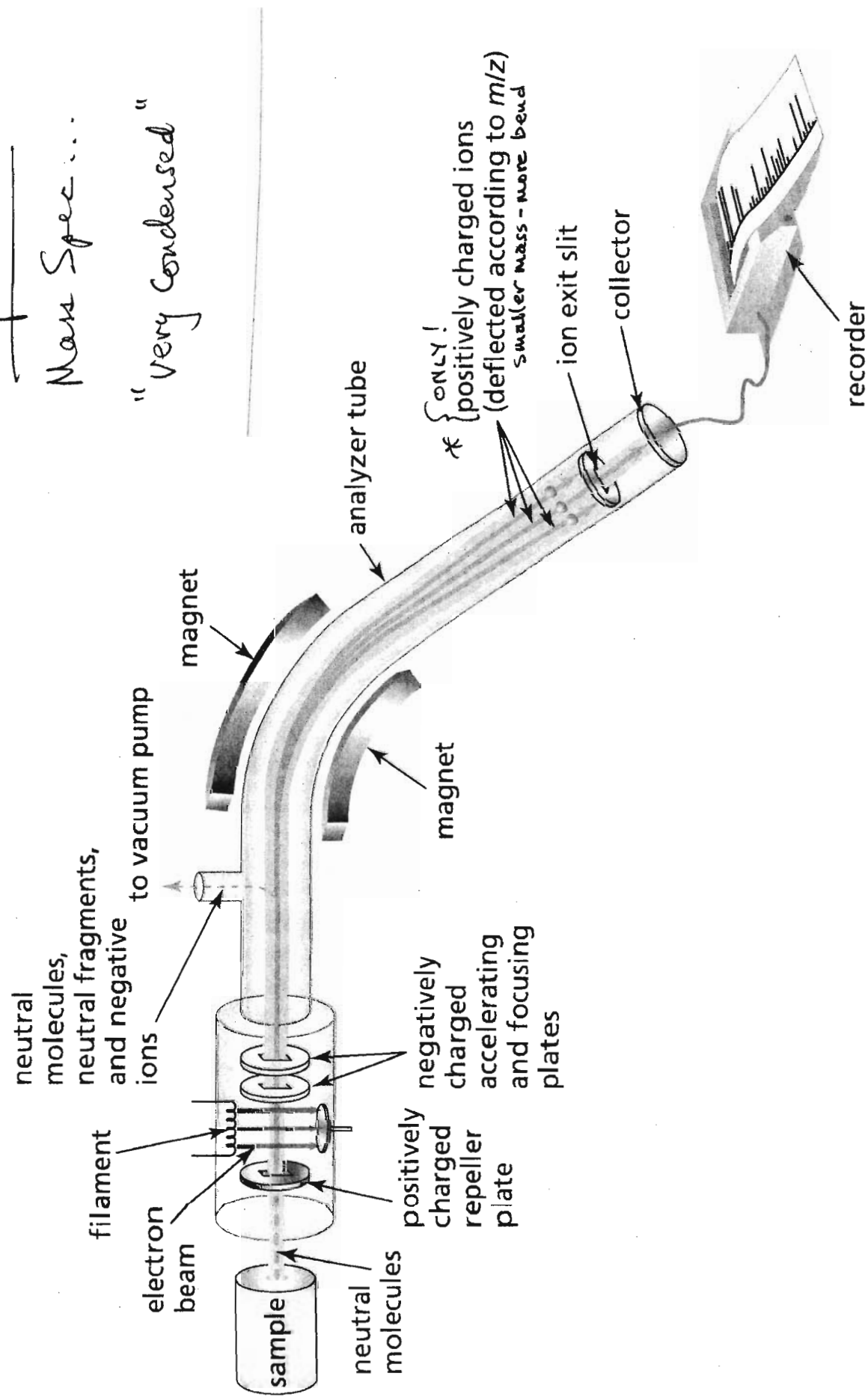


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