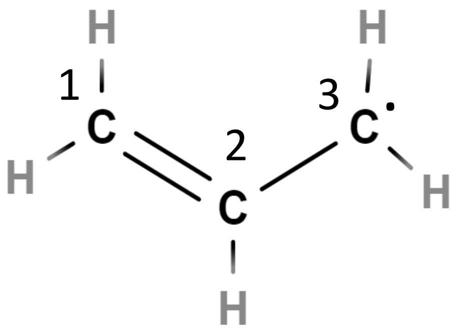
MO di tipo π in idrocarburi
Metodo di Hückel

Radicale allile



Equazione secolare: $\begin{vmatrix} \alpha - E & \beta & 0 \\ \beta & \alpha - E & \beta \\ 0 & \beta & \alpha - E \end{vmatrix} = 0$

$$+\begin{vmatrix} \alpha - E & \beta & 0 \\ \beta & \alpha - E & \beta \\ 0 & \beta & \alpha - E \end{vmatrix} \begin{matrix} \alpha - E & \beta \\ \beta & \alpha - E \\ 0 & \beta \end{matrix} \quad - \begin{vmatrix} \alpha - E & \beta & 0 \\ \beta & \alpha - E & \beta \\ 0 & \beta & \alpha - E \end{vmatrix} \begin{matrix} \alpha - E & \beta \\ \beta & \alpha - E \\ 0 & \beta \end{matrix} \quad =$$

$$= +(\alpha - E)^3 + 0 + 0 - 0 - \beta^2(\alpha - E) - \beta^2(\alpha - E) =$$

$$= +(\alpha - E)^3 - 2\beta^2(\alpha - E) = 0$$

Divido per β^3

$$+\frac{(\alpha - E)^3}{\beta^3} - 2\frac{(\alpha - E)}{\beta} = 0$$

Sostituzione con $\mathrm{x} = \frac{(\alpha - E)}{\beta}$

$$+x^3 - 2x = 0$$

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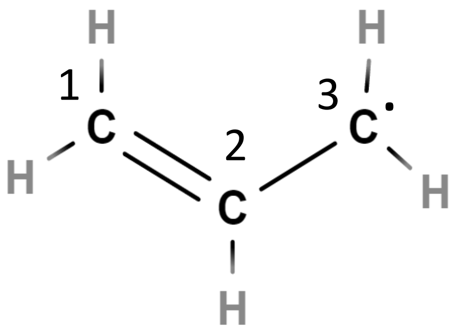


Equazione secolare: $\begin{vmatrix} \alpha - E & \beta & 0 \\ \beta & \alpha - E & \beta \\ 0 & \beta & \alpha - E \end{vmatrix} = 0$

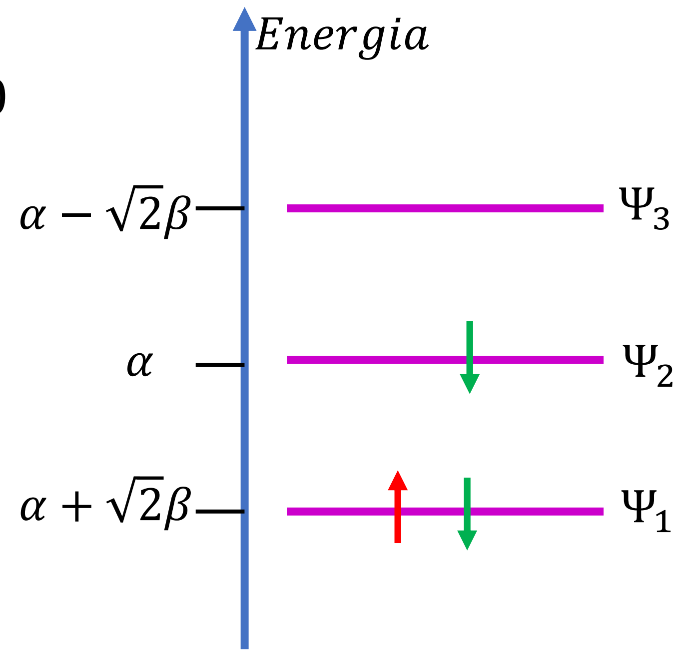
$= +$Sostituzione con $\mathrm{x} = \frac{(\alpha - E)}{\beta}$

$$+x^3 - 2x = 0$$

$x_1 = -\sqrt{2}$ $\qquad E_1 = \alpha + \sqrt{2}\beta$

$x_2 = 0$ $\qquad E_2 = \alpha$

$x_3 = +\sqrt{2}$ $\qquad E_3 = \alpha - \sqrt{2}\beta$



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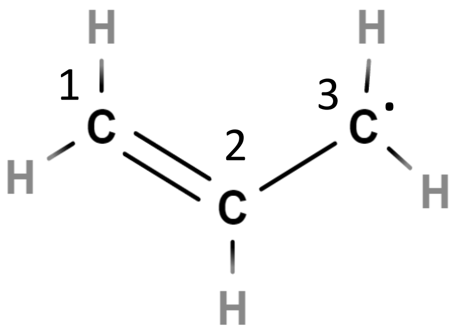

Equazione secolare: $\begin{vmatrix} \alpha - E & \beta & 0 \\ \beta & \alpha - E & \beta \\ 0 & \beta & \alpha - E \end{vmatrix} = 0$

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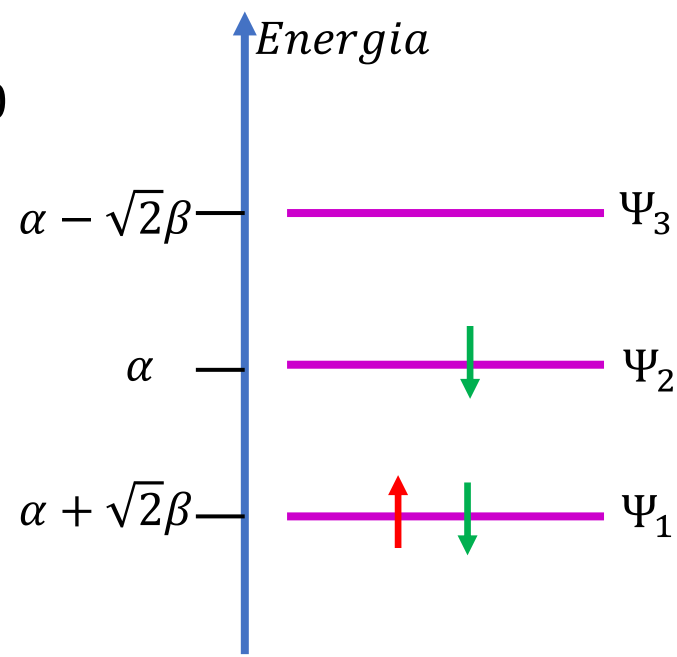
$$+x^3 - 2x = 0$$

$$x_1 = -\sqrt{2} \qquad E_1 = \alpha + \sqrt{2}\beta$$
$$x_2 = 0 \qquad E_2 = \alpha$$
$$x_3 = +\sqrt{2} \qquad E_3 = \alpha - \sqrt{2}\beta$$



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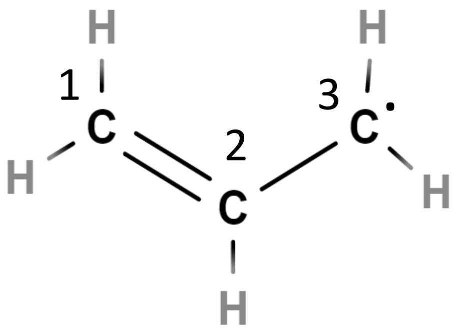
Radicale allile



Equazione secolare:
$$\begin{vmatrix} \alpha - E & \beta & 0 \\ \beta & \alpha - E & \beta \\ 0 & \beta & \alpha - E \end{vmatrix} = 0$$

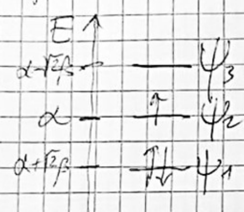
$+(\alpha-E)^3+0+0-0-\beta^2(\alpha-E)-\beta^2(\alpha-E)=$

$=(\alpha-E)^3-2\beta^2(\alpha-E)=0 \qquad x=\dfrac{\alpha-E}{\beta}$

tutto diviso per β^3

$\dfrac{(\alpha-E)^3}{\beta^3}-2\dfrac{\alpha-E}{\beta}=0 \qquad x^3-2x=0$

$x_1=-\sqrt{2} \quad E_1=\alpha+\sqrt{2}\beta$
$x_2=0 \quad E_2=\alpha$
$x_3=+\sqrt{2} \quad E_3=\alpha-\sqrt{2}\beta$



$E_{tot-\pi}=2\alpha+2\sqrt{2}\beta+\alpha$
$=3\alpha+2\sqrt{2}\beta$

ORBITALI MOLECOLARI

$\psi_1 \quad (E_1=\alpha+\sqrt{2}\beta)$

dividiamo per β

$$\begin{vmatrix} \alpha-\alpha-\sqrt{2}\beta & \beta & 0 \\ \beta & \alpha-\alpha-\sqrt{2}\beta & \beta \\ 0 & \beta & \alpha-\alpha-\sqrt{2}\beta \end{vmatrix} \rightarrow \begin{pmatrix} -\sqrt{2} & 1 & 0 \\ 1 & -\sqrt{2} & 1 \\ 0 & 1 & -\sqrt{2} \end{pmatrix}$$

$$\begin{cases} -\sqrt{2}c_1+c_2=0 \\ c_1-\sqrt{2}c_2+c_3=0 \\ +c_2-\sqrt{2}c_3=0 \end{cases} \qquad \begin{cases} c_2=\sqrt{2}c_1 \\ \\ \sqrt{2}c_1-\sqrt{2}c_3=0 \end{cases} \qquad c_2=\sqrt{2}c \quad c_1=c_3=c$$

$\psi_1=c\varphi_1+\sqrt{2}c\varphi_2+c\varphi_3$

IMPONIAMO LA NORMALIZZAZIONE

$1=1\cdot c^2+2c^2+1\cdot c^2=4c^2 \qquad c=\pm 2^{-1}=\pm\frac{1}{2}$

$\psi_1=\frac{1}{2}\varphi_1+\frac{\sqrt{2}}{2}\varphi_2+\frac{1}{2}\varphi_3$

$\int\psi_1^*\psi_1\,d\tau=1=\int c^2\varphi_1^*\varphi_1\,d\tau+2\int c^2\varphi_2^*\varphi_2\,d\tau$ ($c^2\cdot 1$, $2\cdot c^2$)
$+\int c^2\varphi_3^*\varphi_3\,d\tau$ ($1\cdot c^2$)
+ termini nulli perché contengono $\int\varphi_i^*\varphi_j\,d\tau=0$
in altre[...]