

3.27: A Symbolic Huckel MO Calculation Using Mathcad

Enter and solve the butadiene Huckel determinant for energy eigenvalues.

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

Calculate the eigenvectors:

$$\text{eigenvecs} \left(\begin{pmatrix} \alpha - E & \beta & 0 & 0 \\ \beta & \alpha - E & \beta & 0 \\ 0 & \beta & \alpha - E & \beta \\ 0 & 0 & \beta & \alpha - E \end{pmatrix} \right) = 0 \quad \left| \begin{array}{l} \text{simplify} \\ \text{float, 4} \end{array} \right. \rightarrow \begin{pmatrix} .317 & .6013 & -.6013 & -.3717 \\ .6014 & -.3716 & .3716 & .6014 \\ .6014 & .3716 & .3716 & -.6014 \\ .3717 & .6013 & .6013 & .3717 \end{pmatrix}$$

Construct an energy level diagram and show the occupied levels.

Energy	Occupancy	Wave function coefficients
$\alpha - 0.618\beta$	—	($-.3717 \quad .6014 \quad -.6014 \quad .3717$)
$\alpha - 0.618\beta$	—	($-.6014 \quad .3717 \quad .3717 \quad -.6014$)
$\alpha + 0.618\beta$	$_{x o}$	($-.6013 \quad -.3716 \quad .3716 \quad .6013$)
$\alpha + 1.618\beta$	$_{x o}$	($.3717 \quad .6013 \quad .6013 \quad .3717$)

Calculate the π -electron energy:

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

Calculate the delocalization energy:

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

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

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

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