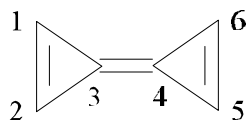


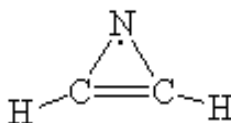
Name _____

1. (12 pts) Consider the Hückel model for the π electrons of



- a) Write the Hückel matrix in terms of α, β .
- b) Write symmetry-adapted basis functions for this system (making clear what reflection plane(s) you are using). (You do *not* have to solve for the Eigenvalues.)

2. (12 pts) Consider the molecule



- a) Write the Hückel Hamiltonian for the π electrons of this system using α for the energies of the carbon p orbitals and α' ($\neq \alpha$) for the energy of the N p orbital. Assume that all nearest neighbor (both C-C and C-N) interactions are given by β .

b) Solve for the Hückel energies in terms of α , α' , and β .

3. (16 pts.) The HOMO of acetylene is π_u and the LUMO is π_g .

a) What electronic states can be made upon exciting an electron from the HOMO to LUMO, assuming the molecule remains linear (give term symbols).

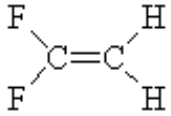
b) Which of the states in part a) is the lowest in energy?

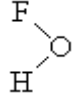
4. (36 pts.) Which of the following statements is true. (Circle those that are *true*.)

a) NaCu has a bond order of 1.

b) The excited state of H₂CO resulting from the HOMO → LUMO transition is of B₁ symmetry.

c) Zn₂ is a van der Waals molecule.

d) The π and π^* orbital of  are of the same symmetry.

e) The point group for  contains only one symmetry operation.

f) The degeneracy of the HOMO of benzene is removed in 1,4-difluorobenzene.

g) NO₂⁺ is strongly bent.

h) Atoms that have a closed subshell, *e.g.*, . . . (ns)², cannot be metallic.

i) In linear triatomic molecules, δ orbitals can be triply degenerate.

5. (6 pts) The linear molecule H-Be-H has the electronic configuration $1\sigma_g^2 1\sigma_u^2 2\sigma_g^2$. If the molecule is bent to 160° with equal H Be bonds, what is the electronic configuration (using the symmetry labels of the appropriate point group).

6. (12 pts) The Be_4 molecule has a tetrahedral structure



Sketch the various MO's, that can be formed from the 2s atomic orbitals and give their symmetries in the T_d group ?.

If you remove an electron from the highest occupied MO, would Be_4 retain its tetrahedral geometry? Why or why not?

7. (6 pts) A diatomic molecule has the electronic configuration $1\pi_u 1\delta_g$ (The closed shell orbitals have not been listed.) Give the term symbols for the various possible electronic states.