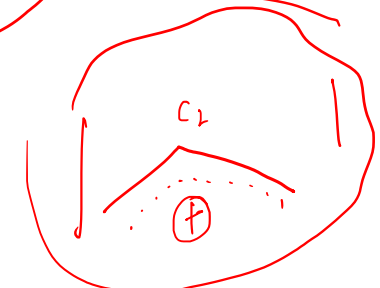
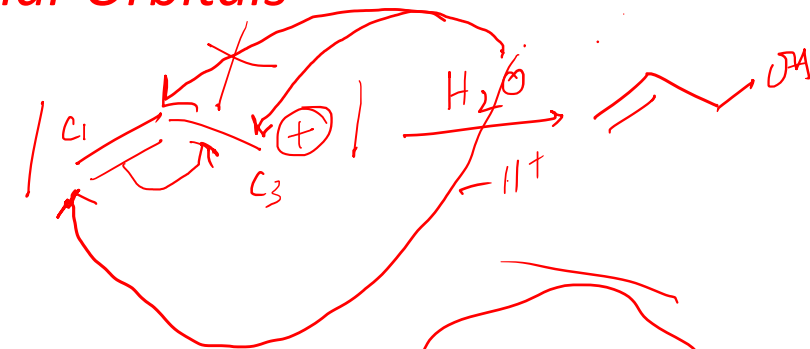
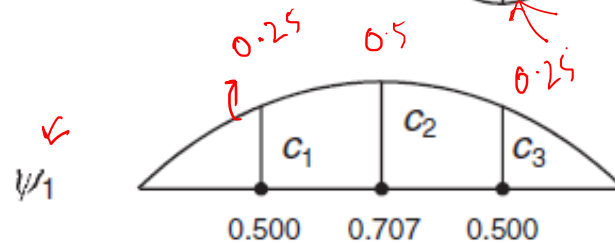
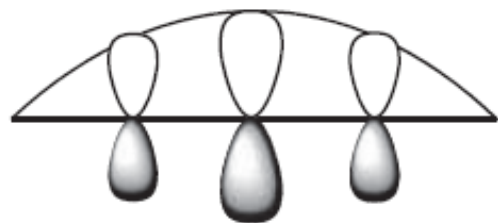
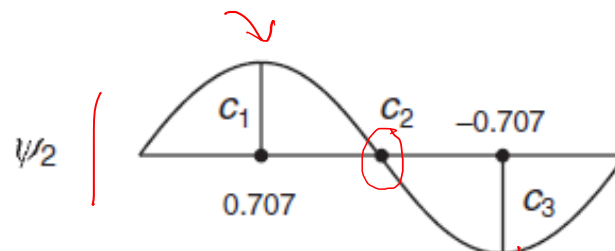
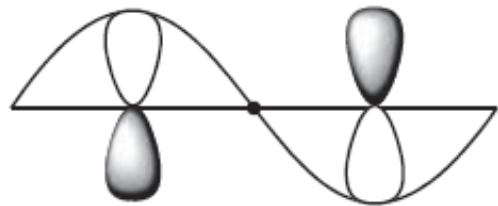
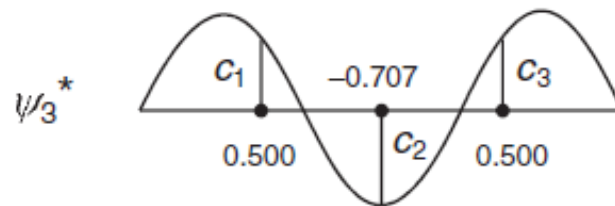
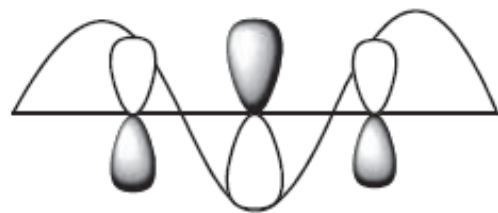
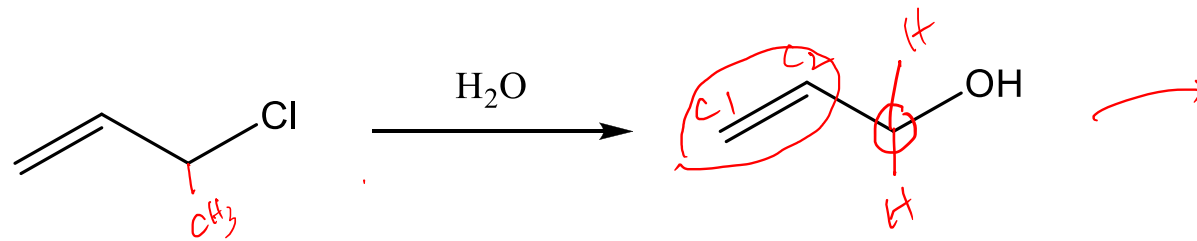
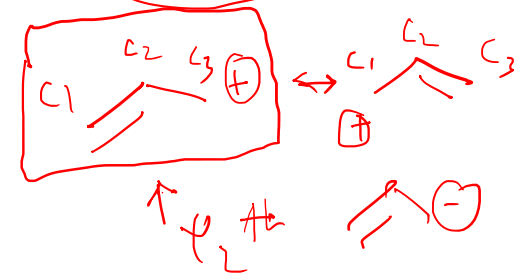


# Regioselectivity Prediction through Molecular Orbitals



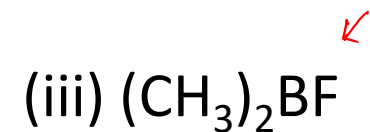
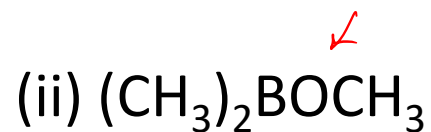
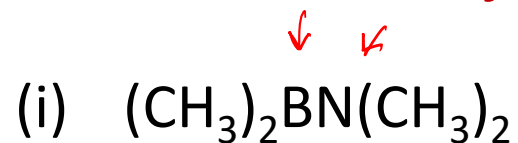
LUMO



HOMO

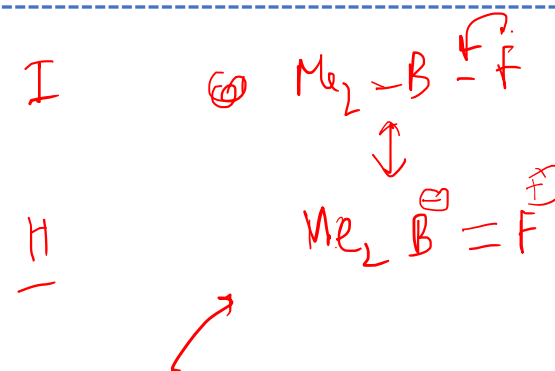
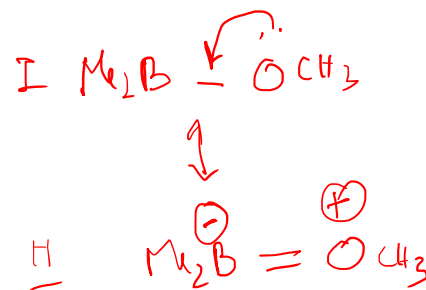
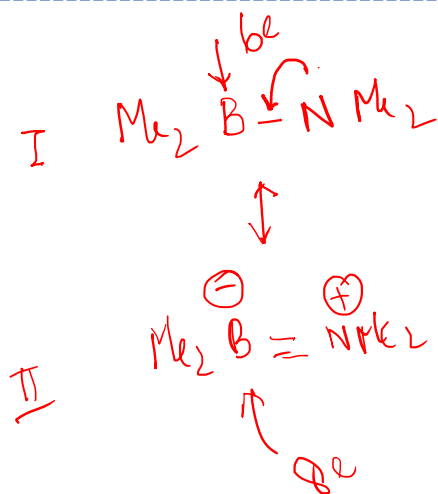
$\psi_1$

Q. Two resonance forms can be written for each of the following structures:



(A) Write the resonance structures

(B) Which forms in each pair of resonance forms is more important?



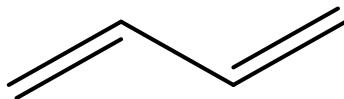
### *A few key points regarding resonance structures*

- ✓ Only electrons move. Atoms never move
- ✓ Only  $\pi$ -electrons (electrons in  $\pi$ -bonds) and lone-pair electrons can move; never move  $\sigma$ -electrons
- ✓ Resonance forms with filled octets are more stable
- ✓ Negative charge should reside on more electronegative atom, positive charge on electropositive atom

## Effect of Conjugation on the $\pi$ -MOs



**Ethylene**

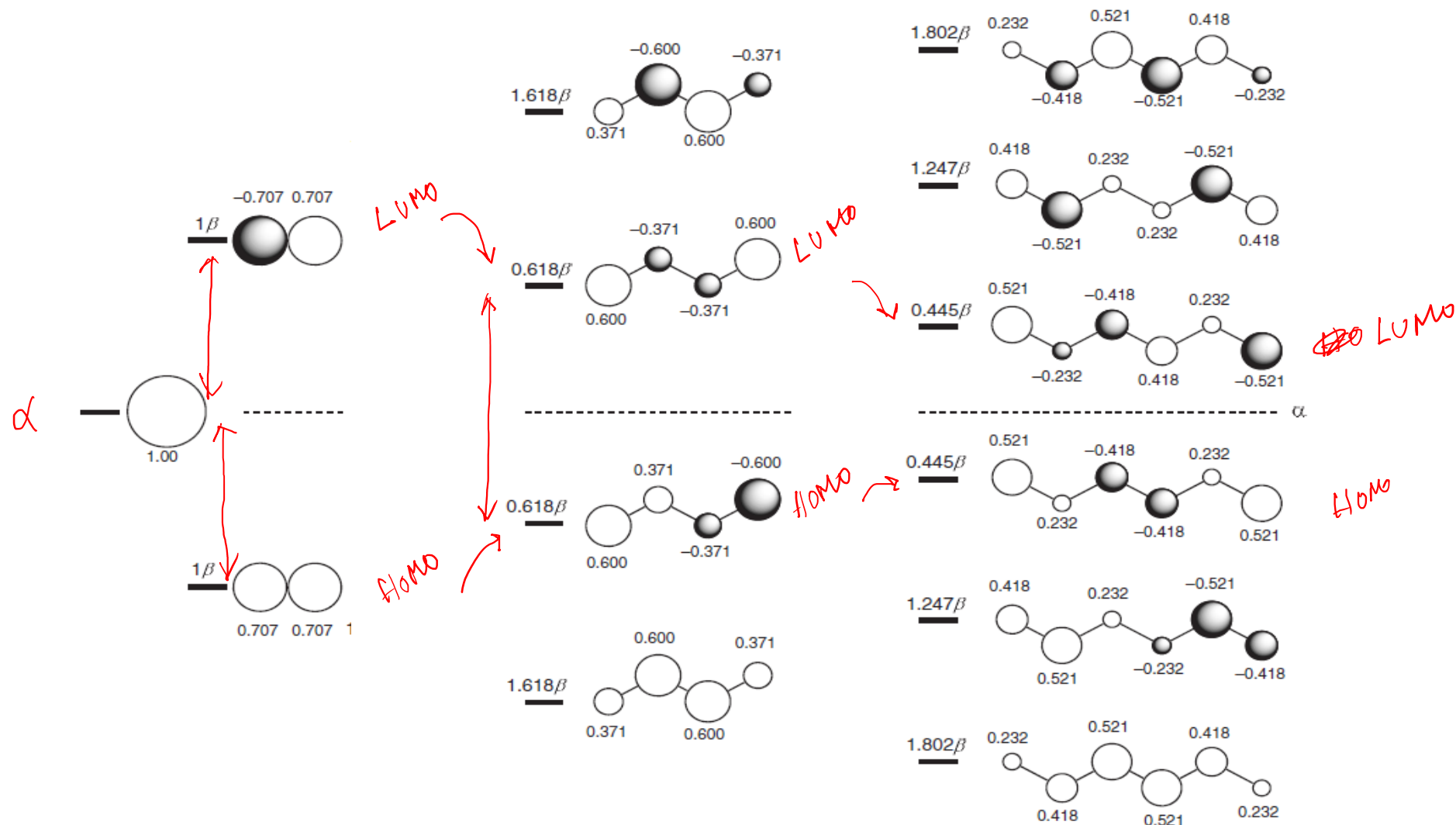


**Butadiene**



**Hexatriene**

- ✓ We have discussed the bonding in ethylene and butadiene
- ✓ As we keep on increasing the number of double bonds in conjugation, what kind of changes do we observe on the  $\pi$ -MOs (especially HOMO and LUMO)?



Ethylene

Butadiene

Hexatriene

HOMO-LUMO gap:

$2\beta$

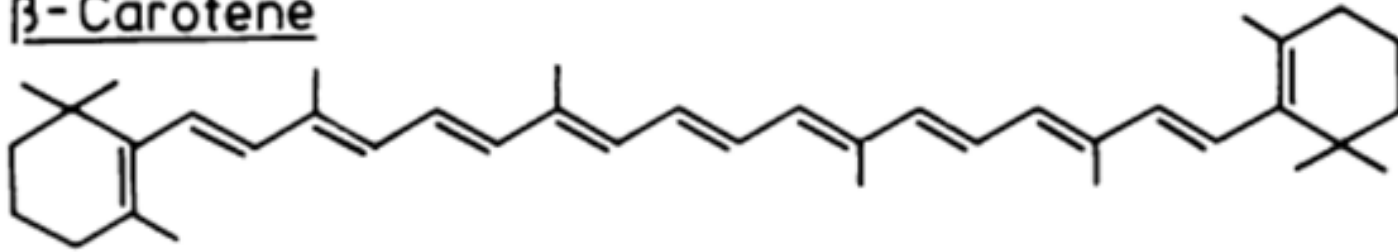
$1.236\beta$

$0.89\beta$

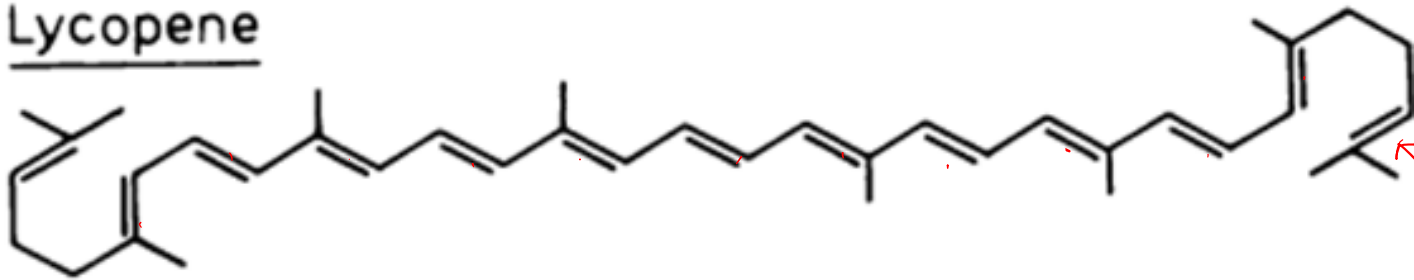
## Delocalization and Conjugation

- An increase in the number of double bonds in conjugation leads to decrease in HOMO-LUMO gap

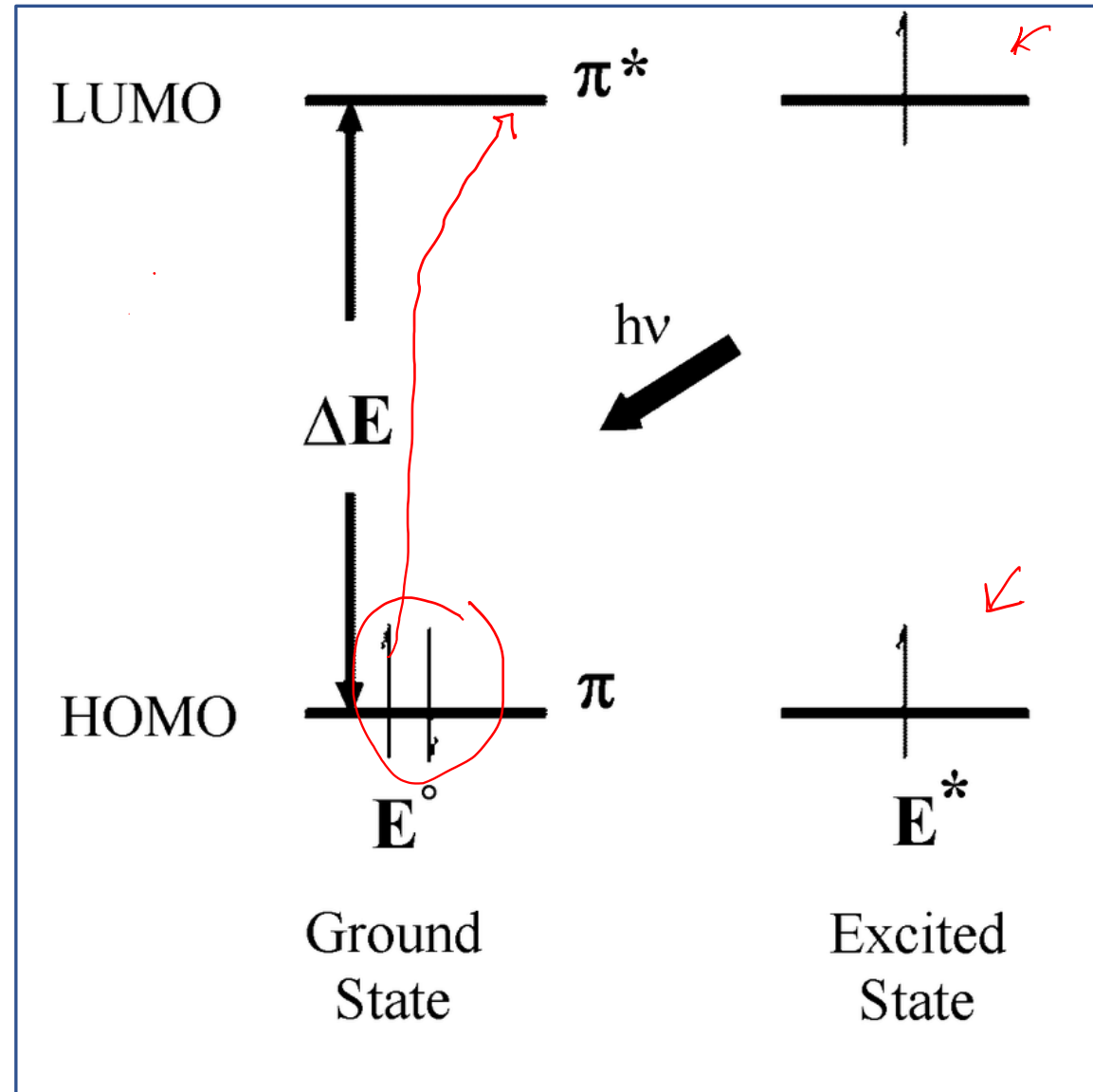
$\beta$ -Carotene



Lycopene

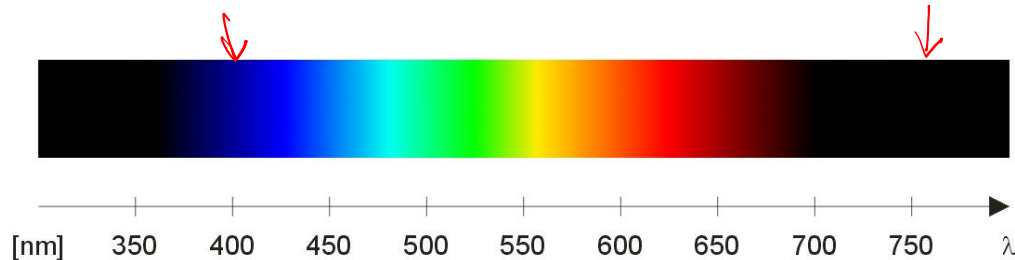


- ✓ Irradiation of light results in the excitation of an electron from HOMO to LUMO



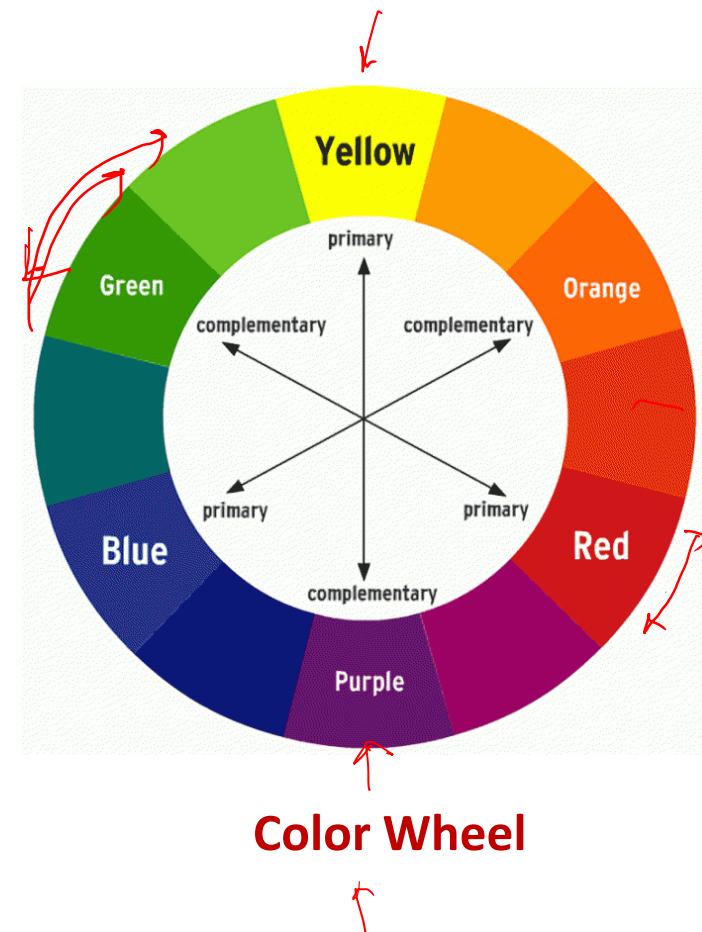
$$\Delta E = h\nu$$
$$= h \frac{c}{\lambda}$$

✓ The color is originated only when the number of double bonds in conjugation is 8 or more



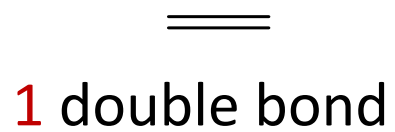
### Approximate wavelengths for different colours

Absorbed frequency, nm	Colour absorbed	Colour transmitted	$R(\text{CH}=\text{CH})_n\text{R}, n =$
200–400	ultraviolet	—	$< 8$
400	violet	yellow-green	8
425	indigo-blue	yellow	9
450	blue	orange	10
490	blue-green	red	11
510	green	purple	
530	yellow-green	violet	
550	yellow	indigo-blue	
590	orange	blue	
640	red	blue-green	

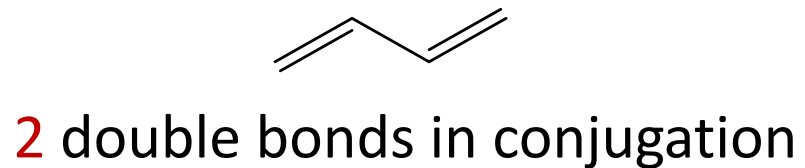




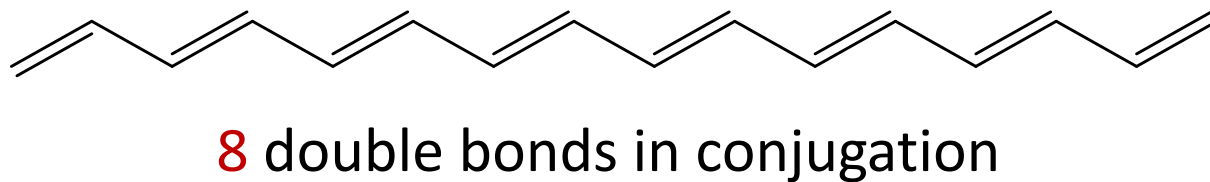
## Absorption



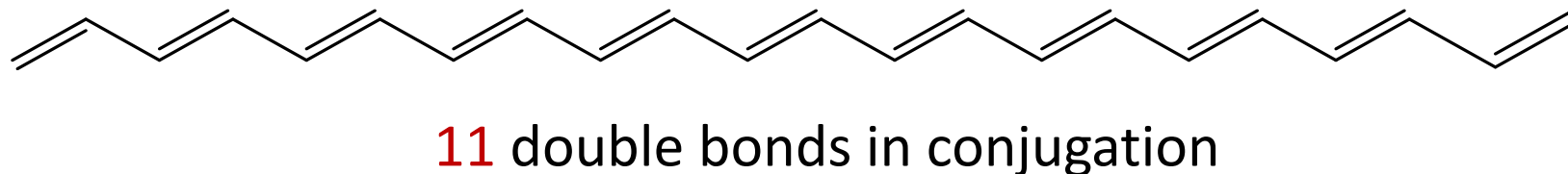
185 nm



215 nm



400 nm



490 nm