SPECIAL TOPICS

(CHEM-291)

Spectroscopy → UV, I.R, NMR, MS
Material chemistry → colloids, liquid crystals
Heterocyclic compounds → furan, pyrrol, pyridine
Biomolecules → carbohydrates, proteins, amino acids
Chemical industry → glass, cement, HNO_3, H_2SO_4

SPECTROSCOPY:

EMP

"Characterize organic compound"

(I.R / U.V) Rays → Org. comp → detector (compounds funtionality).

U.V — visible. — I.R

Q Why red, green & yellow lights used for traffic signal?

Quantum Mechanics:

↳ Quanta → Energy Packets.

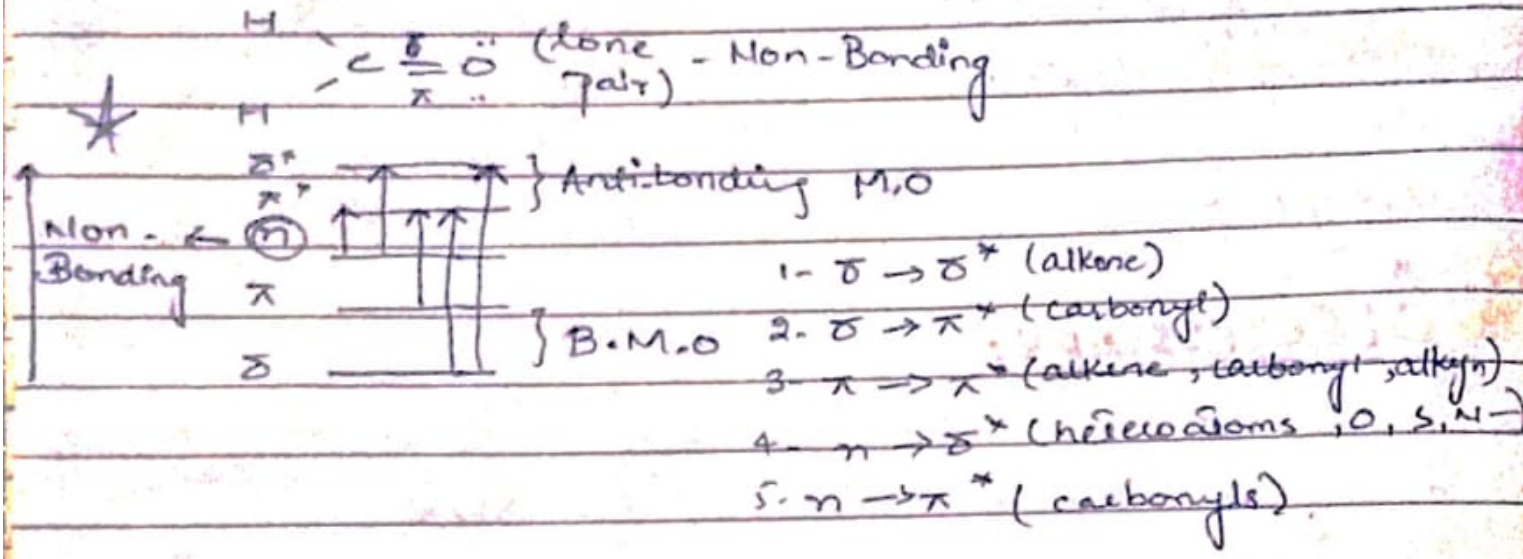
$h = \frac{c}{\lambda}$ $\quad E \propto f$, $\quad E \propto \frac{1}{\lambda}$

high state
↑↓ ~
low state ↳ λ – visible.

Ultraviolet Spectroscopy (180-390 nm)

U.V

=> Electronic Transition - Study in molecule.



Order of Transition Energy

$\sigma \rightarrow \sigma^* > n \rightarrow \sigma^* > \pi \rightarrow \pi^* > n \rightarrow \pi^* > \sigma \rightarrow \pi^*$

Allowed in U.V (+ve result)

other → forbidden.

Lambert Beer Law

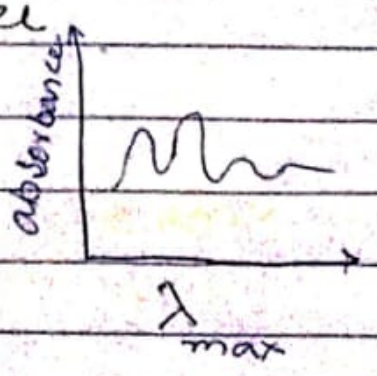
$A = \epsilon C L$

Absorbance
- ε → constant
- C → concentration
- L → length of sample

$A \propto C L$

U.V Spectrophotometer

↳ Instruments.



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λ_{max} — calculate — [theory, experiment - instrument.

Solvent — Should be Transparent
— Should be lack of conjugation.
— Should be cheaper / non-toxic.

Eg. H_2O, C_2H_5OH, n-hexane
↓ ↓ ↓
λ_{max} ⇒ 190nm 205 nm 201 nm.

Q Which solvent is mostly used in U.V?
H_2O, alcohol.

colour loving groups
↳ Chromophores → functional groups.
↳ Molecules which absorb U.V radiations in the range of 180-390nm.
- Mostly, unsaturated org. comp absorb rays of this region.
- Some other groups i.e heteroatoms are also absorbed this system.

→ U.V, we mostly observe transition metals Bio macromolecules, heterocyclic comp.

C=C, C=O → Chromophores.

Substituent
(X) → λ_{max} = 100 nm → change by adding substituent

Chromophore
Shift of λ_{max} toward longer λ → 100↑ ⇒ Bathochromic Shift / Red shift
Smaller → → 100↓ ⇒ Hypsochromic Shift / Blue shift.

→ Chromophore : Light absorb → colours emit
↳ functional groups.

→ Auxochrome : change in λ ↑ ↓
↳ Atoms which alter λ in longer / smaller Shift.

→ How to find λ_{max} theoretically?

Conjugated System → Diene

=  → Conjugate diene

c=c=c 
(Cummulated diene) ↳ Diene - extend.

Homo annular system - prefer over heteroannular

Q conjugation α λ_{max}

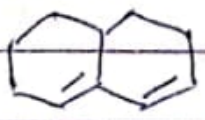
λ_{max} diene < λ_{max} triene.

Wood ward Fieser Rule :

↳ λ_{max} - theoretically calculate

Diene → 3 - Types

1- Acyclic  → 217 (parent value).

2- Cyclic
- Homo Annular  → 2 alternative double bonds in one ring
(Parent value) 253 nm.
- Hetero Annular  2 alternative double bonds in 2 rings.
214 - 417 nm (P.V).

→ Increment Value

1- parent value
2- Extention of conjugation → +30 (one double bond)
3- Exocyclic double Bond = +5
4- Substituent value