Fall 2021 **Chemistry 2600 Final Exam** ____/90 marks

Confidentiality Agreement:
I agree not to discuss (or in any other way divulge) the contents of this exam until after 4:30pm Mountain Time on Saturday, December 11th, 2021. I understand that breaking this agreement would constitute academic misconduct. The minimum penalty would be a mark of 0/90 on this exam.

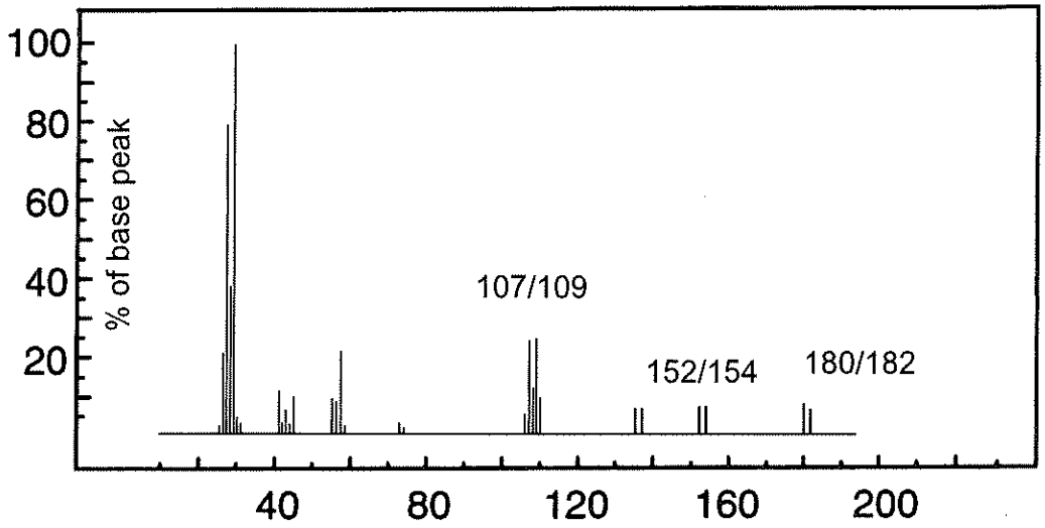
Signature: _____ Date: _____

1) Please read the test carefully before starting. It has 12 pages of questions and a periodic table.
2) You have been given a 6-page Spectroscopy Data Package. **PLEASE DO NOT WRITE ON THE SPECTROSCOPY DATA PACKAGE**! If you need scrap paper, use the back of any page of the test. On questions with spectra, you may also do rough work directly on the spectra.
3) You are allowed to bring one index card (maximum size 3"x5") into the exam with you as a "cheat sheet". This card must be submitted with your exam.
4) You may use a molecular model kit and ruler. You may not have written materials in your model kit.
5) You may use a calculator but only for calculation. No other electronic devices are allowed.
6) **DO NOT WRITE ON ANY QR CODE!!!** Work on pages without a QR code will not be graded.
7) If your work is not legible, it will be given a mark of zero. For full credit, explanations must be complete. In many cases, complete explanations include drawing relevant structures. If delocalization of electrons is invoked, the relevant resonance structures must be drawn.
8) Marks will be deducted for incorrect information added to an otherwise correct answer.
9) You have 9 hours to complete this test.

Question Breakdown

Q1	Q2	Q3	Q4	Q5	Q6	Q7	Q8	Q9						Total
/ 3	/ 2	/ 22	/ 8	/ 7	/ 24	/ 18	/ 5	/ 1						/ 56

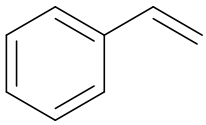
1. The following mass spectrum corresponds to a compound containing one halogen atom. **[3 marks]**



(a) Clearly label the molecular ion on the mass spectrum. *[1 mark]*

(b) Of which element is the halogen atom, and how can you tell? *[2 marks]*

2. For both parts of this question, assume that you are using an instrument capable of resolving all distinct peaks. In other words, do **not** attempt to account for peaks that might coincidentally overlap. **[2 marks]**



(a) How many peaks would you expect to see on the ^{1}H NMR of styrene (drawn above)?

(b) How many peaks would you expect to see on the ^{13}C NMR of styrene (drawn above)?

3. The following page contains spectra for Unknown X ($C_5H_9BrO_2$). **[22 marks]**

(a) Identify Unknown X based on these spectra. Draw your answer in the box provided below.

(b) Use this page to explain your reasoning. **Calculation of integrals is required for full marks.**

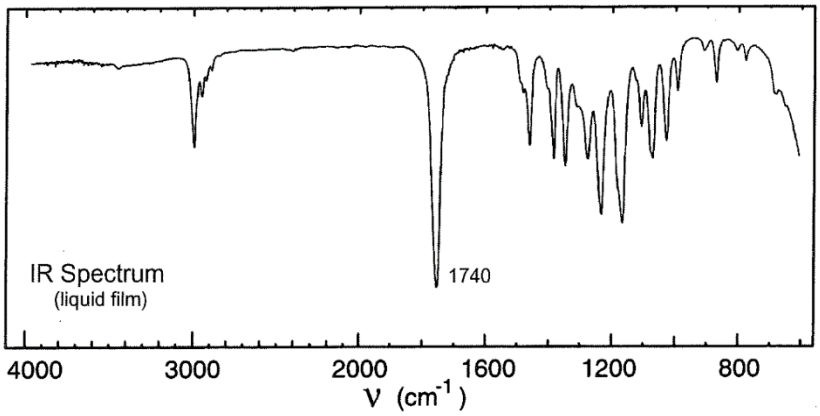
(c) On both NMR spectra, assign as many peaks as you can by numbering the peaks from left to right, drawing Unknown X in the box provided, and labeling each carbon or hydrogen atom with the appropriate peak number. For atoms that cannot be assigned with certainty, list the signals to which they might reasonably correspond.

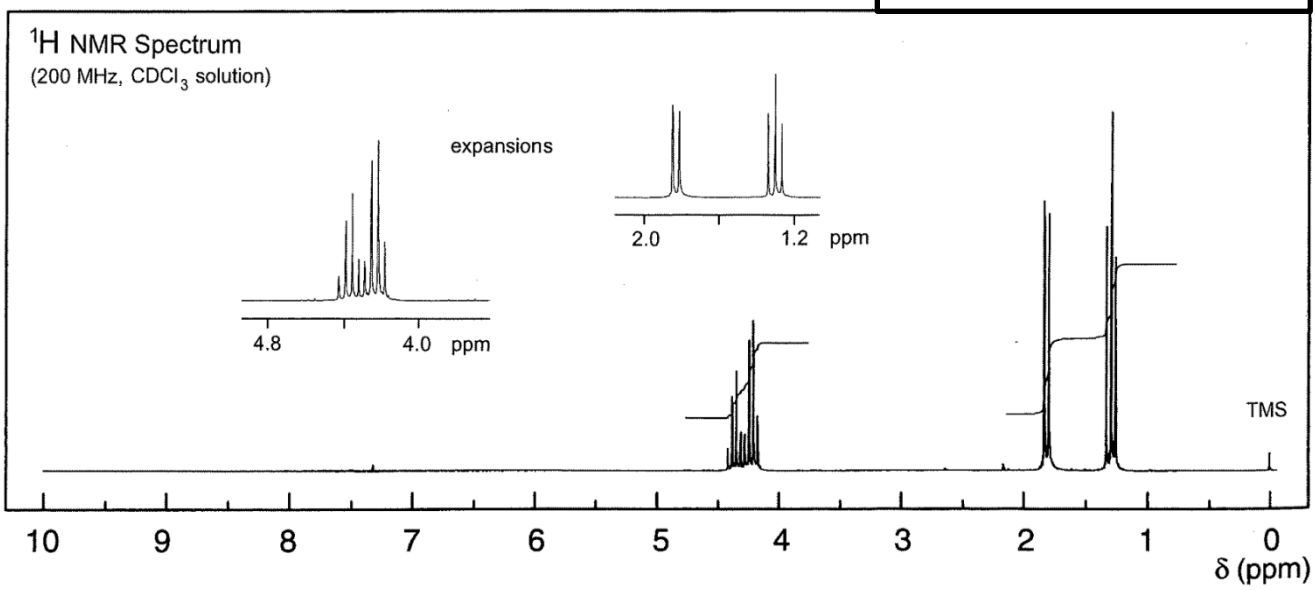
(d) Label any important peaks on the IR, clearly identifying which bond(s) correspond(s) to each peak.

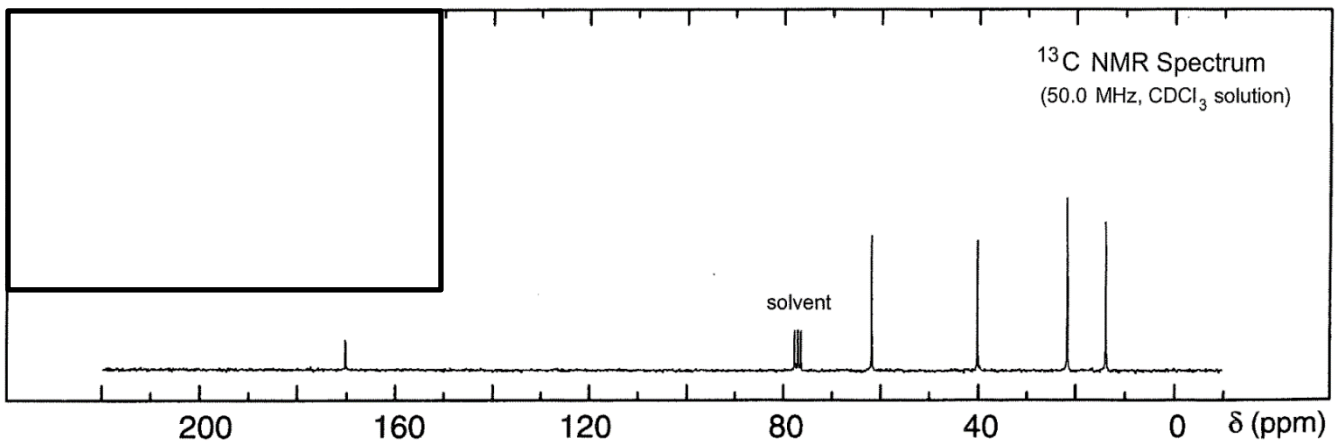
Unknown X:

3. *…continued*

$C_5H_9BrO_2$





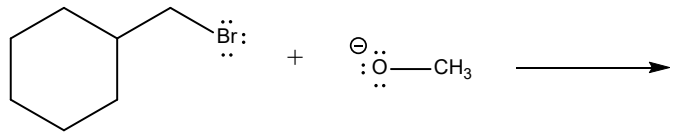


4. Indicate whether you would expect to see a significant amount of reaction according to each mechanism type by circling 'yes' or 'no'. In the bottom row of each table, justify your answer by: **[8 marks]**

- For each 'yes', drawing the organic product(s) that will be observed.
- For each 'no', briefly explaining why you expect little-to-no reaction.

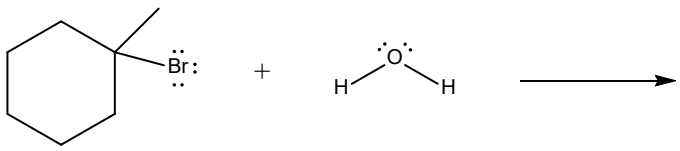
The marks are for the product(s) and/or explanations. The yes/no part is just to help you think.

(a)



S_N1? yes / no	**S_N2?** yes / no	**E1?** yes / no	**E2?** yes / no

(b)



S_N1? yes / no	**S_N2?** yes / no	**E1?** yes / no	**E2?** yes / no

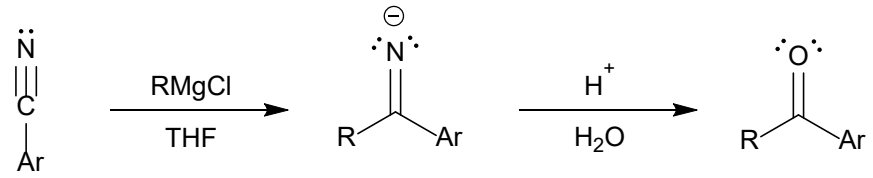
5. Use an argument based on resonance structures (which you must draw) to answer each of the following questions. **[7 marks]**

(a) When cyclopentanone is reacted with a strong base such as LDA, deprotonation always occurs at the carbon atom next to the carbonyl group. Why? *[4 marks]*

(b) 2-methoxy-1,3-butadiene is an electron-rich diene. At which end of the diene is it most electron-rich? Why? *[3 marks]*

6. A chemist wants to make a particular ketone so they can investigate its potential usefulness as a medicine. For the sake of simplicity, we'll use R and Ar to represent the groups on either side of the carbonyl.

One approach would be to react a nitrile with one group attached (**A**) and a Grignard reagent with the other group (RMgCl) then add aqueous acid: **[24 marks]**



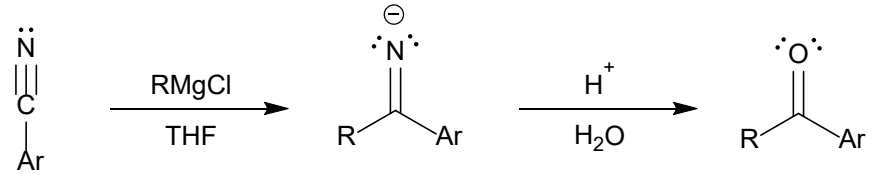
A **B** **C**

(a) At first glance, you might wonder why the chemist couldn't use an ester ($ArCO_2CH_3$) instead of nitrile **A**. Show what would happen if $ArCO_2CH_3$ was reacted with RMgCl. Your answer should include both the mechanism and product of the reaction. You may assume mild acidic work-up. *[8 marks]*

(b) It is possible to use an aldehyde (ArCHO) instead of nitrile **A**; however, an extra step would be needed to convert the product of that reaction into ketone **C**. Show the product of the reaction between ArCHO and RMgCl (before an after mild acidic work-up) **and** show one reagent (or set of reagents) that could be used to convert that product into ketone **C**. *[3 marks]*

continues on next page…

6. *…continued from previous page*

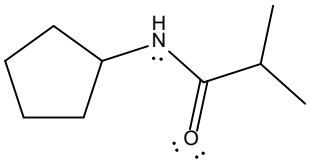


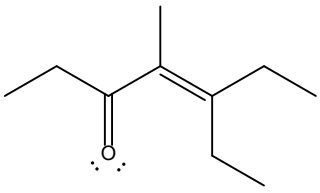
A **B** **C**

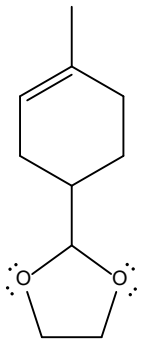
(c) Draw a valid mechanism for the acid-catalyzed conversion of intermediate **B** into ketone **C**. *[13 marks]*
You may use as much H^+ and H_2O as you like.

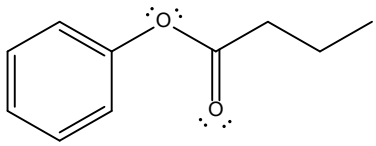
7. Choose any **three** of the molecules below and propose a synthesis for each one. **[18 marks]**

- If your synthesis involves more than one step, write an equation for each step. Show all required reactants. Number steps within a reaction if order of addition is important.
- All organic reactants must be stable compounds containing **no more than five carbon atoms**. They may be **hydrocarbons, alkyl halides or alcohols** and may contain C=C or C≡C bonds. The only exception to this rule is that you are **also allowed** to use **benzene, bromobenzene or phenol**.
- If you wish to use an organic reactant (including Grignard reagent) that does not meet these requirements, you must show how to make it from starting materials that do.
- You may use any inorganic reagents, acids, bases, catalysts, etc.
- Acids, bases, catalysts, etc. do not need to meet the "organic reactant" requirements if the organic part will not be present in the final product.
- Clearly indicate stereochemistry of reaction products where appropriate. Assume that all stereochemistry shown is relative and that you are to make racemic product.
- You are **not** required to show mechanisms for this question.
- There are three pages after this page. Use one of those pages for each synthesis and clearly identify the synthetic target at the top of the page. This page is scrap paper.
- If you give more than three syntheses, I will only mark the first three (ignoring any that are crossed out).









7. *continued…* *[6 marks]*

Synthetic Target #1:

Synthesis:

7. *continued…* *[6 marks]*

Synthetic Target #2:

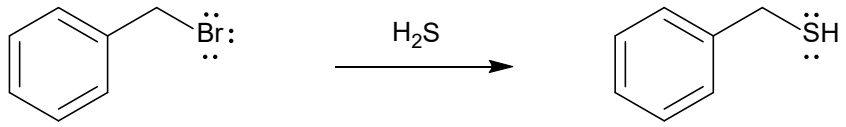
Synthesis:

7. *continued…* *[6 marks]*

Synthetic Target #3:

Synthesis:

8. Looking at the following reaction, it's not immediately obvious whether it would proceed primarily via S_N1 mechanism or S_N2 mechanism. Briefly explain how you could use kinetic data to decide. **[5 marks]**



Your answer should include:

- the rate law expected if the reaction proceeds exclusively via S_N1 mechanism,
- the rate law expected if the reaction proceeds exclusively via S_N2 mechanism,
- clear indication of what experimental parameter(s) would have to be varied, and
- clear indication of how the experimental data would tell you whether you were observing only S_N1 reaction, only S_N2 reaction or a mixture of both.

9. What was the most useful and/or interesting thing you learned in CHEM 2600? **[1 mark]**

…AND THAT'S ALL FOR CHEM 2600.

HAPPY HOLIDAYS!