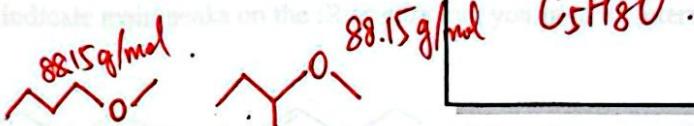


Name Jincheng Hong (Frank)
 Student Number _____
 Practical # _____ TA name _____

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)

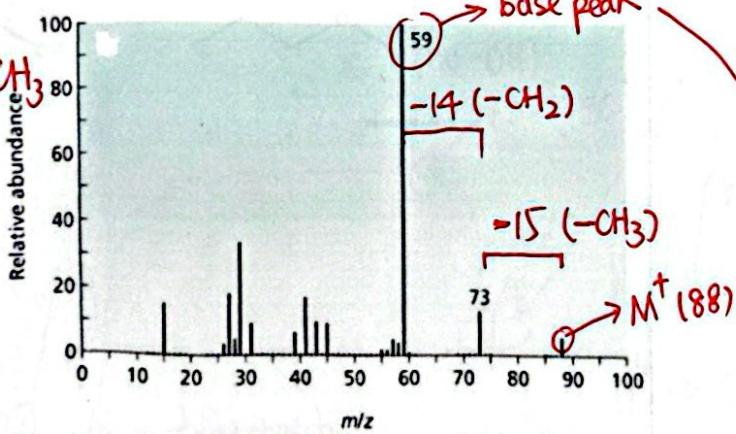
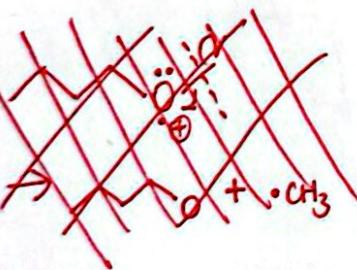
m/z	Intensity	
84 M ⁺	10.00	0 84-16 = 68
85 → (M+1) ⁺	0.56	68 ÷ 13 = 5...3 (H). 5CH + 3H
86 → (M+2) ⁺	0.04	(CH)

Molecular formula:



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 -CH₂CH₃



Name of the compound responsible for the mass spectra above:

2-methoxybutane.

Base peak structure:



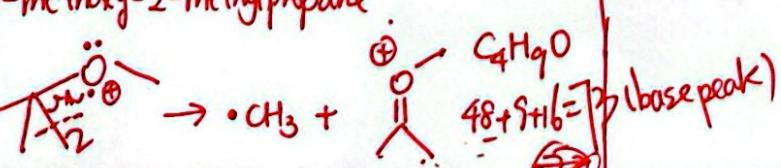
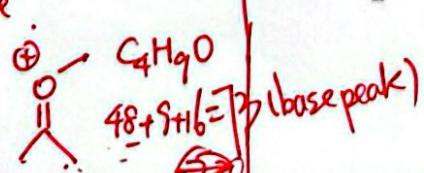
1-methoxybutane



Molar ion peak structure:



2-methoxy-2-methylpropane



if: { 1-methoxybutane : base peak @ 45
 2-methoxy-2-methylpropane : base peak @ 73.

$C_4H_9 = 48 + 9 = 57$ (base peak).
~~Br~~

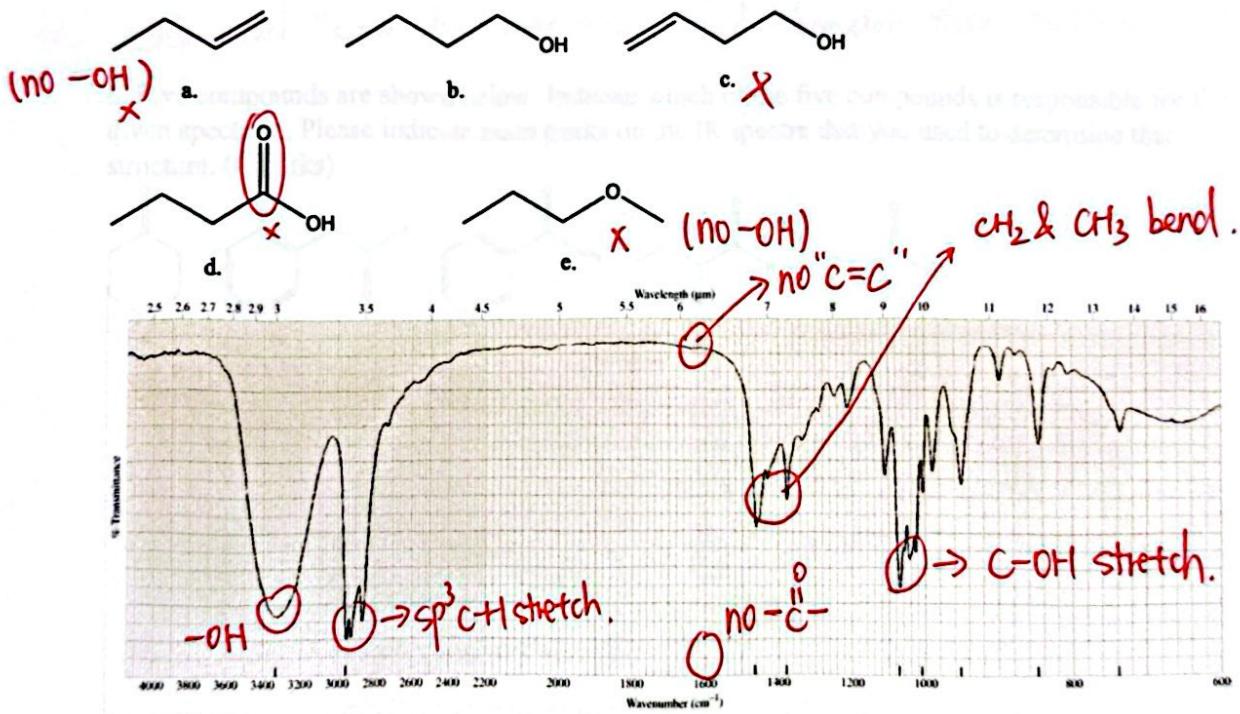
Name _____
 Student Number _____
 Practical # _____ TA name _____

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

Briefly explain your choice for the compound with the smallest wavenumber using the only given spectrum. (4 marks)

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)

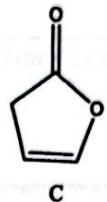
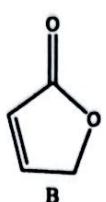
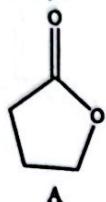


Structure of the compound responsible for the IR spectra above:



Name _____

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

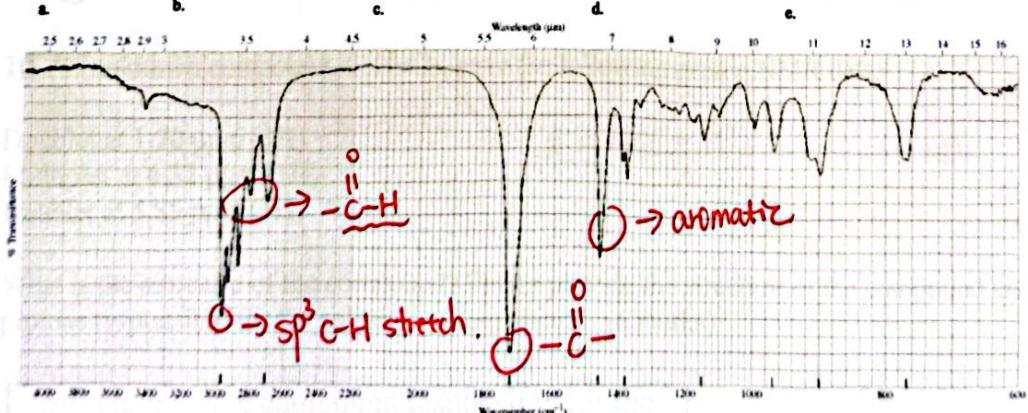
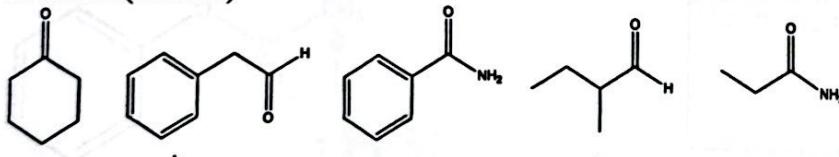


C < B < A (3 marks)

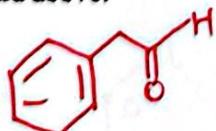
Briefly explain your choice for the compound with the smallest wavenumber using the only space provided below: (3 marks)

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)

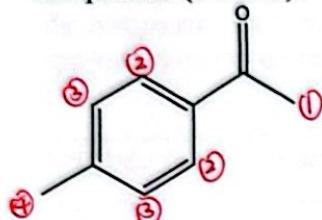


Structure of the compound responsible for the IR spectra above:



Name _____

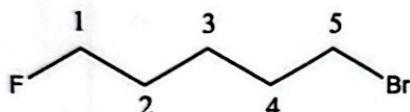
7. How many signals would you expect to see in the ^1H NMR spectrum of the following compound? (2 marks)



Number of signals:

4.

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

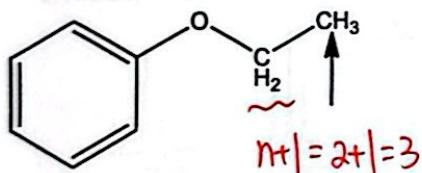


Protons number:

1.

↙ most deshielded.
most electron-withdraw

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



Splitting pattern:

Triplet.

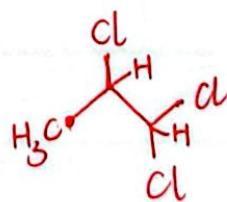
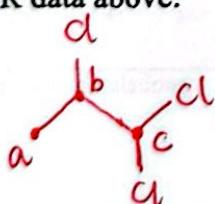
10. An unknown compound, $\text{C}_3\text{H}_5\text{Cl}_3$, gave the following proton NMR data:

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



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 _____

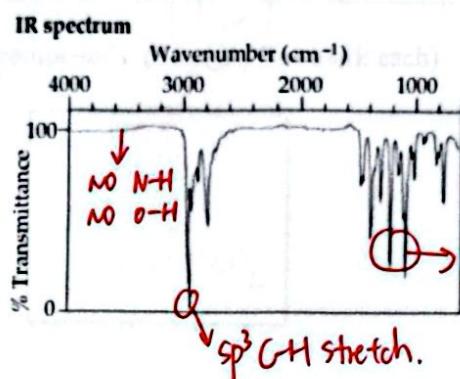
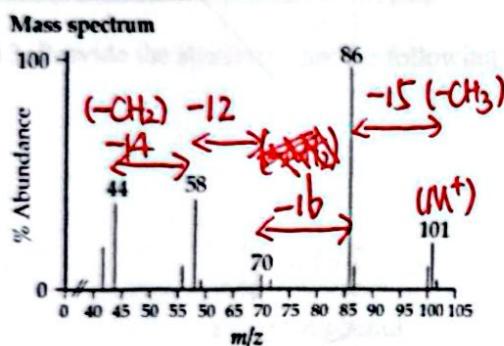
11. An unknown compound was analyzed using several forms of spectroscopy. In addition to the spectral data, the compound revealed the following mass percentages. Please identify structure of the compound based on the information provided. Show your work for the full mark (label all appropriate peaks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

C	H	N
71.22%	14.94%	13.84%

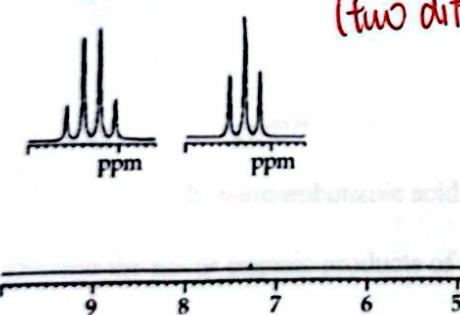
$$C_xH_yNz \quad X:y:Z \approx \frac{71.22}{12} : \frac{14.94}{1} : \frac{13.84}{14} \approx 6 : 15 : 1$$



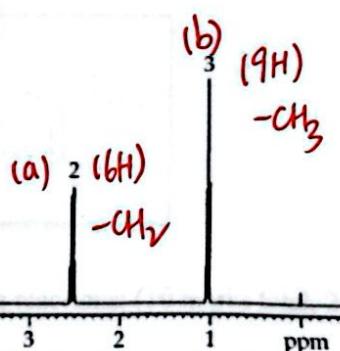
$$12x + 15 + 14 = 72 + 29 \\ = 101 \checkmark$$



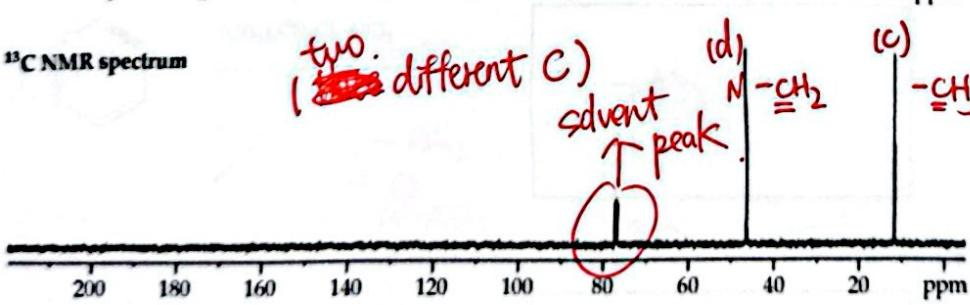
¹H NMR spectrum



(two different H)

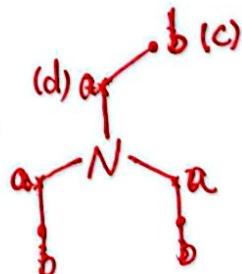


¹³C NMR spectrum



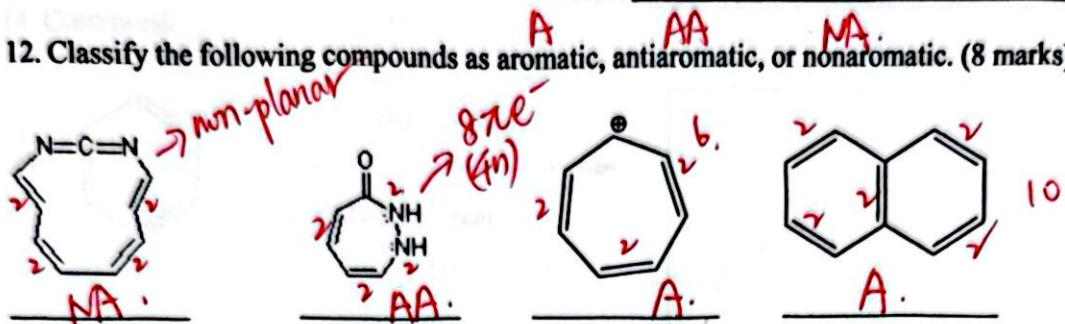
UN number calculations:

Structure:

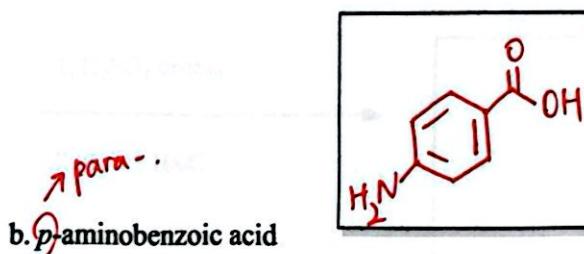
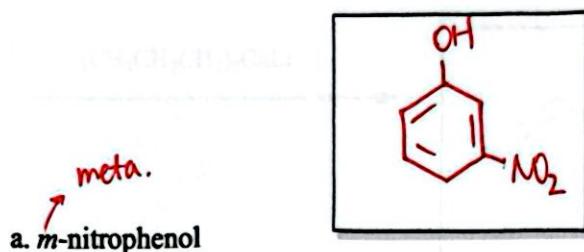


Name _____

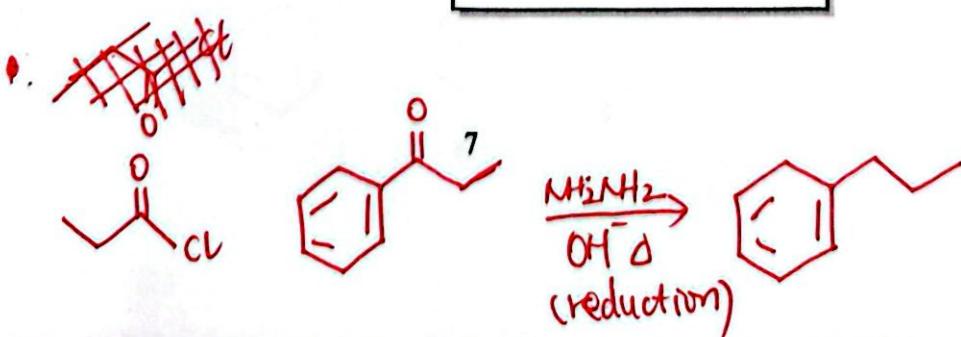
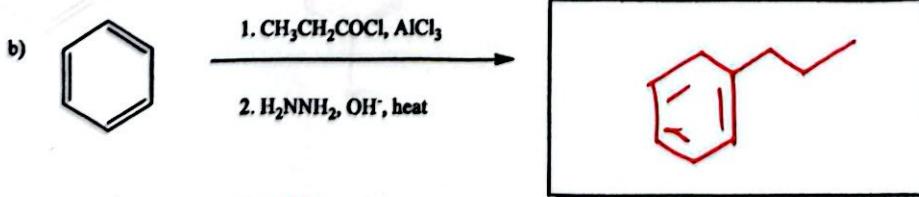
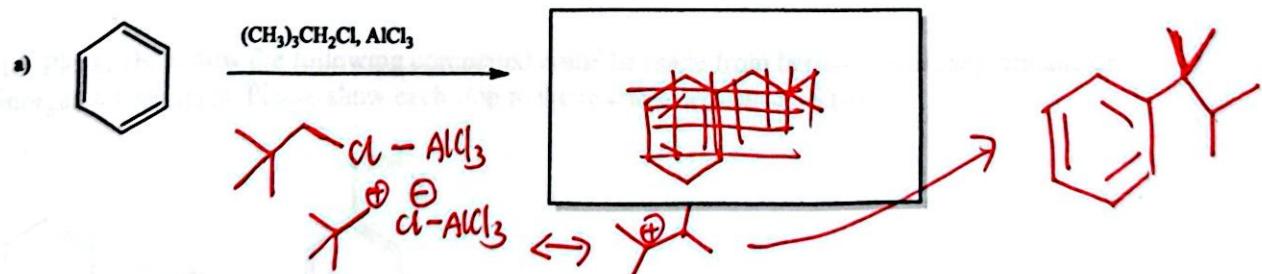
12. Classify the following compounds as aromatic, antiaromatic, or nonaromatic. (8 marks)



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



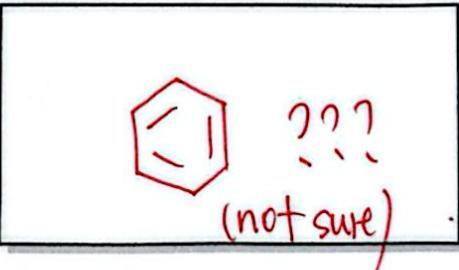
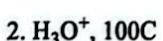
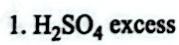
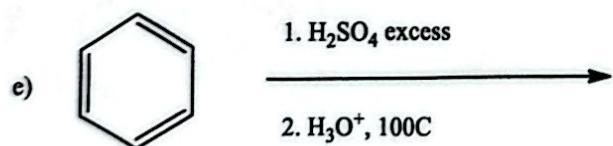
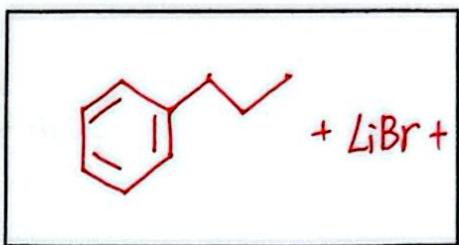
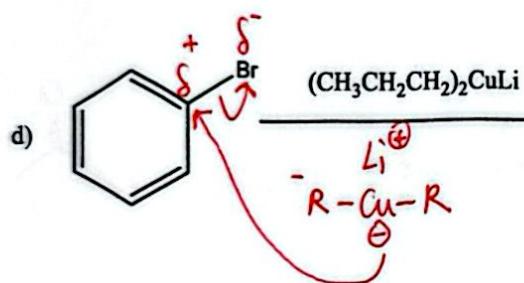
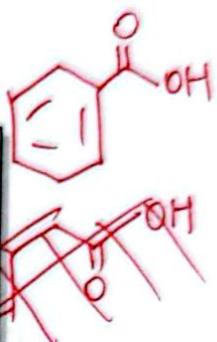
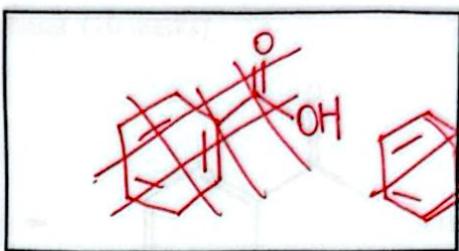
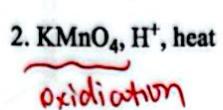
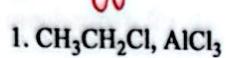
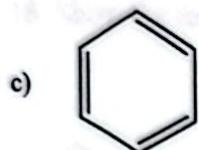
14. Provide the major organic products of the following reactions: (10 marks total, 2 marks each)



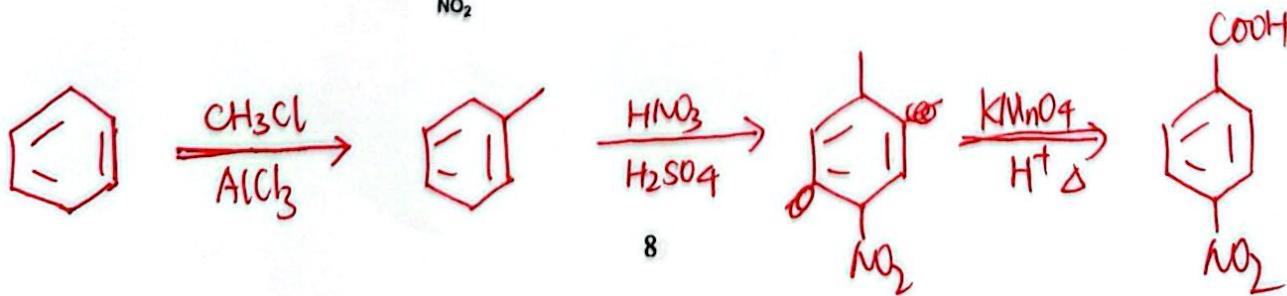
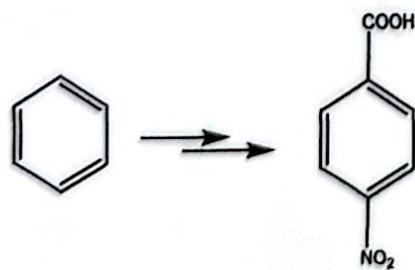


14. Continued:

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)

