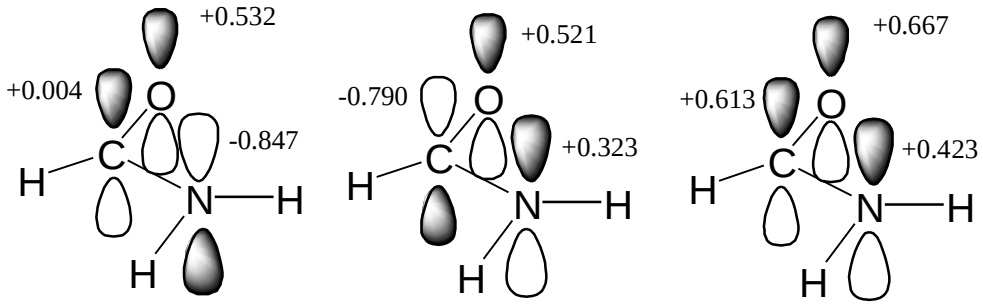
Chemistry 891 **CORE COURSE** **Fall 2002**

QUIZ #2 (100 points)

Answer all questions as completely as you can. Clearly show your work and reasoning.

1. The AM1-RHF ?-molecular orbitals for formamide are shown below, with no particular ordering. (60 pts)



(a) Draw a qualitative energy diagram that shows the orbitals with the correct energy ordering – be sure to label your energy axis.
(b) Put the correct number of electrons in each orbital for your diagram. Show alpha and beta spin properly.
(c) Use your MO diagram to predict which ?-bond in formamide is the *strongest*. Justify using the numbers/diagram as you give it.

2. The ?-molecular orbitals for methylenecyclopropene are shown below in correct energetic order. *Place the correct number of electrons in the diagram for the neutral molecule*, and answer the following question – which molecule has the strongest C2-C3 bond: the neutral hydrocarbon, the radical cation, or the radical anion? *Briefly* explain your answer. (50 pts)