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 Student Number \_\_\_\_\_  
 Practical # \_\_\_\_\_ TA name \_\_\_\_\_

1. Predict the molecular formula of the compound represented below based on the MS data given. Please show your calculations for the full mark. (5 marks)

m/z	Intensity
84 M <sup>+</sup>	10.00
85 → (M+1) <sup>+</sup>	0.56 → 17.0
86 → (M+2) <sup>+</sup>	0.04 → 18.0

0  $84 - 16 = 68$

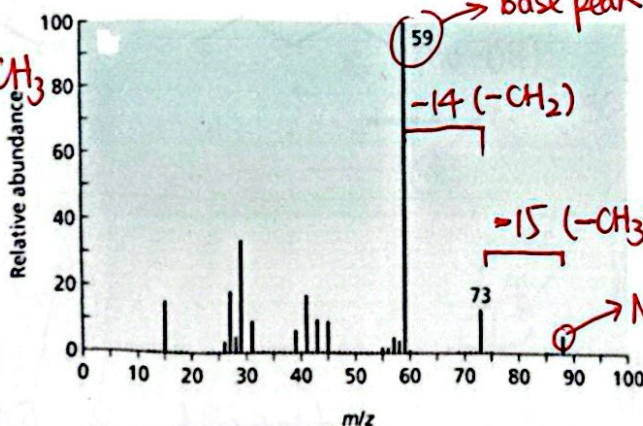
$68 \div 13 = 5 \dots 3 \text{ (H)}$   $5\text{CH} + 3\text{H}$   
 (CH)

Molecular formula:

C<sub>5</sub>H<sub>8</sub>O

2. The mass spectra of 1-methoxybutane, 2-methoxybutane, and 2-methoxy-2-methylpropane were run. Which one of them is responsible for the mass spectrum below? Identify the compound and show structures for the molar ion peak and a base peak. (9 marks total, 3 marks each)

Peak (59): loss of -CH<sub>2</sub>CH<sub>3</sub>



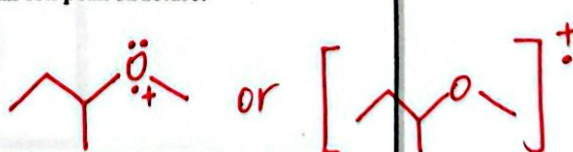
Name of the compound responsible for the mass spectra above:

2-methoxybutane

Base peak structure:

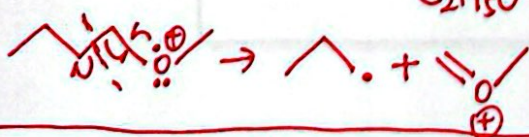


Molar ion peak structure:

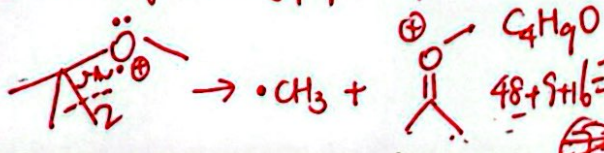


1-methoxybutane

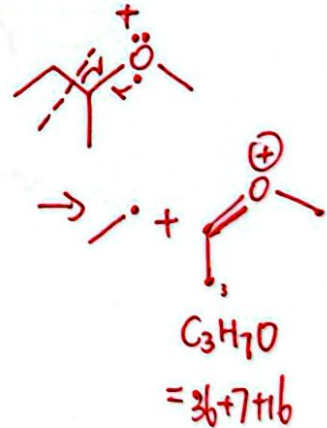
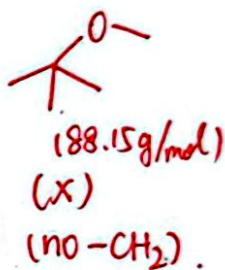
$24 + 15 + 16 = 45$  (base peak)  
 $C_2H_5O$

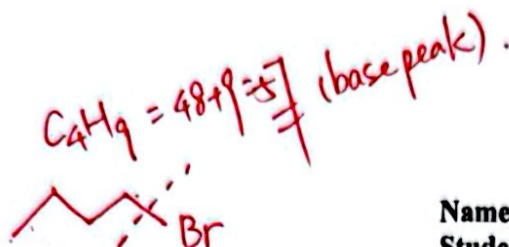


2-methoxy-2-methylpropane



2 if:  $\begin{cases} \text{1-methoxybutane: base peak @ 45} \\ \text{2-methoxy-2-methylpropane: base peak @ 73} \end{cases}$



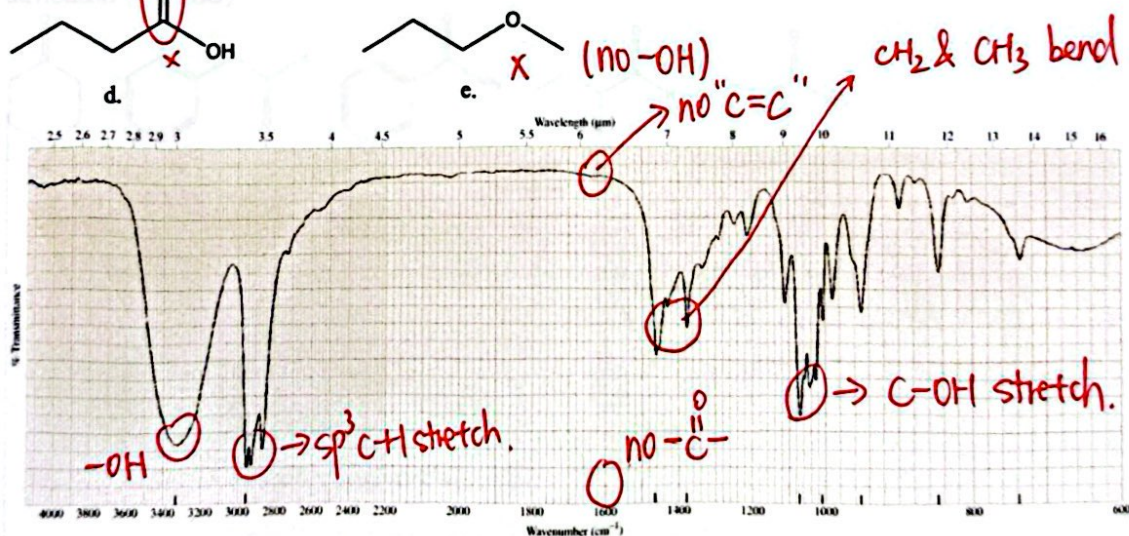
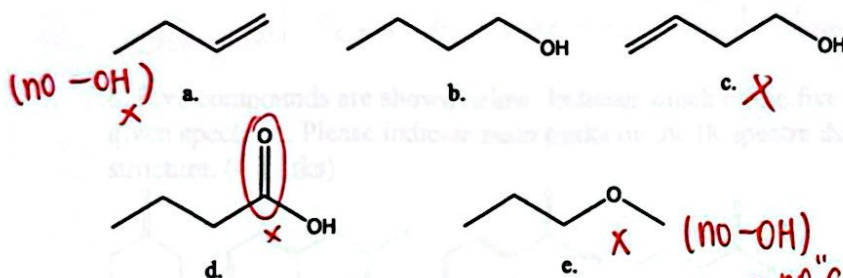


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D 3. Which of the following is/are true about the MS of 1-bromobutane? Please circle the right answer. (3 marks)

- ☒ A) Peaks of approximately equal intensity are observed at  $m/z$  136 and 138.  
☒ B) The major fragmentation occurs by cleavage of the C-Br bond.  
☒ C) The most intense peak occurs at  $m/z$  43.  
☒ D) both A and B  
☒ E) both B and C

4. Five compounds are shown below. Indicate which of the five compounds is responsible for the given spectrum. Please indicate main peaks on the IR spectra that you used to determine this structure. (4 marks)

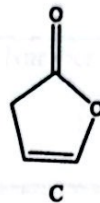
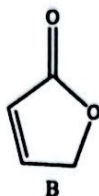
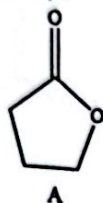


Structure of the compound responsible for the IR spectra above:



Name \_\_\_\_\_

5. List the following compounds in order of decreasing wavenumber of the C=O absorption band: (6 marks total)

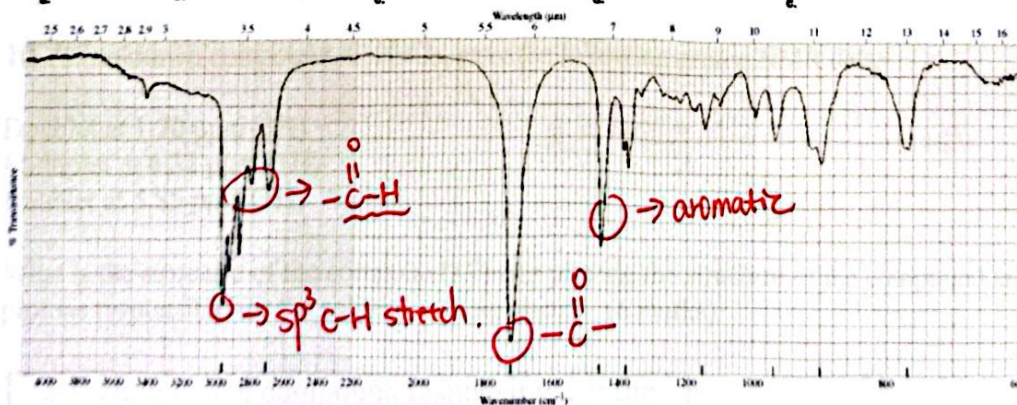
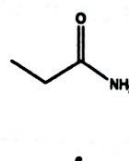
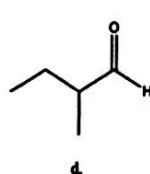
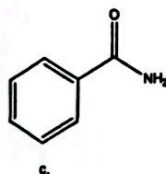
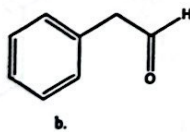
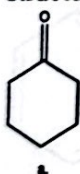


C < B < A (3 marks)

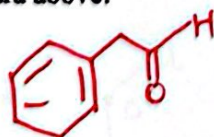
Briefly explain your choice for the compound with the smallest wavenumber using the only space provided below: (3 marks)

Resonance / electrons delocalization lowers the frequency of C=O  
conjugated "C=O" has more single bond character than normal "C=O"

6. Five compounds are shown below. Indicate which of the five compounds is responsible for the given spectrum. Please indicate main peaks on the IR spectra that you used to determine this structure. (4 marks)

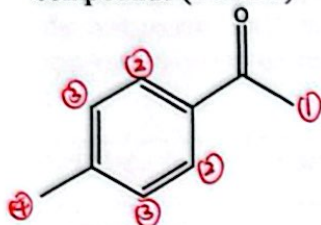


Structure of the compound responsible for the IR spectra above:



Name \_\_\_\_\_

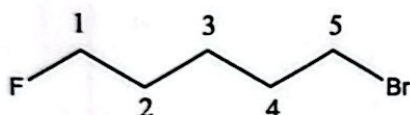
7. How many signals would you expect to see in the  $^1\text{H}$  NMR spectrum of the following compound? (2 marks)



Number of signals:

4.

8. Which of the following protons gives an NMR signal with the highest chemical shift value (farthest downfield)? (2 marks)

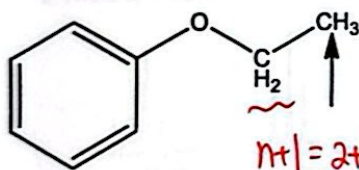


Protons number:

1.

↓ most deshielded.  
most electron-withdrawing

9. What splitting pattern is observed in the proton NMR spectrum for the indicated hydrogens? (2 marks)



Splitting pattern:

Triplet.

$$n+1 = 2+1 = 3$$

10. An unknown compound,  $\text{C}_3\text{H}_5\text{Cl}_3$ , gave the following proton NMR data:

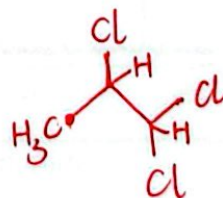
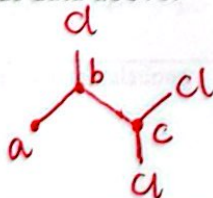
- a Doublet at 1.70 ppm (3H) →  $-\text{CH}_3$
- b Multiplet at 4.32 ppm (1H)
- c Doublet at 5.85 ppm (1H)

$$n = \frac{2 \times 3 + 2 - 5 - 3}{2} = \frac{0}{2} = 0$$



What is the structure of the compound? Please provide the structure of the compound and assign protons responsible for the splitting pattern above. (6 marks)

Structure of the compound responsible for the NMR data above:



Name \_\_\_\_\_

11. An unknown compound was analyzed using several forms of spectroscopy. In addition to the spectral data, the compound revealed the following mass percentages. Please identify structure of the compound based on the information provided. Show your work for the full mark (label all appropriate peaks on each spectrum). (20 marks)

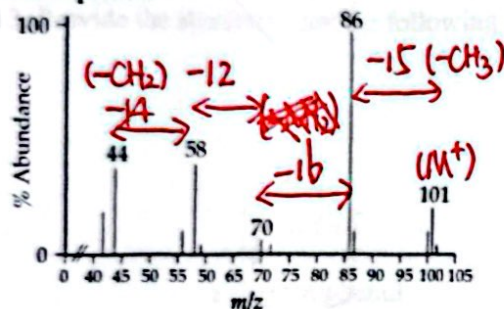
C	H	N
71.22%	14.94%	13.84%

$C_xH_yN_z$   $x:y:z \approx \frac{71.22}{12} : \frac{14.94}{1} : \frac{13.84}{14} \approx 6 : 15 : 1$

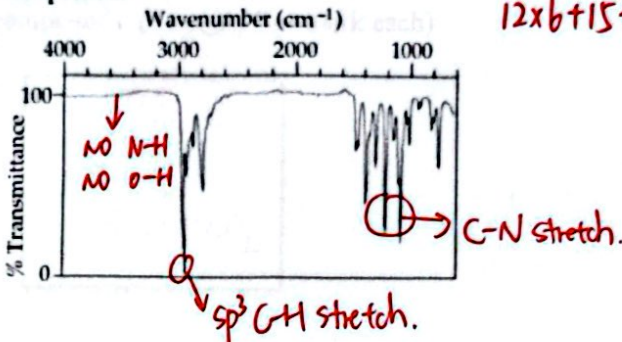


$12 \times 6 + 15 + 14 = 72 + 29 = 101 \checkmark$

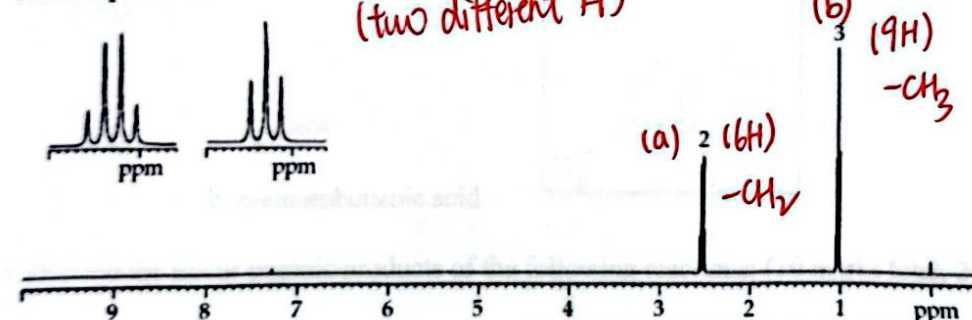
Mass spectrum



IR spectrum



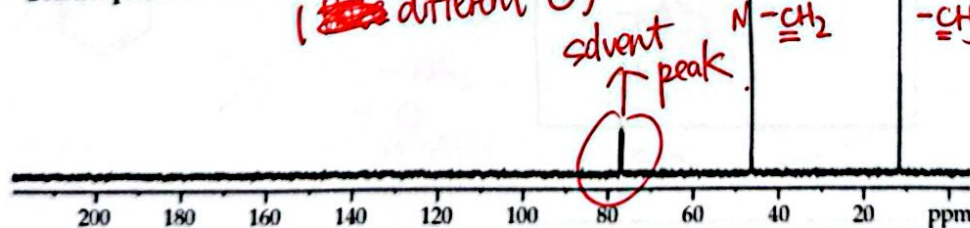
<sup>1</sup>H NMR spectrum



(two different H)

15 H with 2 peaks  
↓  
highly symmetrical

<sup>13</sup>C NMR spectrum



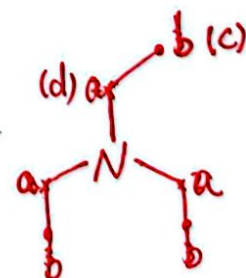
two different C

(d) N-CH<sub>2</sub> (c) -CH<sub>3</sub>

(all <sup>13</sup>C signals should be singlets)

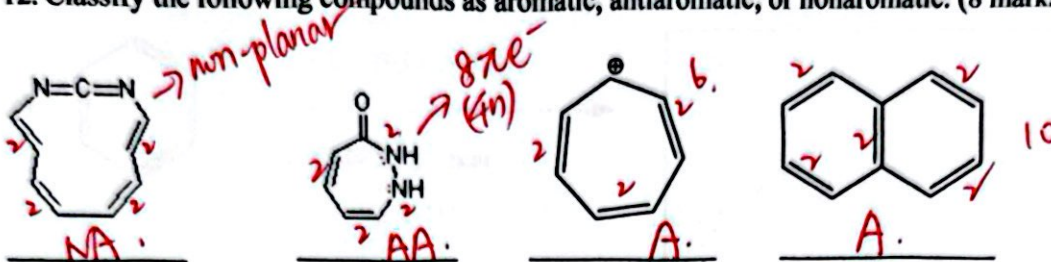
UN number calculations:

Structure:



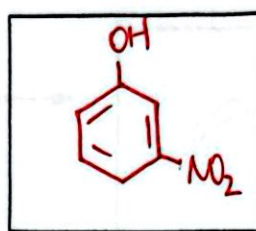
Name \_\_\_\_\_

12. Classify the following compounds as aromatic, antiaromatic, or nonaromatic. (8 marks)

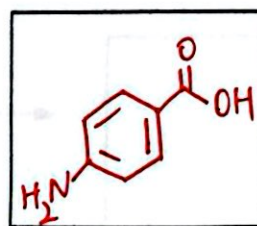


13. Provide the structures for the following compounds: (2 marks, one mark each)

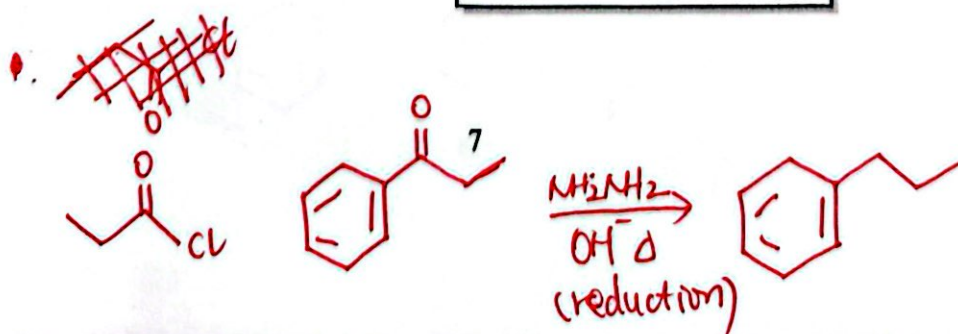
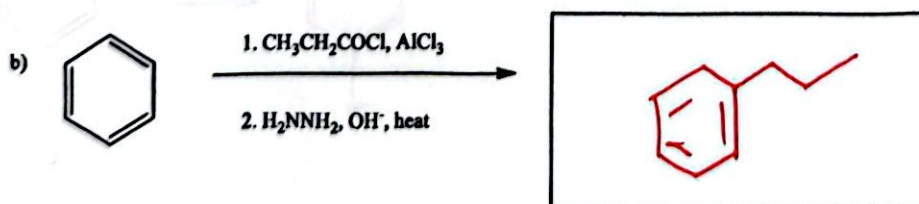
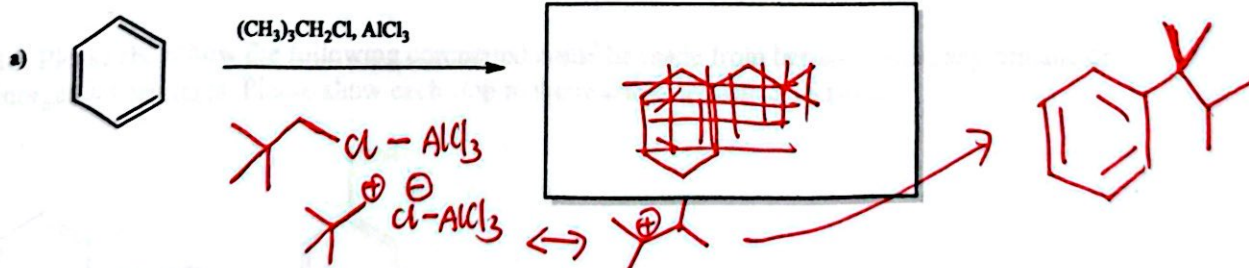
a. *m*-nitrophenol



b. *p*-aminobenzoic acid

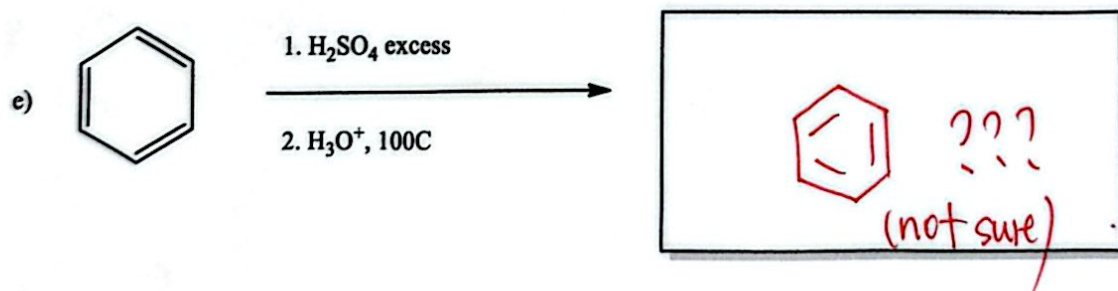
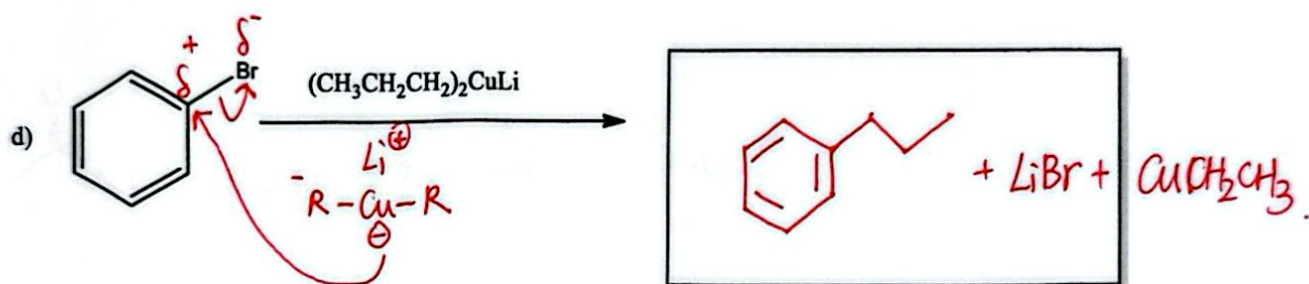
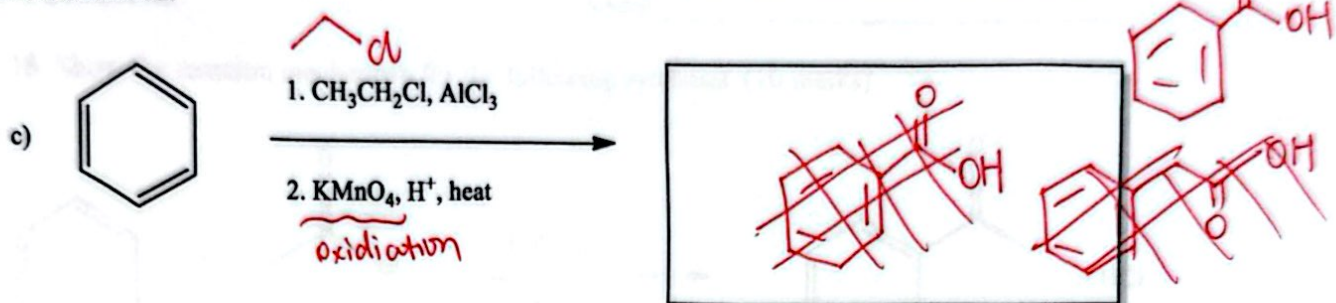


14. Provide the major organic products of the following reactions: (10 marks total, 2 marks each)

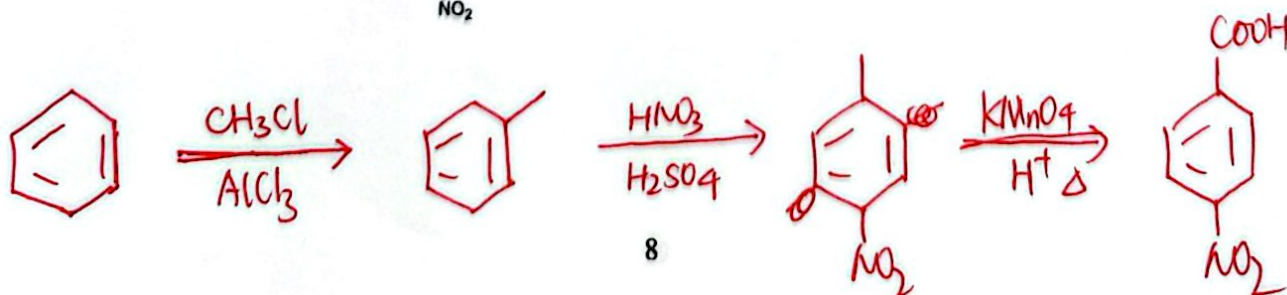
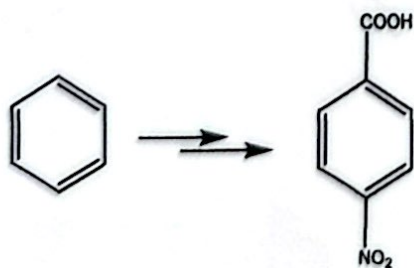


14. Continued:

Name \_\_\_\_\_



15. Please show how the following compound could be made from benzene using any organic or inorganic chemicals. Please show each step in the reaction sequence. (8 marks)



Name \_\_\_\_\_

16. Show the reaction mechanism for the following synthesis. (10 marks)

