ANSWER KEY

Chem 3331 Sammakia Fall 2015 Midterm 1 Name_____

6 1) Provide a definition of the following in one or two sentences (6 pts total):

Electrophile: a reactant that contains an empty orbital that can interact with another molecule that contains a pair of electrons (i.e. a nucleophile) to form a new covalent bond 3

Anti-bonding Molecular Orbital: the out-of-phase combination of 2 atomic orbitals such that there is a resulting node between the 2 nuclei. Antibonding orbitals are at a higher energy than their constituent atomic orbitals. All antibonding orbitals have a corresponding bonding orbital, and the antibonding orbital is raised in energy above its constituent atomic orbitals 3

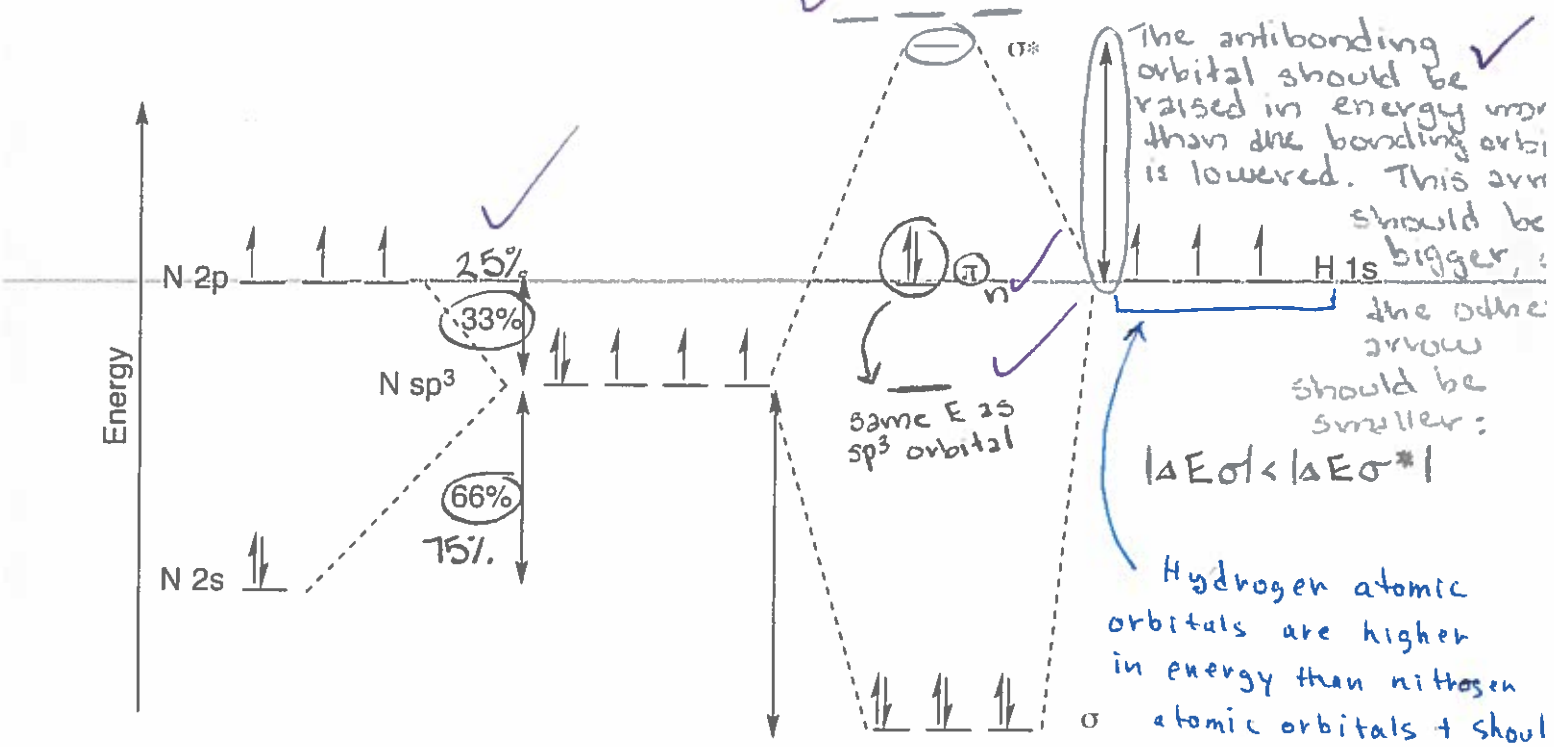
10 2) Below is a molecular orbital diagram for ammonia that contains errors. Circle all the errors and provide a few words describing the error. If you circle things that are not errors. points will be deducted. If your explanation is wrong. points will be deducted (10 pts total).

bonding orbital is lower than d in energ

+10

NH_3

should be 3 antibonding orbitals



The antibonding orbital should be raised in energy mor than the bonding orbi is lowered. This ant should be bigger, the other arrow should be smaller:

$|\Delta E\sigma| < |\Delta E\sigma^*|$

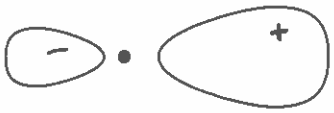
Hydrogen atomic orbitals are higher in energy than nitrogen atomic orbitals + shoul be raised higher on E diagram

3) Are the structures drawn below resonance structures? If they are resonance structures, draw arrows showing the movement of electrons, and circle the most important contributor to the overall structure of the molecule. If they are not resonance structures, explain why not in a few words (4 pts).

They are not resonance structures because the connectivity is not the same. To switch from the first structure to the second, a hydrogen must move from the oxygen to the third (starred) carbon.

+4

4) A carbon sp hybrid orbital is show in the figure below (6 pts total).
a) Write the mathematical sign of the wave function in each lobe of the orbital.
b) Is this considered an atomic orbital or a molecular orbital? Explain your answer in one sentence.

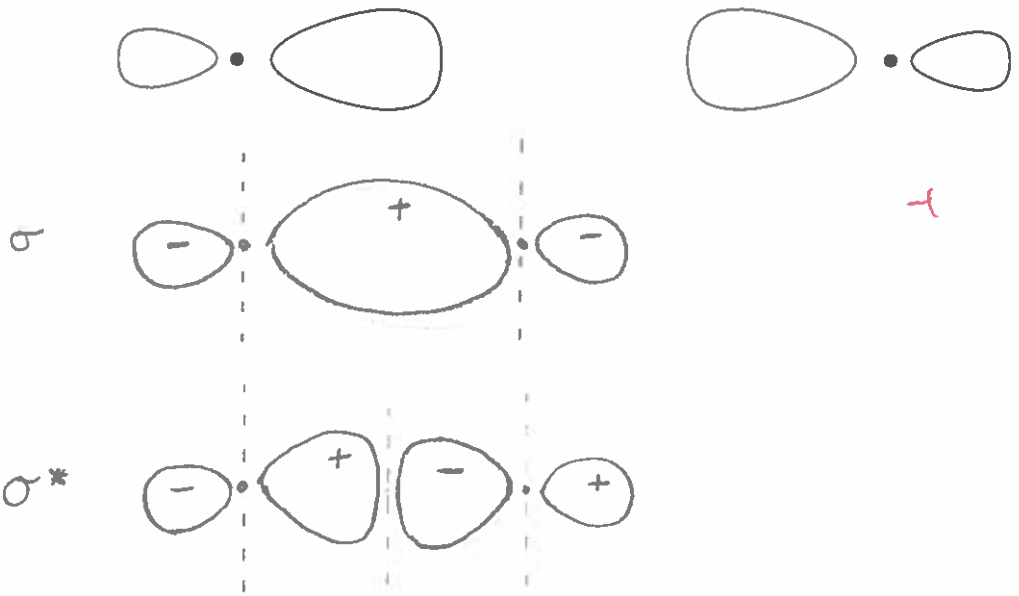


This is an atomic orbital because even though carbon must be bonded to another atom to have that hybridization, this orbital describes only carbon and not its interaction with any other atoms; there is no overlap.

+6

5) Consider two 2sp hybrid orbitals, one on each of two atoms, oriented head-to-head as in the figure below. Imagine bringing the nuclei closer together until the orbitals overlap and a bond is formed. Sketch the shape of the resulting bonding and anti-bonding molecular orbitals. Pay close attention to the following (6 pts total)

- The sizes of the various lobes
- The signs of the wave function at the various lobes
- The location of all nodes in your drawing (indicate this with a dashed line).



+6

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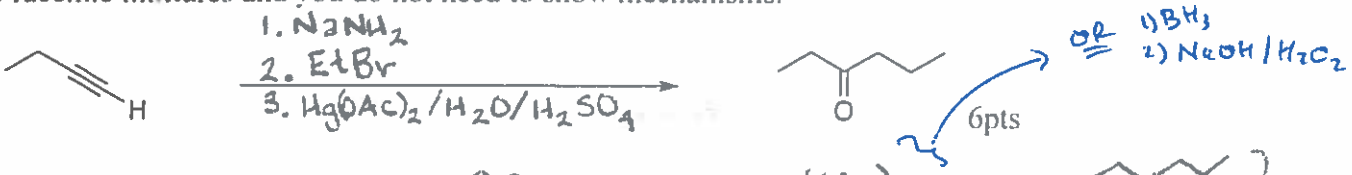
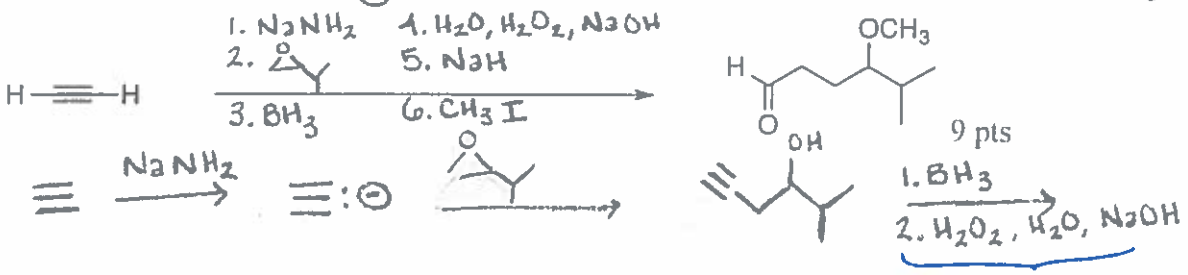
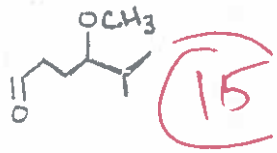
6) Complete the following syntheses using any organic molecule of 5 carbons or less and any reagents you need. You do not have to show the synthesis of the 5-carbon or less molecule you use. If your synthesis requires more than one step, you must provide the product after each step. All chiral products are racemic mixtures and you do not need to show mechanisms.

a) 

b) 



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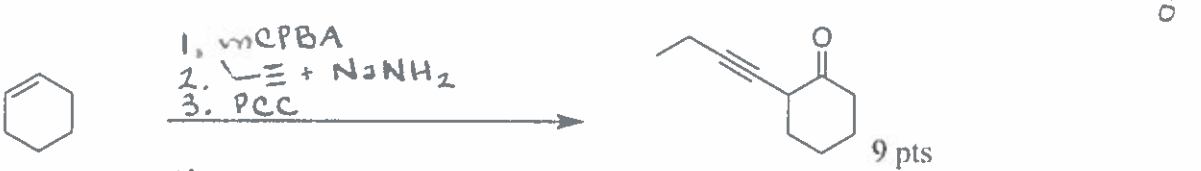
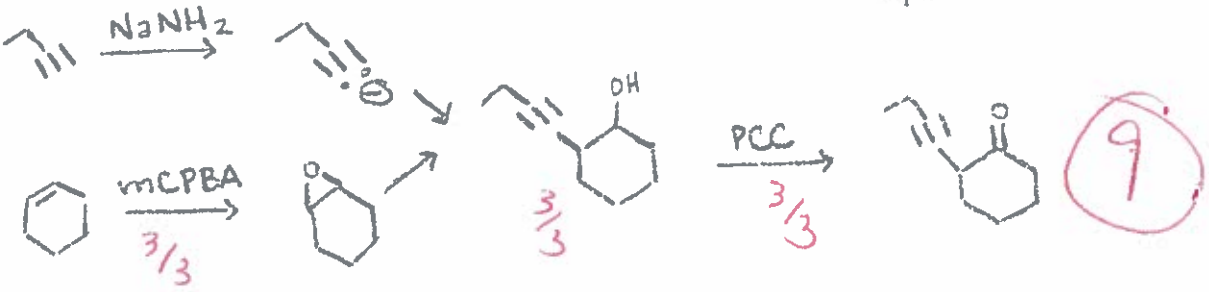
c) 



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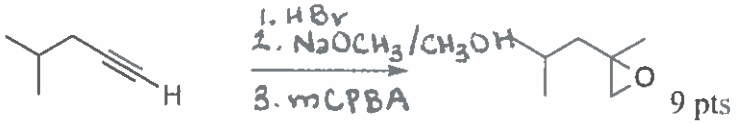
d) 

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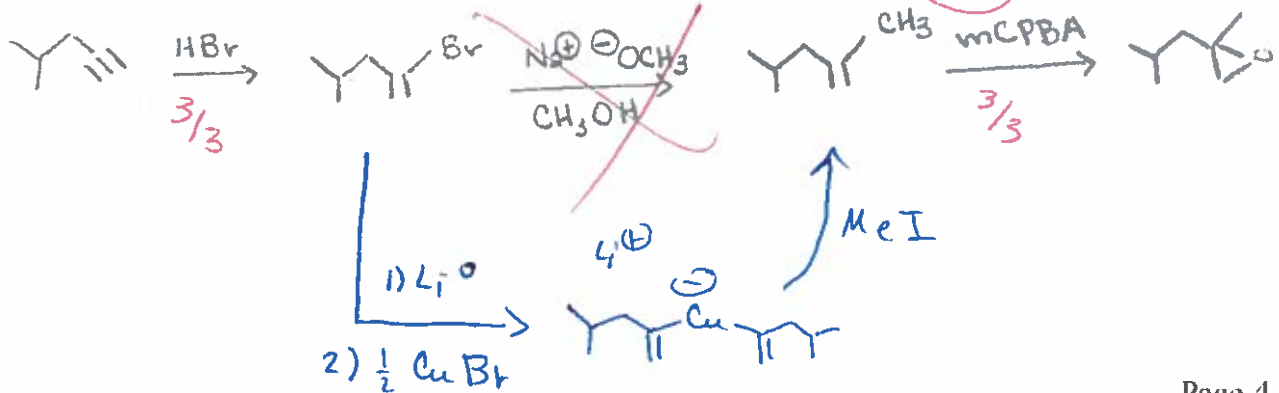

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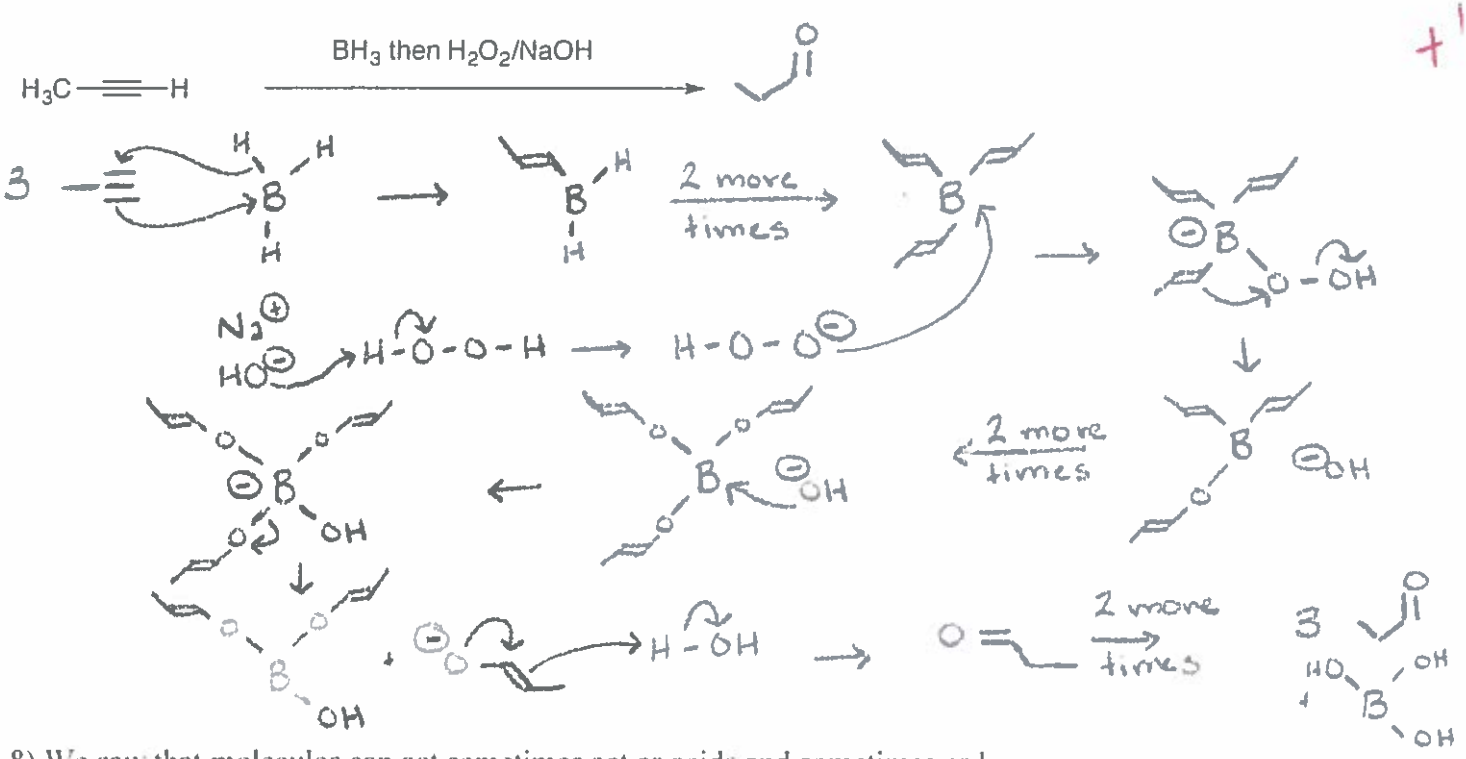
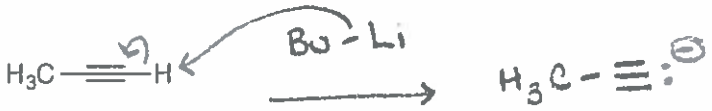
7) Provide the products and mechanisms for the reaction shown below. Show every intermediate with the proper charges and all the arrows required for each step of the reaction including any workup steps (3 pts for product. 10 pts for mechanism)



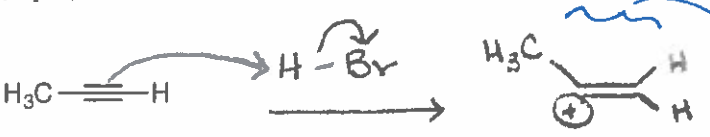
+1

8) We saw that molecules can act sometimes act as acids and sometimes as bases.
a) Give an example of a reaction we have seen this semester where the alkyne shown below acts as a Bronsted acid in the first step of the mechanism. Provide the reagents and the first step of the mechanism (6 pts). ↳ proton donor



+6

a) Give an example of a reaction we have seen this semester where the alkyne shown below acts as a Bronsted base in the first step of the mechanism. Provide the reagents and the first step of the mechanism (6 pts).



Note that the carbon that bears the ⊕ is sp hybridized and ∴ linear.

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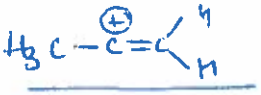

9a) Provide the pKa of the following: H_2O 15.7 acetylene 25 (10 pts total)

9b) What is the equilibrium constant for the reaction shown below:

$K_{eq} = 10^{15.7-25}$

$K_{eq} = 10^{-9.3}$

+10