

HW # 10, Chem 2430

1. Consider the approach of a K atom to a Cl atom. Estimate the distance at which an electron jumps from K to Cl. What is the symmetry of the state at which this jump occurs? Plot the dipole moment function vs. internuclear separation.
2. Conjugation between the rings favors a planar structure for the biphenyl molecule. Use Huckel theory to estimate the stability that derives from the conjugation. Experimentally biphenyl is found to adopt a non-planar structure, with ~ 20 deg distortion from planarity. Can you offer an explanation for this?
3. Consider the molecule p-xylylene (C_8H_8). Show one can use symmetry to simplify the Huckel matrix for this problem, giving at most a 3×3 submatrix. Use your results to calculate the Huckel eigenvalues. Is this molecule predicted to be more or less stable than cyclooctatetraene? Explain your result?
4. The ground state of CO_2 is linear, but CO_2^- at its minimum energy structure has an OCO angle of around 135 deg. Explain this result.