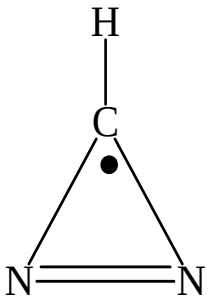
CHM 668 Fall 2004
Exam 1
October 25

The focus of the exam will be on the diazirinyl system:



1. (50 points)

a) Draw an orbital energy diagram for diazirinyl, showing the shapes of orbitals obtained at the Hückel level. Be sure to indicate the alpha level.

b) Compare the MO diagram for diazirinyl to cyclopropenyl, and account for the differences.

c) Write an ROHF wave function for the diazirinyl radical.

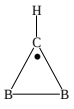
d) For cyclopropenyl radical, we concluded that the system is best represented as a localized radical and a cyclopropenyl double bond,  as opposed to a delocalized radical,  . How should the diazirinyl radical be represented? Support your answer.

2. (40 points) For this part, consider the properties of the diazirinyl anion, formed by one electron reduction of the radical.

a) If I were to tell you that the energy of 2 electrons in a N=N system in Hückel theory is $2\alpha + 3.2\beta$ ($2\alpha - 3.2\beta$ in SHMO), what would you obtain for the delocalization energy in diazirinyl anion?

b) Use the MO coefficients to calculate the C-N π bond orders and the charge densities in the anion. How do you interpret the results?

c) Based on the results in (b), what is the best way to represent the diazirinyl anion structurally? (HINT: you might want to consider multiple resonance structures)

3. (10 points) Suppose instead of diazirinyl, we created the diboracyclopropenyl system: 

What will be the orbital energy diagram? (qualitatively, at least, no need to calculate energies)