

HMO Betrachtung von Benzol

Säkulardeterminante

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

Lösungen

$$E_1 = \alpha + 2\beta$$

$$E_{2/3} = \alpha + \beta$$

$$E_{4/5} = \alpha - \beta$$

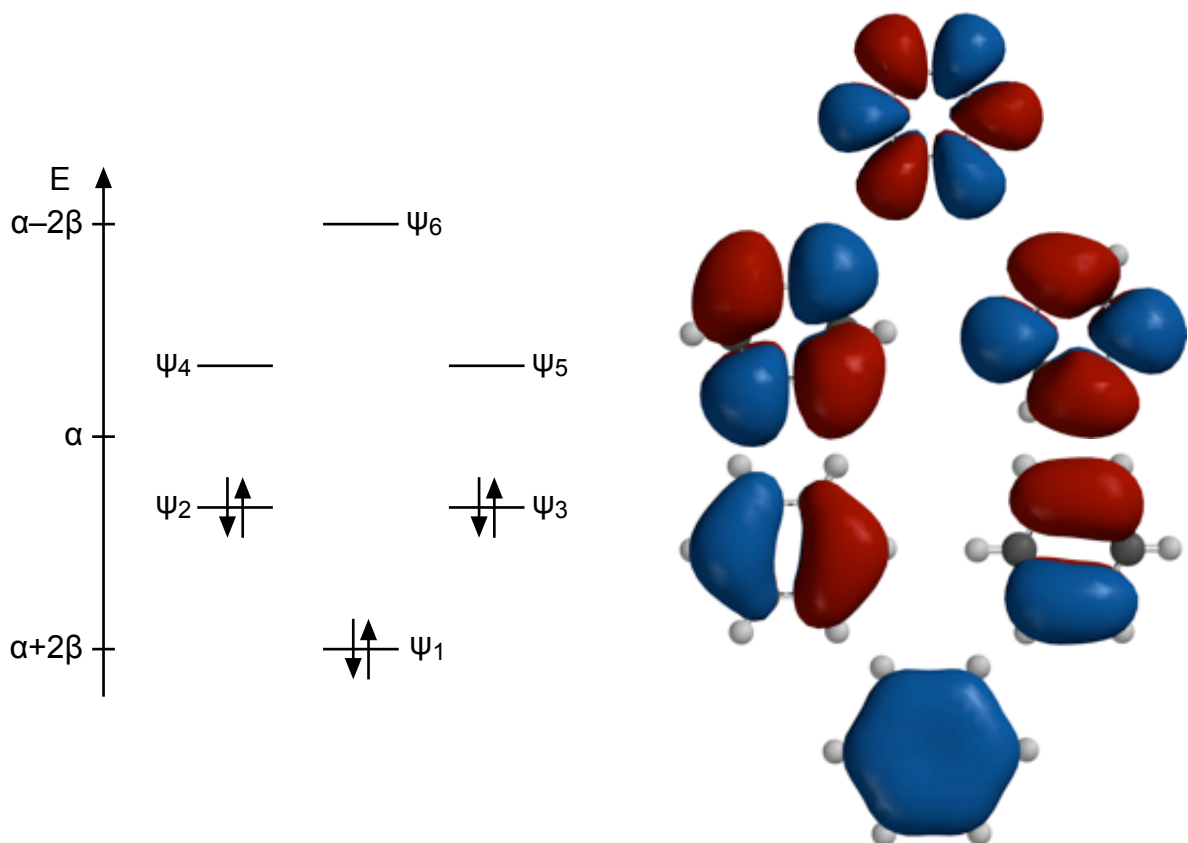
$$E_6 = \alpha - 2\beta$$

Berechnung der Energieniveaus cyclischer konjugierter Polyene beliebiger Ringgröße:

$$E = \alpha + 2\beta \cos \frac{360^\circ r}{n}$$

$$n = \text{Ringgröße}, r = 0, 1, 2 \dots n - 1$$

Termschema



Säkulargleichungen

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

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

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

$$c_C\beta + c_D(\alpha - E) + c_E\beta = 0$$

$$c_D\beta + c_E(\alpha - E) + c_F\beta = 0$$

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

Wellenfunktionen

$$\psi_1 = c_A\Phi_A + c_A\Phi_B + c_A\Phi_C + c_A\Phi_D + c_A\Phi_E + c_A\Phi_F$$

$$\psi_2 = 2c'_A\Phi_A + c'_A\Phi_B - c'_A\Phi_C - 2c'_A\Phi_D - c'_A\Phi_E + c'_A\Phi_F$$

$$\psi_3 = c''_A\Phi_B + c''_A\Phi_C - c''_A\Phi_E - c''_A\Phi_F$$

$$\psi_4 = c''_A\Phi_B - c''_A\Phi_C + c''_A\Phi_E - c''_A\Phi_F$$

$$\psi_5 = 2c'_A\Phi_A - c'_A\Phi_B - c'_A\Phi_C + 2c'_A\Phi_D - c'_A\Phi_E - c'_A\Phi_F$$

$$\psi_6 = c_A\Phi_A - c_A\Phi_B + c_A\Phi_C - c_A\Phi_D + c_A\Phi_E - c_A\Phi_F$$

Orbitalkoeffizienten

$$c_A = \sqrt{\frac{1}{6}}$$

$$c'_A = \sqrt{\frac{1}{12}}$$

$$c''_A = 0,5$$

