Chem. 540
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Hückel Theory – Problem 1

Apply the Hückel approximation to (a) benzene and (b) cyclooctatetraene. In each case set up the Hückel Hamiltonian and use the following expression for the eigenvalues of the Hückel matrix for a cyclic conjugated molecule with an even number N of carbon atoms:

$$E_k = \alpha + 2\beta \cos\frac{2k\pi}{N}, \quad k = 0, \pm 1, \pm 2, \ldots, \tfrac{1}{2}N \quad (N \text{ even})$$

Indicate HOMO and LUMO and give the π binding energy (sum of energies of all π electrons) and the delocalization energy for each of the two molecules.

Further, use a symbolic algebra program to calculate the ground state eigenvectors and discuss your findings.