

Huckel Molecular Orbital Theory - Symbolic Approach

Enter and solve the **butadiene** Huckel determinant for energy eigenvalues:

$$\begin{vmatrix} \alpha - E & \beta & 0 & 0 \\ \beta & \alpha - E & \beta & 0 \\ 0 & \beta & \alpha - E & \beta \\ 0 & 0 & \beta & \alpha - E \end{vmatrix} = 0 \quad \left| \begin{array}{l} \text{solve, E} \\ \text{float, 4} \end{array} \right. \rightarrow \begin{pmatrix} \alpha + .6180 \cdot \beta \\ \alpha - 1.618 \cdot \beta \\ \alpha + 1.618 \cdot \beta \\ \alpha - .6180 \cdot \beta \end{pmatrix}$$

Calculate the eigenvectors:

$$\text{eigenvecs} \begin{pmatrix} \alpha - E & \beta & 0 & 0 \\ \beta & \alpha - E & \beta & 0 \\ 0 & \beta & \alpha - E & \beta \\ 0 & 0 & \beta & \alpha - E \end{pmatrix} \left| \begin{array}{l} \text{simplify} \\ \text{float, 4} \end{array} \right. \rightarrow \begin{pmatrix} .3717 & .6013 & -.6013 & -.3717 \\ .6014 & -.3716 & -.3716 & .6014 \\ .6014 & -.3716 & .3716 & -.6014 \\ .3717 & .6013 & .6013 & .3717 \end{pmatrix}$$

Construct an energy level diagram and show the occupied levels.

Energy	Occupancy	Wave function coefficients
$\alpha - 0.618 \cdot \beta$	_____	(-.3717 .6014 -.6014 .3717)
$\alpha - 0.618 \cdot \beta$	_____	(-.6014 .3717 .3717 -.6014)
$\alpha + 0.618 \cdot \beta$	_____xo_____	(-.6013 -.3716 .3716 .6013)
$\alpha + 1.618 \cdot \beta$	_____xo_____	(.3717 .6013 .6013 .3717)

Calculate the π -electron energy:

$$E_{\pi} = [2 \cdot (\alpha + 1.618 \cdot \beta) + 2 \cdot (\alpha + 0.618 \cdot \beta)] \rightarrow E_{\pi} = 4 \cdot \alpha + 4.472 \cdot \beta$$

Calculate the delocalization energy:

$$E_d = [4 \cdot \alpha + 4.472 \cdot \beta - 2 \cdot (2 \cdot \alpha + 2 \cdot \beta)] \rightarrow E_d = .472 \cdot \beta$$

Calculate the wavelength of the photon required for the HOMO-LUMO transition.

$$\frac{h \cdot c}{\lambda} = (\alpha - 0.618 \cdot \beta) - (\alpha + 0.618 \cdot \beta) \quad \left| \begin{array}{l} \text{solve, } \lambda \\ \text{float, 3} \end{array} \right. \rightarrow -.809 \cdot h \cdot \frac{c}{\beta}$$