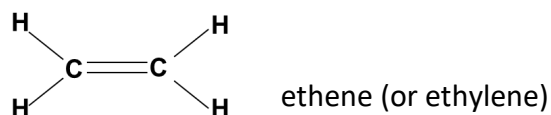


Exercise 13.1 (Hückel molecular orbitals)

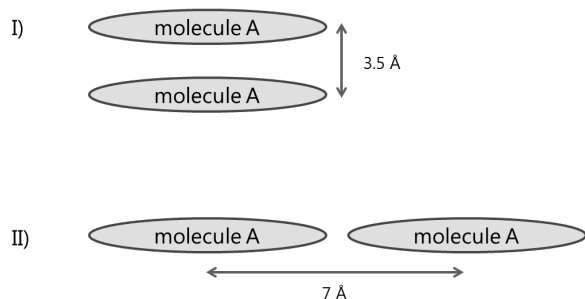


Calculate the energy levels and wave functions of the π molecular orbitals of ethylene using the Hückel model with the Coulombic integral α and transfer integral β as parameters.

- Draw an energy level diagram and sketch the molecular orbitals
- The lowest energy UV-absorption peak of ethylene gas is at a wavelength of about 170 nm. Estimate the value of the transfer integral $|\beta|$ in eV.

Exercise 13.2 (Exciton bands)

An isolated molecule A absorbs at a wavelength of 500 nm and has a transition dipole moment of 5 D oriented along its long molecular axis. When two dye molecules are assembled to form a dimer, the absorption wavelength shifts due to excitonic coupling. Here we are looking at the two dimer structures I) and II).



- Which of the two structures leads to a blue resp. red shift of the absorption band?
- Which of the two dimers is expected to fluoresce? Please explain.
- Calculate the absorption wavelength for both dimers I) and II). Use the point-dipole approximation and take $\epsilon = 3$ for the dielectric constant.