UCB008 - APPLIED CHEMISTRY

THAPAR INSTITUTE
OF ENGINEERING & TECHNOLOGY
(Deemed to be University)

SCBC-TIET

Molecular Spectroscopy Series

Lecture - IV

UV-Visible Spectroscopy – Terms

by

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Learning Outcomes

At the end of this session participants should be able to:

- illustrate the terms used in UV-Visible Spectroscopy

Chromophore

- Isolated covalently bonded groups that shows characteristic absorption in UV-Visible region and even small structural changes brings about change in wavelength of absorption.

or

- The functional groups containing multiple bonds capable of absorbing radiations above 200 nm due to **n-π*** and **π–π*** transitions.

- Examples: C=C, C≡C, N=O, N=N, NO_2, C=O, C=N, C≡N, C=C,C=S, -$CONH_2$, -COOH, etc

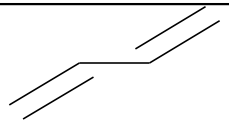
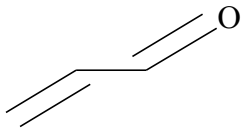
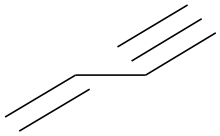
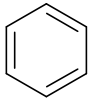
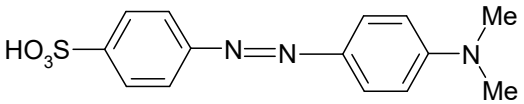
Chromophore

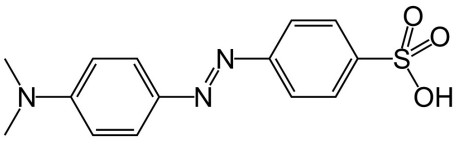
- Non-conjugated alkenes show an absorption below 200 nm and therefore cannot be observed by conventional UV spectrophotometer.

- If these transitions are to be observed, vacuum UV spectrophotometer is required.

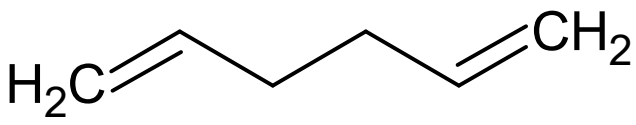
- Non-conjugated carbonyl group compound give a weak absorption band in the 200 - 300 nm due to **n-π^*** transition.

Effect of conjugation on λ_{max}

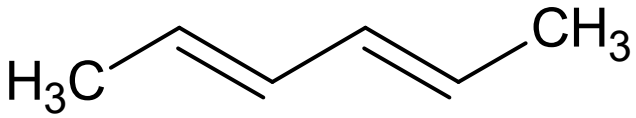
Compound	λ_{max} (nm)
$H_2C=CH_2$	180
	217
	220
	220
	255
	460



Effect of conjugation on λ_{max}



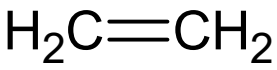
1,5 - hexadiene : λ_{max} = 178 nm



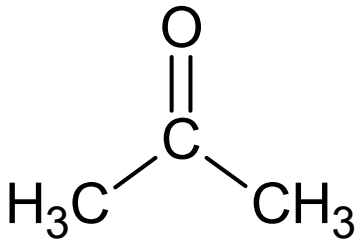
2,4 - hexadiene : λ_{max} = 227 nm

When double bonds are conjugated in a compound, λ_{max} is shifted to longer wavelength.

Effect of conjugation on λ_{max}

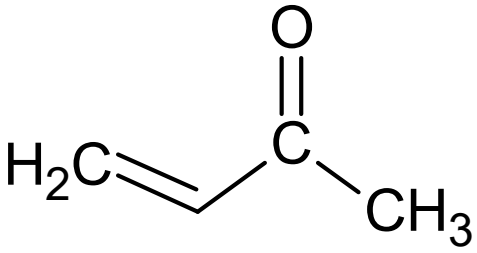


Ethylene has λ_{max} = 171 nm



Acetone has λ_{max} = 279 nm

Conjugation of C=C and carbonyl group shifts the λ_{max} of both groups to longer wavelength.



Crotonaldehyde has λ_{max} = 290 nm

Auxochrome

- The functional group with non-bonding electrons, that does not absorb radiation in UV/visible region, when attached to a chromophore increases the wavelength and intensity of absorption.

OR

- Any group which does not itself act as chromophore but its presence brings about a shift of absorption bands towards red end of the spectrum

Examples: -OH, -OR, $-NH_2$, -NHR, $-NR_2$, -SH etc.

Auxochrome

- Auxochrome when combined with chromophore, modifies the position of absorption band relative to the parent chromophore

Chromophore + Auxochrome

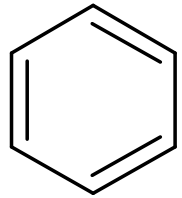
New chromophore having higher λ_{max}

Examples: -OH, -OR, -NH_2 , -NHR, -NR_2, -SH etc.

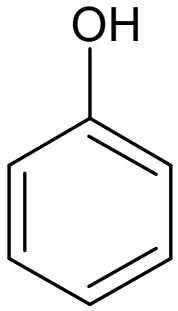
- Auxochrome extends the conjugation of a chromophore by sharing its lone pair of electrons

Auxochrome

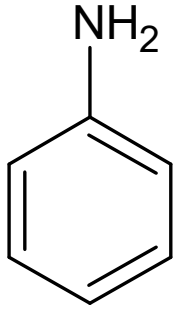
e.g. Benzene λ_{max} = 255 nm



Phenol λ_{max} = 270 nm



Aniline λ_{max} = 280 nm



In the next session.....

- Absorption and Intensity Shifts in UV-Visible Spectroscopy