3.28: A Numeric Huckel MO Calculation Using Mathcad

Enter the number of carbon atoms. $\mathrm{Natoms} = 4$

Enter the number of occupied molecular orbitals. $\mathrm{Nocc} = 2$

Enter the Huckel matrix.

$$H = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \quad H = -H$$

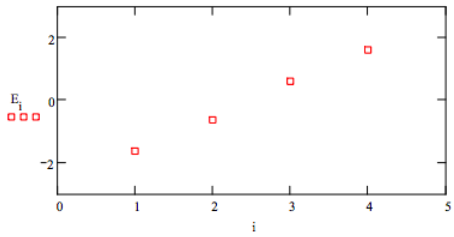
Calculate eigenvalues and eigenvectors:

$$E = \mathrm{eigenvals(H)} \quad \mathrm{Display} = \mathrm{rsort}\left(\mathrm{stack}\left(E^T,\ \mathrm{eigenvecs(H)}\right),\ 1\right)$$

Display eigenvalues and eigenvectors:

$$\mathrm{Display} = \begin{pmatrix} -1.618 & -0.618 & 0.618 & 1.618 \\ 0.372 & -0.602 & 0.602 & -0.372 \\ 0.602 & -0.372 & -0.372 & 0.602 \\ 0.602 & 0.372 & -0.372 & -0.602 \\ 0.372 & 0.602 & 0.602 & 0.372 \end{pmatrix}$$

Display energy level diagram. $\mathrm{E} = \mathrm{sort(E)} \quad \mathrm{i} = 1 \,..\, \mathrm{Natoms}$



Calculate total π-electronic energy:

$$E_\pi = 2\sum_{i=1}^{\mathrm{Nocc}} E_i \quad E_\pi = -4.472$$

Calculate the delocalization energy:

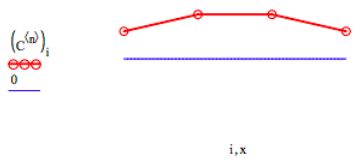
$$E_{deloc} = E_\pi + 2\mathrm{Nocc} \quad E_{deloc} = -0.472$$

Calculate the delocalization energy per atom:

$$\frac{\mathrm{E}_{deloc}}{\mathrm{Natoms}} = -0.118$$

$$C = \mathrm{submatrix}\ (\mathrm{Display},\ 2,\ \mathrm{Natoms} + 1,\ 1,\ \mathrm{Natoms})$$

Enter the number of the molecualr orbital to be plotted.



$$r = 1 \quad s = 1 \quad 2\sum_{i=1}^{Nocc}\left[\left(C^{<i>}\right)_r\left(C^{<i>}\right)_s\right] = 1 \quad \pi - \text{electron density on carbon 1}$$

$$r = 1 \quad s = 2 \quad 2\sum_{i=1}^{Nocc}\left[\left(C^{<i>}\right)_r\left(C^{<i>}\right)_s\right] = 0.894 \quad \pi - \text{bond order between carbons 1 and 2}$$

$$r = 2 \quad s = 3 \quad 2\sum_{i=1}^{Nocc}\left[\left(C^{<i>}\right)_r\left(C^{<i>}\right)_s\right] = 0.447 \quad \pi - \text{bond order between carbons 2 and 3}$$

$$r = 3 \quad s = 4 \quad 2\sum_{i=1}^{Nocc}\left[\left(C^{<i>}\right)_r\left(C^{<i>}\right)_s\right] = 1 \quad \pi - \text{bond order between carbons 3 and 4}$$
