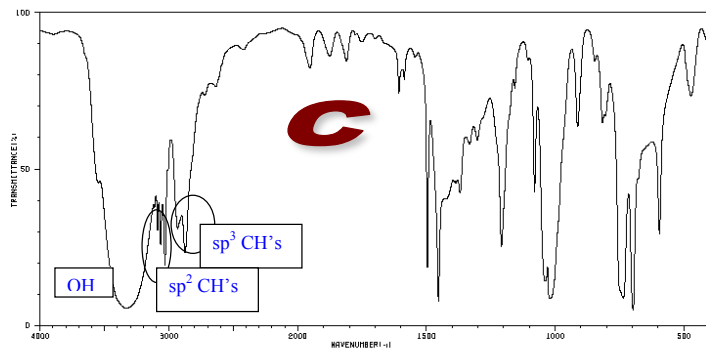
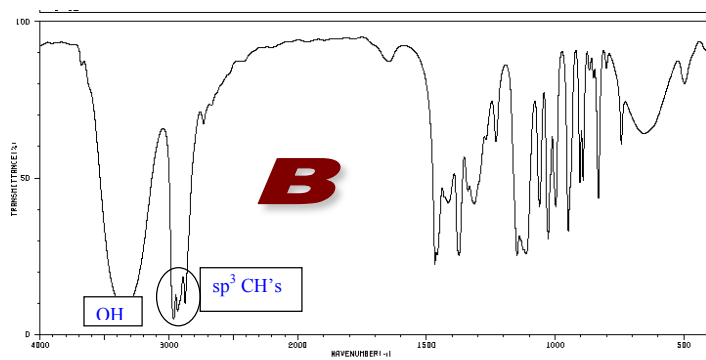


Assignment 5 - Answers
CHM 2120 – Assignment 6 – ANSWERS

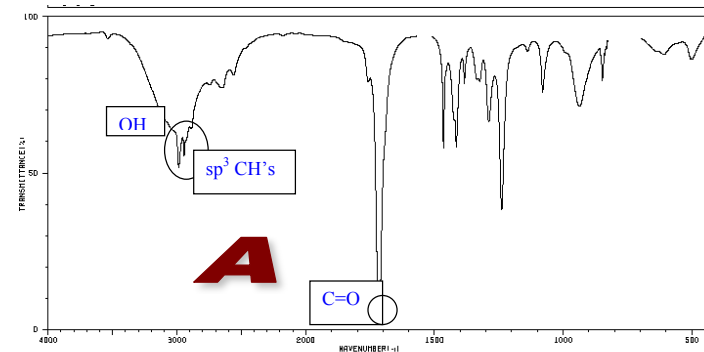
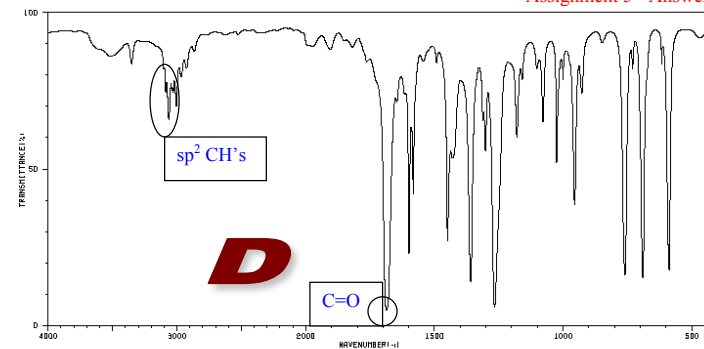
Part A.

1. Associate each of the following IR spectra with one of the following compounds and justify your answer.
 - a. Propanoic acid: look for a carbonyl stretch and a broad OH stretch
 - b. 2-Pentanol: look for an OH peak (broad). No carbonyl peak, no sp^2 CH's.
 - c. Benzyl alcohol; Look for an OH peak and sp^2 CH's. No carbonyl peak.
 - d. Acetophenone: Look for a carbonyl peak and sp^2 CH's. No OH peak.

Note: the key functional groups must be identified. Identifying the peaks on the spectrum directly is a straightforward way to do this.



Assignment 5 - Answers

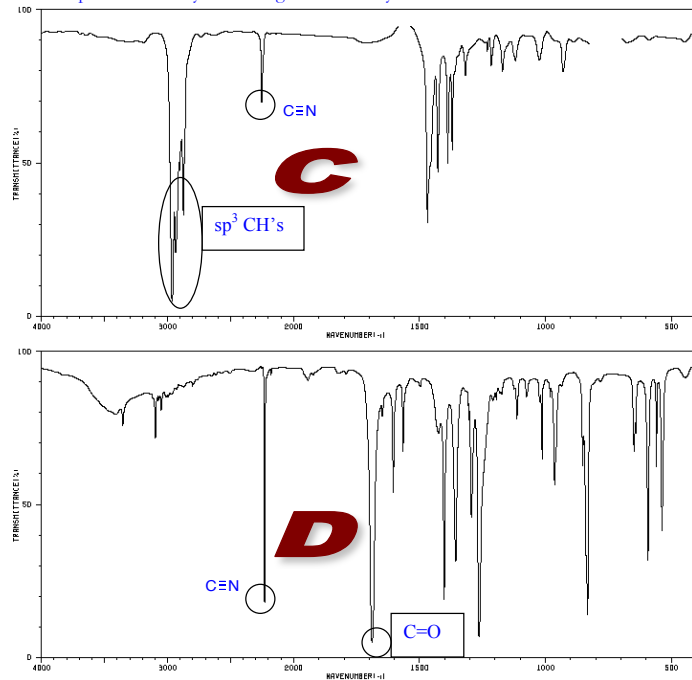


Assignment 5 - Answers

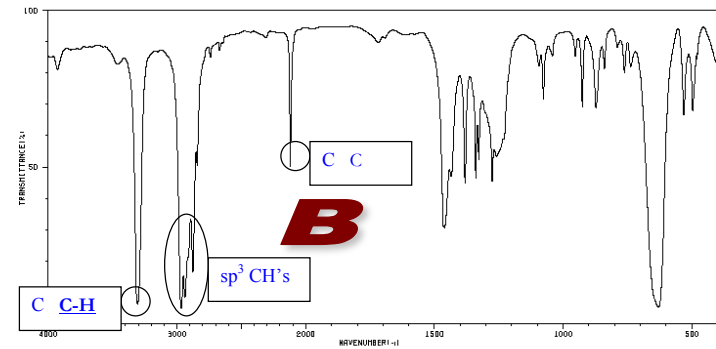
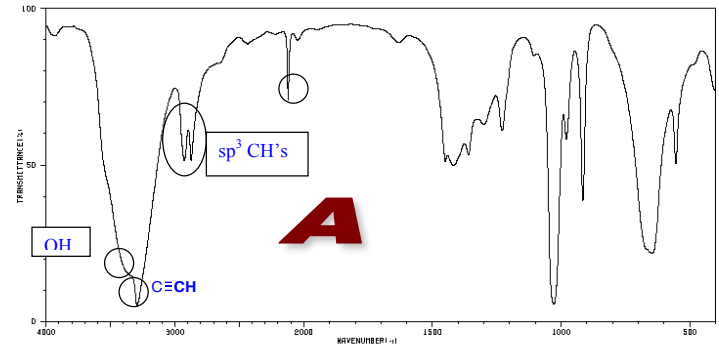
Associate each of the following IR spectra with one of the following compounds and justify your answer.

- e. 2-Propyn-1-ol: Look for an alkyne peak $C \equiv C$ plus an OH peak (broad) and a CH .
- f. 1-Pentyne: Look for an alkyne peak $C \equiv C$ plus CH . No other key groups.
- g. 4-Methylpentanenitrile: Look for a $C \equiv N$. No OH, $C=O$ or CH .
- h. p-Acetylbenzonitrile: Look for $C=O$, $sp^2 CH$'s and $C \equiv N$. No CH .

Note: the key functional groups must be identified. Identifying the peaks on the spectrum directly is a straightforward way to do this.



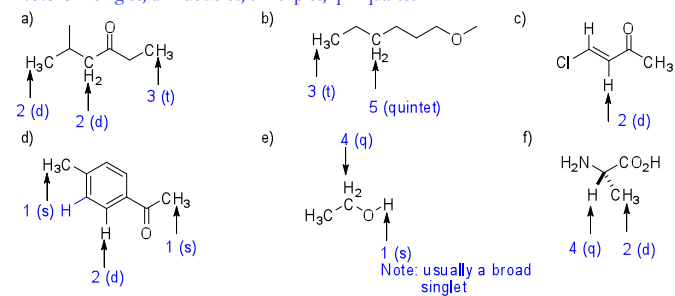
Assignment 5 - Answers



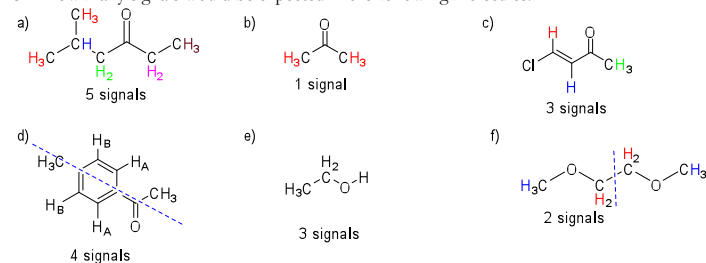
Assignment 5 - Answers

2. Give the number of peaks expected for the indicated protons in each of the following structures:

Note: s = singlet, d = doublet, t = triplet, q = quartet

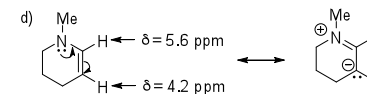
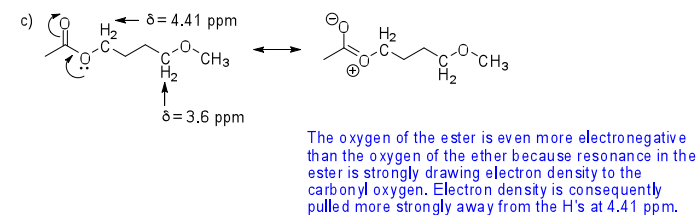
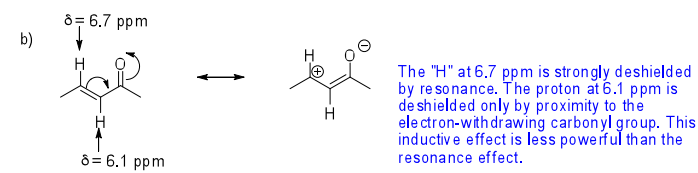
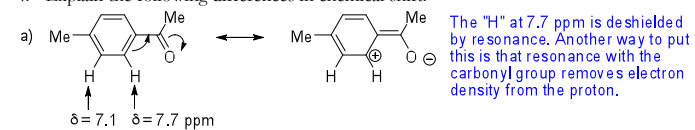


3. How many signals would be expected in the following molecules?



Assignment 5 - Answers

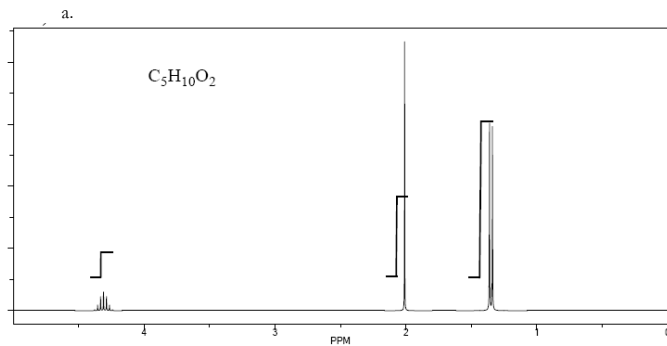
4. Explain the following differences in chemical shift.



Resonance with the nitrogen pushes electron density onto the H at 4.2 ppm, effectively "shielding" it with electrons.

Assignment 5 - Answers

5. Determine the structure of the following unknowns using the table to fill in your answers.

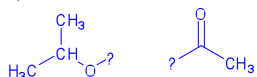


Signal	δ	Integration	Multiplicity	Comments
A	~4.3	1H	m (multiplet) or septet	CH next to O (based on δ)
B	~2.0	3H	s	CH_3 next to $C=O$
C	~1.3	6H	d	2 x CH_3 (identical) next to CH (i.e. an isopropyl group)

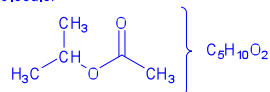
$$DU = [5(2) + 2 - 10]/2 = 1$$

$$\text{Integration: } (6 \text{ mm} + 18 + 34)/10H = 5.8 \text{ mm/H}$$

The pieces:

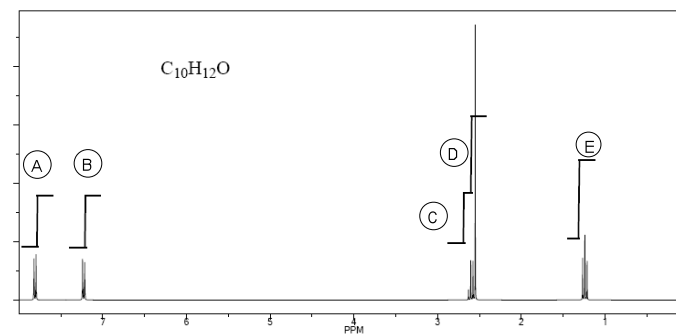


The molecule:

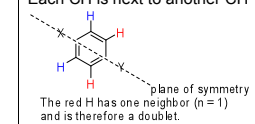


Assignment 5 - Answers

b.



Signal	δ	Integration	Multiplicity	Comments
A	~7.8	2H (CH_2 or 2 x CH)	d	Not all the 2H's can be CH_2 or there wouldn't be enough carbons accounted for in the molecule (there are 10 carbons in the molecule); These H's are in the aromatic region—they can't be CH_2 's — only CH group exist on aromatic rings. Each CH is next to another CH
B	~7.2	2H (CH_2 or 2 x CH)	d	See explanation above
C	~2.7	2H (CH_2 or 2 x CH)	q	CH_2 next to CH_3 (b/c the peak is a quartet); not directly next to O, could be next to $C=O$ (based on δ)
D	~2.6	3H	s	CH_3 next to $C=O$ (based on δ) or on phenyl ring (which acts like an electron-withdrawing group)
E	~1.2	3H	t	CH_3 next to CH_2



$$DU = [10(2) + 2 - 12]/2 = 5$$

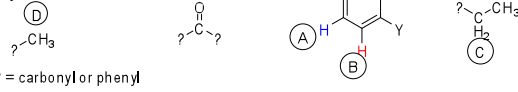
HINT: DU of 4 = phenyl ring...

In this molecule, there is probably a phenyl ring (DU = 4) + one ring or one double bond

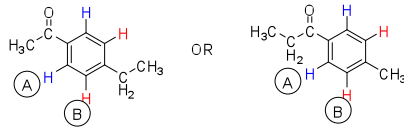
$$\text{Integration: } (11 \text{ mm} + 11 + 11 + 17 + 17)/12H's = 5.6 \text{ mm/H}$$

Assignment 5 - Answers

The pieces:



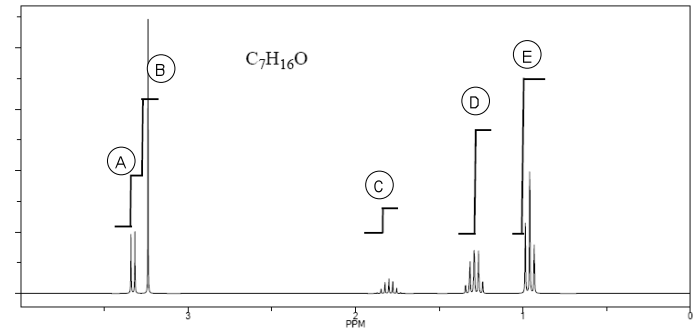
The molecule:



Note: Carbonyl group should be placed at "X". We can tell this because H_A is the most deshielded of the aromatic protons (by resonance with the carbonyl group).

Assignment 5 - Answers

c.

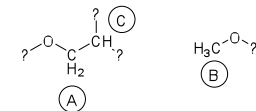


Signal	δ	Integration	Multiplicity	Comments
A	~3.4	2H	d	CH_2 (probably not 2 x CH, but keep this in mind, just in case); next to the CH, next to O (based on δ)
B	~3.3	3H	s	CH_3 isolated, next to O (based on δ)
C	~1.8	1H	m	CH multiplet (hard to say what the neighbors are)
D	~1.3	4H	m	2 x CH_2 (identical—symmetry exists in the molecule); hard to say what the neighbors are
E	~0.9	6H	t	2 x CH_3 , identical in chemical environment, each next to CH_2 (also identical)

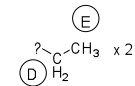
$$\text{DU} = [7(2) + 2 - 16] / 2 = 0 \rightarrow \text{no rings or double bonds}$$

$$\text{Integration: } (12 \text{ mm} + 17 + 6 + 23 + 34) / 16 \text{ H's} = 5.8 \text{ mm/H}$$

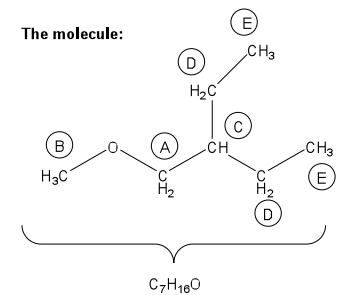
The pieces:



Note: the formula contains only one oxygen

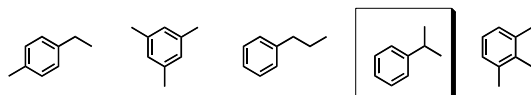


The molecule:



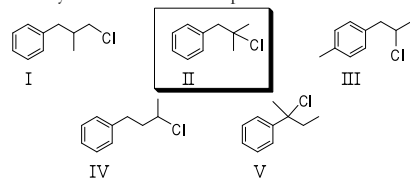
Assignment 5 - Answers

6. Determine the most likely structure of a compound, with the molecular formula C_9H_{12} , which gave a 1H NMR spectrum consisting of:
 a doublet at δ 1.25
 a septet at δ 2.90 and
 a multiplet at δ 7.25



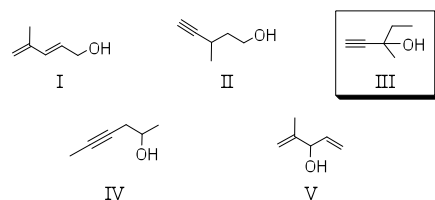
7. A compound with the molecular formula $C_{10}H_{13}Cl$ gave the following 1H NMR spectrum:
 singlet, δ 1.6
 singlet, δ 3.1
 multiplet, δ 7.2 (5H)

The most likely structure for the compound is:



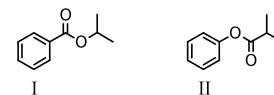
8. Determine the likely structure for a compound A ($C_6H_{10}O$), which is found to decolorize bromine in carbon tetrachloride. Its spectral data is as follows:

1H NMR		IR
triplet, δ 1.0	singlet, δ 2.4	2200 cm^{-1} (sharp)
singlet, δ 1.4	singlet, δ 3.4	3300 cm^{-1} (sharp)
quartet, δ 1.6		3500 cm^{-1} (broad)

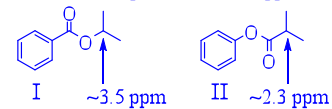


9. Briefly explain how you might distinguish between the following substances by comparing their 1H -NMR spectra:

Assignment 5 - Answers

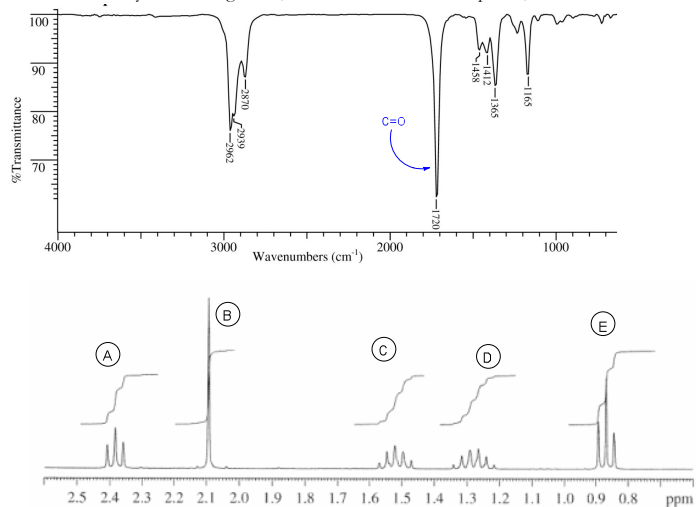


The main difference would likely be in the chemical shift of the methine proton of the isopropyl group. The methine proton in I is likely to be more deshielded, and produce a signal (septet) at about 3.5 ppm, while the analogous proton in II is likely to be found, also as a septet, at about 2.3 ppm.



Assignment 5 - Answers

10. An unknown compound has the formula $C_6H_{12}O$. Elucidate the structure of the molecule by scrutinizing its IR, 1H NMR and ^{13}C NMR spectra, shown below.

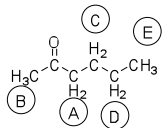


Signal	δ	Integration	Multiplicity	Comments
A	~2.4	2H	Triplet (t)	CH_2 next to CH_2 (based on multiplicity) and next to $C=O$ (based on δ)
B	~2.1	3H	Singlet (s)	CH_3 next to $C=O$ (based on δ)
C	~1.6	2H	Multiplet (m)	CH_2
D	~1.3	2H	Multiplet (m)	CH_2
E	~0.9	3H	Triplet (t)	CH_3 next to CH_2 (based on multiplicity)

$DU = [6(2) + 2 - 12]/2 = 1 \rightarrow C=O$ (based on IR)

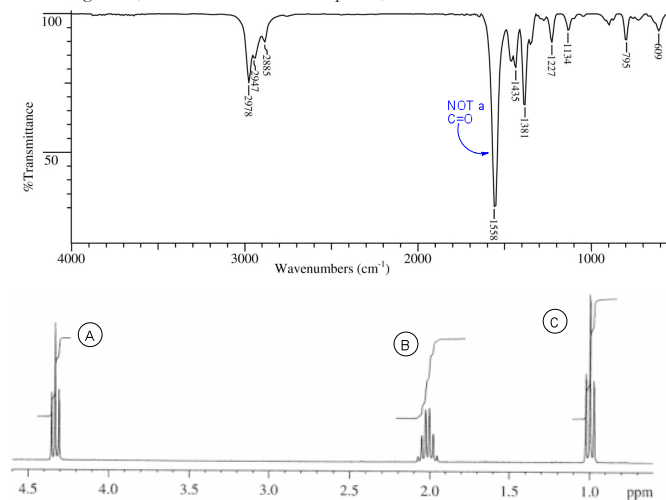
Integration: $(9\text{ mm} + 13 + 10 + 10 + 14) / 12\text{ H's} = 4.7\text{ mm/H}$

The molecule:



Assignment 5 - Answers

An unknown compound, I, has the formula $C_3H_7NO_2$. Elucidate the structure of I by scrutinizing its IR, 1H NMR and ^{13}C NMR spectra, shown below.



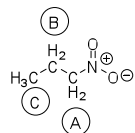
Assignment 5 - Answers

Signal	δ	Integration	Multiplicity	Comments
A	~4.4	2H	Triplet (t)	CH ₂ , next to CH ₂ (based on multiplicity), next to O or NO ₂ (based on δ)
B	~2.0	2H	M	CH ₂
C	~1.0	3H	t	CH ₃ , next to CH ₂

DU = [3(2) + 2 + 1 - 7] / 2 = 1 → NOT a C=O based on IR... maybe NO₂?

Integration: (17 mm + 17 + 26) / 7H's = 8.6 mm/H

The molecule:



Assignment 5 Answers

Part B. Identify the compound represented in each of the ¹H NMR spectra

1. 2-pentanone



2. Pentanal



3. 3-pentanone



4. Methyl propanoate



5. Ethyl acetate



6. Butanoic acid



7. 3-methyl butan-2-one



8. isopropyl acetate



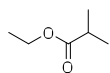
9. methyl isobutyrate



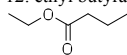
10. isopropyl propionate



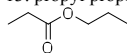
11. ethyl isobutyrate



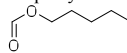
12. ethyl butyrate



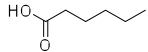
13. propyl propionate



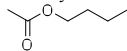
14. pentyl formate



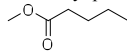
15. hexanoic acid



16. butyl acetate



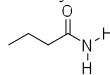
17. methyl pentanoate



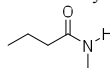
18. *N,N*-dimethylpropionamide



19. butyramide



20. *N*-methylbutyramide



21. 1-propanol



22. 2-propanol



Assignment 6 – NMR, IR
ANSWERS

23. propanal



24. 1-bromobutane



25. 2-iodobutane



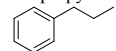
26. 1-chloro-2-methylpropane



27. 2-chloro-2-methylpropane



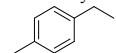
28. propylbenzene



29. isopropylbenzene



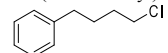
30. 1-ethyl-4-methylbenzene



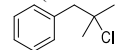
31. 1,3,5-trimethylbenzene



32. (4-chlorobutyl)benzene

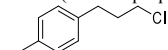


33. (2-chloro-2-methylpropyl)benzene

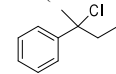


Assignment 6 – NMR, IR
ANSWERS

34. 1-(3-chloropropyl)-4-methylbenzene



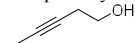
35. (2-chlorobutan-2-yl)benzene



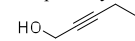
36. 3-methylpent-1-yn-3-ol



37. pent-3-yn-1-ol



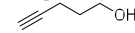
38. pent-2-yn-1-ol



39. 2-methylbut-3-yn-2-ol



40. pent-4-yn-1-ol



41. 1-methoxypropane



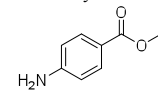
42. ethoxyethane or diethyl ether



43. *N*-methylpropan-1-amine

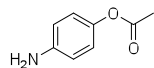


44. methyl 4-aminobenzoate

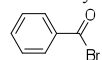


45. 4-aminophenyl acetate

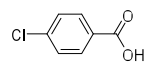
Assignment 6 – NMR, IR
ANSWERS



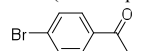
46. benzoyl bromide



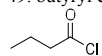
47. 4-chlorobenzoic acid or *p*-chlorobenzoic acid



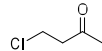
48. 1-(4-bromophenyl)propan-1-one



49. butyryl chloride



50. 4-chlorobutan-2-one



51. 2-aminopropanoic acid or alanine

