

Homework 11, Due May 6

1. The molecular orbitals of a linear H_3 molecule can be approximated as linear combinations of 1s atomic orbitals of the hydrogen atoms. Write down the secular equation and the corresponding secular determinant for this system, assuming the diagonal elements of the Hamiltonian matrix are equal and denoted as α and the off diagonal elements are non-zero and denoted as β . Describe how to determine the energies and wavefunctions of the molecular orbitals.
2. The HF bond has the largest contributions from the 1s orbital of H and the 2pz from F. Express the molecular orbitals using these two atomic orbitals and determine the LCAO coefficients and the energies using variational theory. Assume $S = 0.30$, $\alpha(H1s) = -13.6$ eV, $\alpha(F2pz) = -18.6$ eV, $\beta = -8.35$ eV.