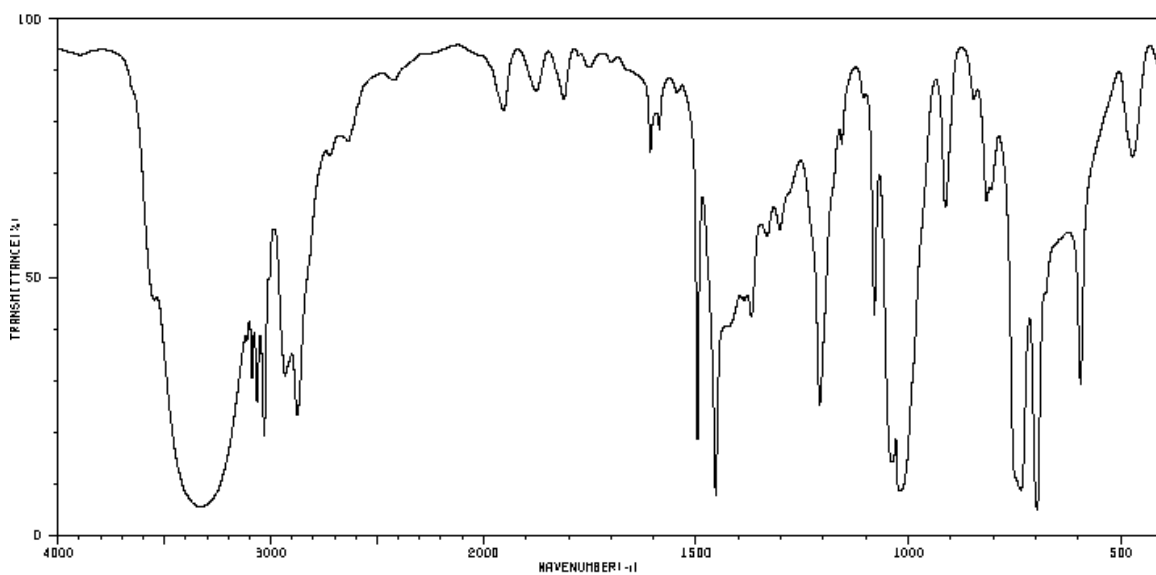
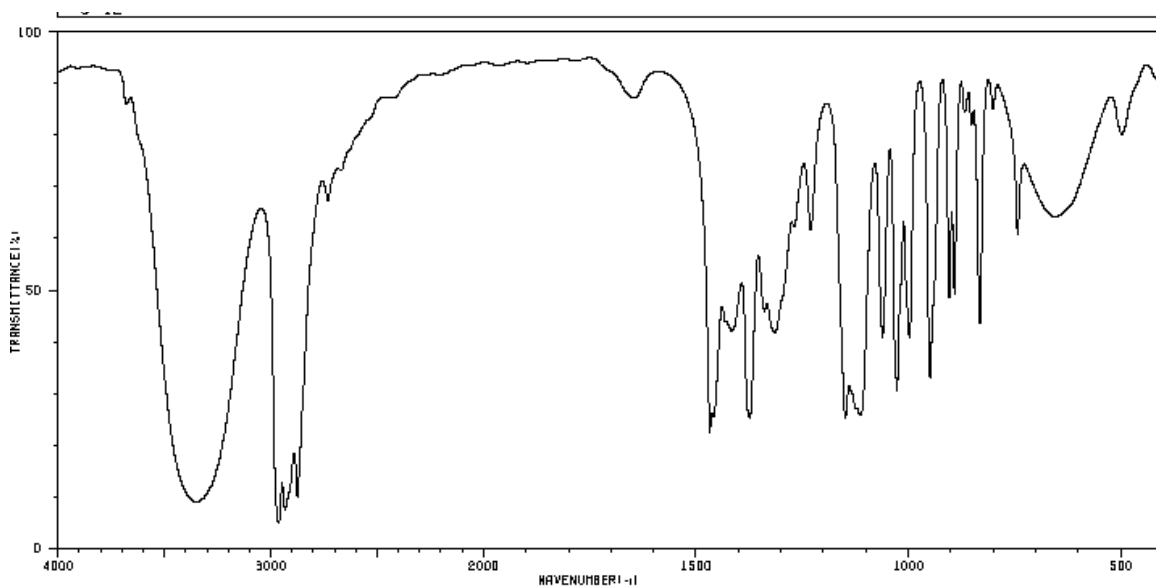


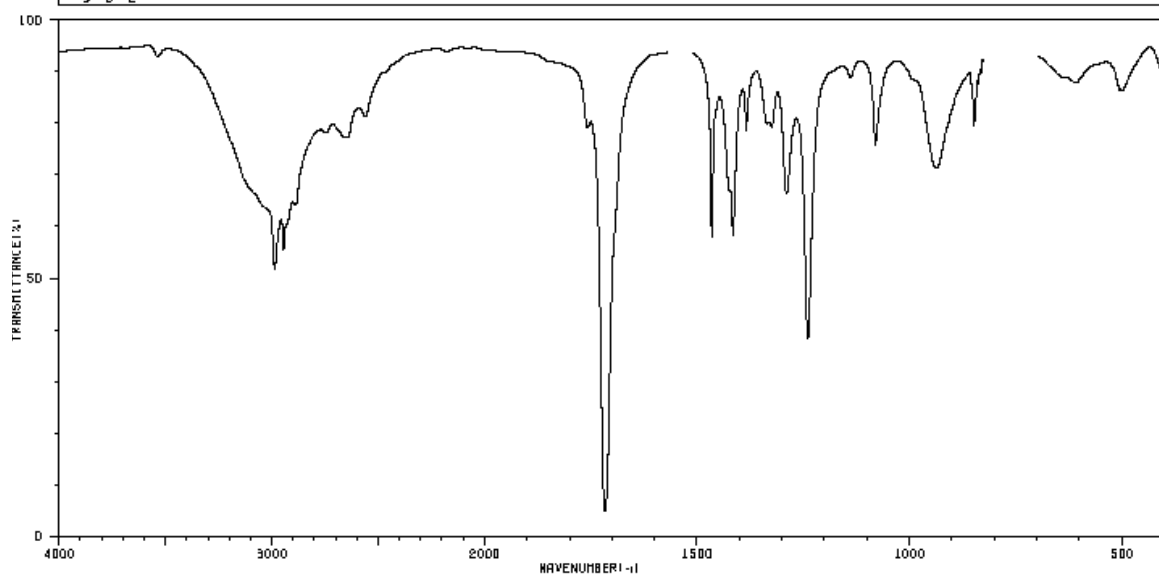
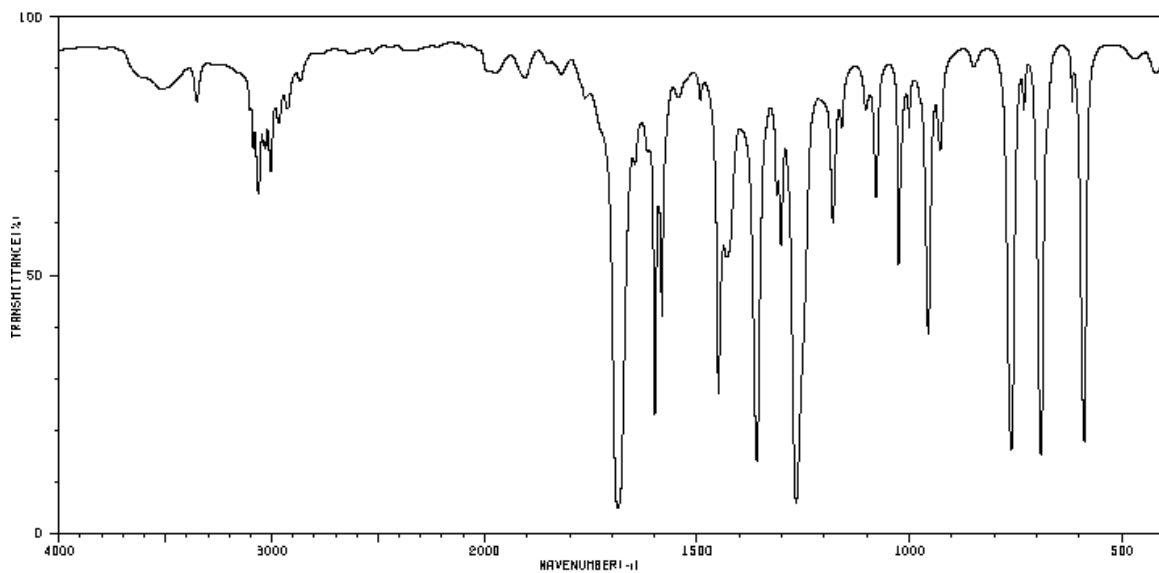
## CHM 2120 – Problem set 3

### In this assignment:

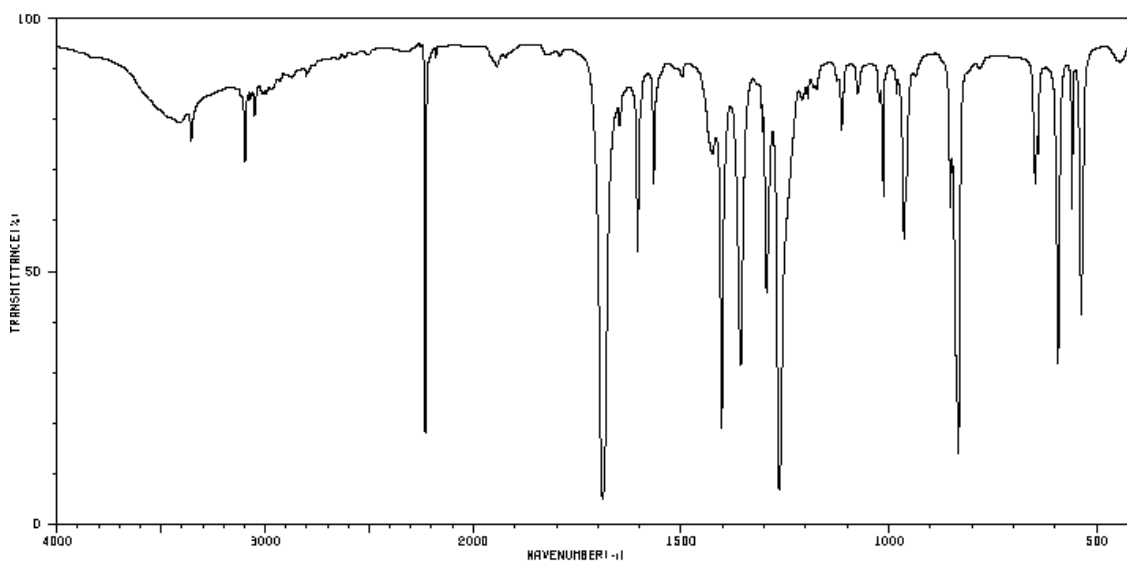
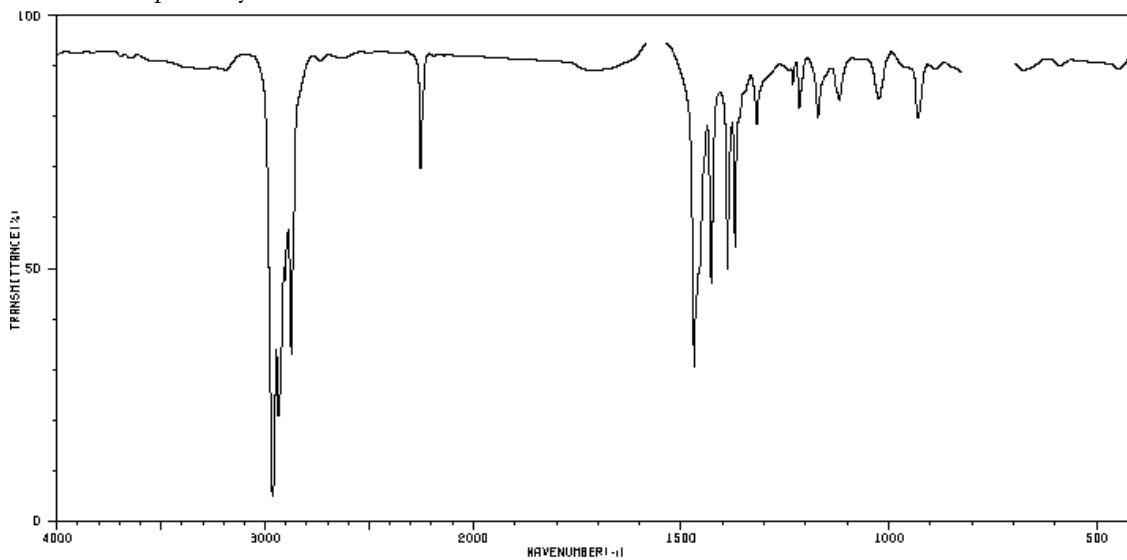
- NMR spectroscopy
  - IR spectroscopy
  - Problem-solving and structure identification
1. Associate each of the following IR spectra with one of the following compounds and justify your answer.
- a. Propanoic acid
  - b. 2-Pentanol
  - c. Benzyl alcohol
  - d. Acetophenone



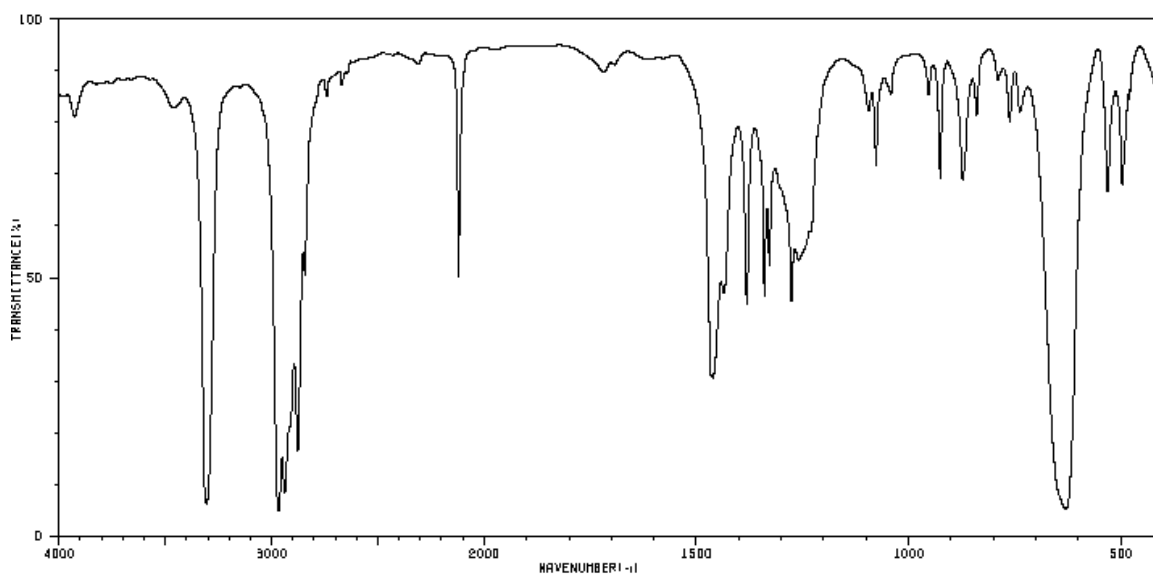
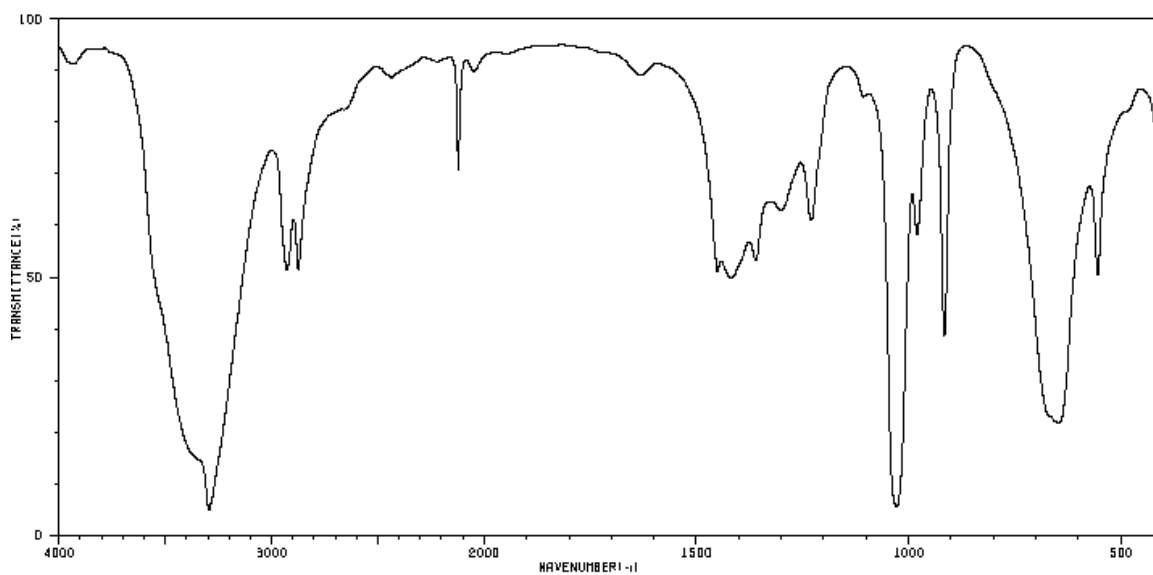
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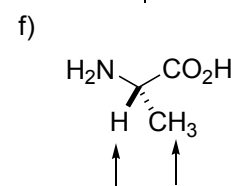
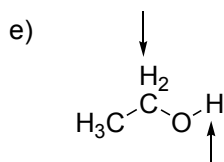
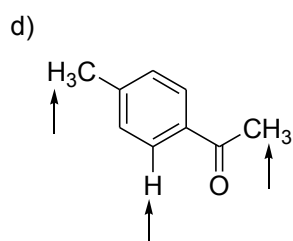
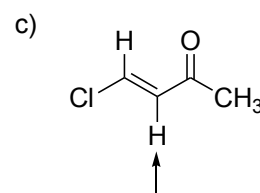
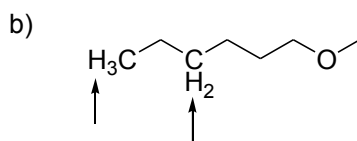
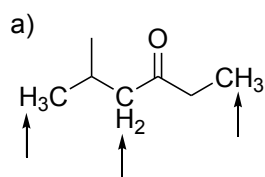
2. Associate each of the following IR spectra with one of the following compounds and justify your answer.
- 2-Propyn-1-ol
  - 1-Pentyne
  - 4-Methylpentanenitrile
  - p-Acetylbenzotrile



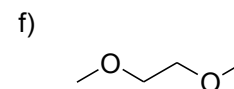
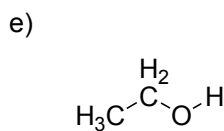
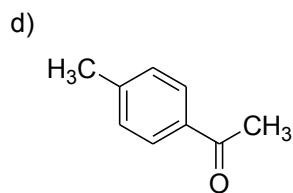
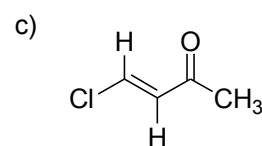
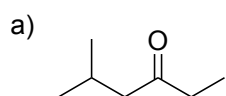
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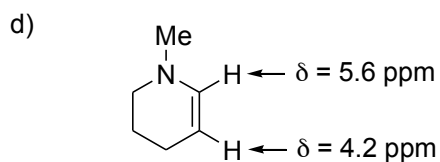
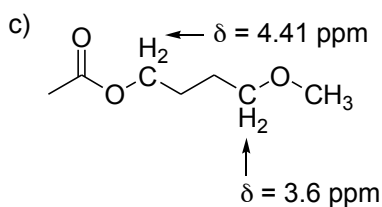
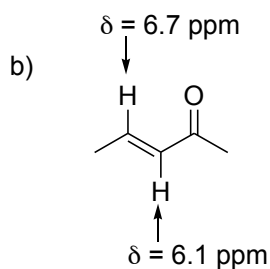
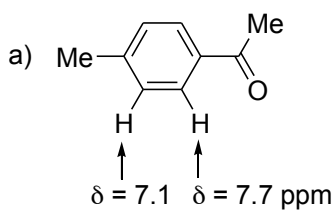
3. Give the number of peaks expected in the  $^1\text{H}$  NMR for the indicated protons in each of the following structures:



4. How many signals would be expected in the  $^1\text{H}$  NMR of the following molecules?

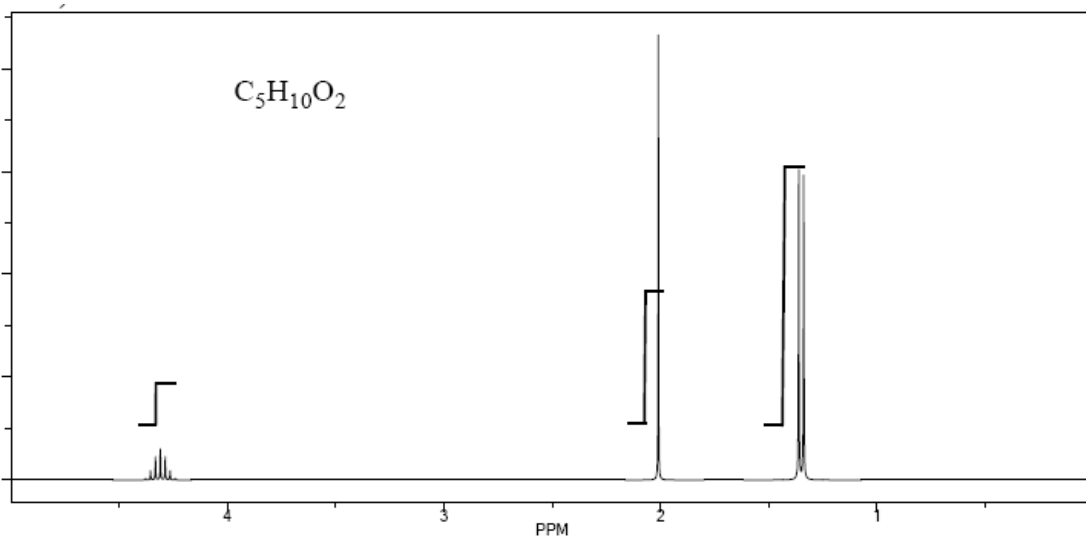


5. Explain the following differences in chemical shift.



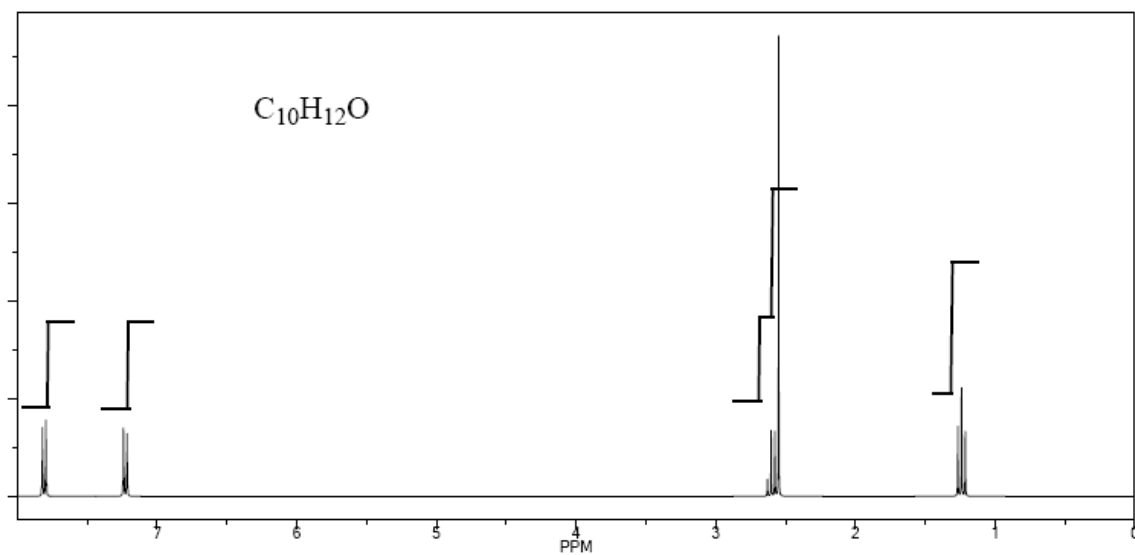
6. Determine the structure of the following unknowns using the table to fill in your answers.

a.



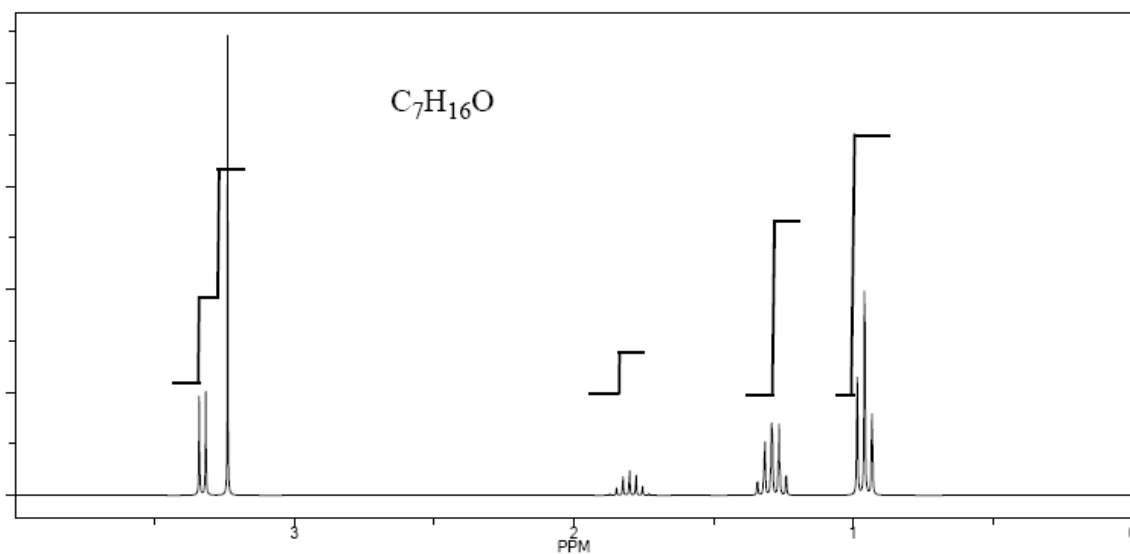
Signal	$\delta$	Integration	Multiplicity	Comments
A				
B				
C				

b.



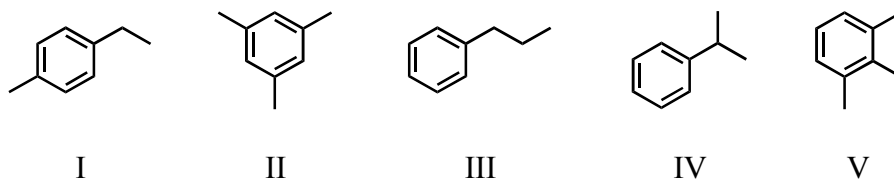
Signal	$\delta$	Integration	Multiplicity	Comments
<b>A</b>				
<b>B</b>				
<b>C</b>				
<b>D</b>				
<b>E</b>				

c.



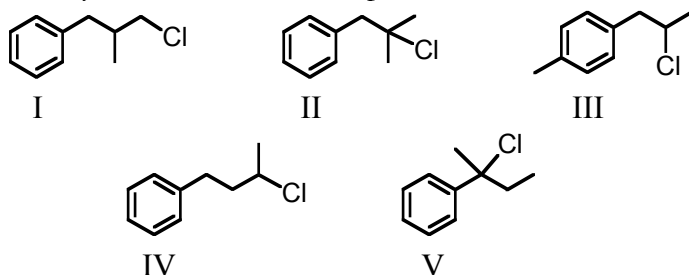
Signal	$\delta$	Integration	Multiplicity	Comments
<b>A</b>				
<b>B</b>				
<b>C</b>				
<b>D</b>				
<b>E</b>				

7. 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  $\delta$  1.25
  - a septet at  $\delta$  2.90 and
  - a multiplet at  $\delta$  7.25



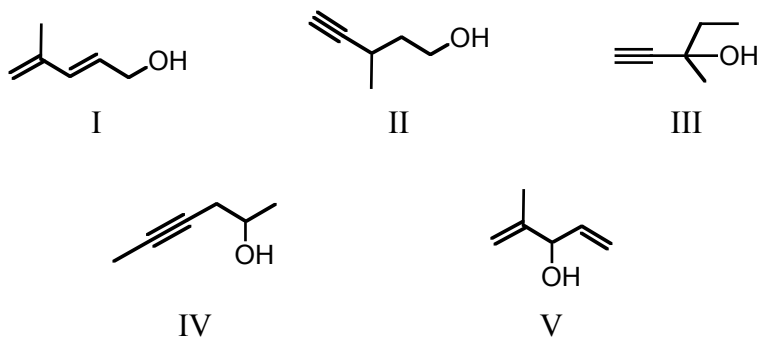
8. A compound with the molecular formula  $C_{10}H_{13}Cl$  gave the following  $^1H$  NMR spectrum:
- singlet,  $\delta$  1.6
  - singlet,  $\delta$  3.1
  - multiplet,  $\delta$  7.2 (5H)

The most likely structure for the compound is:

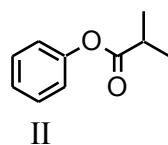
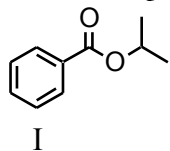


9. Determine the likely structure for a compound A ( $C_6H_{10}O$ ), which is found to decolorize bromine in carbon tetrachloride. Its spectral data is as follows:

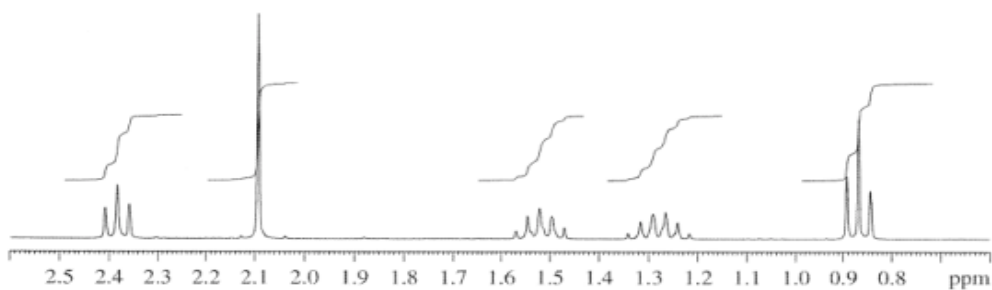
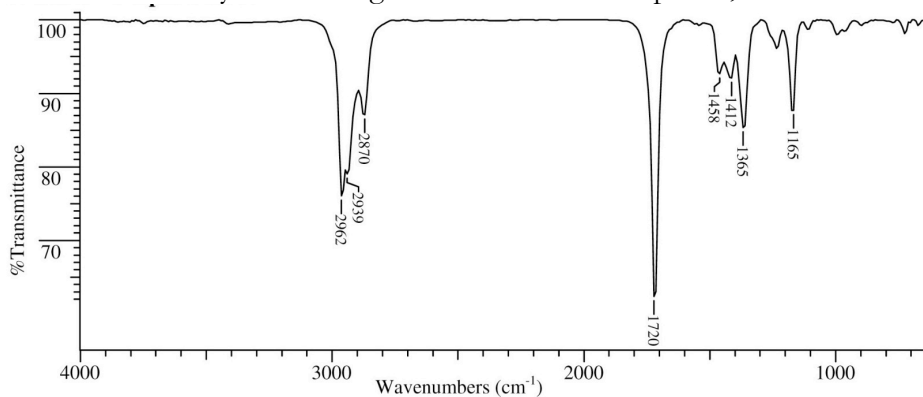
<u><math>^1H</math> NMR</u>		<u>IR</u>
triplet, $\delta$ 1.0	singlet, $\delta$ 2.4	2200 $cm^{-1}$ (sharp)
singlet, $\delta$ 1.4	singlet, $\delta$ 3.4	3300 $cm^{-1}$ (sharp)
quartet, $\delta$ 1.6		3500 $cm^{-1}$ (broad)



10. Briefly explain how you might distinguish between the following substances by comparing their  $^1\text{H-NMR}$  spectra:

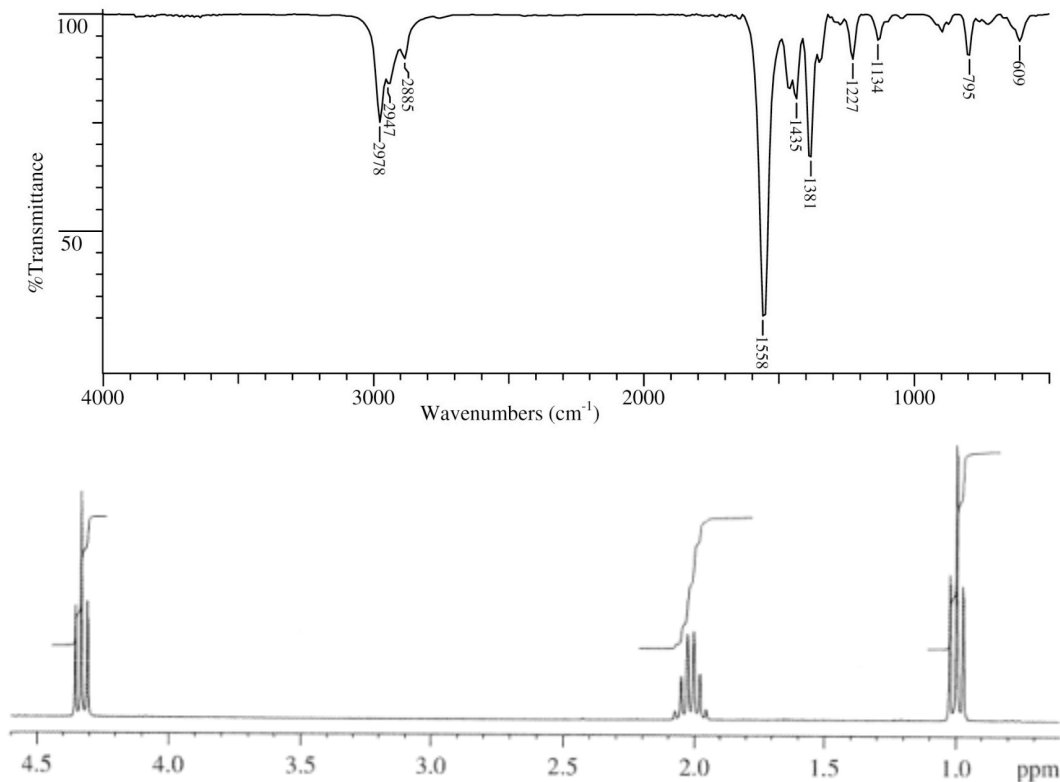


11. An unknown compound has the formula  $\text{C}_6\text{H}_{12}\text{O}$ . Elucidate the structure of the molecule by scrutinizing its IR and  $^1\text{H NMR}$  spectra, shown below.



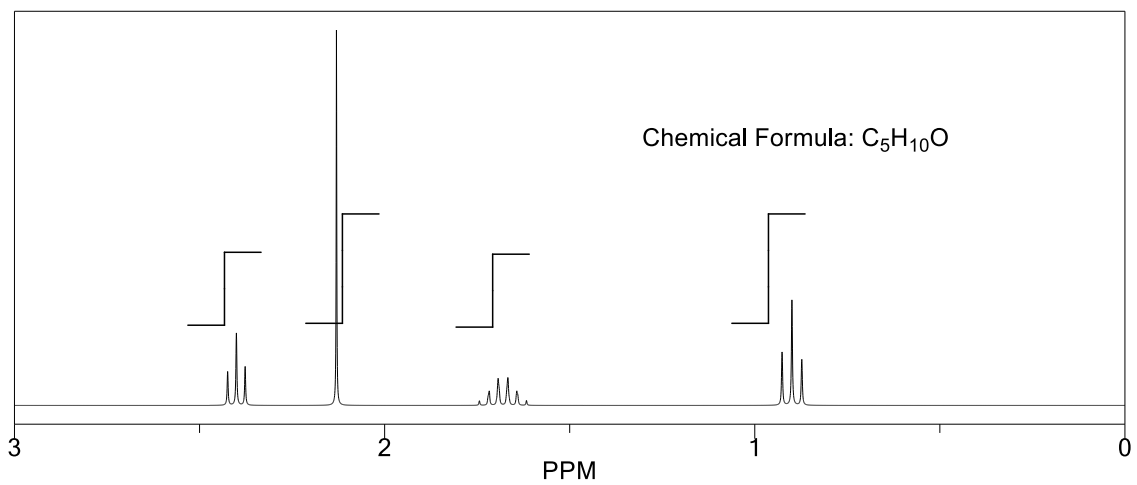
Signal	$\delta$	Integration	Multiplicity	Comments
<b>A</b>				
<b>B</b>				
<b>C</b>				
<b>D</b>				
<b>E</b>				

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

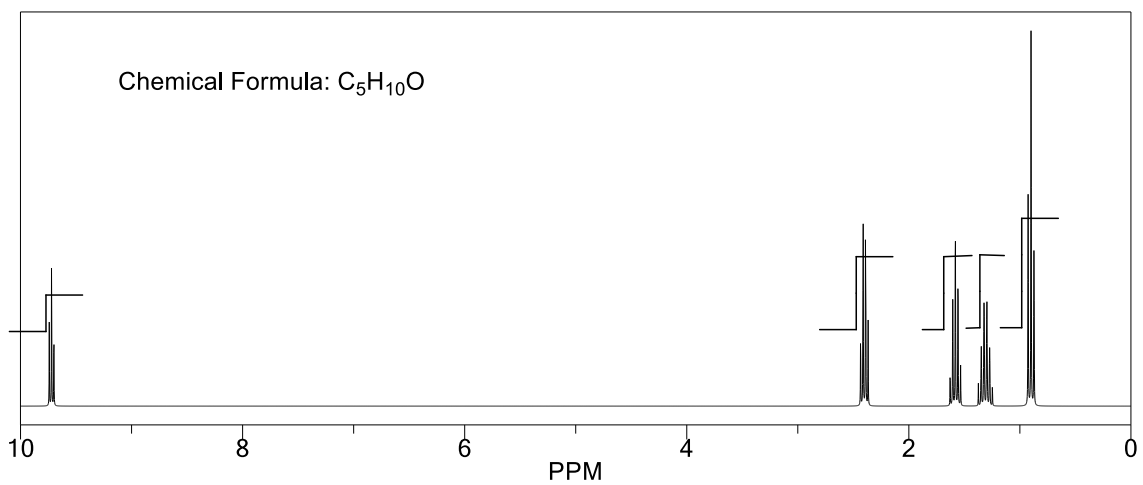


Signal	$\delta$	Integration	Multiplicity	Comments
<b>A</b>				
<b>B</b>				
<b>C</b>				

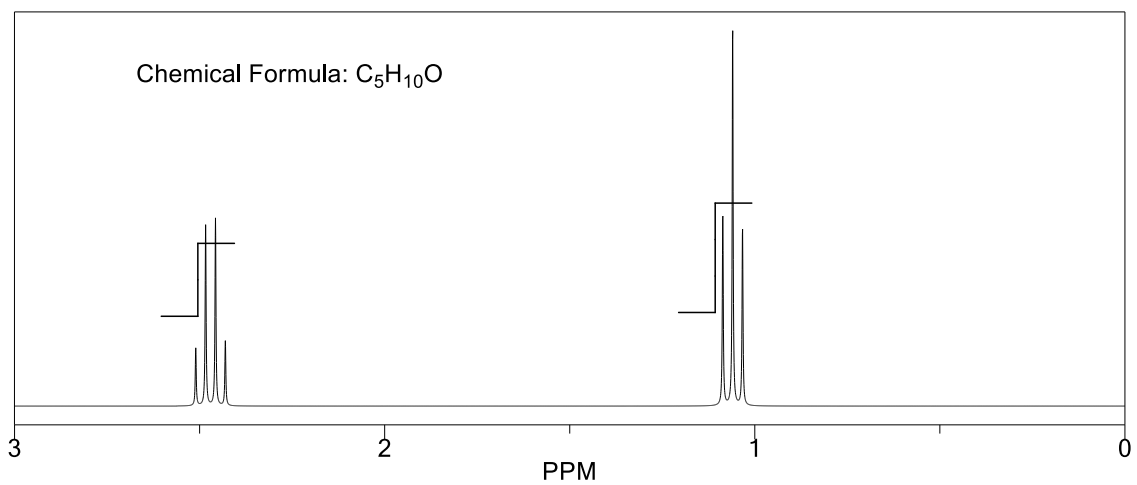
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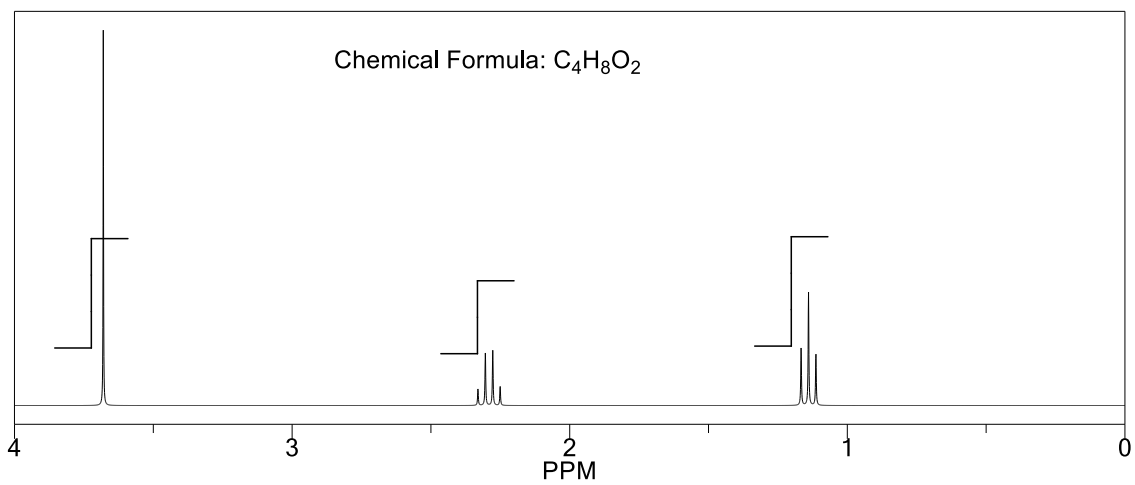
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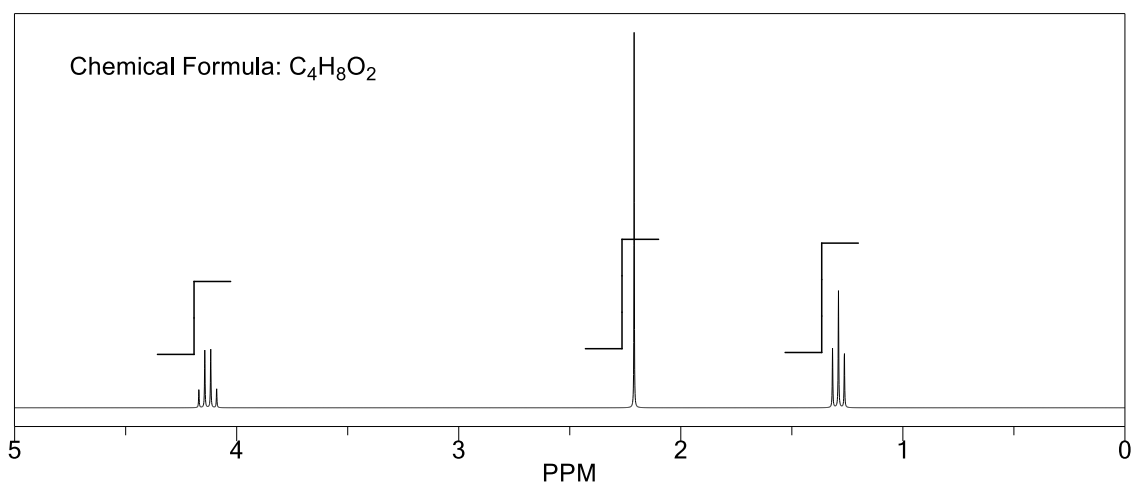
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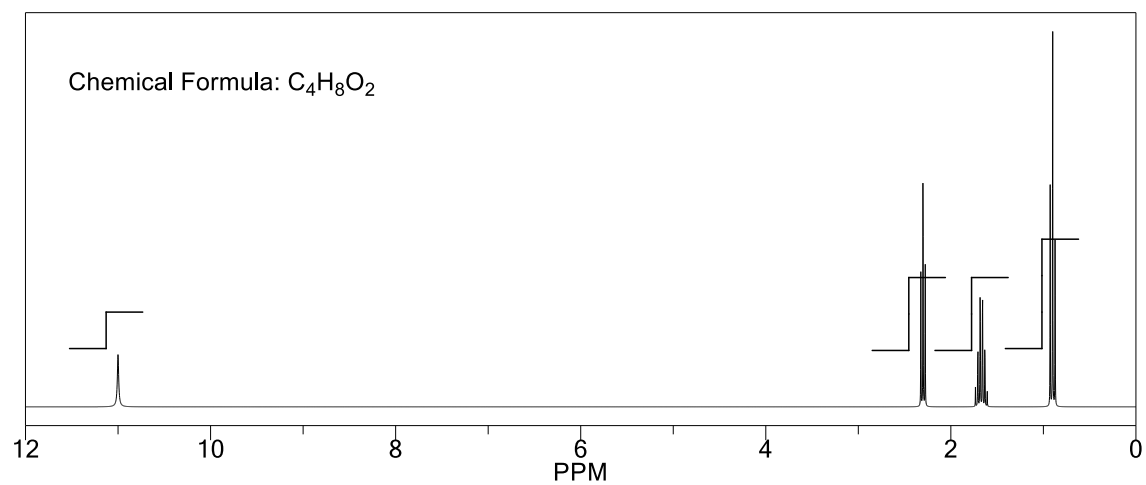
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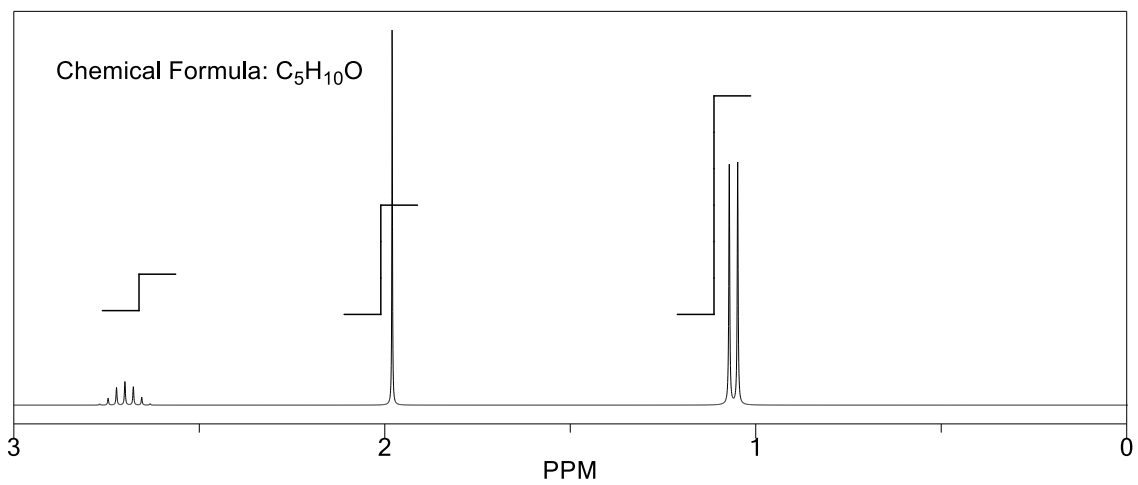
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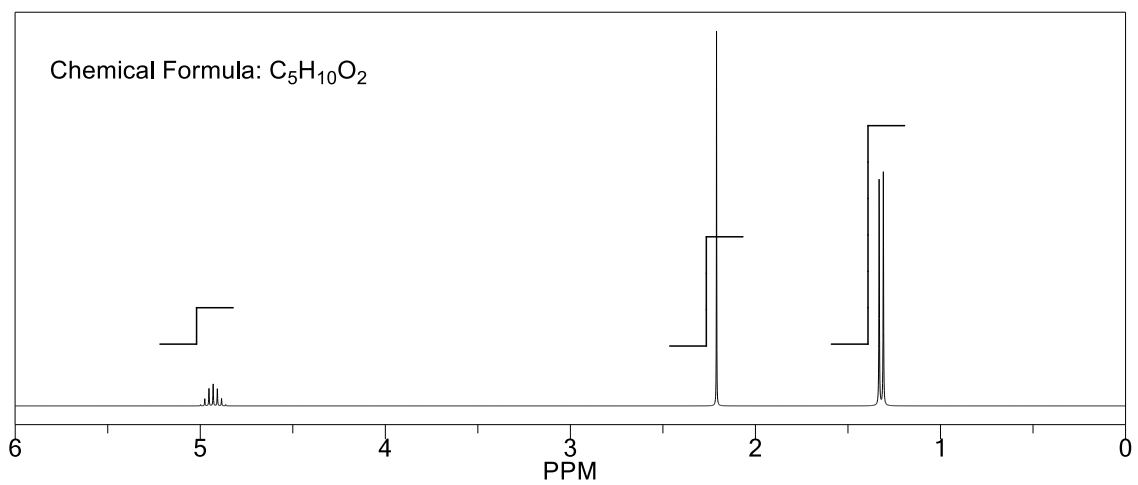
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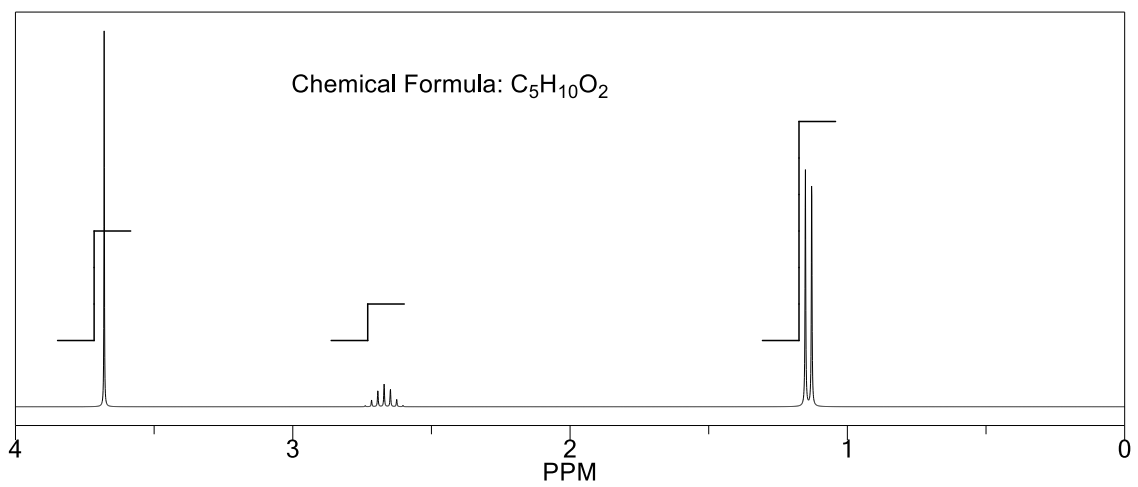
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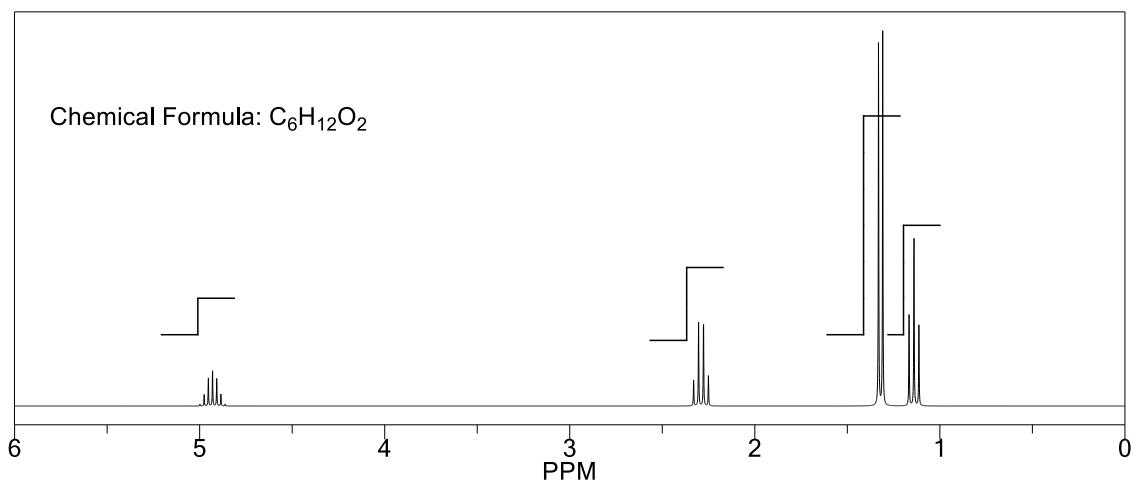
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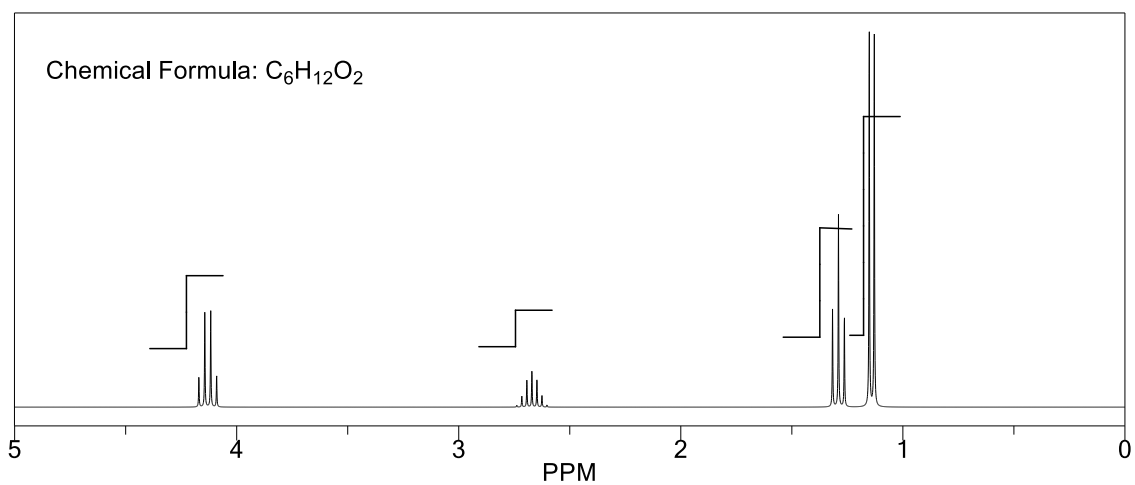
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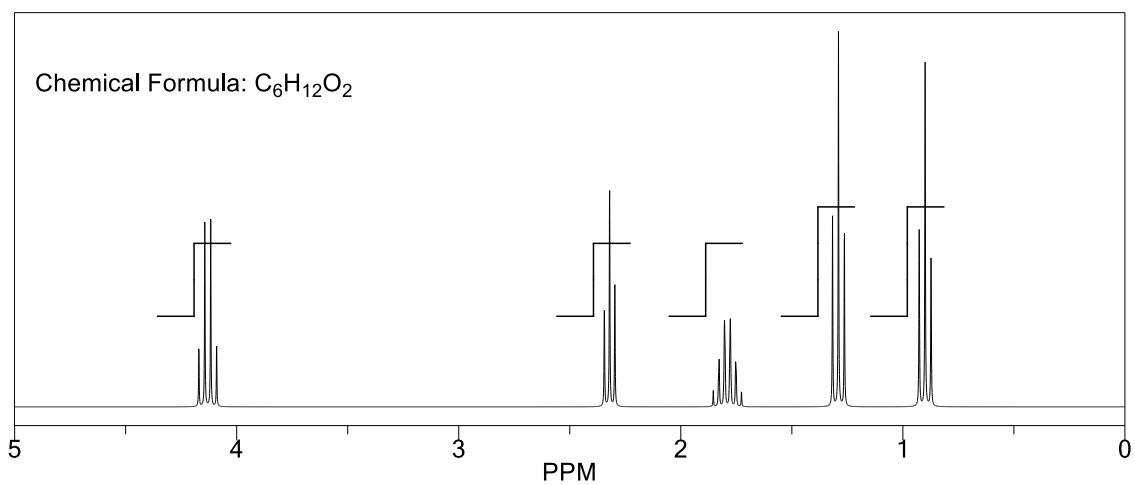
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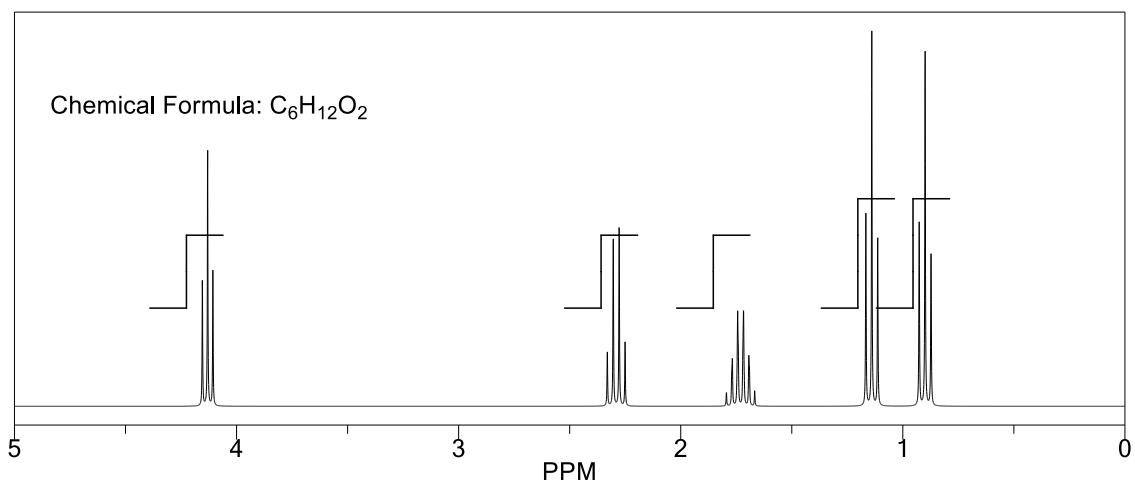
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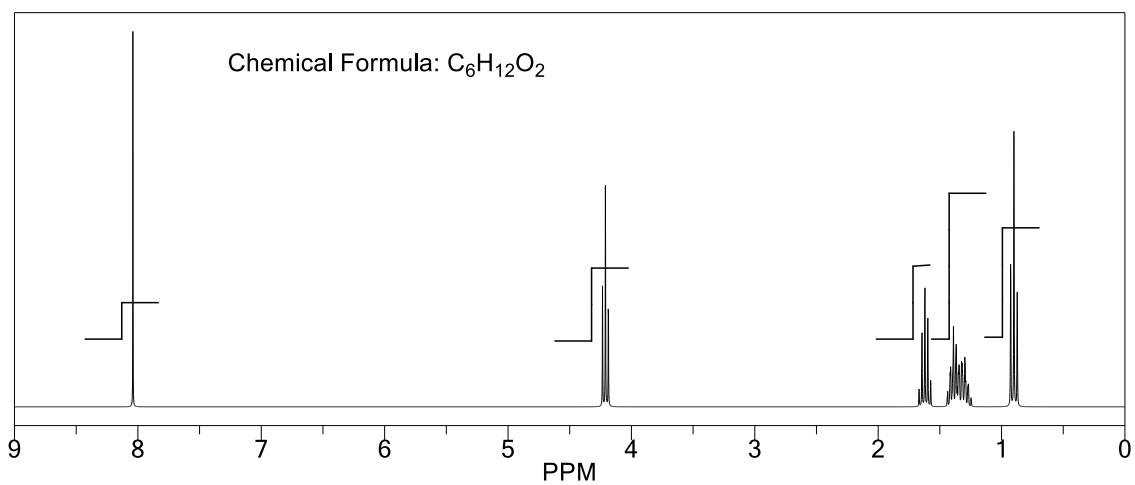
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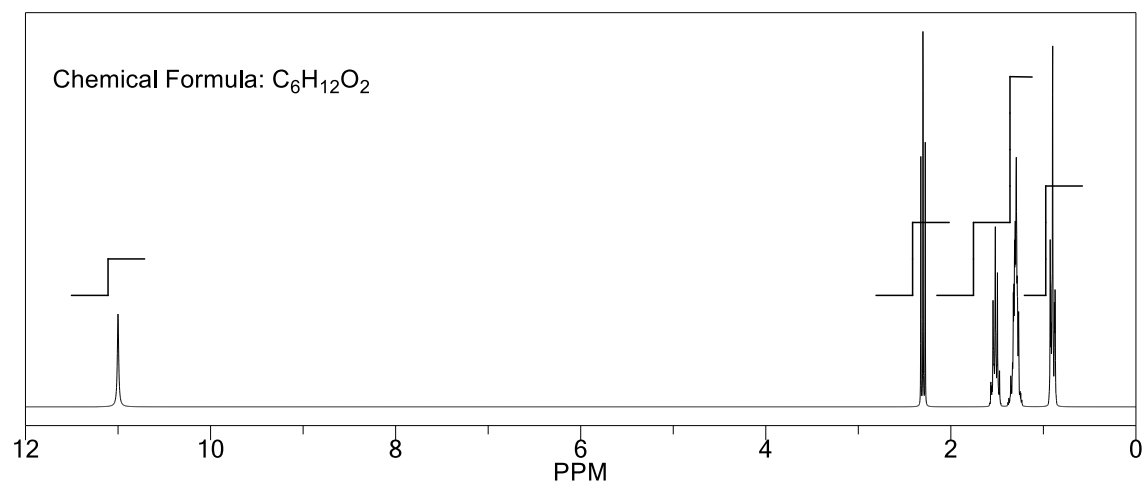
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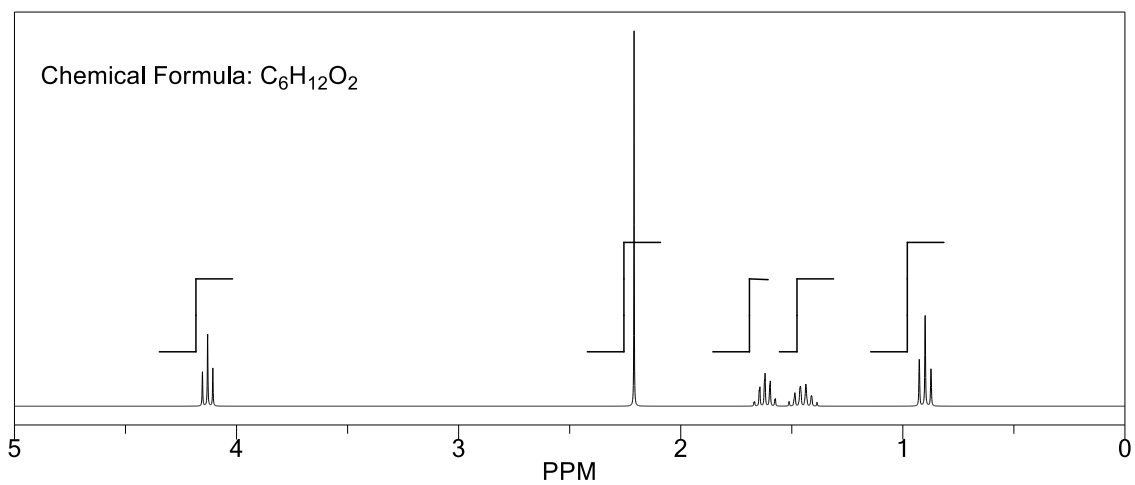
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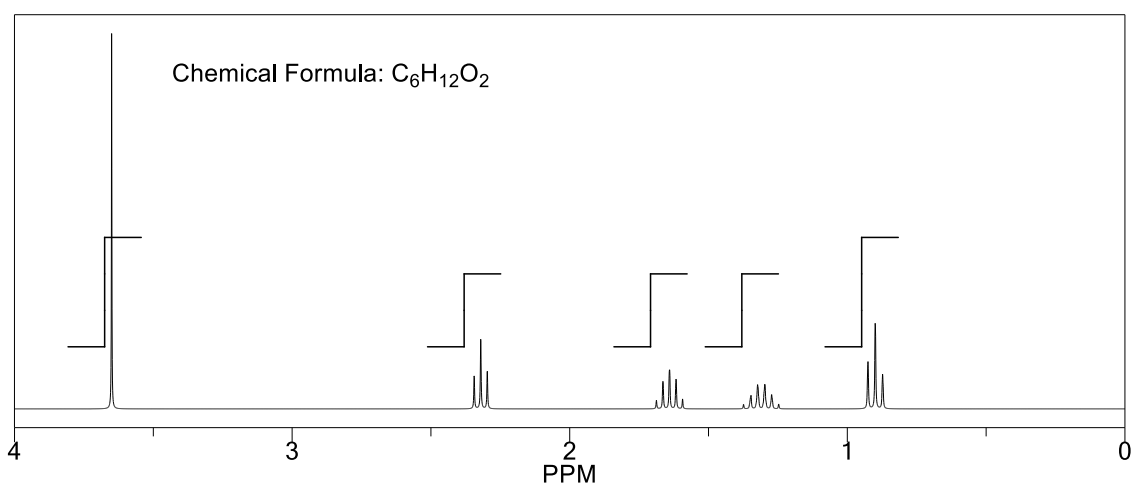
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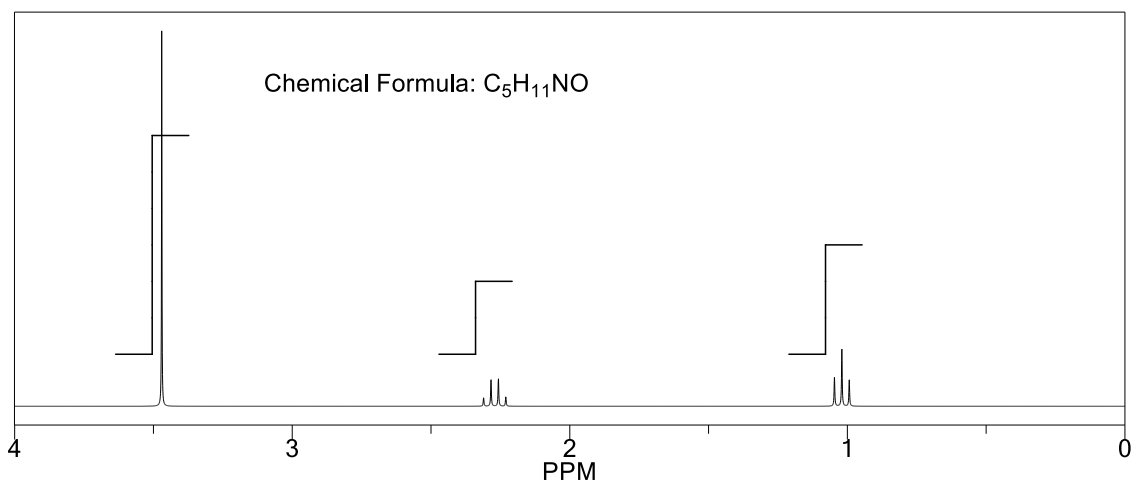
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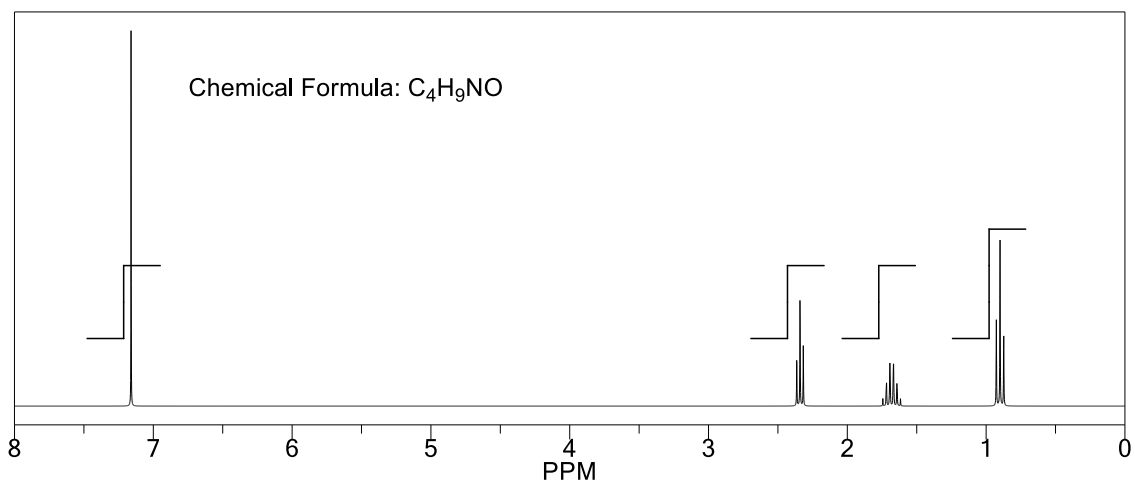
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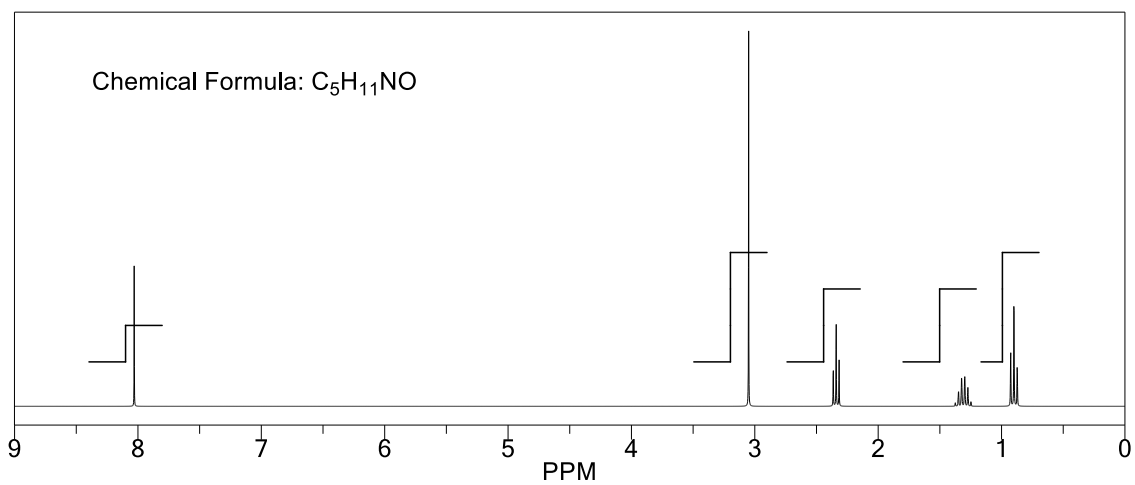
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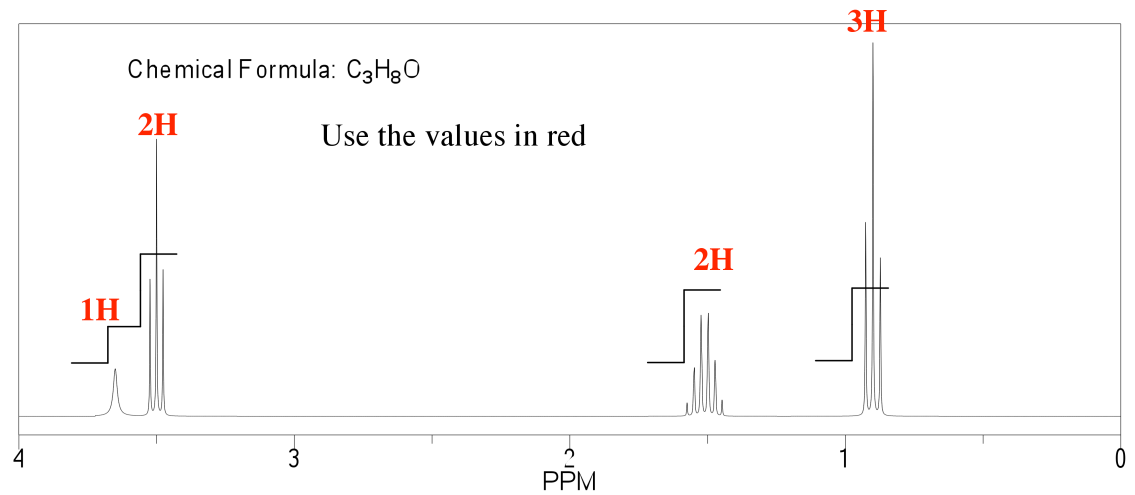
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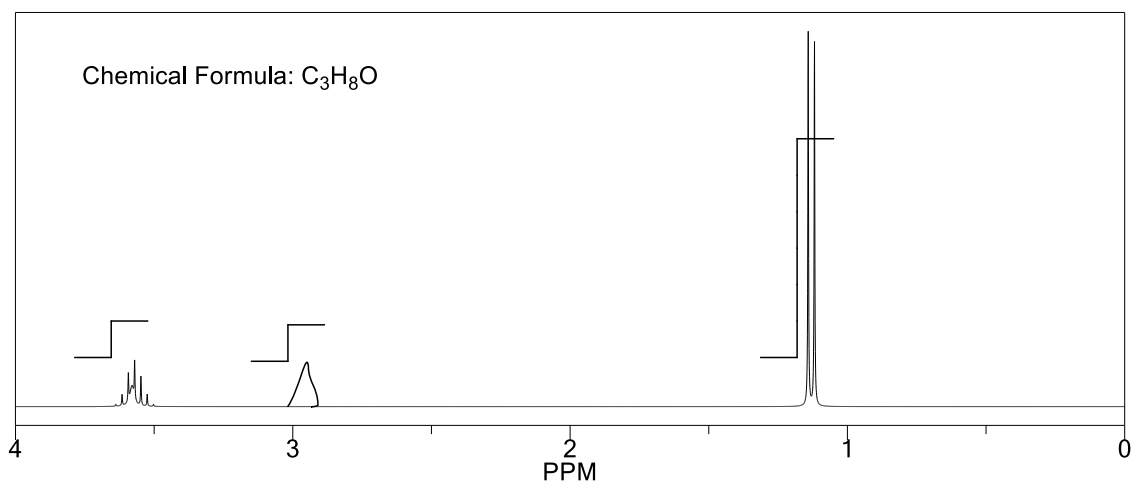
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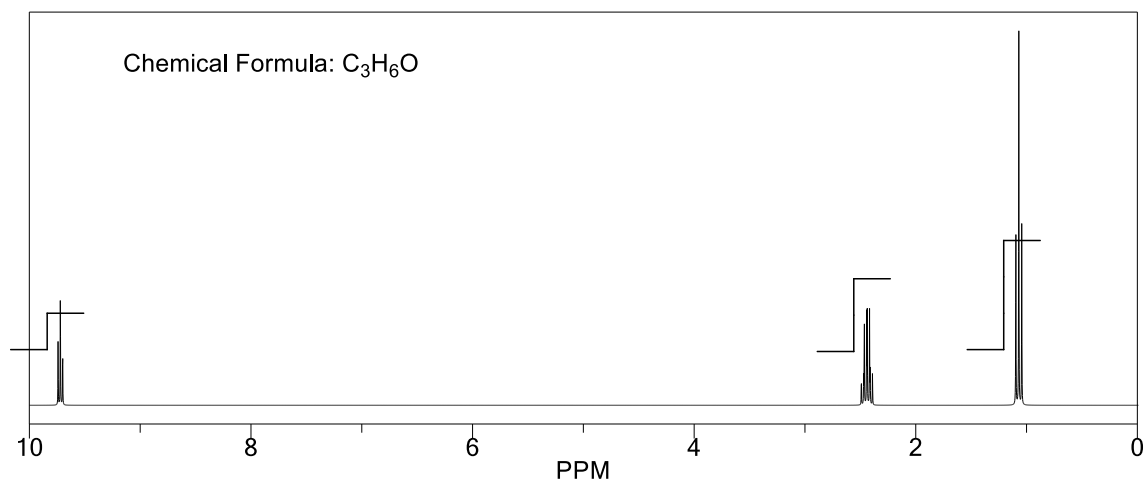
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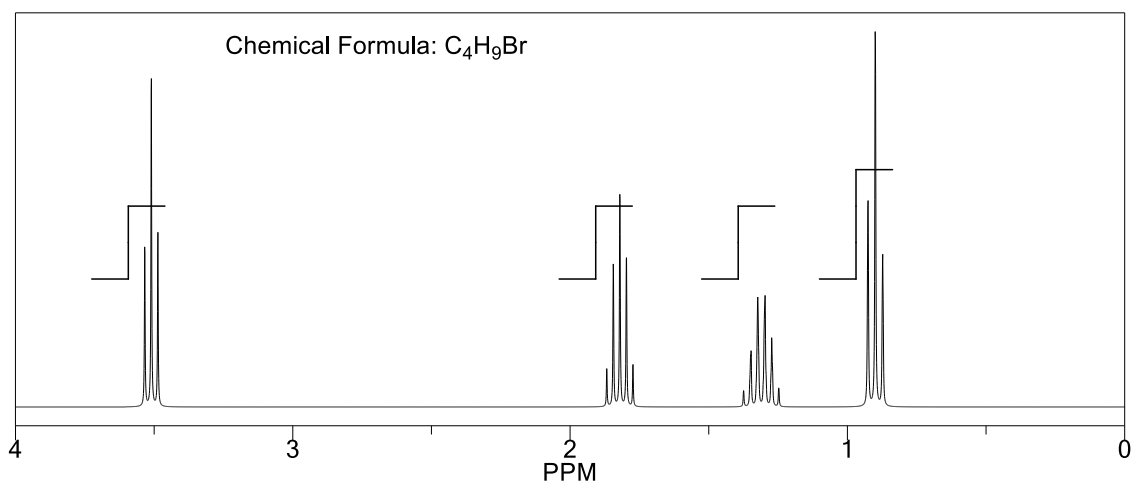
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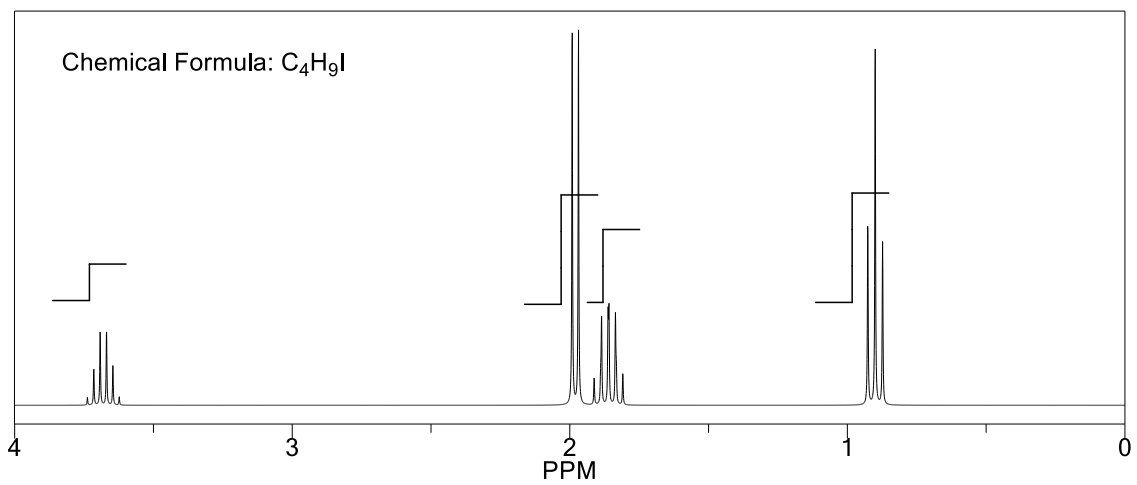
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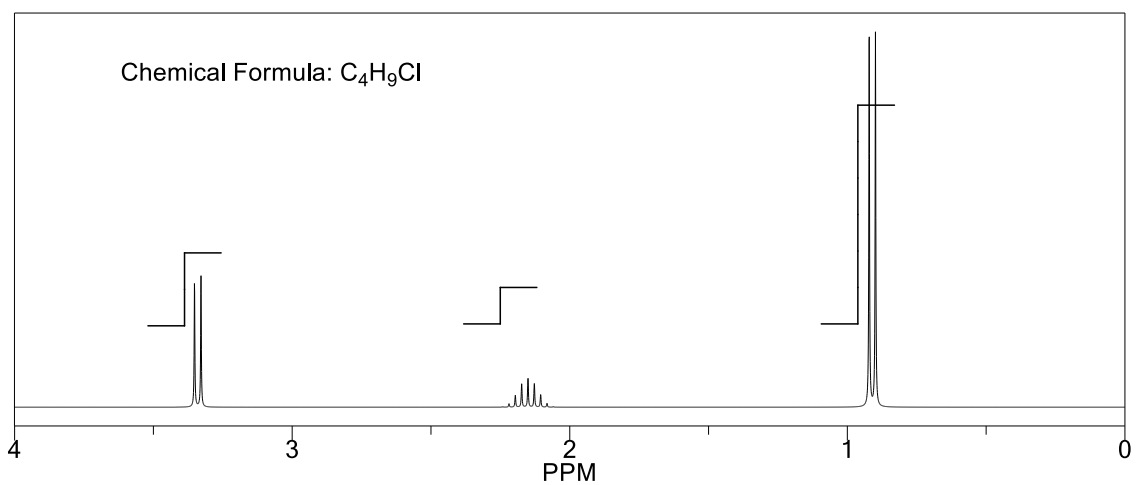
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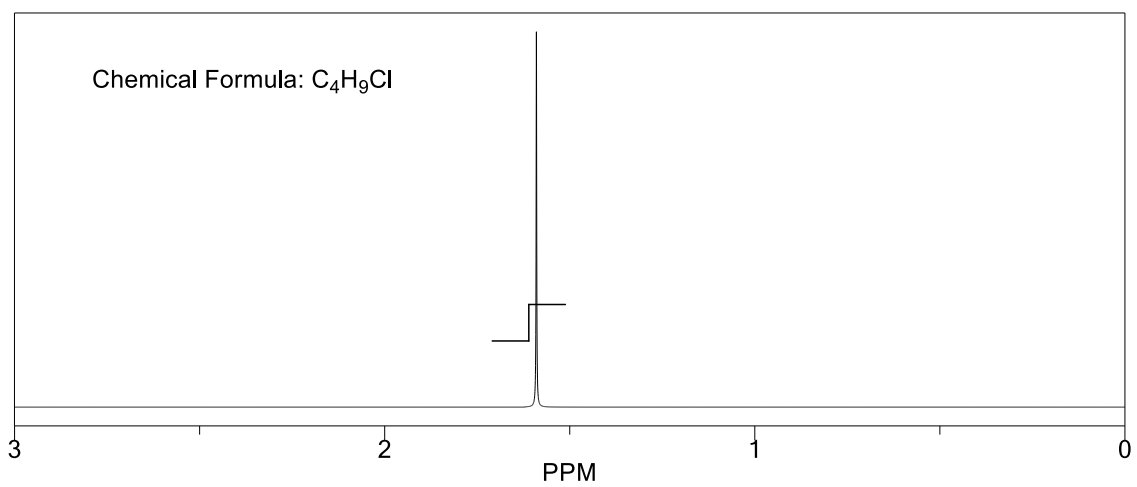
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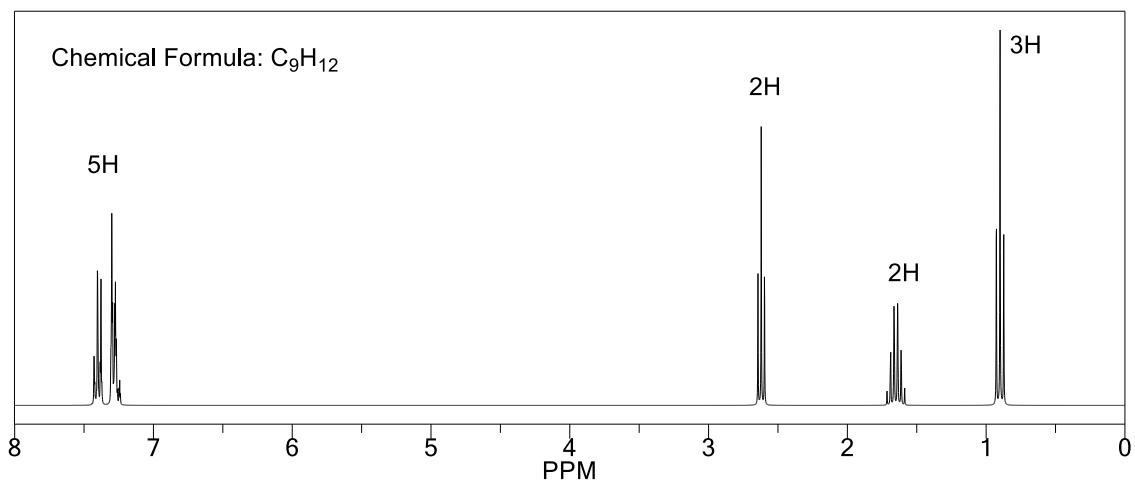
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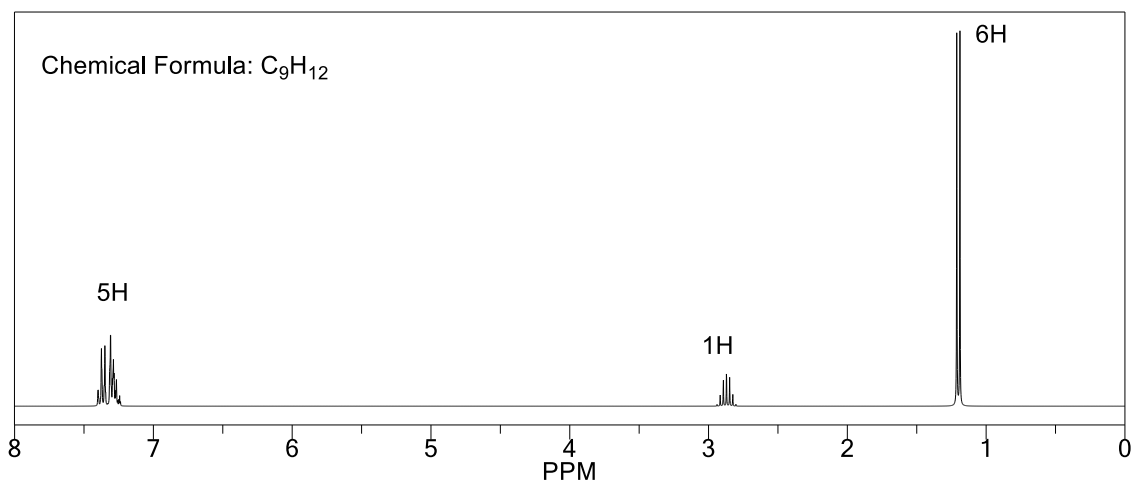
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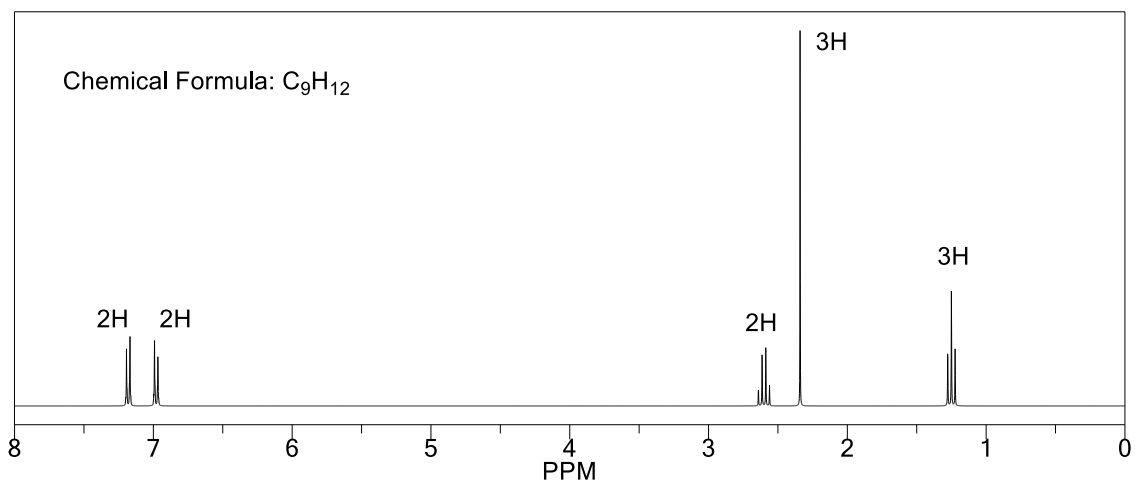
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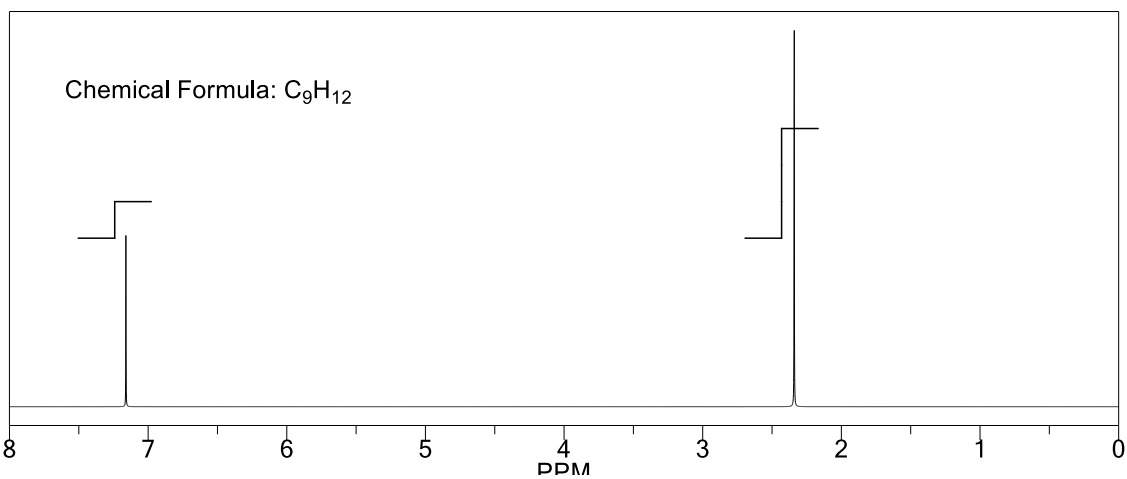
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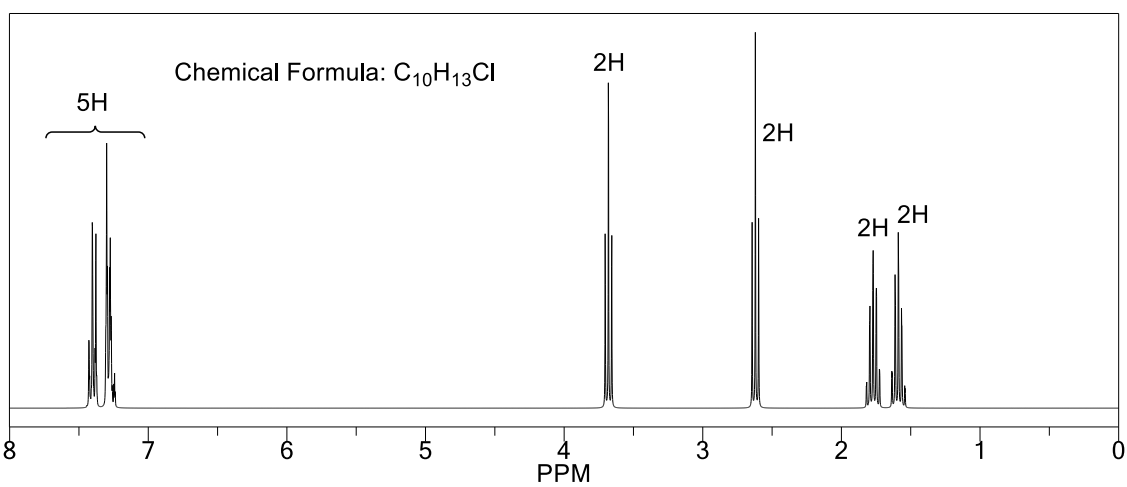
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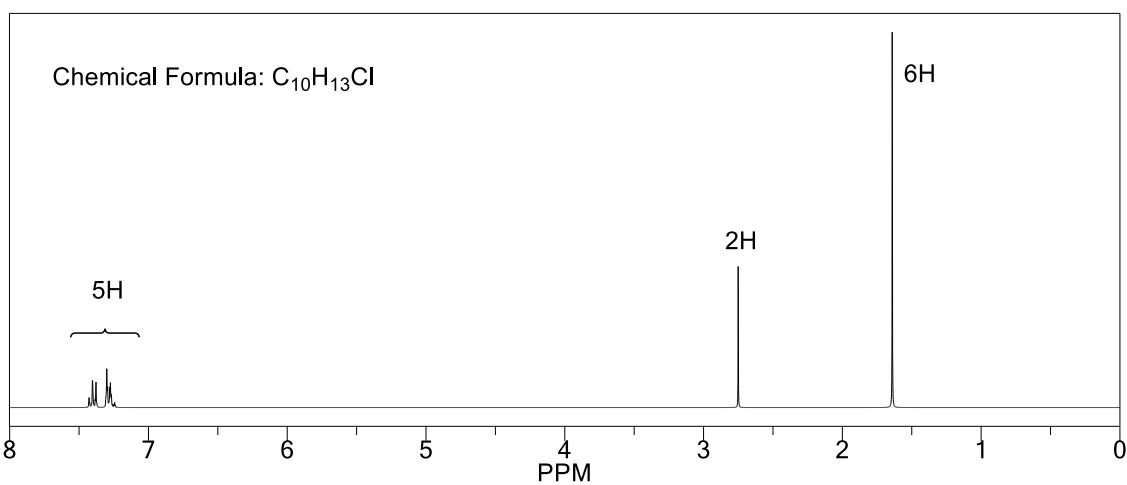
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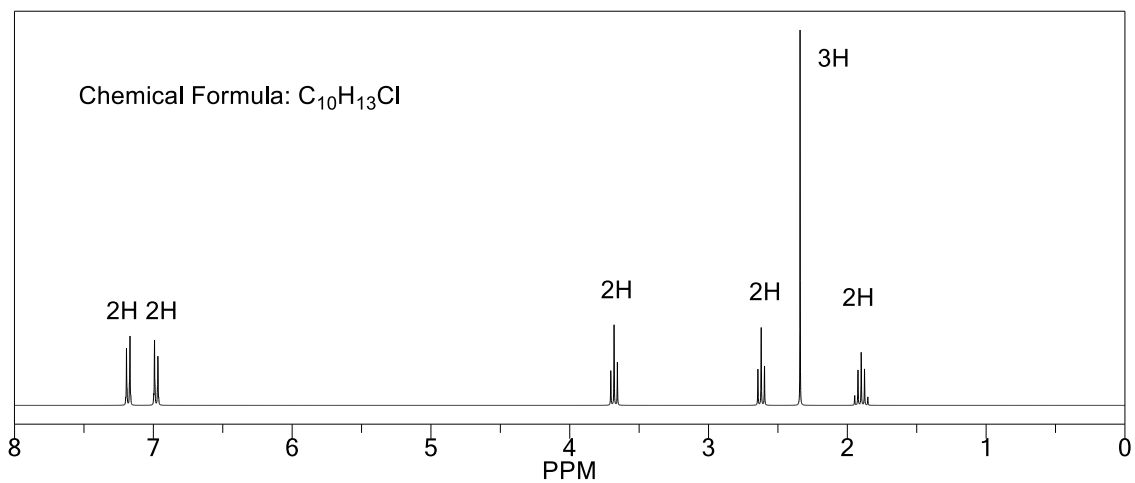
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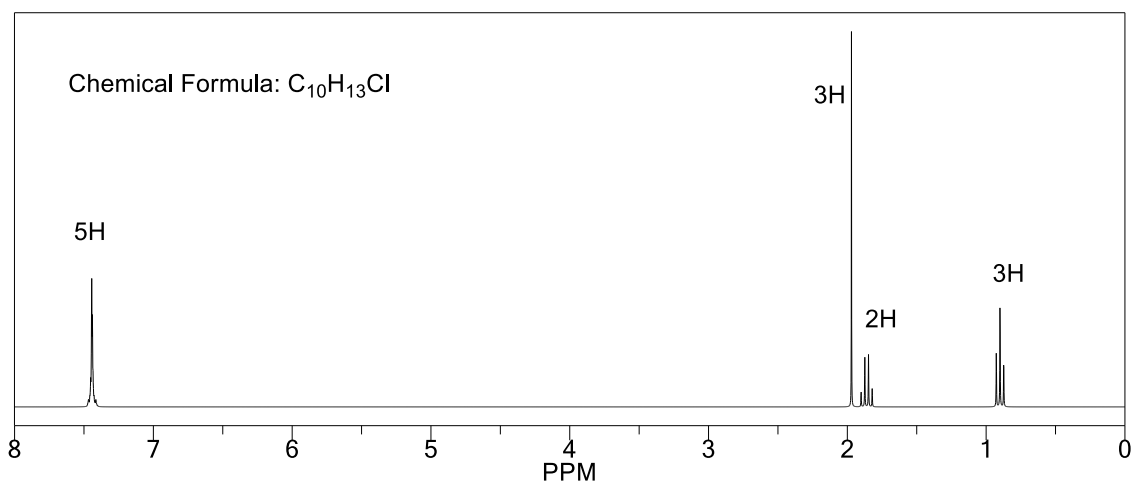
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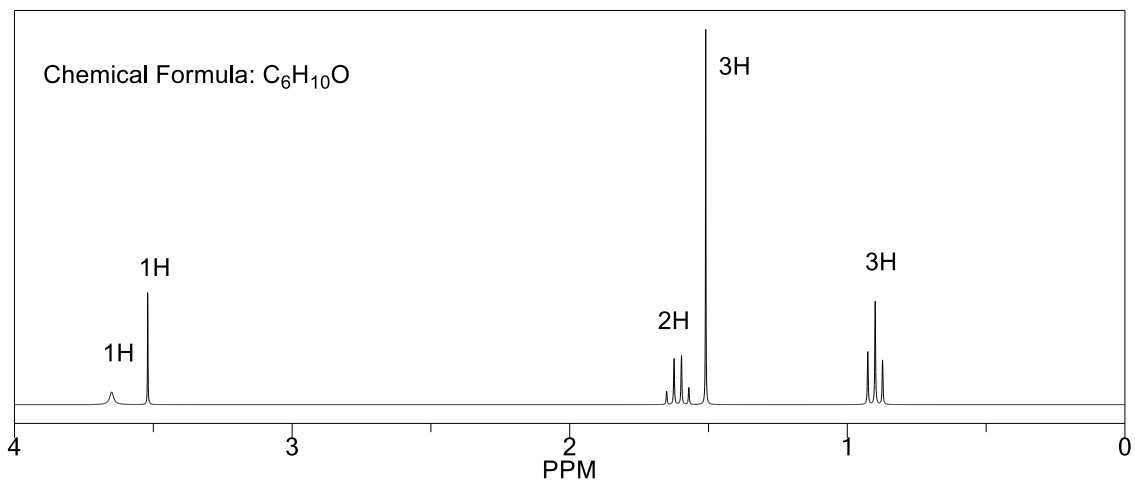
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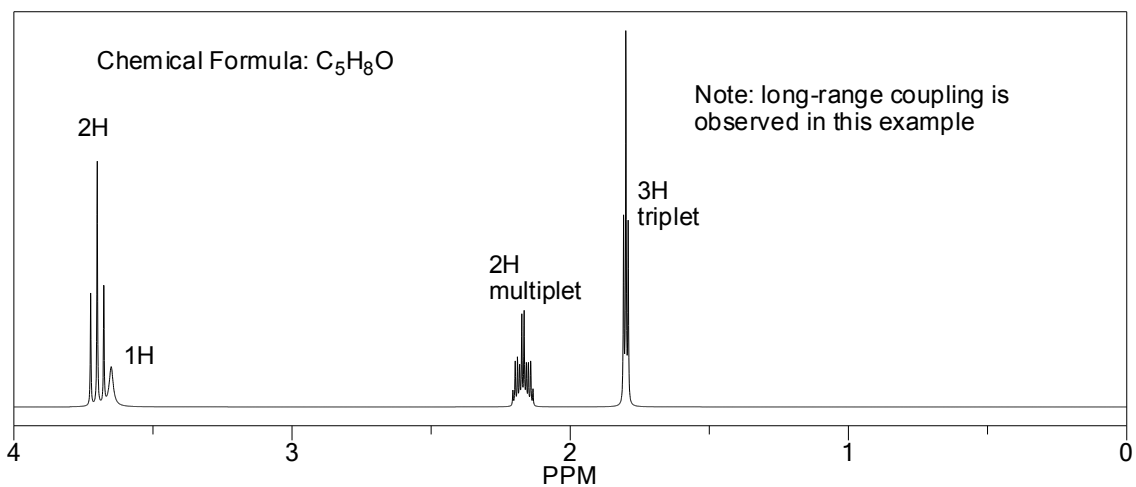
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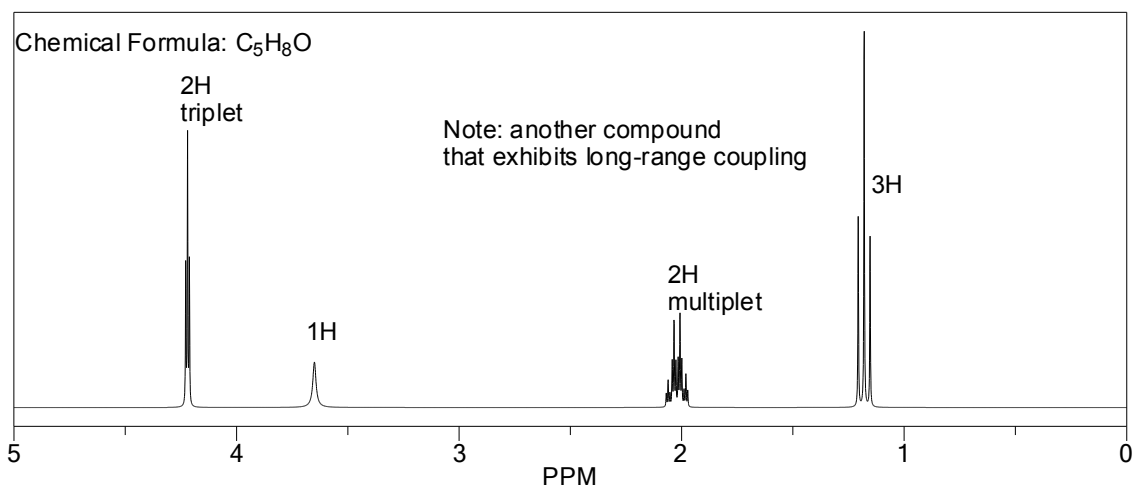
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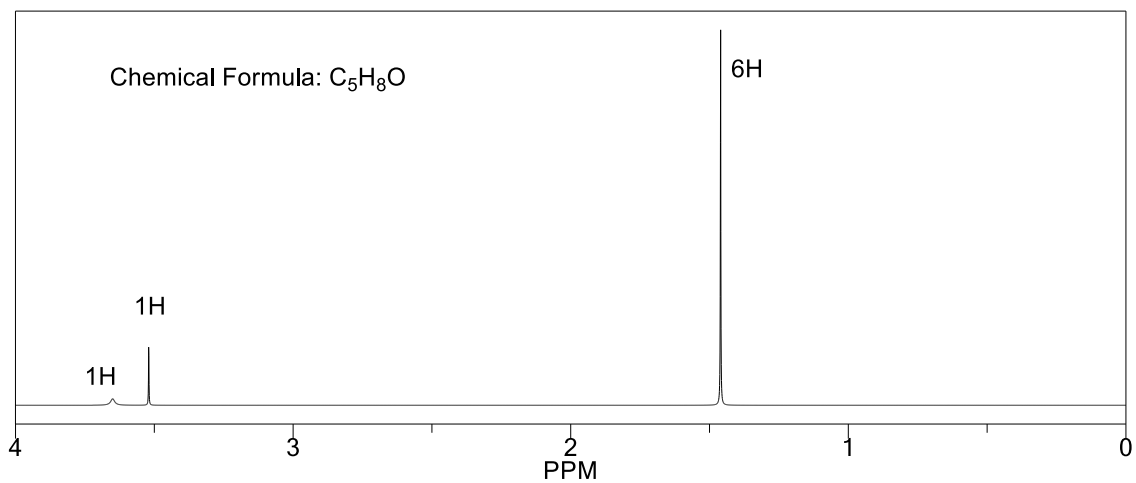
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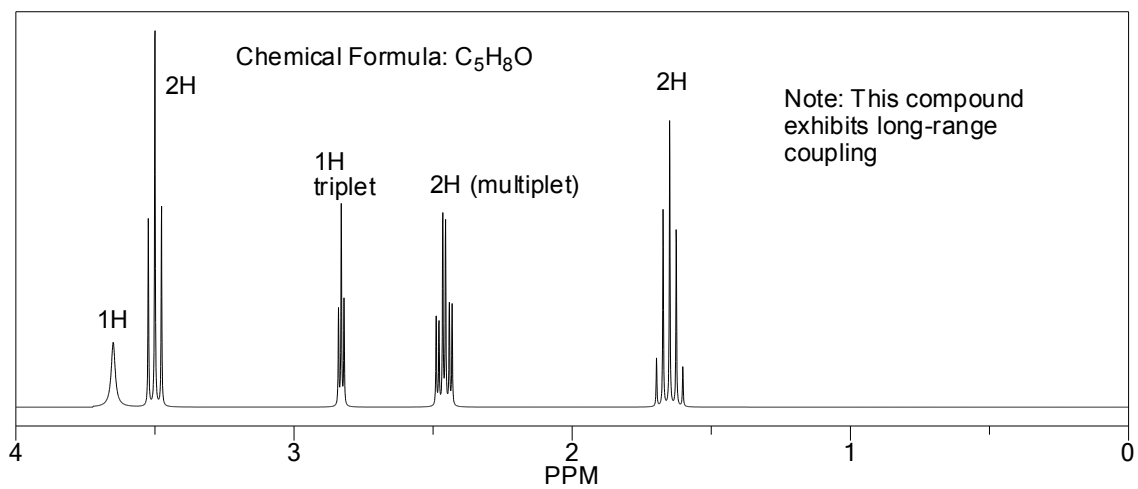
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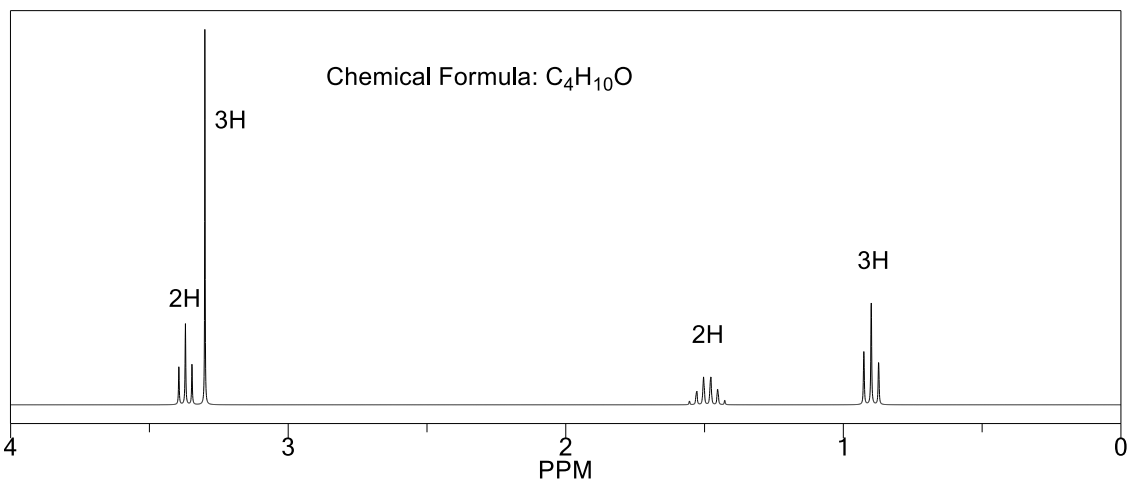
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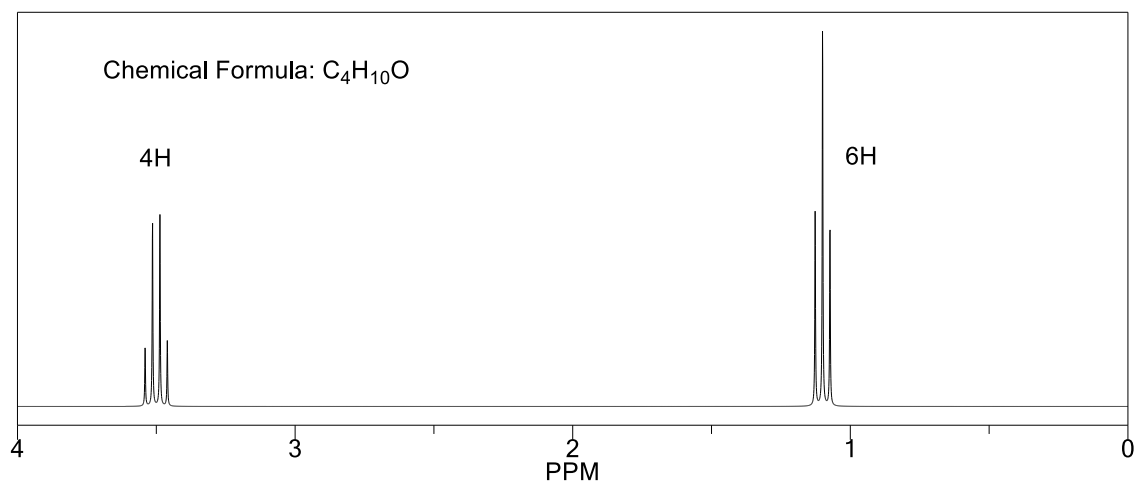
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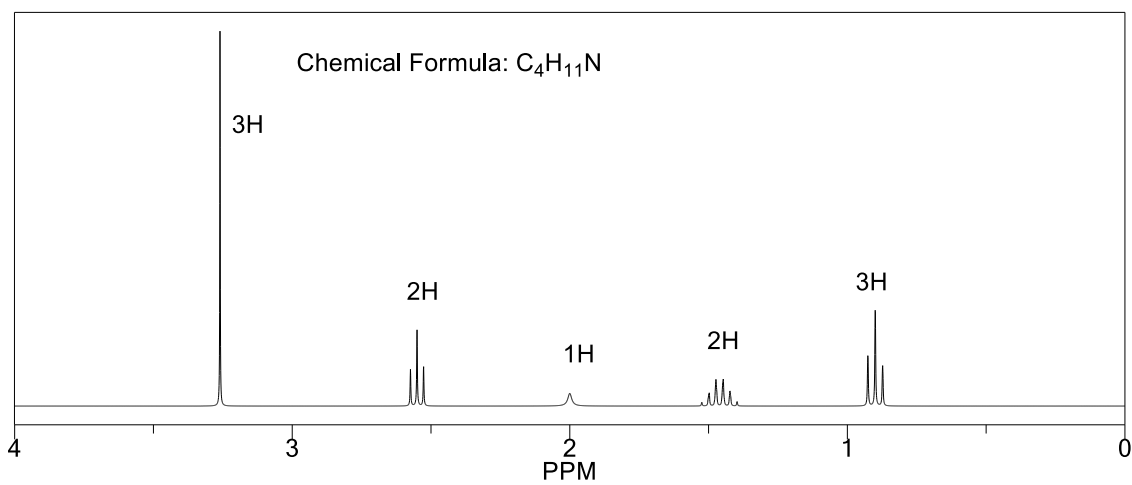
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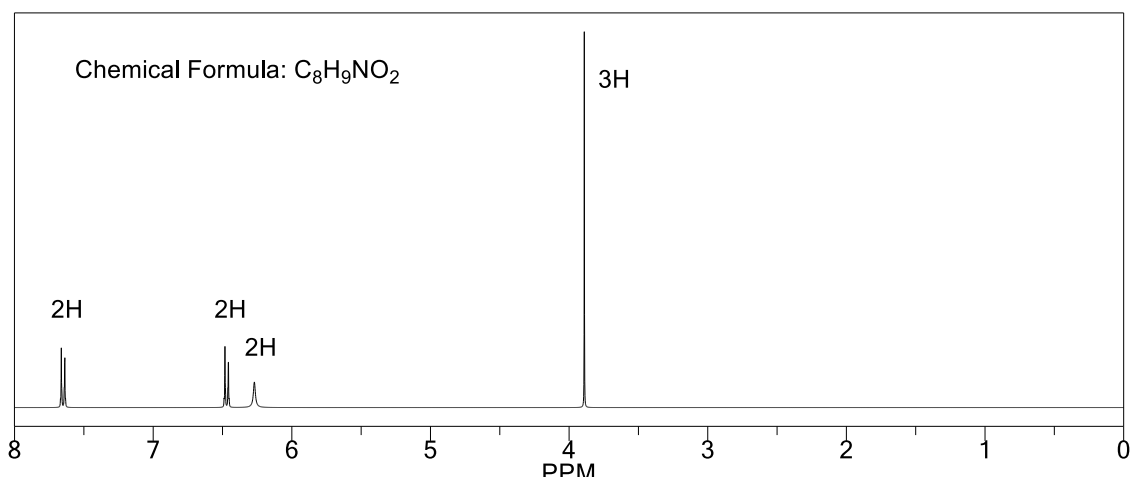
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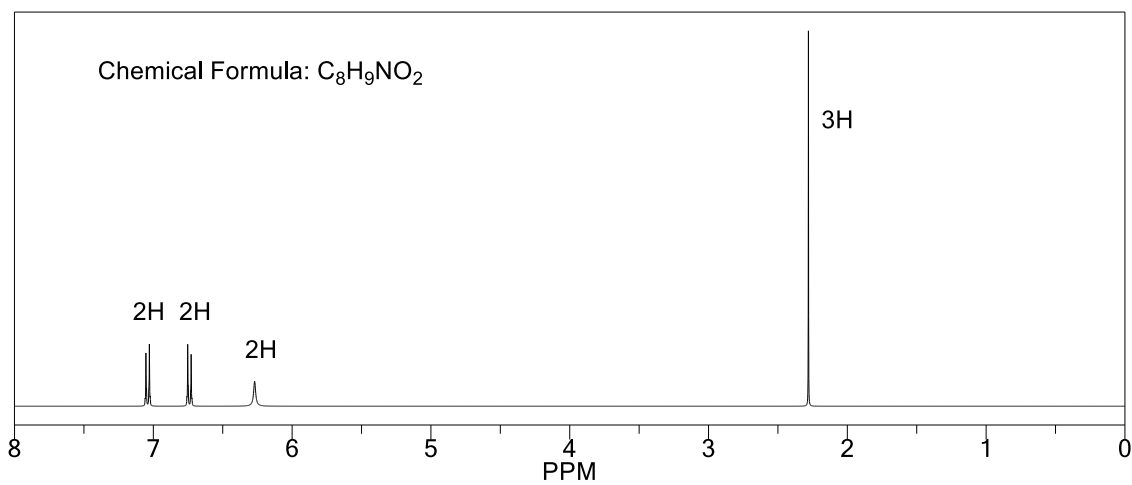
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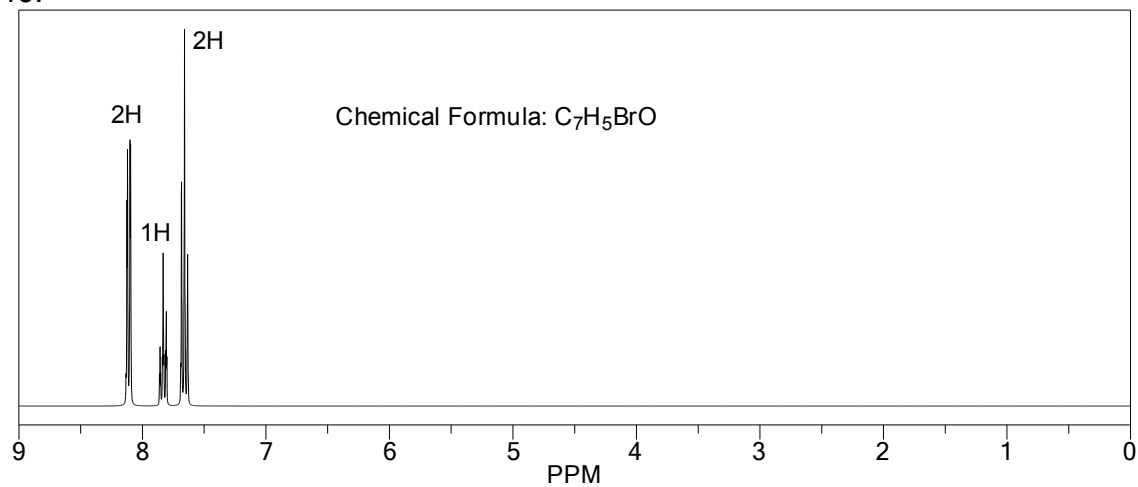
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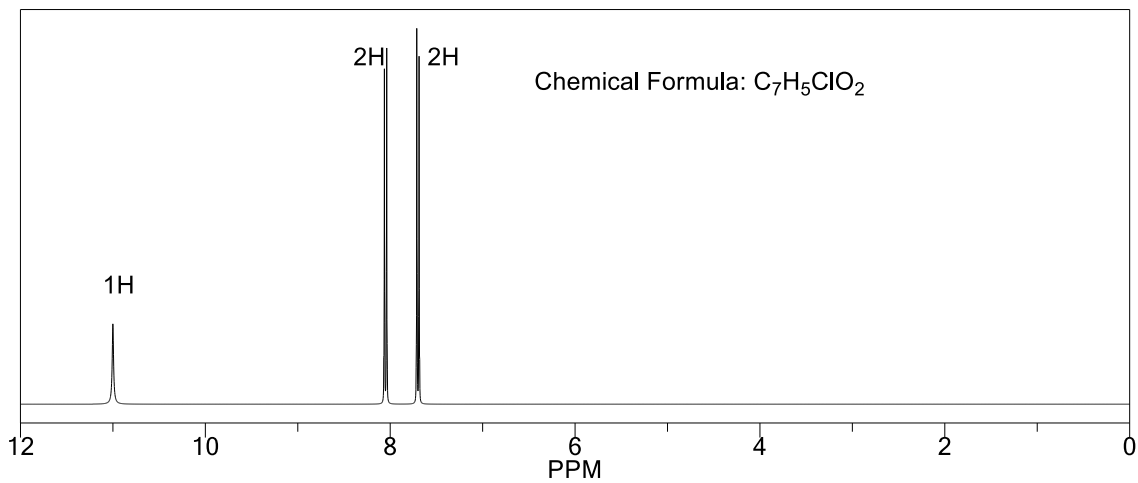
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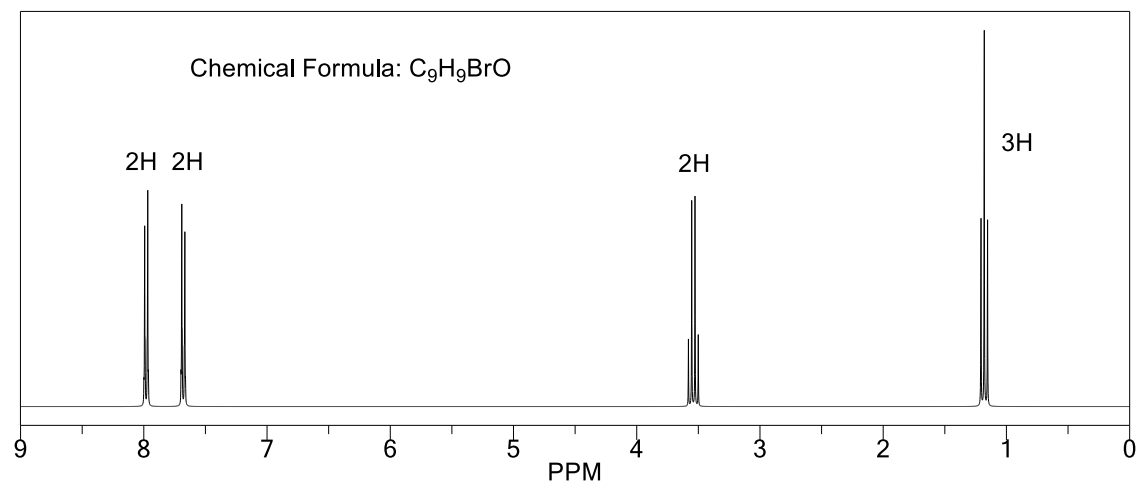
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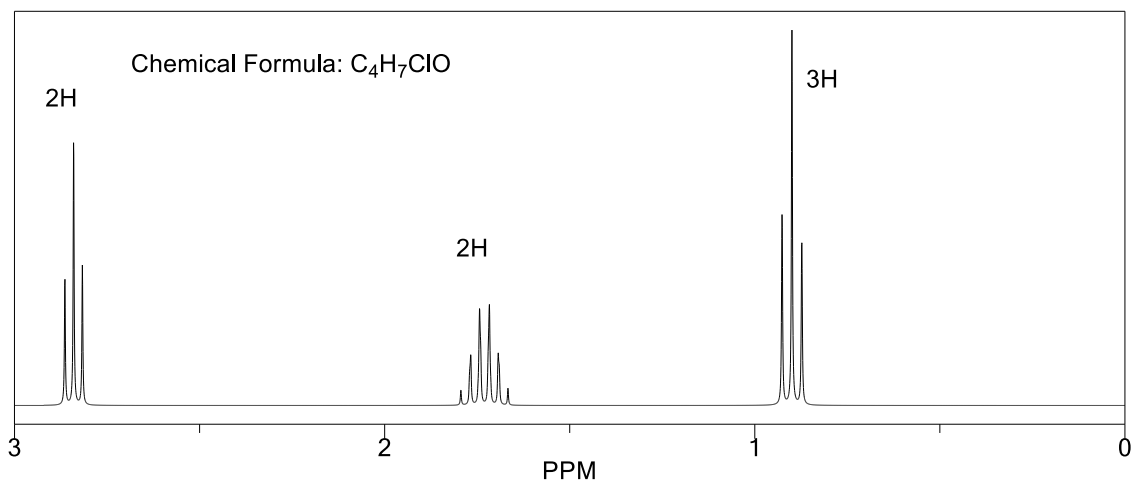
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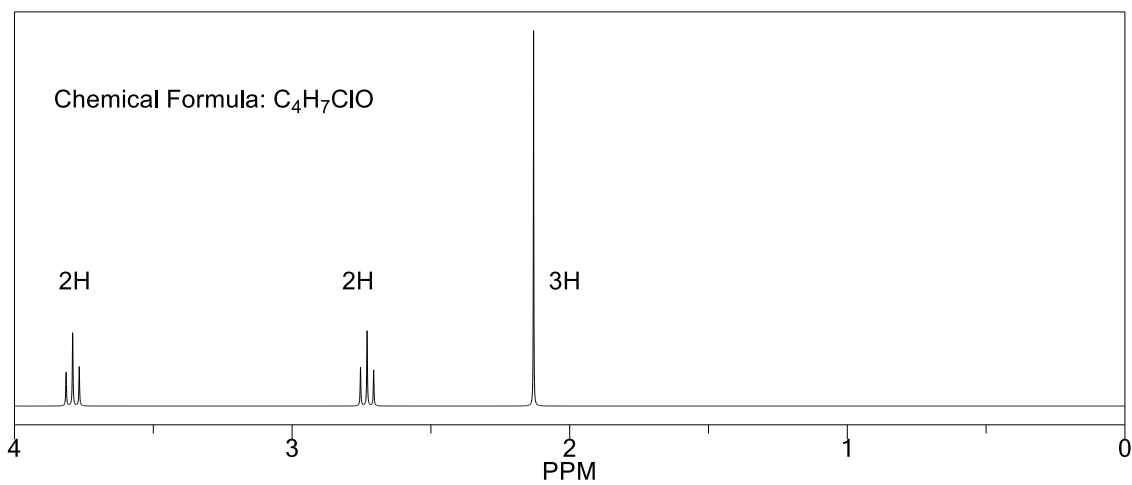
48.



49.



50.



51.

