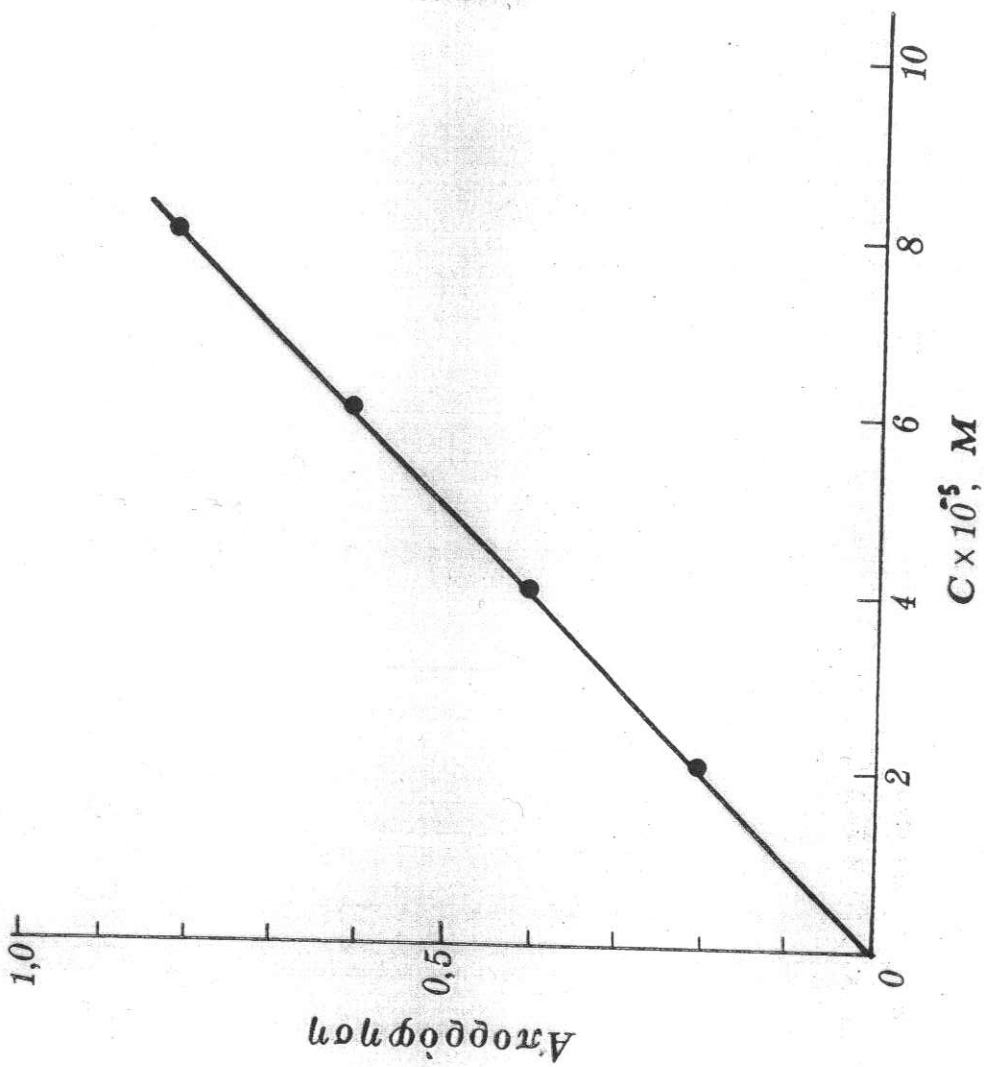
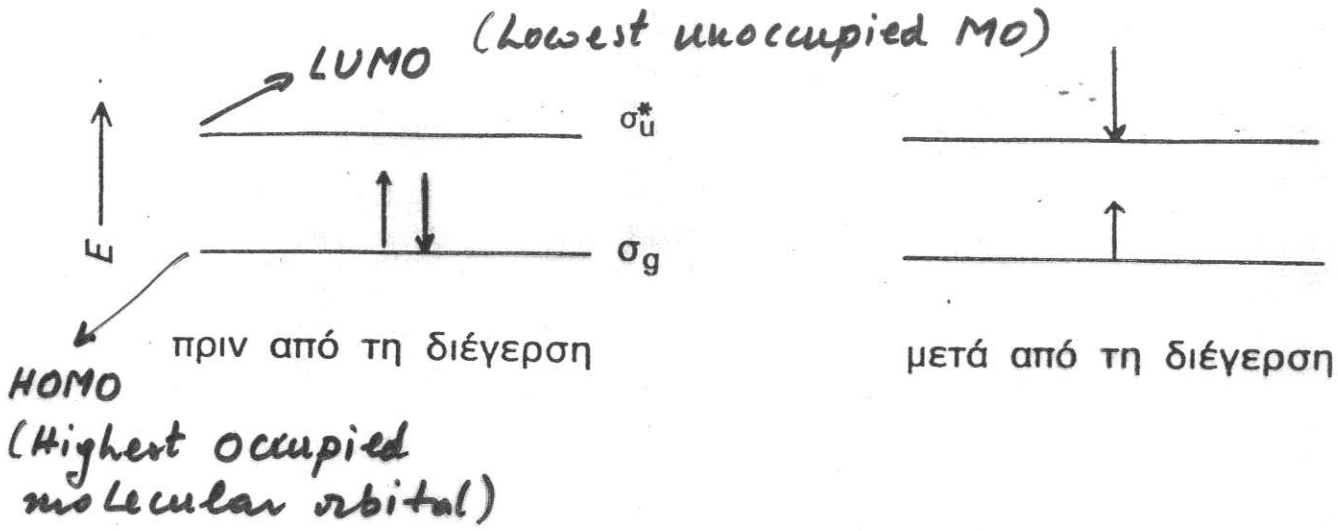
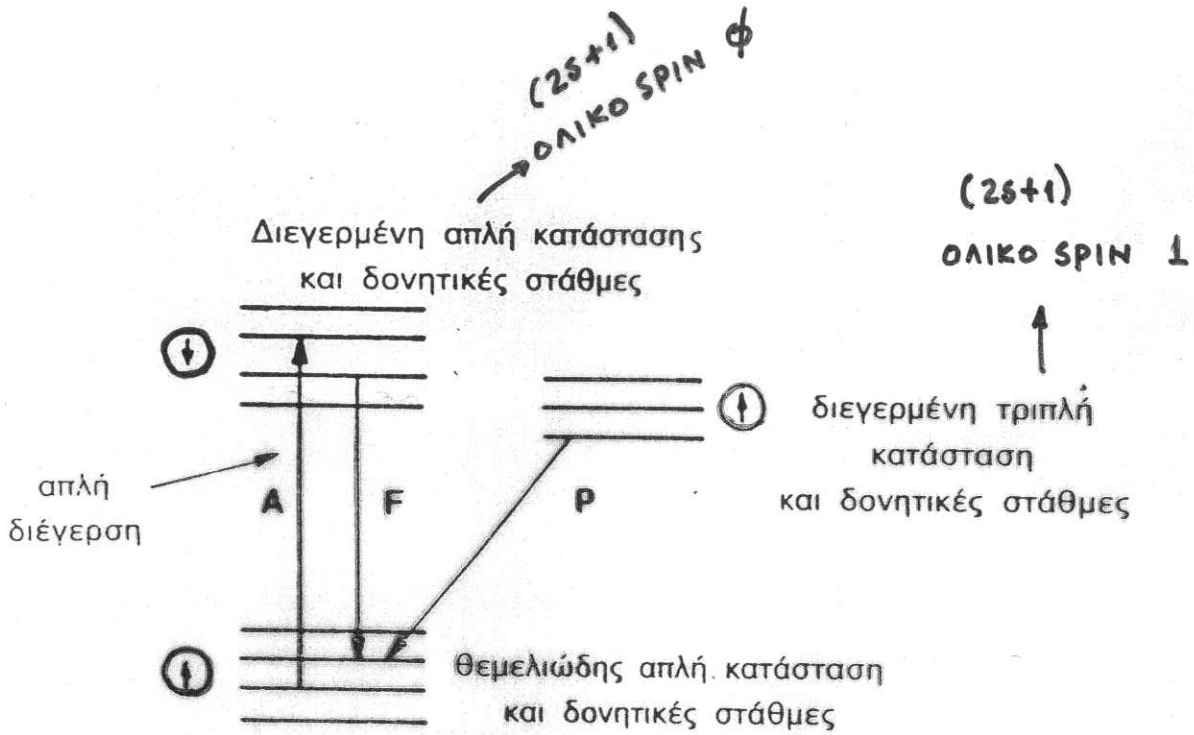
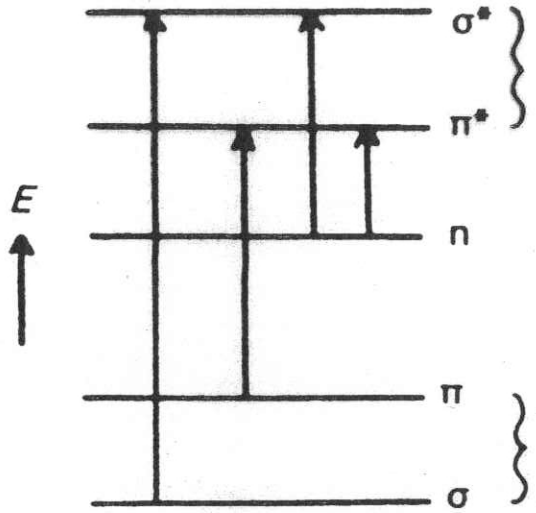

Απορρόφηση
1,0
0,5
0
2
4
6
8
10
C × 10^5, M





Τύποι ηλεκτρονικών διεγέρσεων - αποδιεγέρσεων.



Αντιδεσμικά τροχιακά $E = \alpha - x\beta$

μη δεσμικό τροχιακό $E = \alpha$

Δεσμικά τροχιακά $E = \alpha + x\beta$

Συνηθισμένοι τύποι ηλεκτρονικών διεγέρσεων.

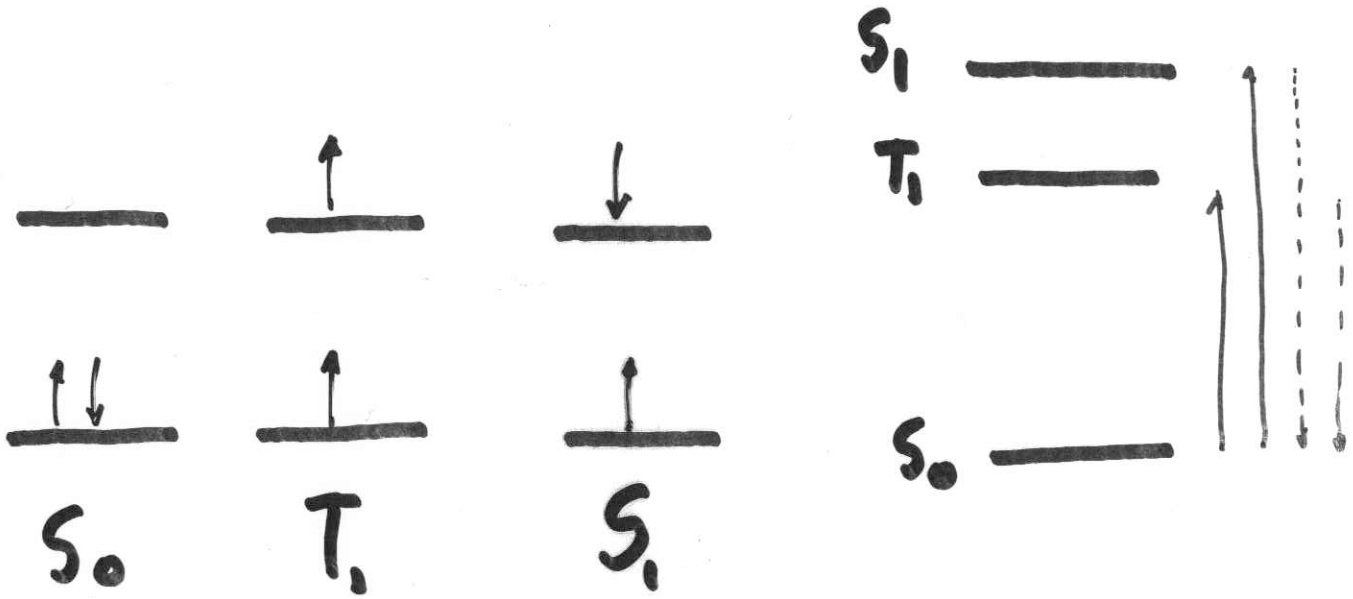
Κανόνες επιλογής

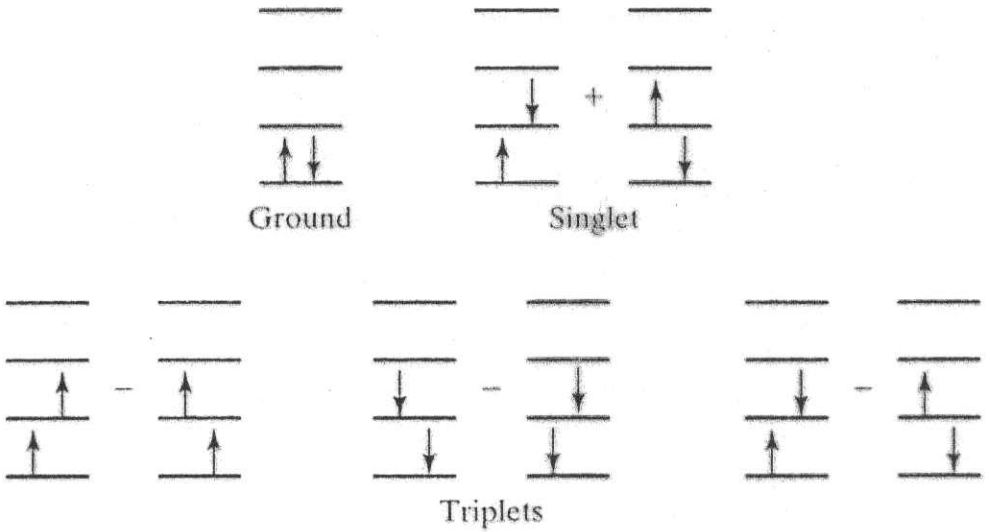
(1) Το συνολικό spin και η πολλαπλότητα spin $(2S+1)$ δεν θα πρέπει να μεταβάλλονται κατά τη μετάπτωση.

Επιτρέπονται: $S \rightarrow S$, $T \rightarrow T$

(2) Αποκλεισμός μεταπτώσεων μεταξύ συμμετρικών τροχιακών (symmetry exclusion - κανόνας Laporte)

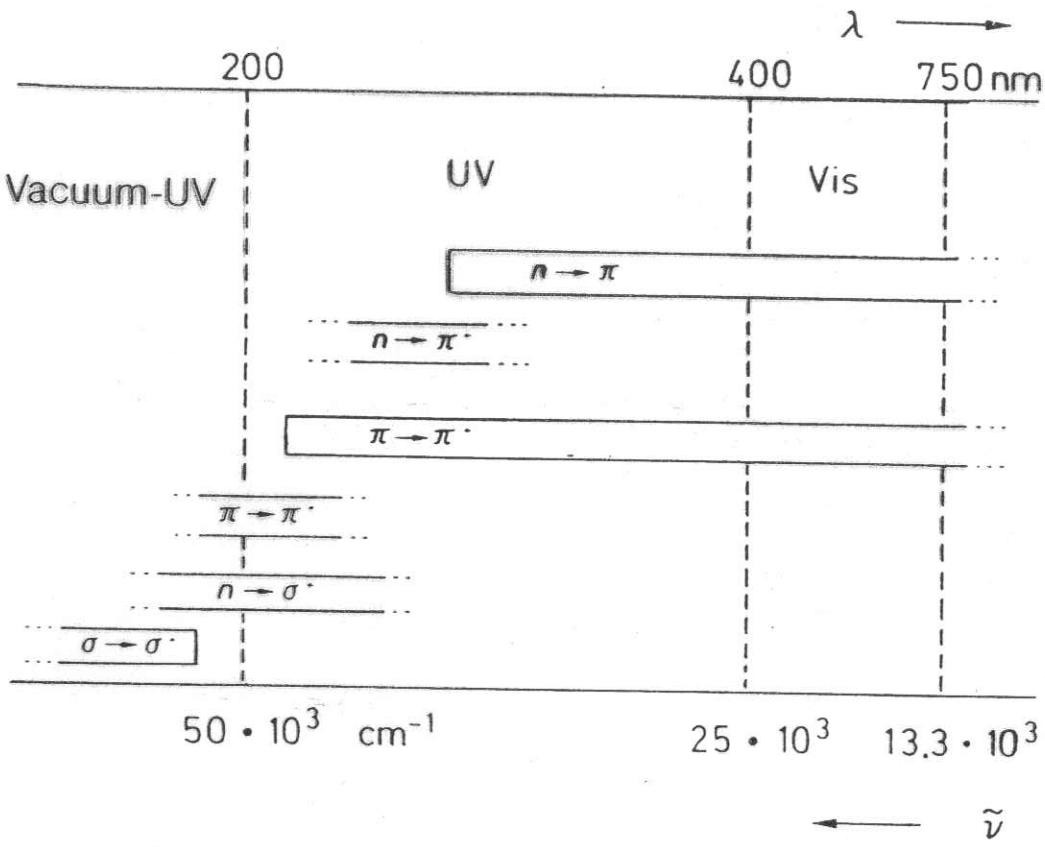
Επιτρέπονται: $g \rightarrow u$, $u \rightarrow g$


S1
T1
S0
S0
T1
S1

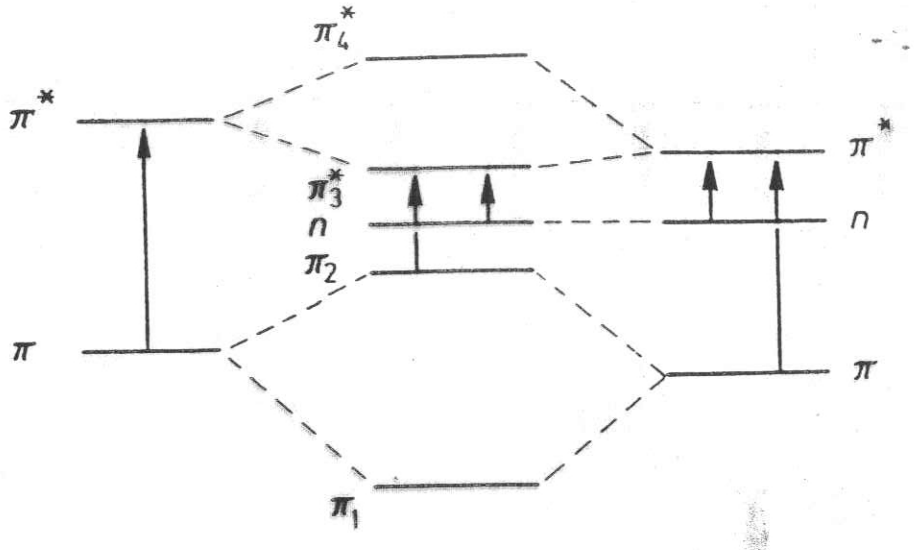


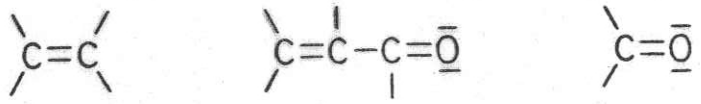
H_2

Diagrams for the space parts of the ground state, first singlet state, and first triplet states (three) for the hydrogen molecule. The signs are for the space parts with the spins denoted by the direction of the arrows.



Absorption regions of various electron transitions





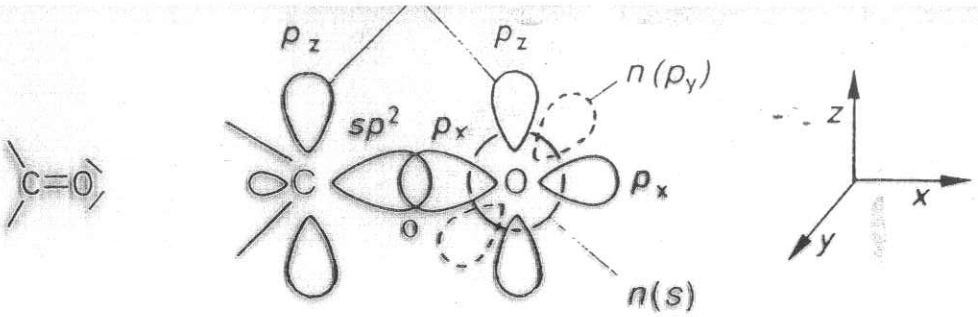
Energy diagram of the electronic transitions in conjugated enones compared to alkenes and saturated carbonyl compounds

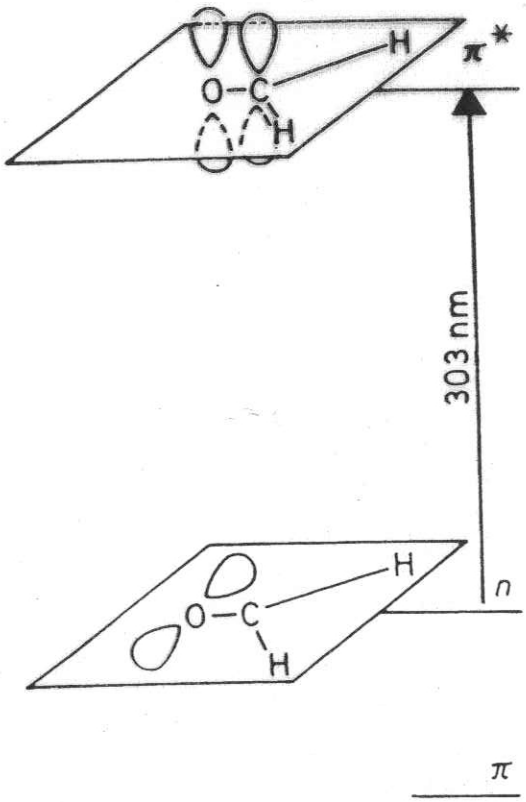
Absorption maxima of the long wavelength $\pi \rightarrow \pi^*$ transition in the vinylogous series $C_6H_5-(CH=CH)_n-CO-R$ (in methanol)

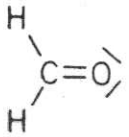
n	R = H		R = C_6H_5	
	λ_{max} (nm)	ε_{max}	λ_{max} (nm)	ε_{max}
0	244	12000	254	20000
1	285	25000	305	25000
2	323	43000	342	39000
3	355	54000	373	46000
4	382	51000	400	60000

Absorptions of isolated chromophoric groups (lowest energy transitions)

Chromophore	Transition	Example	λ_{max} [a] (nm)	ε_{max} [a]
C–H	$\sigma \rightarrow \sigma^*$	CH_4	122	strong
C–C	$\sigma \rightarrow \sigma^*$	$H_3C—CH_3$	135	strong
–$\bar{O}$–	$n \rightarrow \sigma^*$	H_2O	167	1500
	$n \rightarrow \sigma^*$	$H_3C—OH$	183	200
	$n \rightarrow \sigma^*$	$C_2H_5—O—C_2H_5$	189	2000
–$\bar{S}$–	$n \rightarrow \sigma^*$	$H_3C—SH$	235	180
	$n \rightarrow \sigma^*$	$H_3C—S—CH_3$	228	620
	$n \rightarrow \sigma^*$	$C_2H_5—S—S—C_2H_5$	250	380
–$\bar{N}$–	$n \rightarrow \sigma^*$	NH_3	194	5700
	$n \rightarrow \sigma^*$	$C_2H_5—NH_2$	210	800
	$n \rightarrow \sigma^*$	$C_2H_5—NH—C_2H_5$	193	3000
	$n \rightarrow \sigma^*$	$(C_2H_5)_3N$	213	6000
–Hal	$n \rightarrow \sigma^*$	$H_3C—Cl$	173	200
	$n \rightarrow \sigma^*$	$H_3C—Br$	204	260
	$n \rightarrow \sigma^*$	$H_3C—I$	258	380
	$n \rightarrow \sigma^*$	CHI_3	349	2170
C=C	$\pi \rightarrow \pi^*$	$H_2C=CH_2$	165	16000
	$\pi \rightarrow \pi^*$	$C_2H_5—CH=CH—C_2H_5$	185	7940
–C≡C–	$\pi \rightarrow \pi^*$	$HC\equiv CH$	173	6000
	$\pi \rightarrow \pi^*$	$H—C\equiv C—C_2H_5$	172	2500
C=$\bar{O}$	$n \rightarrow \pi^*$	$H_3C—CH=O$	293	12
	$\pi \rightarrow \pi^*$	$H_3C—\overset{\overset{O}{\|\|}}{C}—CH_3$	187	950
	$n \rightarrow \pi^*$	$H_3C—\overset{\overset{O}{\|\|}}{C}—CH_3$	273	14
C=$\bar{S}$	$n \rightarrow \pi^*$	$H_3C—\overset{\overset{S}{\|\|}}{C}—CH_3$	460	weak
C=$\bar{N}$–	$\pi \rightarrow \pi^*$	$H_3C—CH=N—OH$	190	8000
	$n \rightarrow \pi^*$	$H_3C—CH=N—OH$	279	15
–$\bar{N}$=$\bar{N}$–	$n \rightarrow \pi^*$	$H_3C—N=N—CH_3$	353	240
		$H_3C—N=N—CH_3$	343	25
–$\bar{N}$=$\bar{O}$	$n \rightarrow \pi^*$	$(H_3C)_3C—NO$	300	100
		$(H_3C)_3C—NO$	665	20





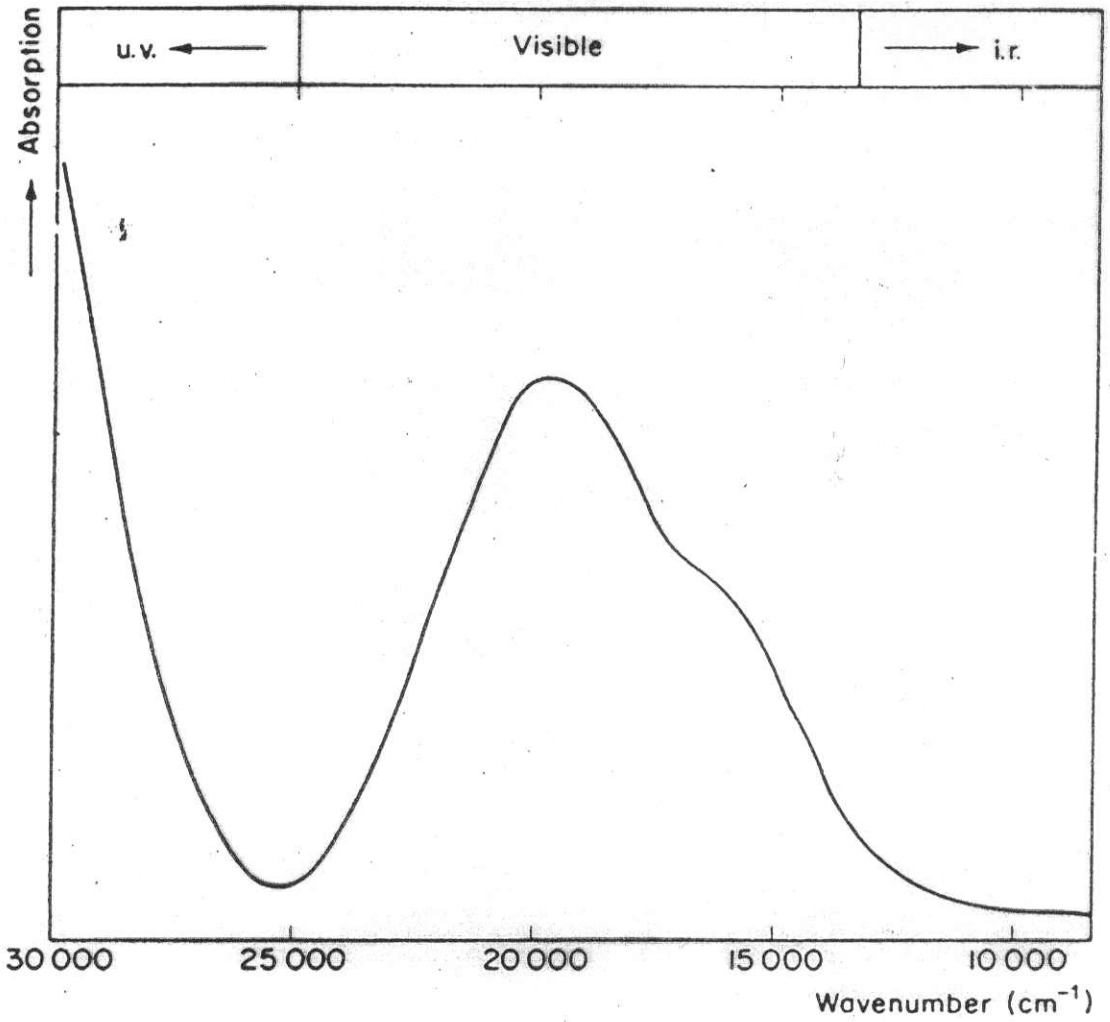


λ_{max} = 303 nm

ε_{max} = 18

$n \rightarrow \pi^*$ Transitions in saturated carbonyl compounds

Compounds	λ_{max} (nm)	ε_{max}	Solvents
Acetaldehyde	293	12	Hexane
Acetone	279	15	Hexane
Acetyl chloride	235	53	Hexane
Acetic anhydride	225	50	Isooctane
Acetamide	205	160	Methanol
Acetic acid ethyl ester	207	70	Petrol ether
Acetic acid	204	41	Ethanol



The visible absorption spectrum of the $[Ti(H_2O)_6]^{3+}$ ion