HMO Betrachtung von 1,3,5-Hexatrien

Säkulardeterminante

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

Lösungen

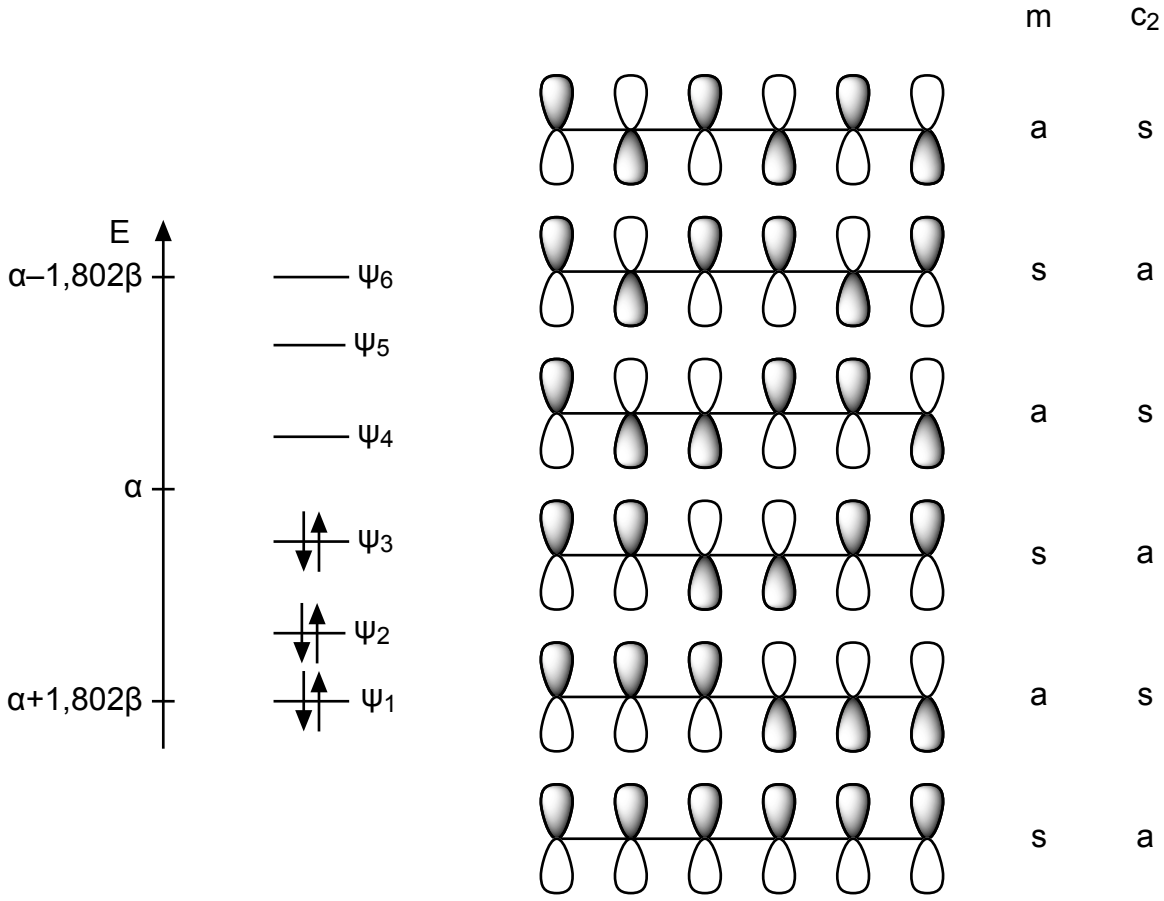
$$E_1 = \alpha + 1{,}802\beta$$
$$E_2 = \alpha + 1{,}247\beta$$
$$E_3 = \alpha + 0{,}445\beta$$
$$E_4 = \alpha - 0{,}445\beta$$
$$E_5 = \alpha - 1{,}247\beta$$
$$E_6 = \alpha - 1{,}802\beta$$

Berechnung der Energieniveaus linearer konjugierter Polyene beliebiger Länge:

$$E = \alpha + 2\beta \cos\frac{180\,r}{n+1}$$

n = Länge der konjugierten Kette, *r* = 1,2,3 ... n

Termschema



vereinfachte Darstellung mit Atomorbitalen

Säkulargleichungen

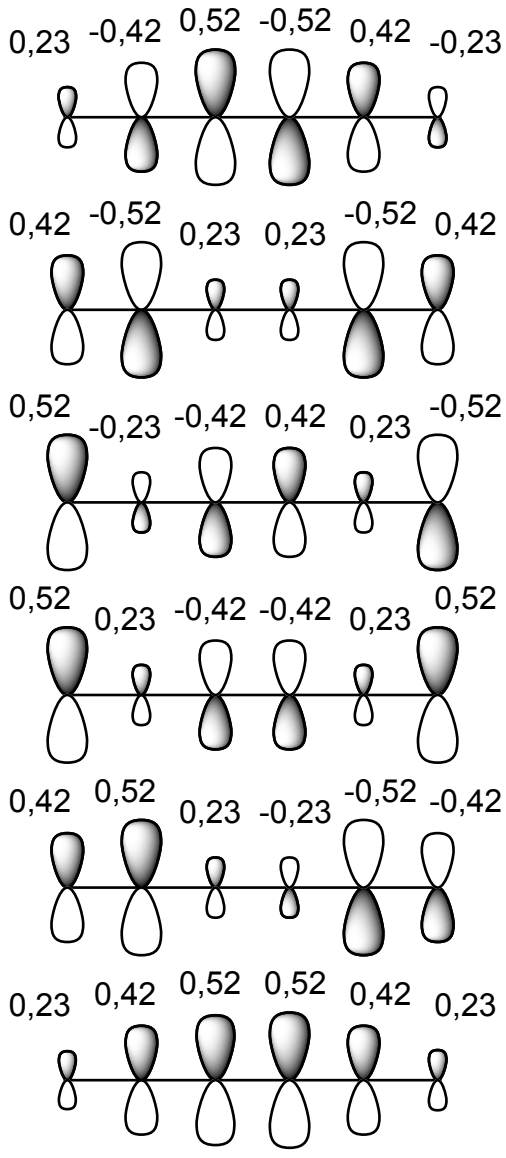
$$c_A(\alpha - E) + c_B\beta = 0$$
$$c_A\beta + c_B(\alpha - E) + c_C\beta = 0$$
$$c_B\beta + c_C(\alpha - E) + c_D\beta = 0$$
$$c_C\beta + c_D(\alpha - E) + c_E\beta = 0$$
$$c_D\beta + c_E(\alpha - E) + c_F\beta = 0$$
$$c_E\beta + c_F(\alpha - E) = 0$$

Wellenfunktionen

$$\psi_1 = c_A\Phi_A + 1{,}802c_A\Phi_B + 2{,}247c_A\Phi_C + 2{,}247c_A\Phi_D + 1{,}802c_A\Phi_E + c_A\Phi_F$$
$$\psi_2 = c'_A\Phi_A + 1{,}247c'_A\Phi_B + 0{,}555c'_A\Phi_C - 0{,}555c'_A\Phi_D - 1{,}247c'_A\Phi_E - c'_A\Phi_F$$
$$\psi_3 = c''_A\Phi_A + 0{,}445c''_A\Phi_B - 0{,}802c''_A\Phi_C - 0{,}802c''_A\Phi_D + 0{,}445c''_A\Phi_E + c''_A\Phi_F$$
$$\psi_4 = c''_A\Phi_A - 0{,}445c''_A\Phi_B - 0{,}802c''_A\Phi_C + 0{,}802c''_A\Phi_D + 0{,}445c''_A\Phi_E - c''_A\Phi_F$$
$$\psi_5 = c'_A\Phi_A - 1{,}247c'_A\Phi_B + 0{,}555c'_A\Phi_C + 0{,}555c'_A\Phi_D - 1{,}247c'_A\Phi_E + c'_A\Phi_F$$
$$\psi_6 = c_A\Phi_A - 1{,}802c_A\Phi_B + 2{,}247c_A\Phi_C - 2{,}247c_A\Phi_D + 1{,}802c_A\Phi_E - c_A\Phi_F$$

Orbitalkoeffizienten

$c_A = 0{,}232$ $\quad$ $c'_A = 0{,}418$ $\quad$ $c''_A = 0{,}521$



Berechnung der Orbitalkoeffizienten linearer konjugierter Polyene beliebiger Länge:

$$c_{jr} = \sqrt{\frac{2}{n+1}}\, sin\frac{180\, rj}{n+1}$$

j = Position des Kohlenstoffatoms in der Kette, *r* = Nummer des Molekülorbitals, *n* = Länge des konjugierten Systems