29_Hückel Calculations of Heteroatomic Aromatics

ChemActivity 15

Hückel Molecular Orbital (HMO) theory was developed for the conjugated \( \pi \)-system of carbon atoms. As HMO developed, chemist wanted to apply the theory to systems containing non-carbon atoms. HMO is successfully applied to aromatic heteroatom systems by adjusting the integrals of the secular determinant. By fitting heteroatom integrals to experimental data, HMO theory does a nice job of describing the orbitals of these chemically interesting systems.

Due Friday

Furan is another example of a heteroatomic aromatic.

1. Use the heteroatomic \( \pi \) energies table to create the secular determinant for furan, use \( \alpha = -13.6 \text{ eV} \) and \( \beta = -1.42 \text{ eV} \) for carbon. Solve the secular determinant for the \( \pi \) molecular orbitals energies of furan.

2. Using these energies, make a molecular orbital diagram similar to the one we constructed for imidazole.

3. Using the last page from today’s notes as a guide, solve for the AO coefficients for the furan molecular orbitals.

4. Sketch the five \( \pi \) molecular orbitals of furan in a similar way to the orbitals for imidazole. This is show in CA15 (pg. 142).

5. Determine the \( \pi \) electron charge on each atom in furan from their AO coefficients.

6. Draw the resonance structures for furan. Do these resonance structures predict a similar charge distribution?