Huckel Molecular Orbital Theory - Symbolic Approach

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

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

Calculate the eigenvectors:

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

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:

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

Calculate the delocalization energy:

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

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

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