CHM 2120A
Midterm #2
November 14, 2018

First Name: _____ Last Name: _____

Student Number: _____

Approximate total number of marks: 97
The marks are given as a guide and are subject to change.
You can write in pen or in pencil.
The use of molecular models is permitted but they cannot be shared.
The use of calculators or other electronic devices is not permitted.
The final page has a pK_a table, ^1H chemical shift table, and IR table; it can be detached.

Read carefully:

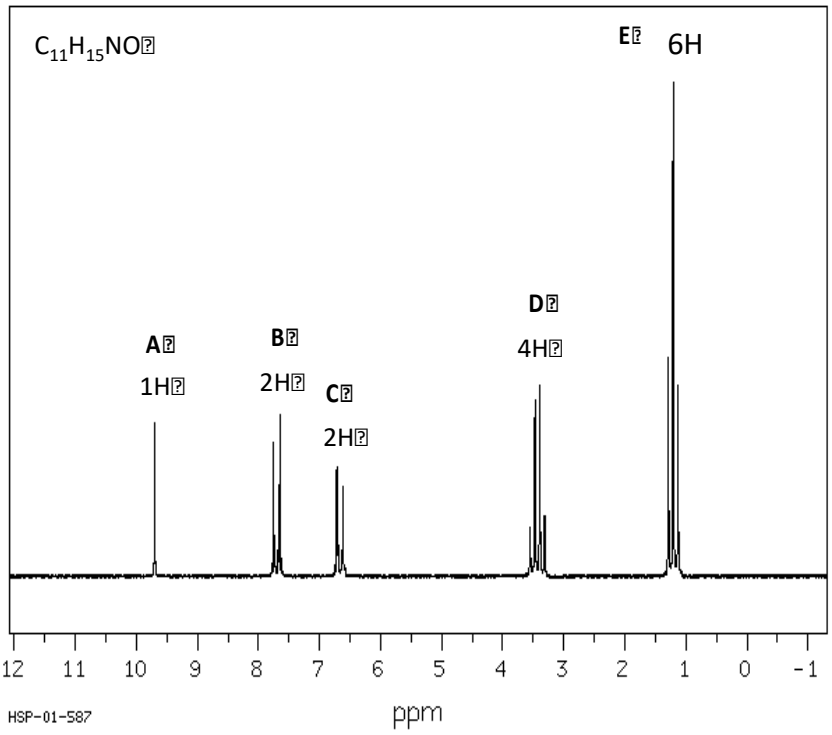
Cellular phones, unauthorized electronic devices or course notes (unless an open-book exam) are not allowed during this exam. Phones and devices must be turned off and put away in your bag. Do not keep them in your possession, such as in your pockets. If caught with such a device or document, the following may occur: academic fraud allegations will be filed which may result in your obtaining a **0** (zero) for the exam.

By signing below, you acknowledge that you have read and ensured that you are complying with the above statement.

Signature: _____

1a	2a	3b	4b	5b	6b	7b	8		1b	2b	3a	4a	5a	6a	7a	0
1 H																2 He
3 Li	4 Be										5 B	6 C	7 N	8 O	9 F	10 Ne
11 Na	12 Mg										13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
55 Cs	56 Ba	57 La	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
87 Fr	88 Ra	89 Ac	104 Rf	105 Ha	106 106												

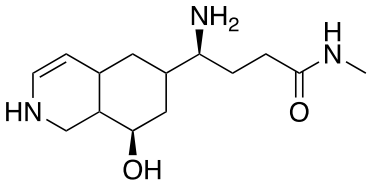
1. Determine the structure of the following unknown, which has molecular formula of $C_{11}H_{15}NO$. The ^1H NMR spectrum is below. Circle your final answer. **(6 points)**



Signal	δ (ppm)	Integra-tion	Multipli-city	Ideas (not marked)
A				
B				
C				
D				
E				

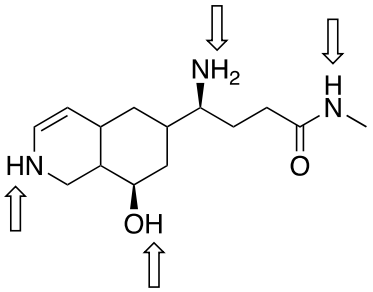
2.

a. Point to the **most** nucleophilic atom in the compound below. **(1 point)**
b. Circle the **least** nucleophilic atom in the compound below. **(1 point)**

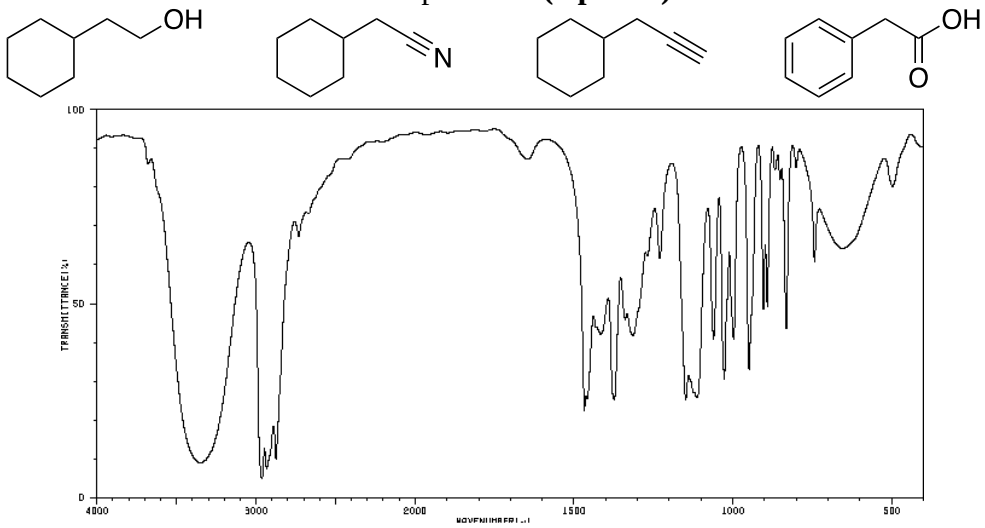


c. Justify your ranking in part a. **(4 points)**

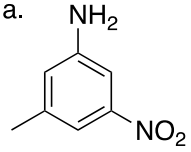
3. Estimate the pK_a value of each indicated proton. **(4 points)**

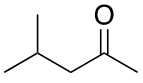


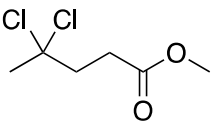
4. Circle the molecule that best fits the IR spectrum. **(2 points)**



5. How many signals are expected in the ^1H NMR spectrum for each of the following molecules? **(3 points)**

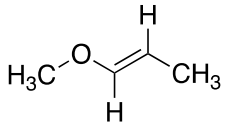
a.


b.


c.


6.

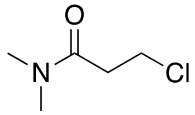
a. Assign all the signals listed from the ^{1}H NMR spectrum below by writing the letter of each signal beside the corresponding proton(s): **(3 points)**



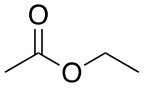
Assignment	Shift (ppm)
A	6.5
B	5.2
C	3.8
D	1.6

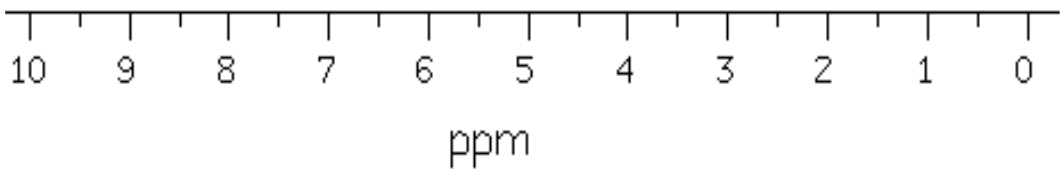
b. Justify your assignment of signals A and B. Use structures to support your explanation **(5 points)**

7. The ^{1}H NMR spectrum of following compound has two different signals for the methyl groups. Explain why there are two different signals even through the methyl groups are on the same atom. Draw structures to support your explanation. **(4 points)**



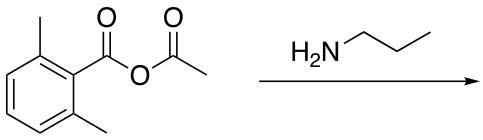
8. Draw the expected 1H NMR spectrum for the compound shown below, including number of signals chemical shift, multiplicity, relative peak intensity, and integration. **(5 points)**



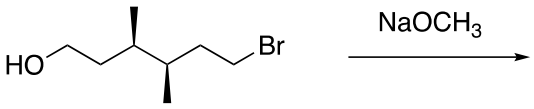


9. Draw the major organic product(s) OR reagents for each of the following reactions. **(3 points each: 12 points)**

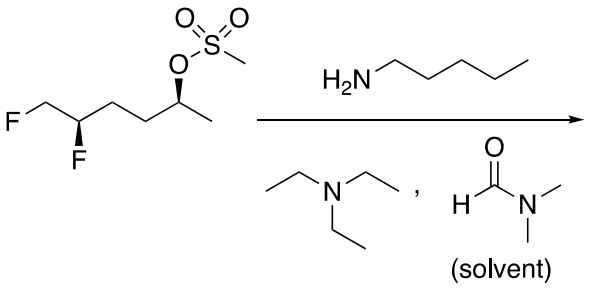
a.



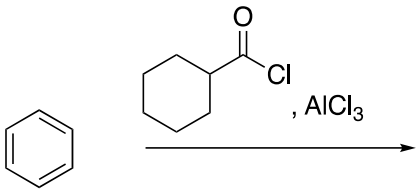
b.



c.

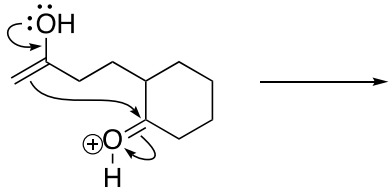


d.



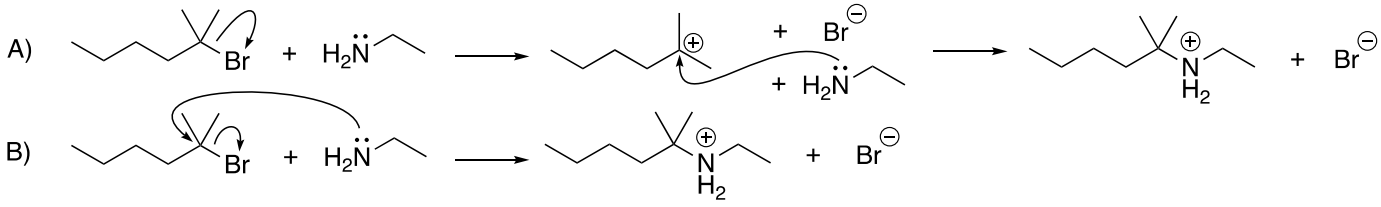
10.

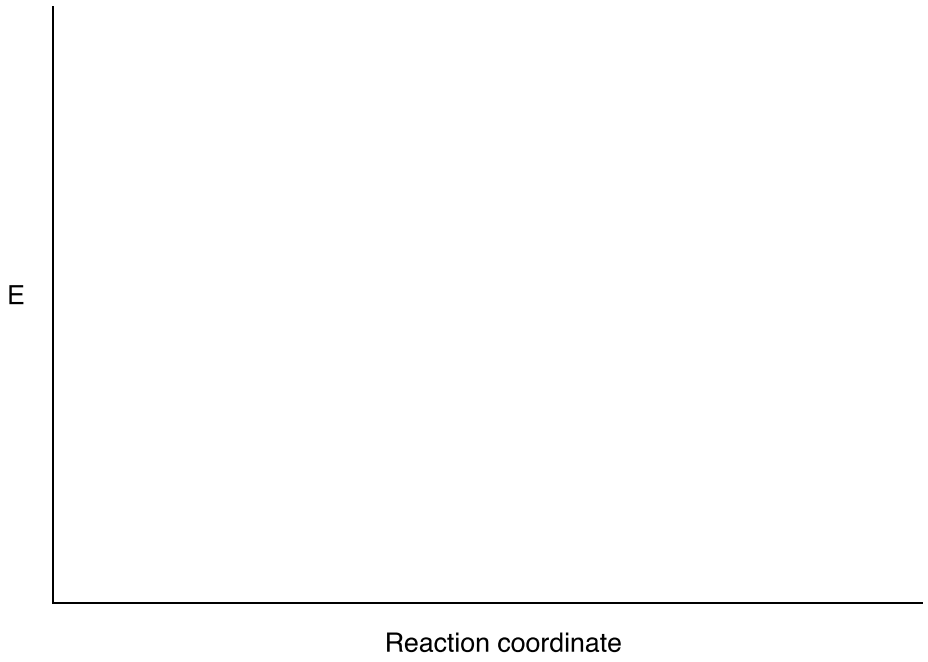
a. Draw the product of the reaction step below (one step only). **(3 points)**
b. Map the atoms and electrons directly involved in the reaction. **(2 points)**



11.

a. Draw and label the reaction coordinate diagram for the two proposed reaction mechanisms shown below, including for each reaction the transition states, activation energy of the rate determining step, reactants, intermediates, and products, as applicable. **(9 points)**



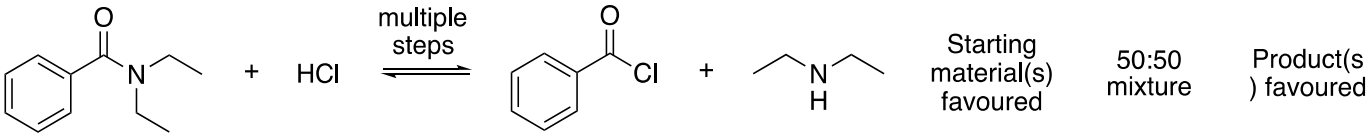


b. Which mechanism is most likely for the reaction shown? _____ **(1 point)**

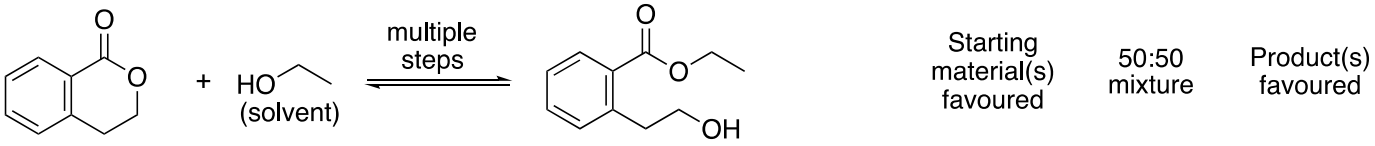
c. Justify your answer in part b, using your reaction coordinate diagram as part of your explanation. **(4 points)**

12. Predict the direction of each of the equilibrium shown below (for c, circle the predominant species at equilibrium). **(4 points)**

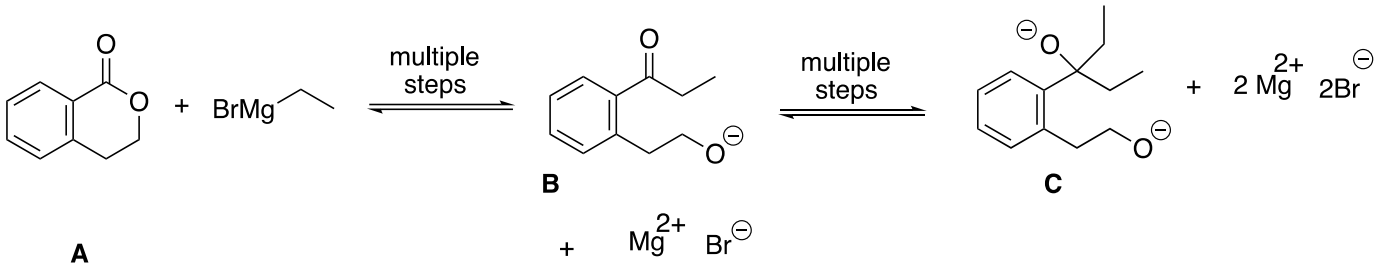
a.



b.



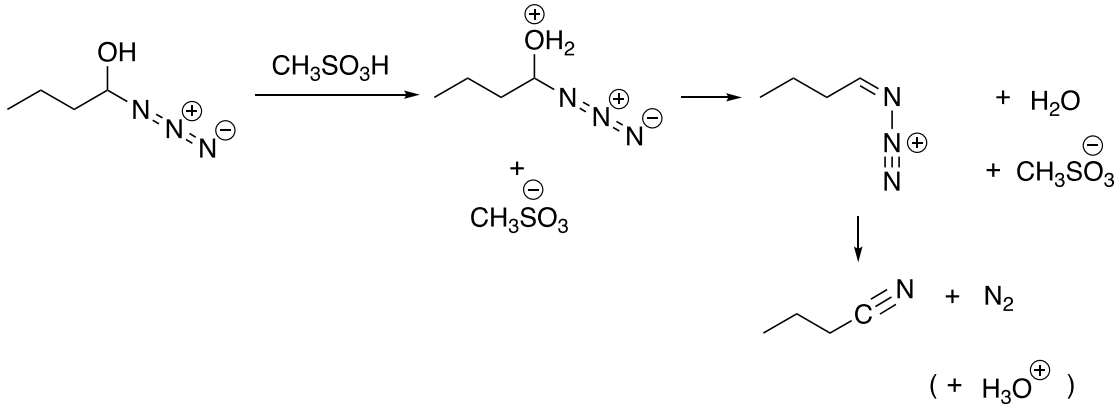
c.



13.

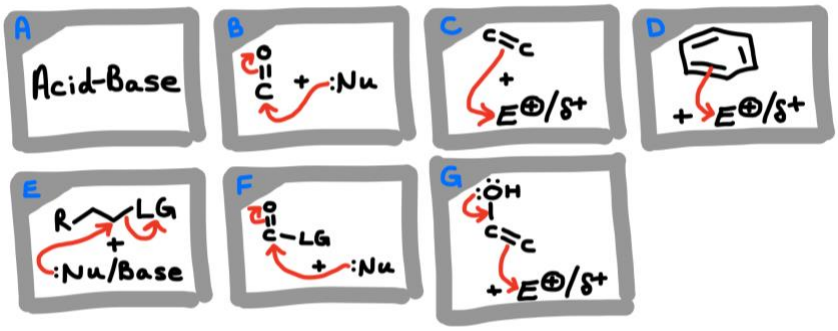
a. Add curved arrows to show the movement of electrons in each of the reaction steps below. **(8 points)**

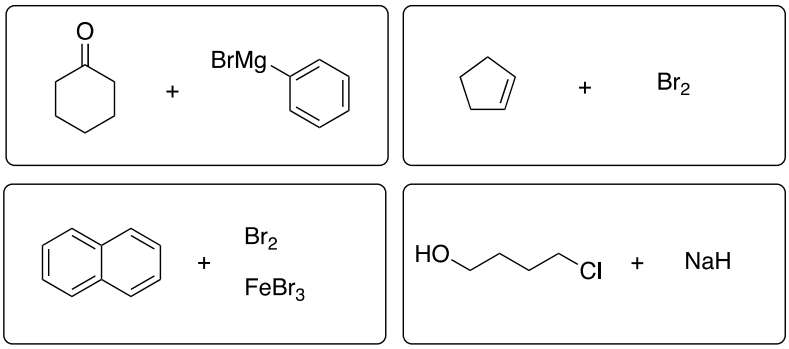
b. Around the reacting centres, add non-bonding electrons and draw the carbon and hydrogen atoms explicitly. **(2 points)**



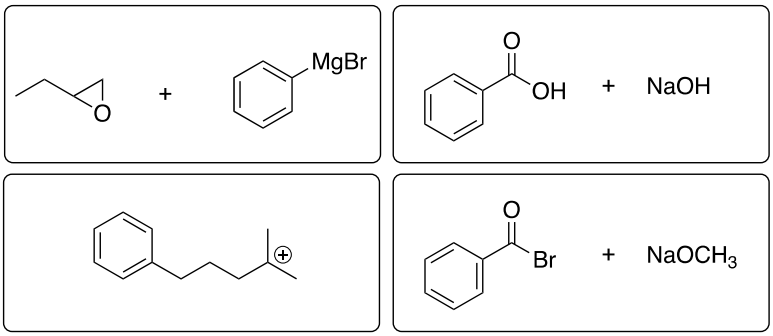
14.

a. Categorize each of the following reactions using the categories provided below. **(4 points)**

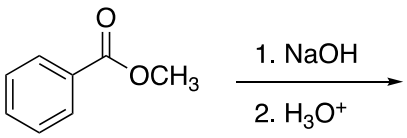




b. Circle the reaction(s) below that fit into category **F**. **(2 points)**

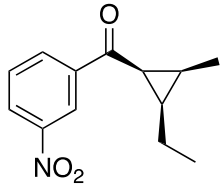


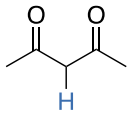
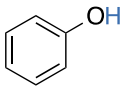
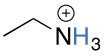
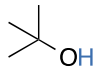
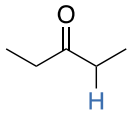
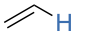
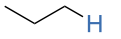
15. Draw the mechanism and products of the following reaction. **(8 points)**



BONUS!!!

How many signals are expected in the ^{1}H NMR spectrum of the compound below? **(2 points)** _____

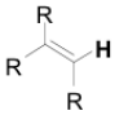
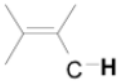
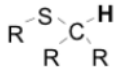
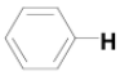
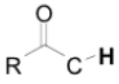
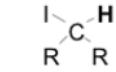
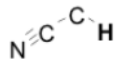
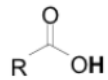
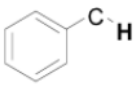
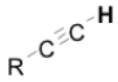
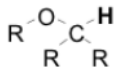
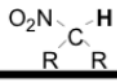


Acid	pK_a value (H_2O solvent)	Acid	pK_a value (H_2O solvent)
HI	-10		9
H_2SO_4	-3		
HBr	-9		9.9
HNO_3	-1.3		
HCl	-8		10.6
HF	3.17	H_2O	15.7
	-3.8		17
	-2.6		20
	-6.2		24
H_3O^+	-1.7	H_2	36
$CH_3OH_2^+$	-2.2	NH_3	38
	4.76		50
			51

IR Key Absorptions (cm^{-1}):

C-H Alkyl	C-H	2850-2960	m, sharp
C-H sp^2	C-H	just >3000	m, sharp
Alcohol	R**O-H**	3200-3650	s, broad
Carboxylic acid	RC(=O)**O-H**	2500-3300	s, broad
Amine	R2**N-H**	3300-3500	s, broad
*Carbonyl	R2**C=O**	1650-1780	s, sharp
Nitrile	R**C≡N**	2220-2260	v, sharp
Alkynyl	C≡**C-H**	~3300	m, sharp
Alkynyl	**C≡C**	2100-2260	v, sharp

Typical proton NMR chemical shifts

RCH_n	0.7 - 1.7		2.2 - 2.9		4.5 - 7.0
	1.6 - 2.6		2.0 - 3.0		6.5 - 8.0
	2.1-2.5		2.0 - 4.0		9.0 - 10.0
	2.1 - 3.0		2.7 - 4.1		11.0 - 12.0
	2.3 - 2.7		3.1 - 4.1		
	1.7 - 2.7		4.2 - 4.8	OH, NH: variable	
			3.0 - 5.0		
			4.1 - 4.3		

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