

Chemistry 3A –Exam #1

Student Name: _____

Student ID Number: _____

Point Breakdown

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Problem 2 _____ / 16

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Problem 5 _____ / 18

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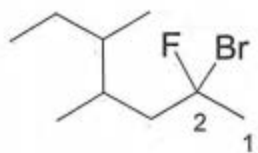
Total _____ / 150

Check that you have 9 pages with questions on them.

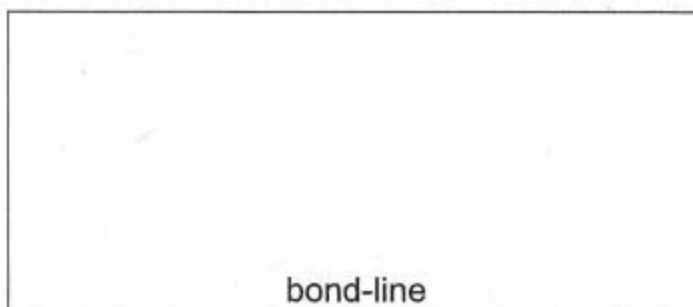
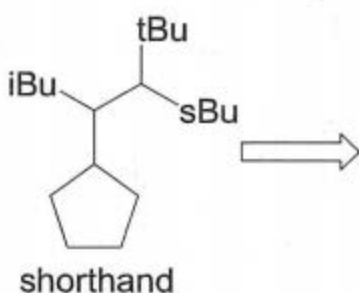
You will have 120 minutes for this exam.

**REMEMBER: Opposites attract,
formal charges are required, and
the octet rule is super important**

1. A. Provide a systematic name for the following molecule. Use common names where appropriate. Continue numbering the carbons based on the first 2 carbons. (2 pts)



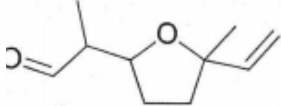
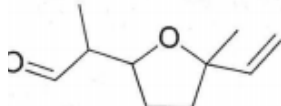
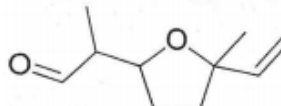
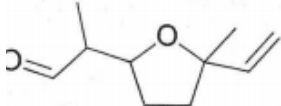
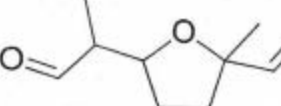
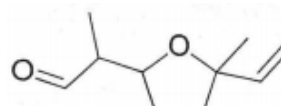
1. B. Specifically show the full bond-line structure of the molecule below. For example, instead of "Me", use an end of a line. (2 points)



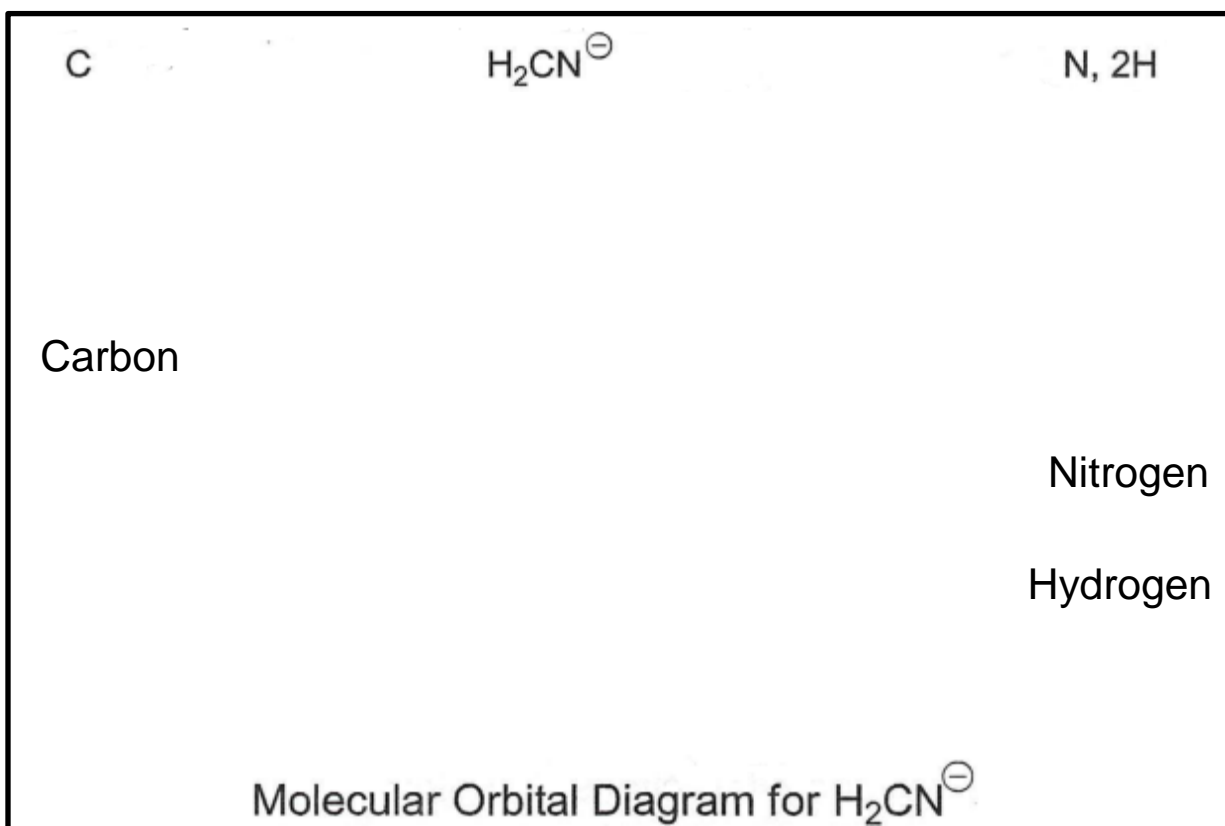
1. C. Provide a systematic name for the molecule you drew in 1.B. above. Part of the name has been provided for you. Make sure your number scheme matches the name provided. (2 points)

2,6-dimethyl- _____ octane

1. D. Lilac Aldehyde has many functional groups. On the molecule in each box, circle the functional groups or types of atoms named. If it is not present, write NONE. (12 points)

 two tertiary carbons	 aldehyde	 all sp^2 hybridized atoms
 all primary carbons	 alcohol oxygen	 ether oxygen

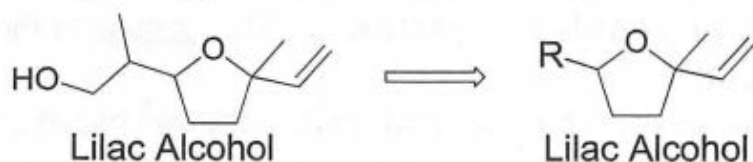
2. Construct the molecular orbital diagram for the molecule H_2CN^- , using the following guidelines and labeling schemes. The carbon is the central atom. (16 pts)
- Assume the nitrogen and carbon atoms are both sp^2 hybridized.
 - Indicate the relative energy levels of any atomic and hybrid orbitals on both sides of the diagram and label them (s, sp^2 , etc.).
 - Clearly indicate which orbitals are being combined to make MOs
 - Label all of the MO levels (σ_{CH} , π_{CN} , π^*_{CN} , n.b. N, etc.)
 - Fill the MOs with the correct number of electrons
 - Label the HOMO and LUMO



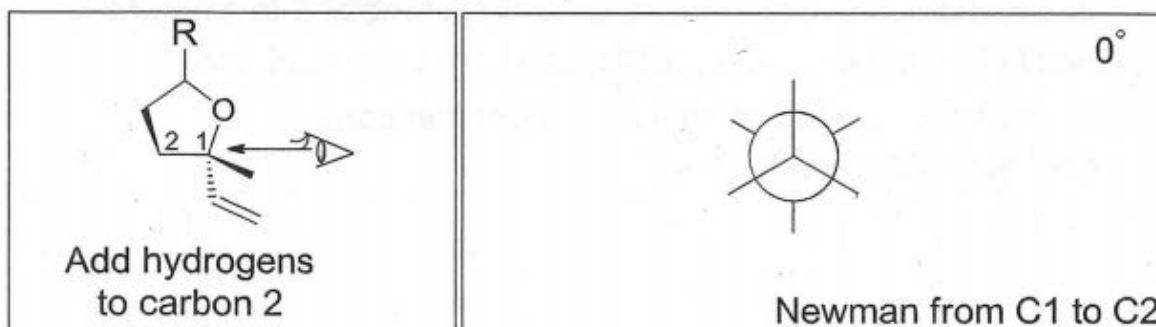
- g. Draw the 3D representation of H_2CN^- below. Feel free to use our template from class. You must clearly show all formal charges.



3. Lilac Alcohol is responsible for the distinctive scent of lilacs.

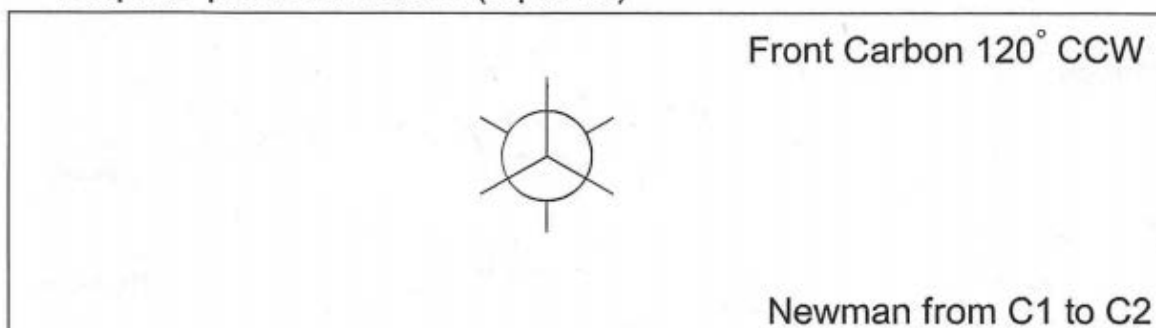


3. A. Add the hydrogen atoms, with proper tetrahedral shape, to carbon 2 of Lilac Alcohol below. (2 points)



3. B. Draw a Newman Projection along the C1-C2 bond as indicated by the eye. Use the projection template provided above. (3 points)

3. C. Rotate the front carbon 120 degrees counter clockwise using the template provided below. (3 points)



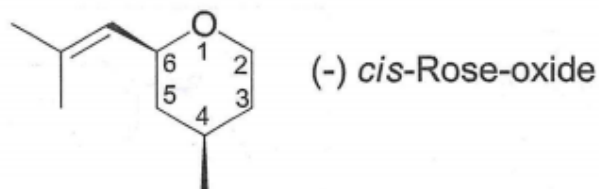
3. D. Describe the steric interactions at 0° and 120° . Use the abbreviations "Me" for the methyl group, "Alk" for the alkene, "O" for the oxygen, and "ring" for the oxa-cyclopentane ring. Use "E" and/or "G" for eclipsing and/or gauche interactions. (6 points)

Rotation Angle	Steric Interactions
Front Carbon 0°	
Front Carbon 120° CCW	

3. E. Is it possible to rotate the front carbon 120° CW? Explain. (4 pts)

Yes / No because:	(3 word limit)
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4. (-) *cis*-Rose-oxide is the molecule responsible for the characteristic scent of roses. It is a very minor, but potent, component of roses.



4. A. Draw the substituents of (-) *cis*-Rose-oxide in the proper orientation on the chair structure provided below. (3 points)
4. B. Draw the chair-flipped structure in the box to the right. (3 points)
4. C. Using the data provided at the bottom of the page, calculate the ΔG of the chair-flip. Please take substituent-substituent interactions into account. Place that value in the appropriate box. Show your work to receive any credit. (5 points)
4. D. Based on your ΔG , add an appropriate equilibrium arrow. (2 points)

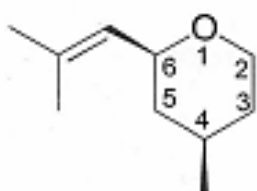
 Chair	$\Delta G =$ <div style="border: 1px solid black; height: 20px; width: 100%; margin-top: 5px;"></div>	 Chair-flipped structure
equilibrium arrow		

Show work:

Substituent	ΔG° (kcal/mol)	Substituent	ΔG° (kcal/mol)
Me _{eq} → ax	1.70	eq → ax	1.80

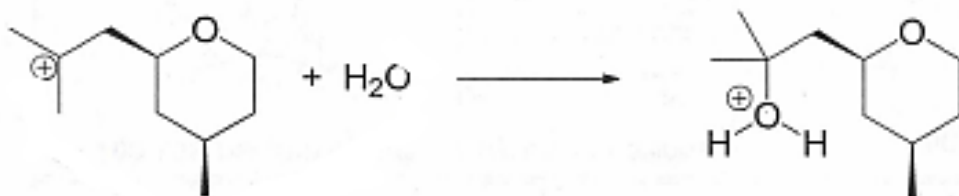
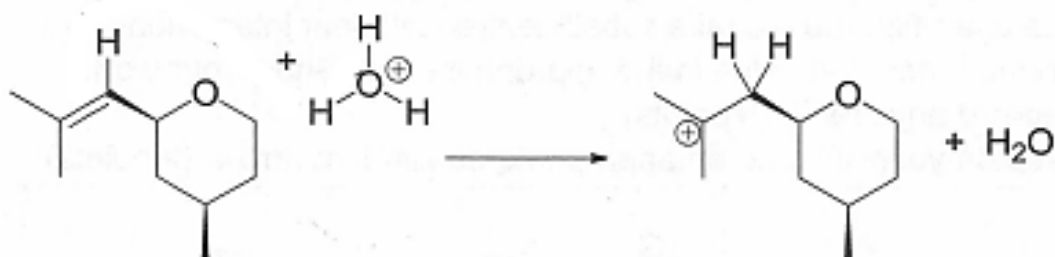
Substituent-substituent interaction	Gauche: Me,	1,3-diaxial: Me,
Energy Cost	3.0 kcal/mol	2.5 kcal/mol

4. E. There are two possible *trans*-Rose-oxide structures. Draw one of them in the box below. (3 points)

(-) *cis*-Rose-oxide

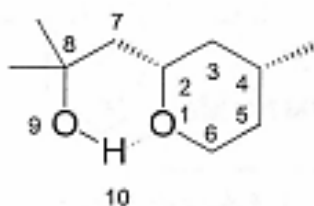
One possible *trans*-Rose-oxide

4. F. Draw the necessary electron-pushing arrows. (10 points)



4. G. Draw the compound below in an all chair conformation with an intramolecular hydrogen bond AS A DOTTED LINE between the alcohol proton (10) and the oxygen of the ring (1). (5 points)

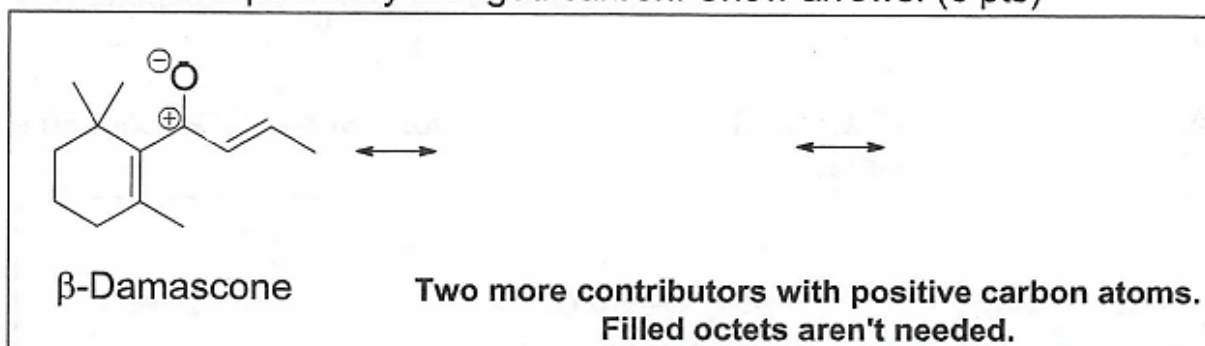
Flat-Ring



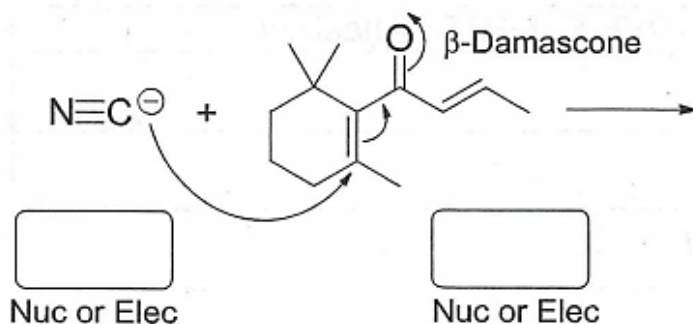
Chairs clearly showing intramolecular H-Bond between (10) and (1).

hint: it looks like *trans*-decalin

5. A. Draw two more resonance contributors of β -Damascone, a scent molecule in roses. Filled octets aren't necessary. Each contributor needs a positively charged carbon atom. Show arrows. (6 pts)



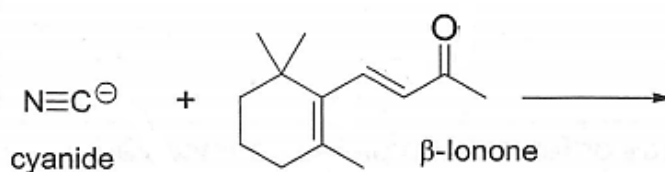
5. B. Label the nucleophile, "Nuc", and electrophile, "Elec", in the reaction below. (2 points)



5.C. Draw product.

5. C. Show the product of the reaction above. (3 points)

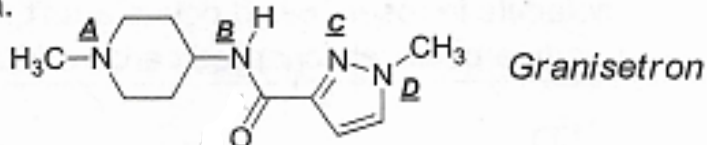
5. D. Draw the product of the following two reactants creating a new bond between the partial positive carbon in the ionone ring and cyanide. Show the negative charge on oxygen in the product. (3 points)



5.D. Draw product.

5. E. Add electron-pushing arrows to the reaction described in 5.D. (4 pts)

6. Granisetron is an antiemetic drug given to patients following chemotherapy to treat vomiting and nausea.



6. A. Define Bronsted Base in 8 words or fewer. Don't worry about complete sentences. (4 points)

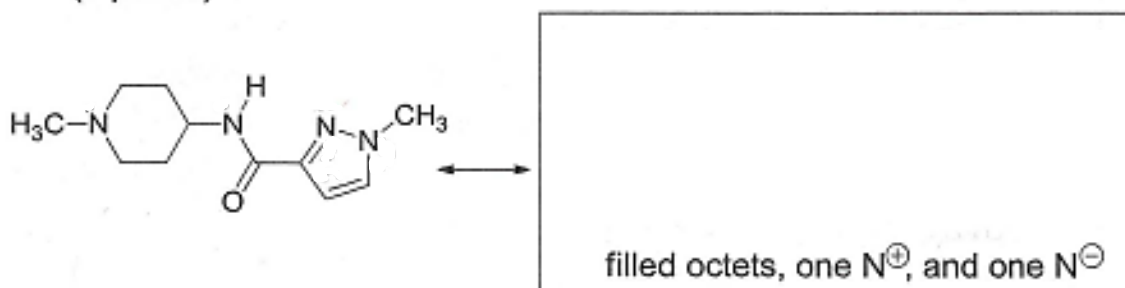
6. B. Indicate whether the INDUCTIVE EFFECT increases, decreases, or does not affect the basicity of each nitrogen atom in Granisetron. (8 points)

Nitrogen Atom	Effect of INDUCTIVE EFFECT on basicity
<u>A</u>	
<u>B</u>	
<u>C</u>	
<u>D</u>	

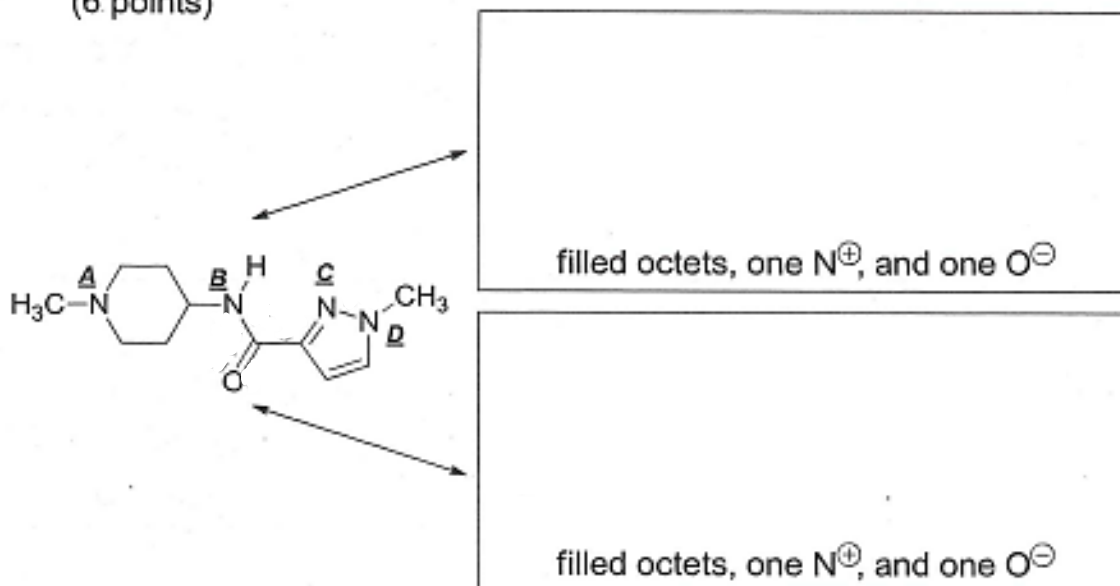
6. C. Based on the INDUCTIVE EFFECT, which nitrogen is most basic of Granisetron? Explain in 25 words or fewer. (5 points)

6. D. Define Nucleophile in 8 words or fewer. Complete sentences are not necessary. (4 points)

6. E. Draw a resonance contributor of Granisetron with filled octets, one negatively charged nitrogen atom, and one positively charged nitrogen. (3 points)



6. F. Draw two resonance contributors of Granisetron with filled octets, one negatively charged oxygen atom, and one positively charged nitrogen. (6 points)



6. G. Indicate whether RESONANCE increases, decreases, or does not affect the nucleophilicity of each nitrogen atom in Granisetron. (8 pts)

Nitrogen Atom	Effect of RESONANCE on nucleophilicity
<u>A</u>	
<u>B</u>	
<u>C</u>	
<u>D</u>	

6. H. Which two nitrogen atoms of Granisetron are least nucleophilic based on resonance? Explain in 25 words or fewer. (5 points)

6. I. Show the products of the electron-pushing arrows. (6 points)

