

CHEMISTRY 161 - Section A3

MIDTERM - October 17, 2006 - Dr. John C. Vederas

150 Points - 80 Minutes

Part	Points		PRINT LAST NAME:
I	56		KEY
II	35		
III	28		ID NUMBER (If Known):
IV	31		
Total	150		SIGNATURE:

Before you begin be sure that your exam has **11** consecutively numbered pages including this cover sheet. **Do not begin until told to do so.** When you begin, please **print** your name **on each page** of this exam in the upper right hand corner. Loose pages without names will be discarded. Illegible answers will be marked as incorrect. No books, notes, or unauthorized communications are permitted. If you have any questions or problems, please raise your hand. Do not leave your seat without permission. **Models are permitted but may not be handed to another and NO CALCULATORS or other electronic devices are to be used.** Slide rules are permitted.

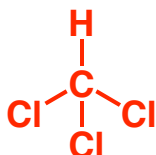
GOOD LUCK

Answers in Red

I. Structure and Nomenclature - 56 Points

A. Draw structures for which names are given, or name the given structures by any correct (systematic or common) nomenclature. Be sure to give cis or trans (or if appropriate Z or E) assignment to the isomer where indicated by asterisks (***). (4 points each)

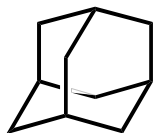
1. chloroform



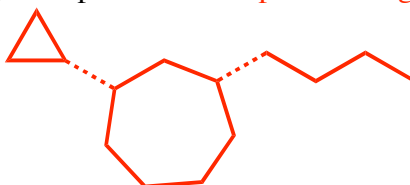
2. neopentyl iodide



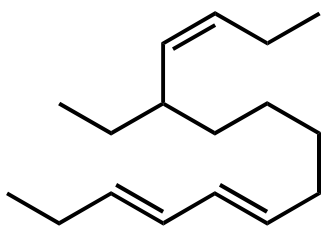
3.

**Adamantane**

*** 4. cis-1-cyclopropyl-3-butylcycloheptane 2 pts if wrong or no stereochemistry



*** 5.

**11-ethyl-3E, 5E, 12Z-pentadecatriene** (will accept cis/trans)

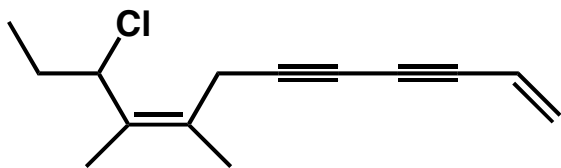
1 pt off each error up to 4

*** 6.

**trans-2-methyl-1-pentylcyclohexane**or **trans-1-methyl-2-pentylcyclohexane**

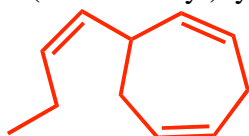
2 pts if wrong or no stereochemistry

*** 7.



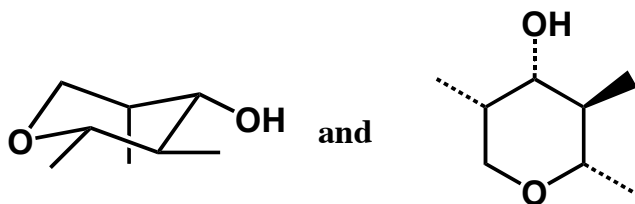
10-chloro-8,9-dimethyldodeca-1,8Z-dien-3,5-diyne
1 pt off each error up to 4

*** 8. 6-(cis-1-butenyl)cyclohepta-1,4-diene



B. Determine whether the following pairs of structures are identical, structural isomers, or stereoisomers.
(4 points each)

1.

___ **Identical** ___

2.

___ **Structural Isomers** ___

3.

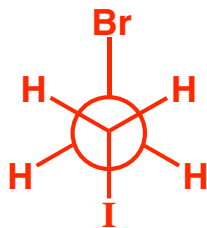
___ **Structural Isomers** ___

4.

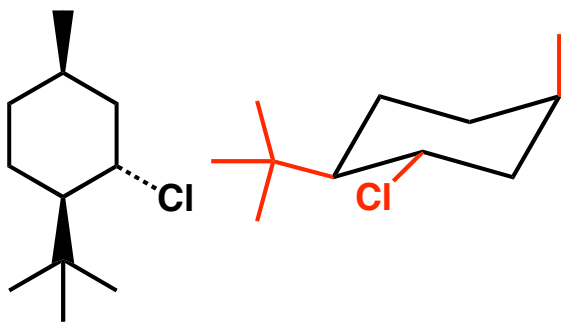
___ **Identical** ___

C. Conformation

1. Draw the Newman projection showing the most stable conformation of 1-bromo-2-iodoethane. (2 pts)

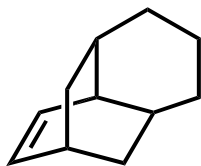


2. Draw the most stable conformation of the molecule shown below. Use the template provided for your drawing. If you make an error, please redraw the template. (2 pts)



3. For the structure below, provide:

the molecular formula (C_xH_y) and specify the number of degrees of unsaturation. (4 pts).



$C_{11}H_{16}$ 4 degrees of unsaturation

II. Quantitative Analysis and Definitions - 35 points

A. Briefly define (10 words or less) each of the following concepts - (3 points each)

1. sigma orbital **A molecular orbital that is made from atomic orbitals with s component**

2. Lewis acid **A substance that accepts a pair of electrons**

3. LCAO **Linear Combination of Atomic Orbitals**

B. Aspirin is a widely-used analgesic, antipyretic (lowers body temperature) and anticoagulant drug. It contains only carbon, hydrogen and oxygen. Quantitative analysis gave: C 60.00 %; H 4.48 %

1. Show how to calculate the empirical formula and obtain the correct result. (14 pts)
2. If the molecular weight is 180, what is the molecular formula? Show calculation. (2 pts)

$$100\% - 60.00\% \text{ C} - 4.48\% \text{ H} = 35.52\% \text{ O}$$

Divide each percentage by atomic weight to get crude ratios, then divide each crude ratio by smallest crude ratio, finally multiply by integer (1, 2, 3, 4...) to get integral ratios

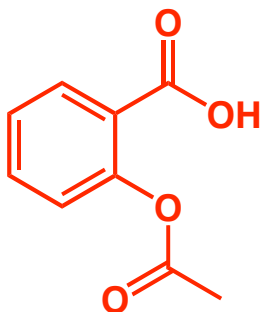
$$60.00 \div 12 = 5.00 \quad 4.48 \div 1 = 4.48 \quad 35.52 \div 16 = 2.22$$

$$5.00 \div 2.22 = 2.25 \quad 4.48 \div 2.22 = 2.00 \quad 2.22 \div 2.22 = 1.00$$

$$2.25 \times 4 = 9 \quad 2.00 \times 4 = 8 \quad 1.00 \times 4 = 4 \quad \text{Empirical Formula is } \mathbf{C_9H_8O_4}$$

Empirical Weight = (12 x 9) + (1 x 8) + (16 x 4) = 180 Hence Molecular Formula is also $\mathbf{C_9H_8O_4}$

Aspirin Structure (cannot be determined from information given) is:



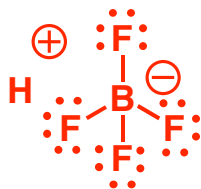
C. Circle the appropriate letter to indicate whether each of the following statements is true (T) or false (F). No penalty for guessing. (Similar to previous exams but be cautious) (1 point each - total 10 points)

1. ΔG is negative for an endothermic reaction T **F**
2. Resonance forms are not rapidly interconverting molecules **T** F
3. About 150 to 200 kcal/mole of energy are available at room temperature T **F**
4. Steric effect is caused by mutual repulsion of atoms having inert gas configuration of electrons **T** F
5. A completely pure organic compound may have different physical properties depending on whether it was made by chemists or isolated from Nature T **F**
6. The atomic number of an atom is always the total number of protons in the nucleus **T** F
7. The net dipole of CCl_4 is the vector sum of the individual bond dipoles **T** F
8. If ΔG is 0 there are equal amounts of starting material and product at equilibrium **T** F
9. The structure of a molecule determines all of its physical and biological properties **T** F
10. Neopentane has a high mp but lower bp than n-pentane **T** F

III. Atomic Structure and Molecular Structure - Energy Diagrams - 28 Points

A. Fluoroboric Acid (HBF_4) is a very powerful acid.

1. Based on your understanding of 1st and 2nd row elements in the periodic table, draw its molecular structure. Be sure to show all bonds and any lone pairs of electrons that may be present. (3 points)



Charges optional in this structure

2. Determine the formal charge on the boron. Use any method, but show calculations. (2 points)

B has	5 protons	+5
	2 1s electrons	-2
	½ 8 electrons shared	-4
	TOTAL	-1 is formal charge on boron

3. Calculate the formal charge on a fluorine. Use any method, but show calculations. (2 points)

F has	9 protons	+9
	2 1s electrons	-2
	½ 2 electrons shared	-1
	6 electrons lone pairs	-6
	TOTAL	0 is formal charge on fluorine

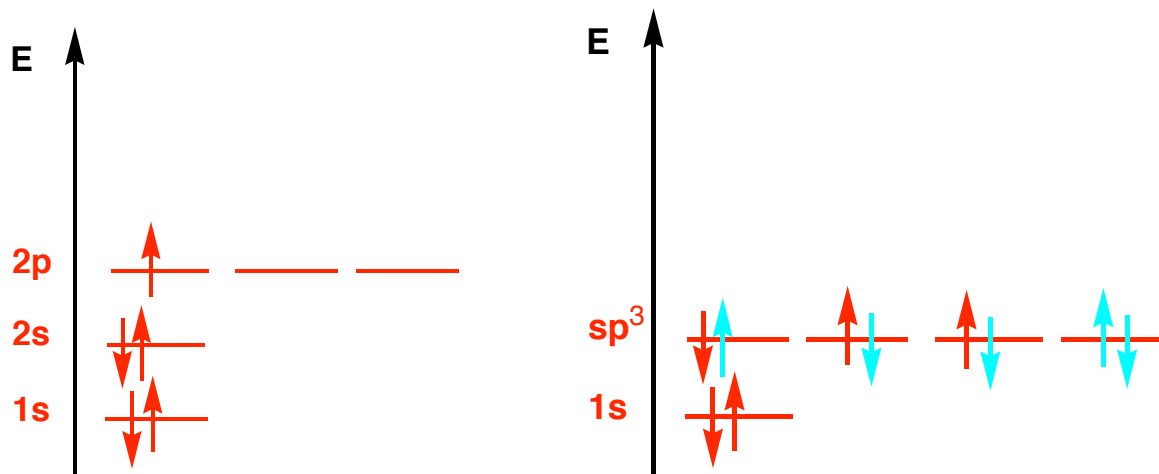
4. Calculate the formal charge on hydrogen. Use any method, but show calculations. (2 points)

H has	1 proton	+1
	0 electrons	0
	TOTAL	+1 is formal charge on hydrogen

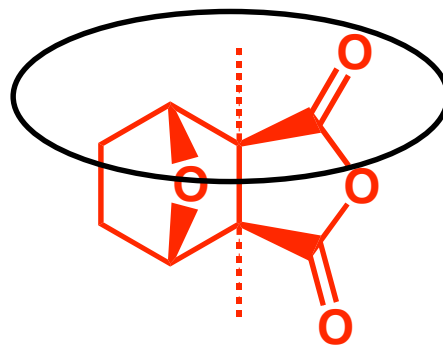
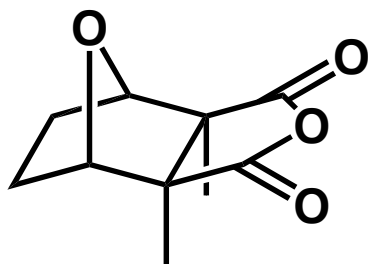
5. What is the hybridization of boron in HBF_4 and what are the bond angles ? (2 points)

boron is sp^3 F-B-F angles are 109 degrees

6. Draw two energy diagrams: one depicting all of the atomic orbitals of a boron atom by itself and another indicating the electronic structure of boron in HBF_4 . Be sure to label each orbital. (6 pts)

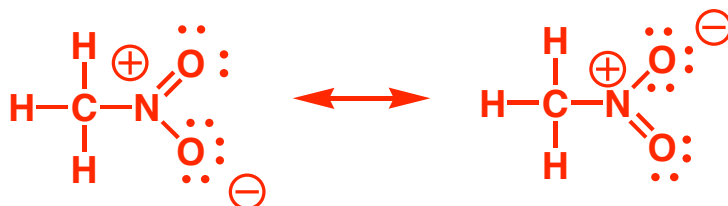


B. The monoterpene shown below is a toxic isoprenoid that acts as a defense substance for a beetle, *Cantharis vesicatoria*, also known as Spanish fly. It has been used as an aphrodisiac. Redraw the molecule in flat projection using the six-membered ring provided as a template. Be sure to indicate correct stereochemistry by using dashed and bold lines as necessary. Then circle one isoprene unit in the flat structure. If you make an error, please redraw the six-membered ring carefully below. (6 pts)



C. The molecular formula (and linear structure) of nitromethane is CH_3NO_2 . Draw the structure in full to show all bonds, lone pairs and formal charges that are not zero. Then draw an equally good resonance form.

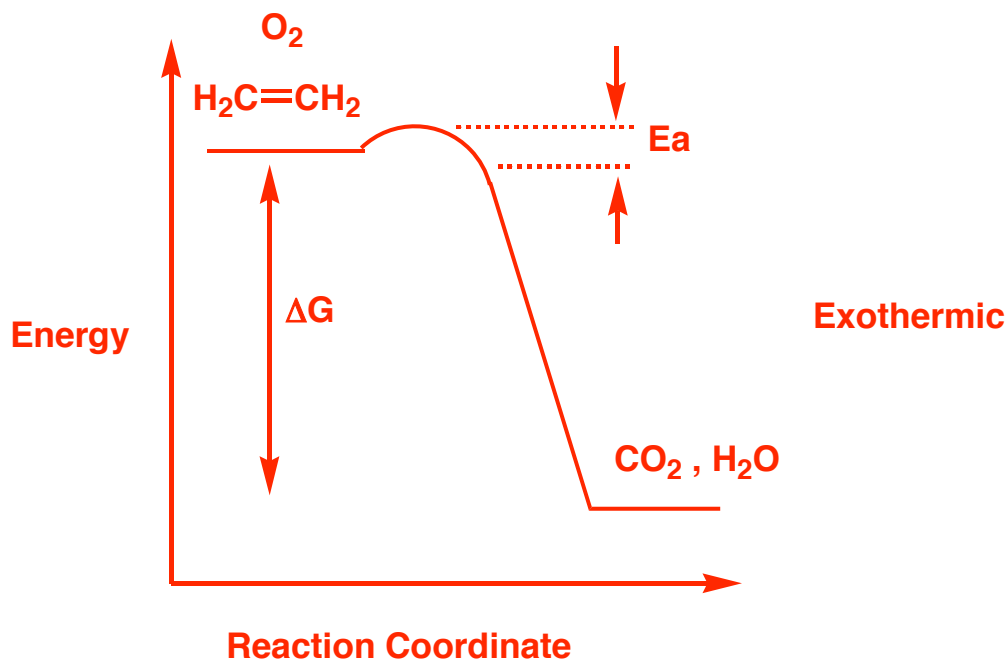
(5 points)



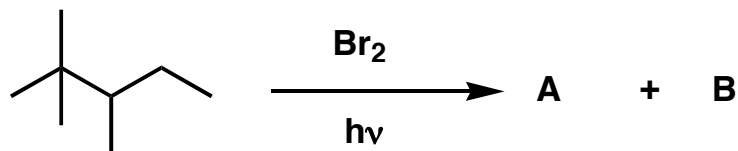
IV. Reactions and Mechanism - (31 points)

A. Write a balanced equation for the complete reaction of ethylene with oxygen (4 points). Draw a simple energy diagram for this process. Be sure to label both axes, label the starting materials and products (give their structures) in the correct locations. Also label the ΔG , the activation energy (E_a) and indicate in your drawing whether the reaction is exothermic or endothermic.

(12 points)



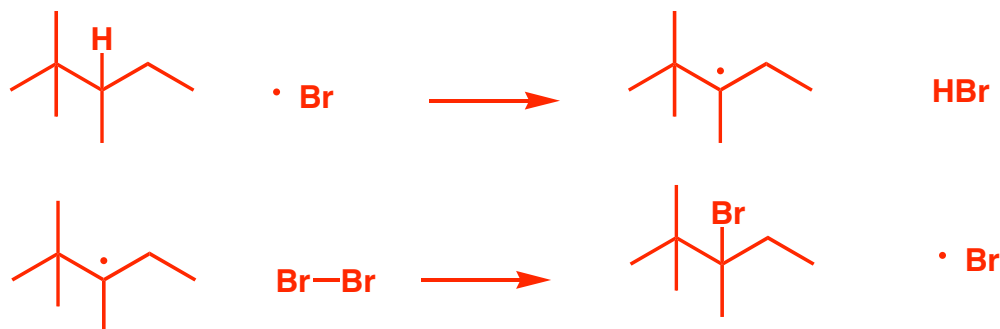
B. Examine the overall reaction shown below and answer the questions that follow.



1. Assuming there is one equivalent of Br_2 for each equivalent of alkane, show the structures of the two major products A and B. (3 points)



2. Write the two propagation steps for the reaction. (6 points)



3. Write one possible termination step for the above reaction. (2 points)

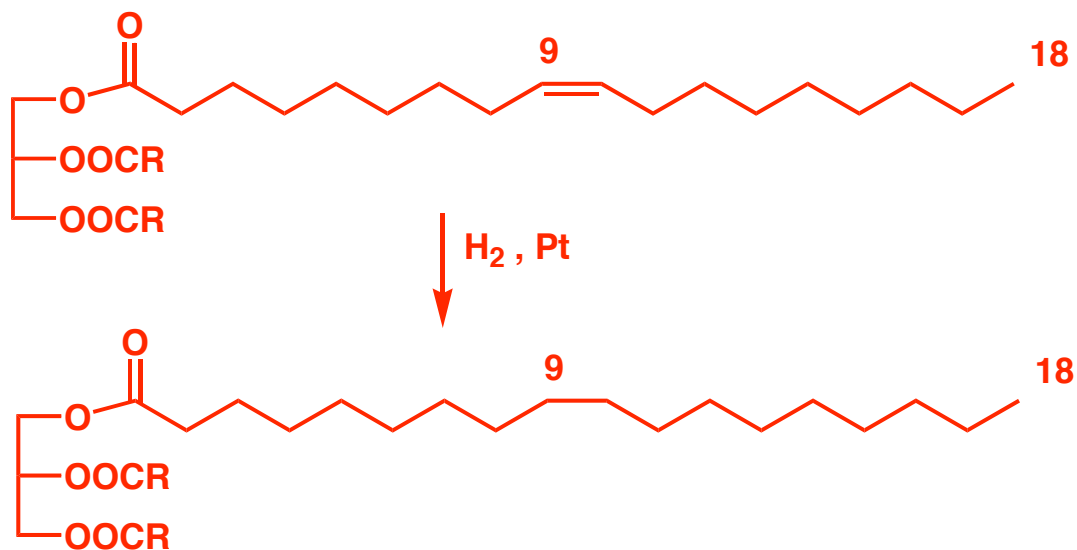
Any combination of two radicals to make stable species, for example:



4. Write the initiation step for the above reaction. (2 points)



C. Draw a chemical structure of a mono-unsaturated fat with at least one 18 carbon chain shown in full (others can be R groups). Then show the reaction that converts this into a saturated fat and the structure of the product (i.e. saturated fat). (6 pts)



Extra Credit (3 points): Who won the Nobel Prize in Chemistry this month ? **No partial credit here**

Roger Kornberg (Stanford University) only last name is necessary for credit