CHM 2120A
Midterm #1
October 7, 2020

ANSWERS

First Name: _____ Last Name: _____

Student Number: _____

Approximate total number of marks: 70
The marks are given as a guide and are subject to minor changes.

Instructions:

1. You can write the midterm digitally, on blank paper, or on a printed copy of the midterm.
2. When finished, submit your midterm to this assignment space in PDF format. If you are scanning papers, please use a scanner or app that scans to PDF. The Dropbox app is one option.

Academic integrity rules for Midterm 1:

1. Work individually, without consulting or working with anyone else
2. Open book: you may consult text or internet sources, except where answers are explicitly posted (e.g., Discord, Chegg)
3. You may not post questions/answers or ask for answers

Important! **If you become aware of academic dishonesty** during the midterm, report it to Dr. Flynn by email or anonymously.

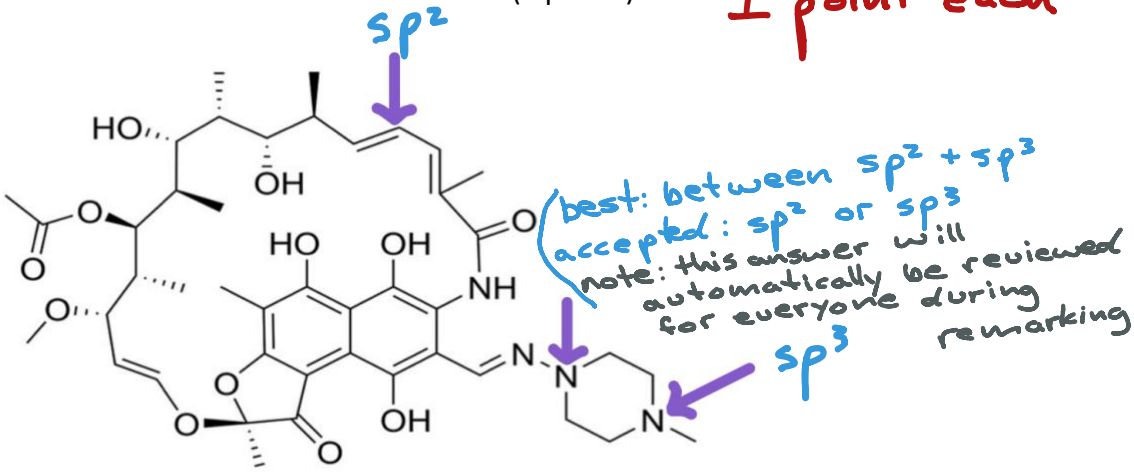
Please sign below to attest that you have read and agree to the rules for academic integrity for this midterm:

Signature: _____

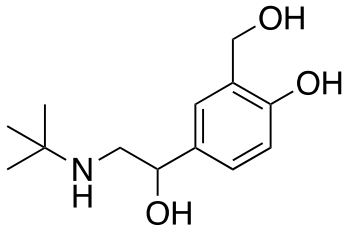
- Have questions during the midterm? You can:
  - Post your question on Piazza (preferred)
  - Contact Dr. Flynn via Zoom
  - Email Dr. Flynn (confidential messages only)

1. What is the hybridization of each of the indicated atoms? (3 points)

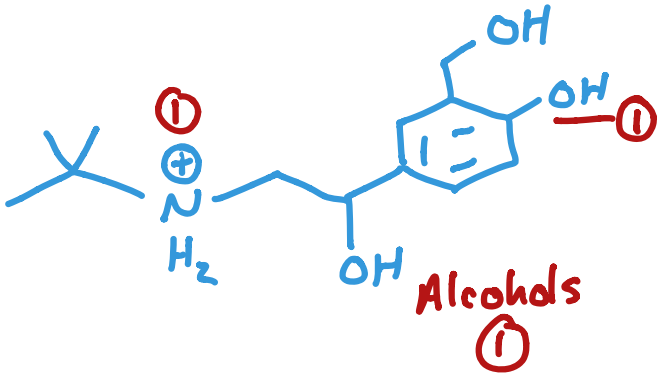
1 point each



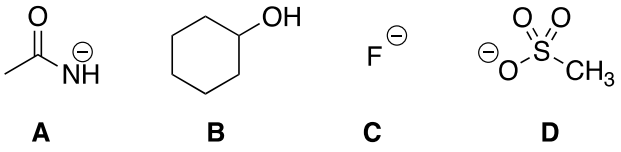
2. Draw the predominant form of Ventolin, drawn below, at pH 7. (3 points)



Ventolin (asthma)



3. Rank the following compounds in order of increasing leaving group ability (worst to best) (3 points)



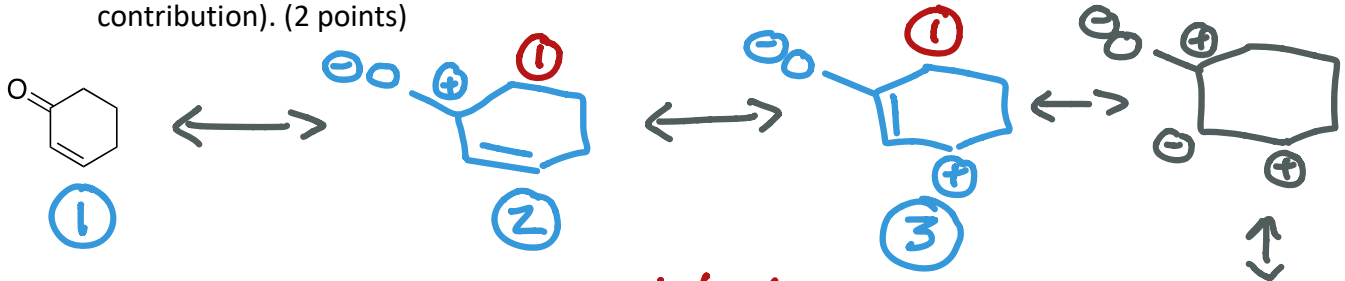
A **B** **C** **D**

A < C < B < D

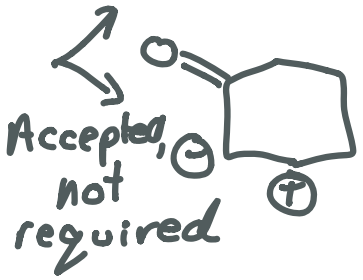
worst best

4.

a. Draw two additional resonance structures for the molecule below. (2 points)
b. Rank all the structures in order of their contribution to the resonance hybrid (1=greatest contribution). (2 points)



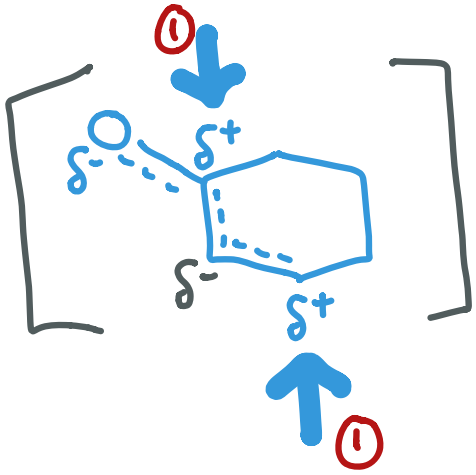
Ranking -1 per error/switched ranking



Accepted, not required

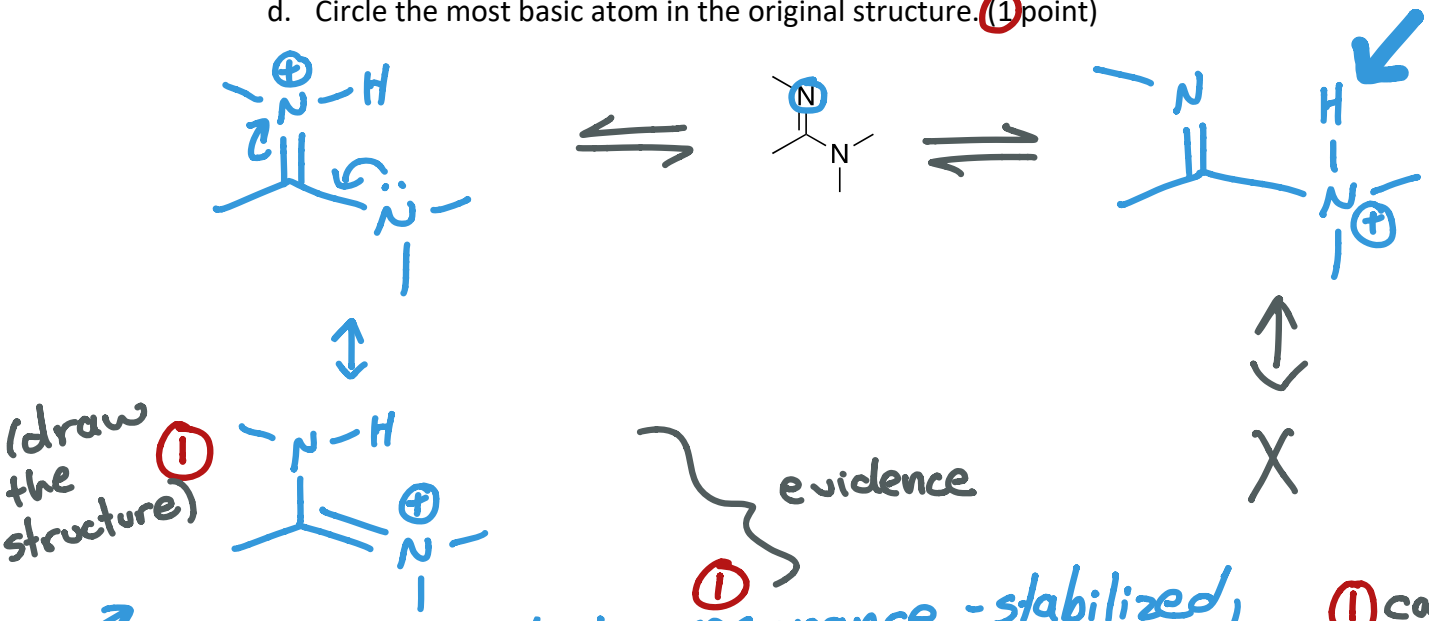
c. Draw the resonance hybrid structure. (3 points)
d. Point to the electrophilic sites on the hybrid (with an arrow). (2 points)

(1) Base structure
(1) Partial bonds
(1) Partial charges



→ aspects in grey are optional

5. For the following reaction:
   a. Protonate each nitrogen atom, drawing separate structures to show each conjugate acid. (2 points) → 1 point per structure
   b. Point to the most acidic proton. (1 point)
   c. Justify your answer in part b, using chemical reasons in your answer and at least linear causal reasoning. (4 points)
   d. Circle the most basic atom in the original structure. (1 point)



(draw the structure) 1

evidence 1

X

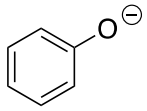
conjugate acid is resonance-stabilized, (least acidic) which spreads out the negative charge making it a weaker acid than the other conjugate acid, which is not resonance-stabilized, and is instead DE-stabilized by the neighbouring electron withdrawing group.

1 causal reasoning

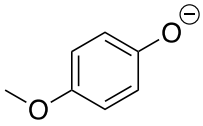
compare 1

6.

a. Compare the following bases and circle how each factor affects each base's relative stability. (5 points)



A

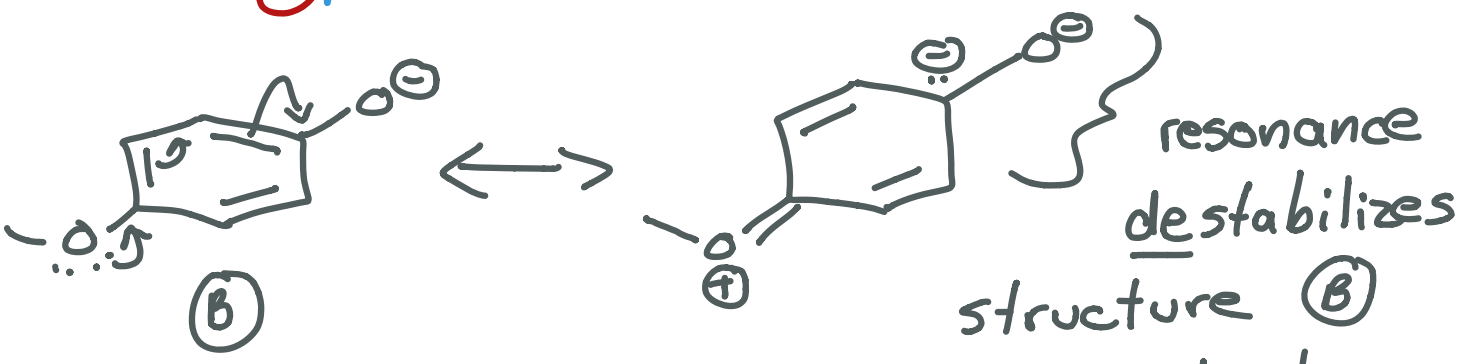


B

Electronegativity	Stabilizes **A** more than **B**	Stabilizes **B** more than **A**	Not relevant
Atom size	Stabilizes **A** more than **B**	Stabilizes **B** more than **A**	Not relevant
Resonance	Stabilizes **A** more than **B**	Stabilizes **B** more than **A**	Not relevant
Hybridization	Stabilizes **A** more than **B**	Stabilizes **B** more than **A**	Not relevant
Inductive effects	Stabilizes **A** more than **B**	Stabilizes **B** more than **A**	Not relevant

b. Given that the conjugate acid of **A** has a pK_a value of 18 and the conjugate acid of **B** has a pK_a value of 19 (both determined in dimethylsulfoxide as solvent), which factor(s) dominate the relative stability in this case? (1 point)

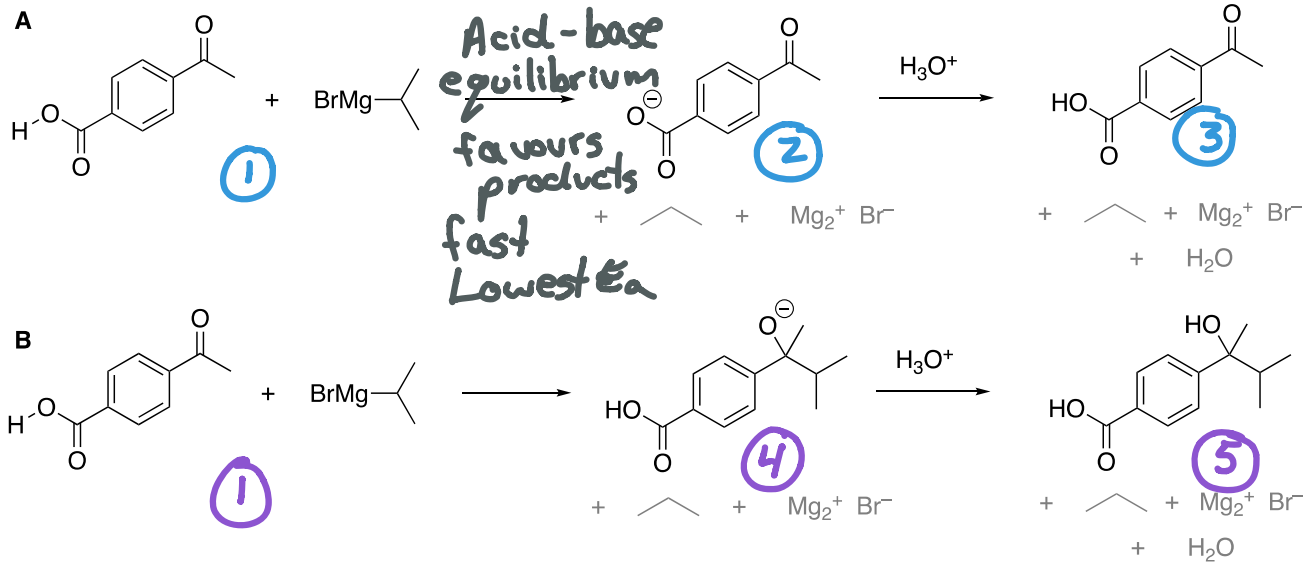
(1) Resonance

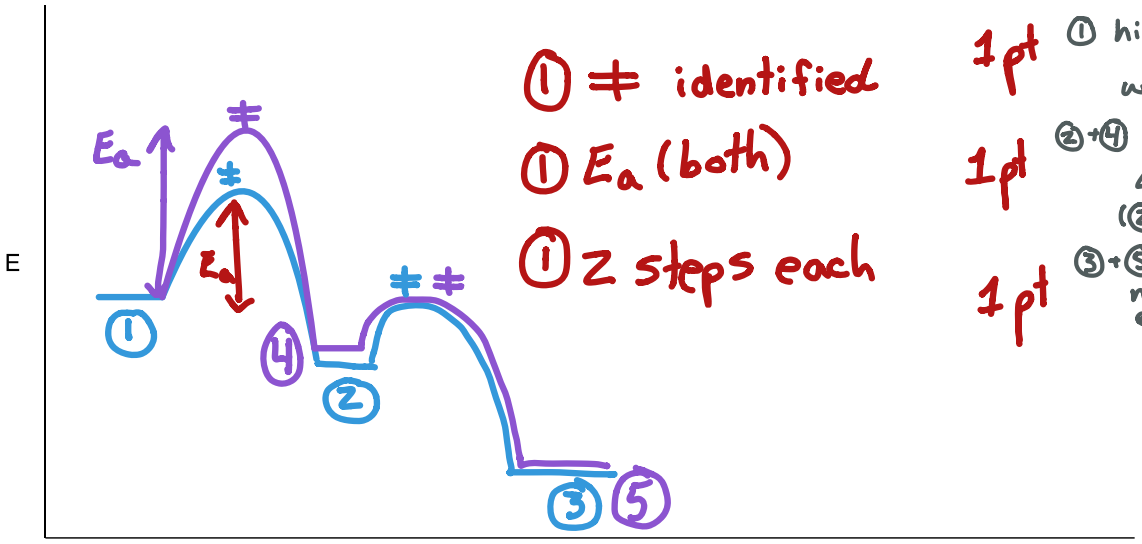


resonance destabilizes structure (B) making structure (A) more stable by comparison

7.

a. Draw and label the reaction coordinate diagram for reaction mechanisms **A** and **B**, including for each mechanism, the: transition states, activation energy of the rate determining step, reactants, intermediates, and products, as applicable. (6 points)





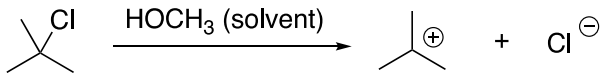
a. Which mechanism is most plausible for the reaction shown? A (1 point)

b. Justify your answer in part b, using your reaction coordinate diagram as part of your explanation. (3 points)

The first step in reaction (A) is an acid-base reaction that favours products, suggesting that it's the fastest first step, therefore with the lowest E_a (shown on RCD).

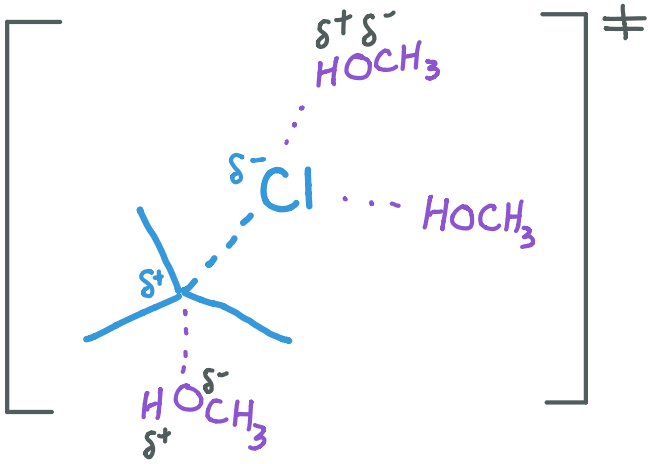
The second step in each reaction is similar (acid-base), and so is not relevant in comparing rxns.

8. For the single step of the reaction shown below:



a. Draw the transition state structure. Be sure to draw in solvent molecules, too. (4 points)

square brackets + transition state symbol (‡) should be drawn but are not marked for this question



① Floating point

① partial bond

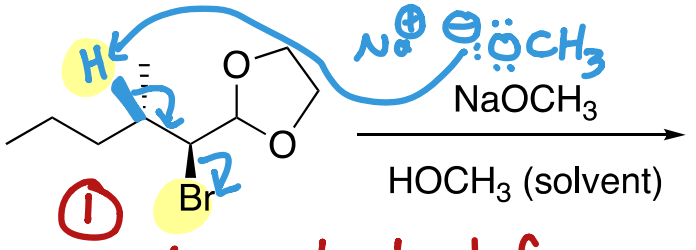
① partial charges

① solvent, with correct orientation

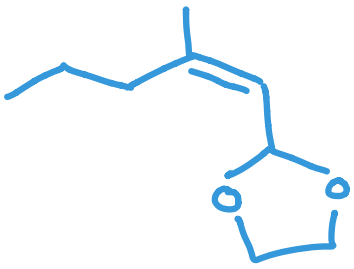
b. What is the role of solvent in that reaction step? (3 points)

① stabilize the charges as they form through hydrogen-bonding ① (for the leaving group) and dipole-dipole/dipole-ion (one of the two) ① interactions (as the carbocation forms)

a. Draw the electrophile in the Newman projection of its reactive conformation. (3 points)
b. Draw the mechanism and the major organic product; you can draw the mechanism on the original structure or on the Newman projection. (2 points)



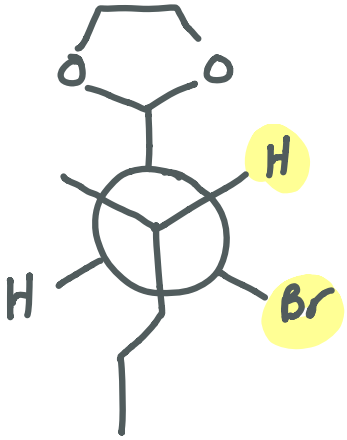
(1) Arrows (must start from electrons, not charges or atoms)



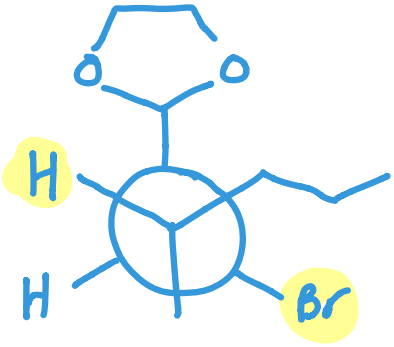
+ $Br^{\ominus}$ $Na^{\oplus}$

(1) product – correct constitutional isomer

(1) correct configuration (Z)



original conformation



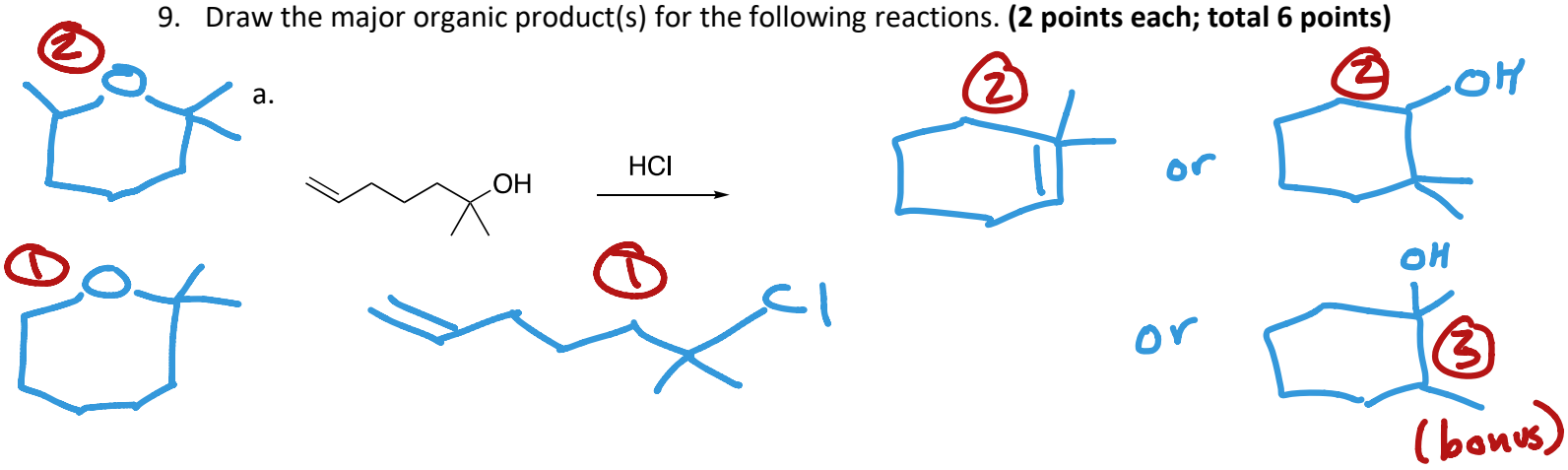
reactive conformation

(1) correct molecule

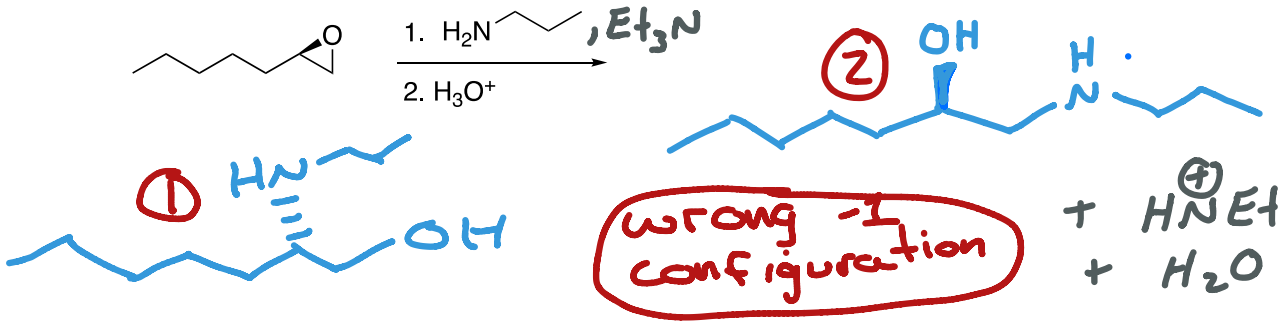
(1) H + Br antiperiplanar

9. Draw the major organic product(s) for the following reactions. **(2 points each; total 6 points)**

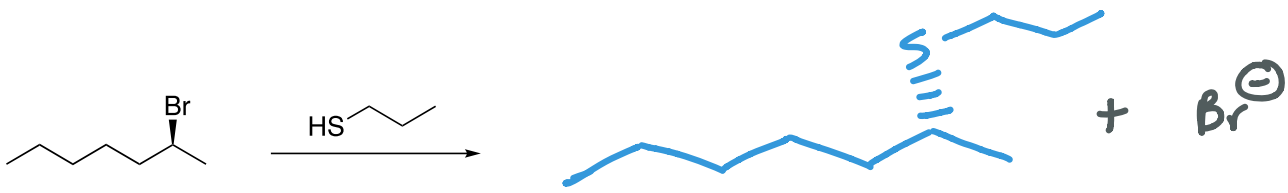
a.



b.



c.



(1) SN2

(1) correct configuration