Quiz 9.3 – Molecular Orbital Theory: Polyatomic Molecules

Name:
Resonance in 1,3,5 hexatriene
\circ Show the Hückel theory determinant for 1,3,5 hexatriene. You may either show the matrix populated with α and β terms, or the simplified matrix with only $1{\rm s}$ and $0{\rm s}$
 Solve for the energy levels (You may use WolframAlpha or similar software to either find the determinant or diagonalize the matrix) and draw the energy level diagram
\circ Give the total bonding energy of the π system, as well as the resonance stabilization energy

Resonance in benzene

\circ Show the Hückel theory determinant for benzene. You may either show the matrix populated with α and β terms, or the simplified matrix with only $1{\rm s}$ and $0{\rm s}$
o Solve for the energy levels (You may use WolframAlpha or similar software to either find the determinant or diagonalize the matrix) and draw the energy level diagram
\circ Give the total bonding energy of the π system, as well as the resonance stabilization energy
\circ Compare these values to those found for 1,3,5 hexatriene and comment on why they are different