HMO Betrachtung von Ethen

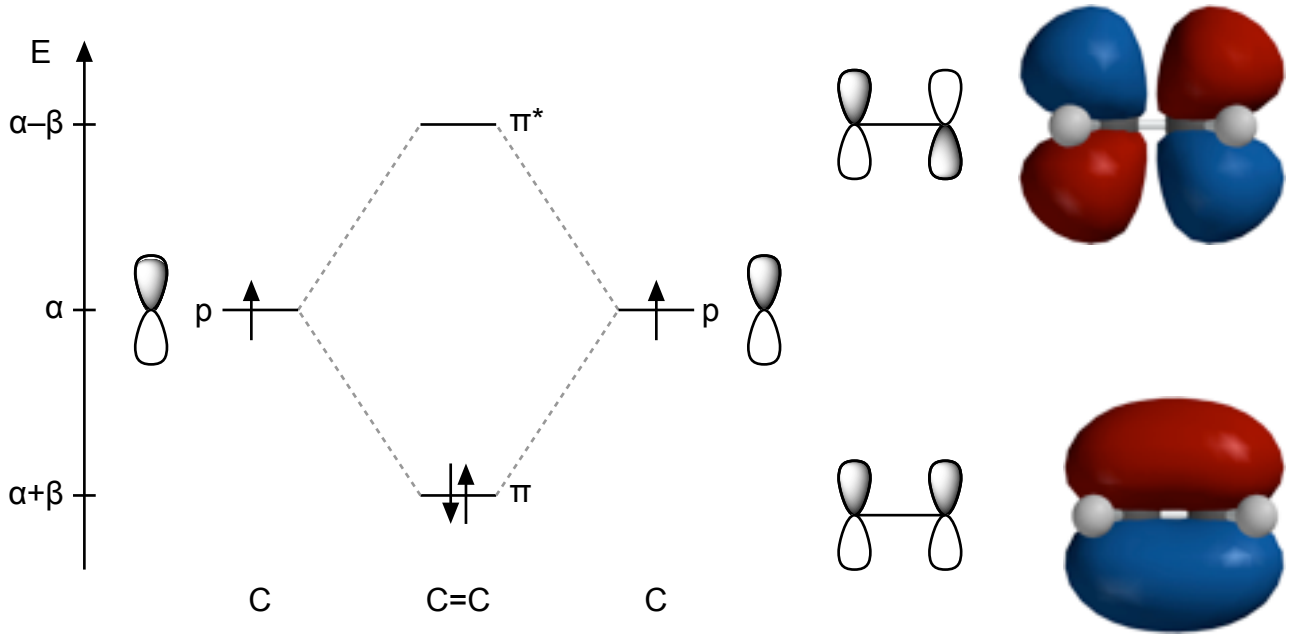
Säkulardeterminante

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

Lösungen

$$E_1 = \alpha + \beta$$
$$E_2 = \alpha - \beta$$

Termschema



Säkulargleichungen

$$c_A(\alpha - E) + c_B\beta = 0$$
$$c_A\beta + c_B(\alpha - E) = 0$$

Lösungen

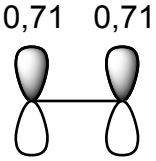
$$c_A = c_B$$
$$c_A = -c_B$$

Wellenfunktionen

$$\psi_1 = c_A\Phi_A + c_A\Phi_B$$
$$\psi_2 = c'_A\Phi_A - c'_A\Phi_B$$

Orbitalkoeffizienten

$$c_A = \sqrt{0{,}5}$$



$$c'_A = \sqrt{0{,}5}$$