→ 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}

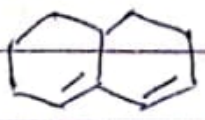
λ_{max} diene < λ_{max} triene.

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).

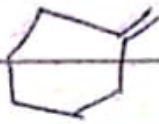
→ Increment Value

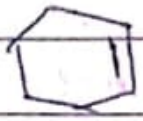
1- parent value
2- Extention of conjugation → +30 (one double bond)
3- Exocyclic double Bond = +5
4- Substituent value

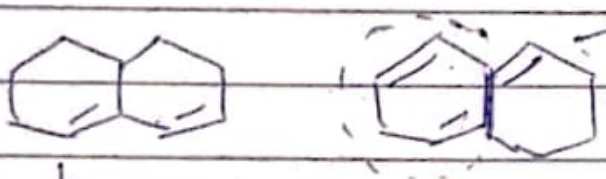
(R) alkyl → +5 OR → +6 SR → +30

$OCOCH_3$ → 0 X → +5 NR_2 → +60

Homo annular → 253.

Exocyclic double bond  (outside cycle)

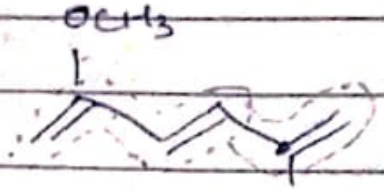
Endocyclic double bond  (inside cycle)



→ Calculate λ_{max}.

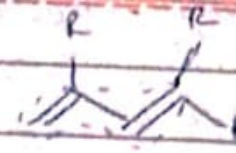
- P-value = 217nm
- extra conjugation = 0
- exocyclic = 0
- Substituent (X) = +5

λ_{max} = 222nm



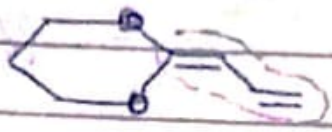
- P. value = 217nm
- extra conjugation = +30
- Exocyclic = 0
- Substituent (OCH_3) = +6
- C_2H_5 = +5

λ_{max} = 258nm.



- P-value = 217
- Extention of conjugation = 0
- Exocyclic = 0
- Substituent = R x 3 = 15

λ_{max} = 232 nm



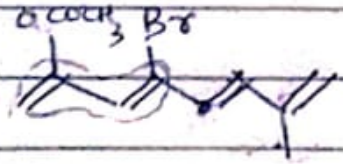
- P. value = 217
- Extra conjugation = 0
- Exocyclic = +5
- Substituent = 10

λ_{max} = 232nm

Heteroannular cyclic diene.

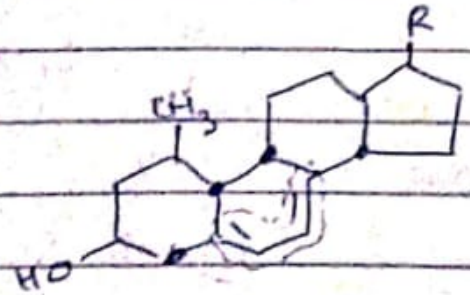
- P. value = 214 nm
- Extra conjugation = 0
- Exocyclic = +5
- Substituent = 15

λ_{max} = 234 nm



- P value = 217
- E. conj = +60
- Exo = 0
- Sub = +5
  +5
  +0

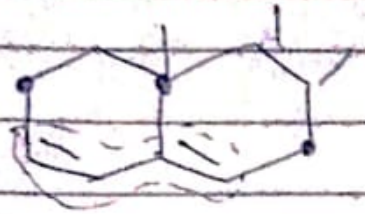
λ_{max} = 287 nm



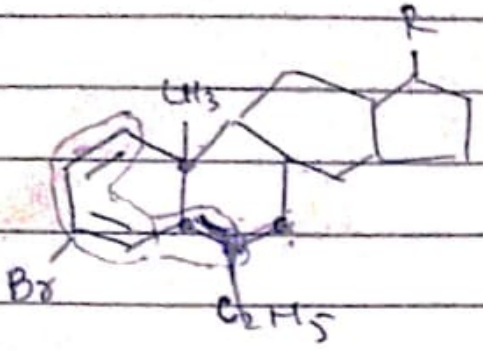
- P. value = 253nm
- E. conj = 0
- Exo = +5+5
- Sub = 20 + ~~5+5+6~~

λ_{max} = ~~294nm~~ 283nm

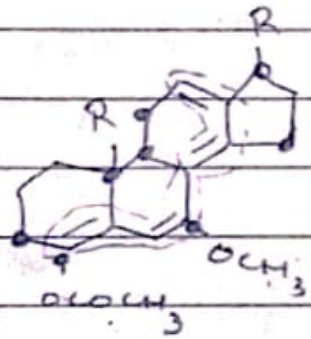
$\frac{283}{46}$



P. value = 214 nm
ε conj = 0
ε x o = + 5
Sub = + 15
λ_{max} = 234 nm



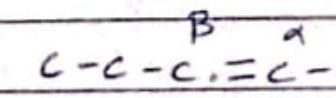
P = 253
ε . C = 30
ε x o = 5
Sub = 15 + 5
λ_{max} = 308 nm



P. value = 253 nm
ε . conj = + 60
ε x o = + 20
Sub = 30 + 6
λ_{max} = 369 nm

253
116
369

α-β unsaturated carbonyl system.



1- Acyclic = 215 nm
2- 6 membered cyclic ketone = 215 nm
3- -COOH / COR = 195 nm
4. 5 membered cyclic ketone = 202 nm
5- 5 membered cyclic aldehyde 207 nm.

Increment value:

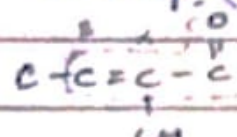
Homodienes = + 39
Conjugation = + 30
exocyclic = + 5

δ^{++} δ^{+} δ γ β α O

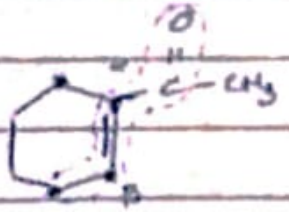
C = C - C = C - C = C - C - R

functional group	α	β	γ	δ	δ^{+}	δ^{++}
OH	35	30	30	20	20	20
OR	35	30	17	31	31	31
O_{Ac}	6	6	6	06	06	06
Cl	15	12	12	12	12	12
-R	10	12	18	18	18	18
-Br	25	30	25	25	25	25

Examples

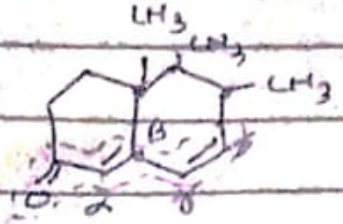


P. value = 215
Conjugation = 0
Exocyclic = 0
Substituent = R - α = 10, β = 12
λ_{max} = 237 nm

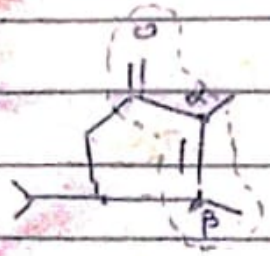


P value = 215nm
Conj = 0
Exocyclic = 0
Sub = R = α = 10, β = 12
λ_{max} = 237 nm

P - value = 215nm
Conj = 0
Exocyclic = + 5
Sub α = R = 10, β = 12
λ_{max} = 242 nm

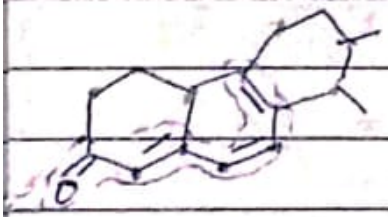


P. value = 215nm
Exocyclic = +5
Sub R = α = 0 β = 12 γ = 18
λ_{max} = 280nm



P. value = 202nm
conjugation = 0
Sub α = R = +10, β = 2R = 12×2
λ_{max} = 236nm.

P value = 202nm
Conjugation = 0
Exocyclic = +5, +5 = 10
Sub β = R = 24 α = 10
λ_{max} = 246nm.

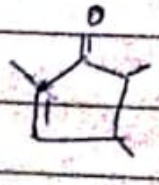


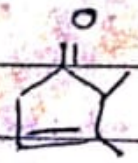
P. value = 215nm
Conjugation = +30, +30
Exocyclic = +5, +5
Sub = 12 + 18 + 18 + 18
= 346 + 139
↳ Homodiene
λ_{max} = 385nm.

Q: A yclic ketone has λ_{max} = 235nm
Identify its structure.

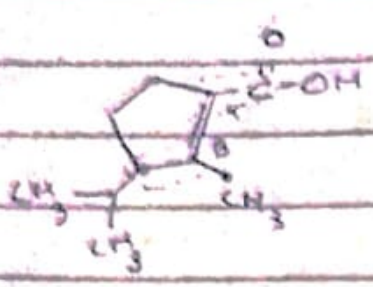
(a) 

P.V = 202
Conj = 0
Exo = 0
Sub α = 10 β = 24
λ_{max} = 236nm

(b) 

(c) 

-COOH



P. value = 105 nm

Sub = α = 10 β = 24

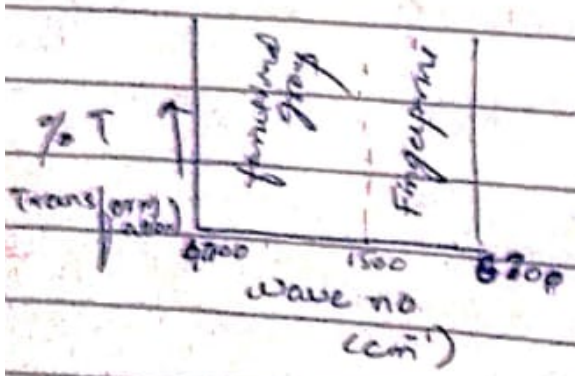
λ_{max} = 229 nm

λ_{max}

- acetaldehyde = 290nm
- acetic acid = 208nm
- amide $-\overset{O}{\overset{\|}{C}}-NH_2$ = 220nm
- Acid chloride = 220nm

Infrared Spectroscopy (F.T-IR)

- Fourier Transform Infrared Spectroscopy
- 670-4000 cm^{-1}
- Also called vibrational spectroscopy.
  Because in vibrational mode of atom molecules should be observed.



2- Regions
- fingerprint region (670-1500 cm^{-1})
- functional group region (1500-4000 cm^{-1})