Fall 2021 **Chemistry 2600 Midterm #1** ____/50 marks

Confidentiality Agreement:
I agree not to discuss (or in any other way divulge) the contents of this exam until after 8:30pm Mountain Time on Thursday, October 14th, 2021. I understand that breaking this agreement would constitute academic misconduct. The minimum penalty would be a mark of 0/50 on this exam.

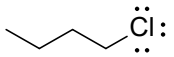
Signature: _____ Date: _____

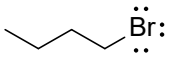
1) Please read the test carefully before starting. It has 5 pages of questions and a periodic table.
2) You have been given a 6-page Spectroscopy Data Package. **PLEASE DO NOT WRITE ON THE SPECTROSCOPY DATA PACKAGE**! If you need scrap paper, use the back of any page of the test. On questions with spectra, you may also do rough work directly on the spectra.
3) You may use a molecular model kit and ruler. You may not have written materials in your model kit.
4) You may use a calculator but only for calculation. No other electronic devices are allowed.
5) **DO NOT WRITE ON ANY QR CODE!!!** Work on pages without a QR code will not be graded.
6) 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.
7) Marks will be deducted for incorrect information added to an otherwise correct answer.
8) You have 2 hours to complete this test.

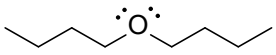
Question Breakdown

Q1	**Q2**	**Q3**	**Q4**	**Q5**									**Total**
/ 8	/ 4	/ 3	/ 10	/ 25									/ 50

1. You find an unlabeled bottle in the back of the chemical cabinet. In order to decide how best to dispose of it, you analyze it by ^{1}H NMR and ^{13}C NMR. That convinces you that it is one of the following three compounds: **[8 marks]**

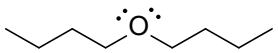


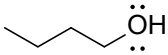
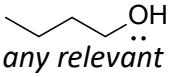




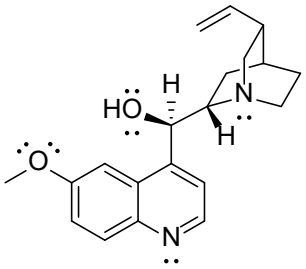
The lab next door offers to let you use their mass spectrometer to analyze your mystery compound since that should let you choose definitively between these three options.

(a) Describe what you would expect to see in the molecular ion region of a mass spectrum for each of these three compounds. Be specific. Your answer should address two factors. *[5 marks]*

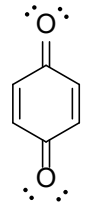
(b) Your friend points out that  contains a lot more hydrogen atoms than the other two options. Why can't you use the integrals on the ^{1}H NMR to distinguish between this option and the other two? *[1 mark]*

(c) Your friend also wonders why you haven't included  on your list of options. Which of the two types of NMR let you eliminate this compound as an option? How did it do that? *In other words, how would that spectrum for*  *be different from the spectrum for any of the three compounds in part (a). Describe any relevant peaks.* *[2 marks]*

2. On another shelf of the cabinet, you find a small bottle whose label has been partially obscured. It must say either “quinine” or “quinone”, but you can’t tell which. **[4 marks]**



quinine

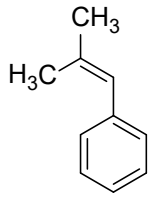


quinone

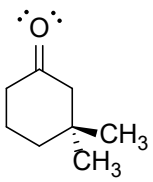
How could you use IR to quickly decide which compound was in the bottle? Your answer must include one peak that would be produced by quinine (but not quinone) and one peak that would be produced by quinone (but not quinine). For each peak, identify a wavenumber range where it would be expected and the bond responsible for that peak.

3. On each molecule, two CH_3 groups have been explicitly drawn. Identify whether those two CH_3 groups are homotopic, enantiotopic, diastereotopic or constitutionally different. **[3 marks]**

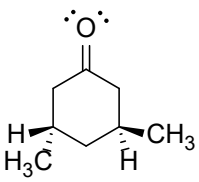
(a)



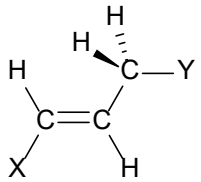
(b)



(c)

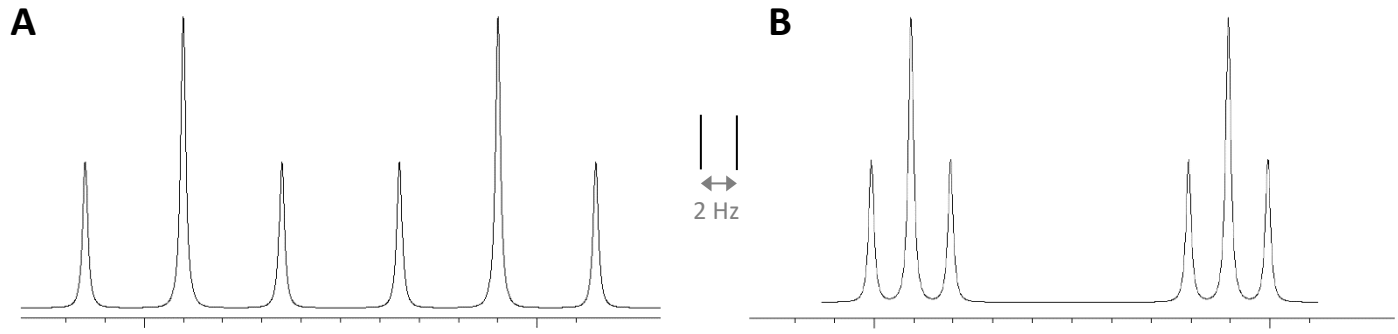


4. When the following molecule is analyzed by ^{1}H NMR, three signals are observed. **[10 marks]**



X and Y contain no hydrogen atoms.

Two of those signals are shown below (labeled "A" and "B"). The distance between adjacent "ticks" along the bottom of each spectrum is 2 Hz.



(a) Both signals have the same splitting pattern (with different coupling constants). *[2 marks]*
Name the splitting pattern.

(b) Measure or calculate the coupling constants for each signal. Label each diagram with the appropriate coupling constants, clearly indicating which lines were used to measure/calculate each coupling constant. *[4 marks]*

(c) Clearly identify which hydrogen atom(s) generated each of the two signals shown above. *[2 marks]*

(d) What does the third signal on the ^{1}H NMR look like? Sketch a picture and name the splitting pattern. *You are not expected to predict chemical shift since you do not know what "X" and "Y" are.* *[2 marks]*

5. The following page contains spectra for Unknown X ($C_{14}H_{12}O_3$). **[25 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:

5. *…continued*

$C_{14}H_{12}O_3$

