H-NMR Spectroscopy

- The NMR spectrometer reads signals and plots them on a graph (NMR Spectrum).

- This technique used to identify the carbon-hydrogen framework of an organic compound.

Information that H-NMR Spectrum tells us:

- The **position** of the signals show how shielded or deshielded the proton is.
- The **Number** of the signals show how many different kinds of protons are present.
- Signal **Splitting** show the number of protons on adjacent atoms.
- The **Intensity (Integration)** of the signal show the number of protons of that type.

The position of the signals

- The position of the signals in an NMR specrum are based on how far they are from the signal of the reference compound (TMS) and based on chemical shift.
- Chemical Shift, having units of parts-per-million (**ppm**), and designated by the symbol (**δ**).

Principles that affect Shielding and Deshielding

- **1-Electronegativity**:

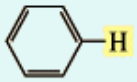
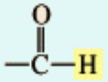
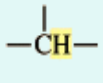
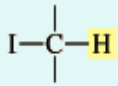
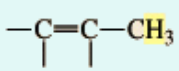
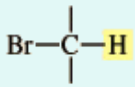
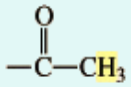
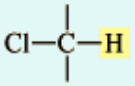
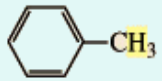
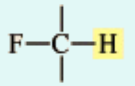
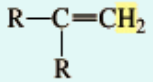
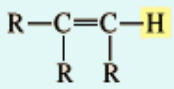
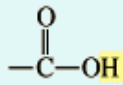
- Protons bound to carbons bearing electron withdrawing groups are deshielded based on the magnitude of the withdrawing effect.

- Electronegativity F>O>Cl>Br>I

2-Hybridization effects:

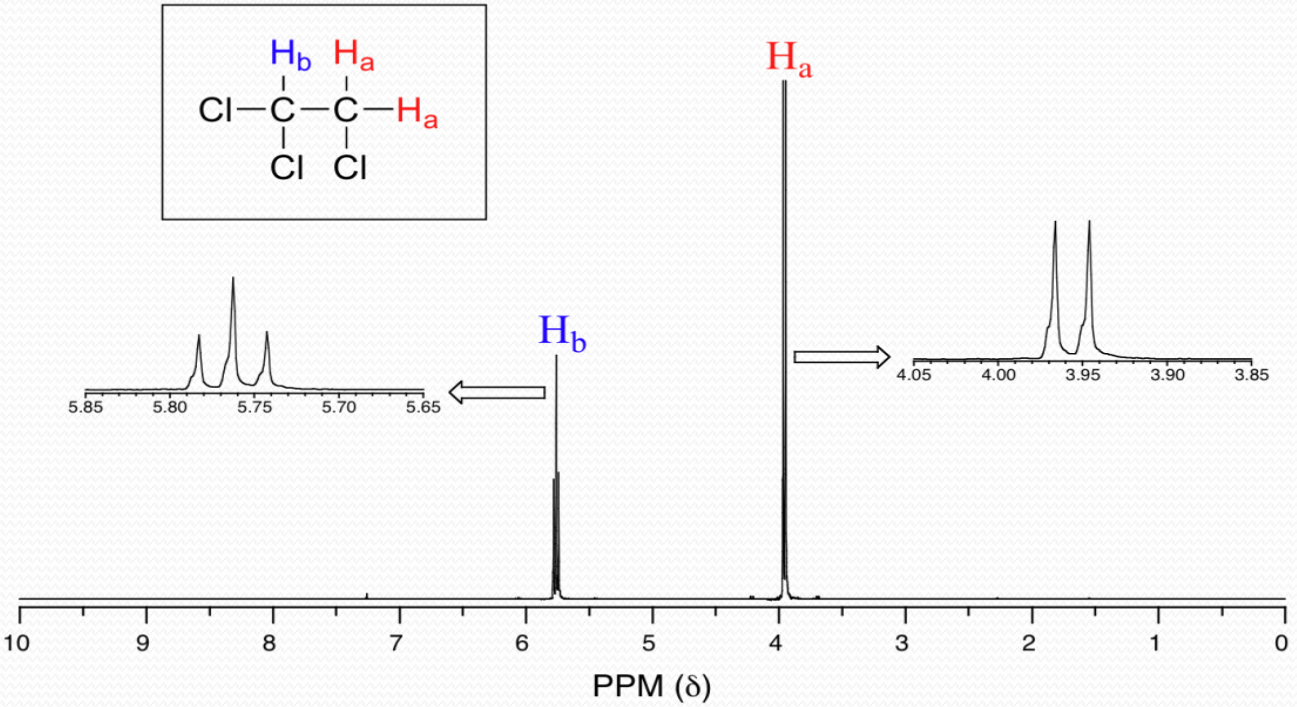
- The greater the S- character, the more tightly bound the electrons are to carbon.
- (SP=50%S ,SP^2=33%S and SP^3=25%S)

PROTON CHEMICAL SHIFTS

Type of proton	Approximate chemical shift (ppm)	Type of proton	Approximate chemical shift (ppm)
$(CH_3)_4Si$	0		6.5–8
$-CH_3$	0.9		
$-CH_2-$	1.3		9.0–10
	1.4		2.5–4
	1.7		2.5–4
	2.1		3–4
	2.3		4–4.5
$-C\equiv C-H$	2.4	RNH_2	variable, 1.5–4
$R-O-CH_3$	3.3	ROH	variable, 2–5
	4.7	ArOH	variable, 4–7
	5.3		variable, 10–12

The Number of the signals

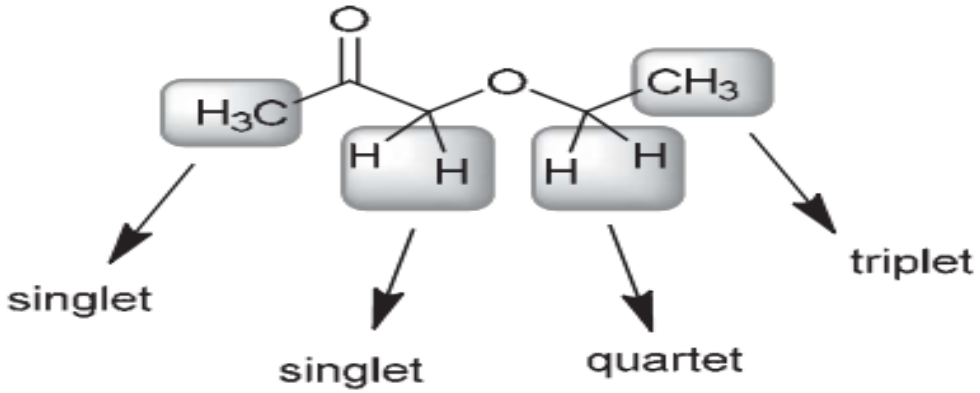
- Nuclei in same magnetic environment = **equivalent**
- Number of signals = number of equivalent proton sets

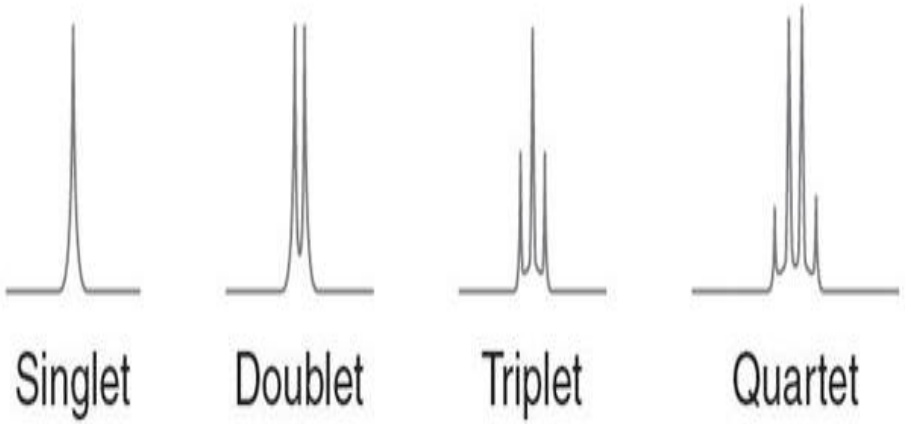


Splitting of signals

- Splitting of signals is caused by protons attached to adjacent carbons.
- **N+1 Rule:**
- N=the number of equivalent protons attached to the adjacent carbons.

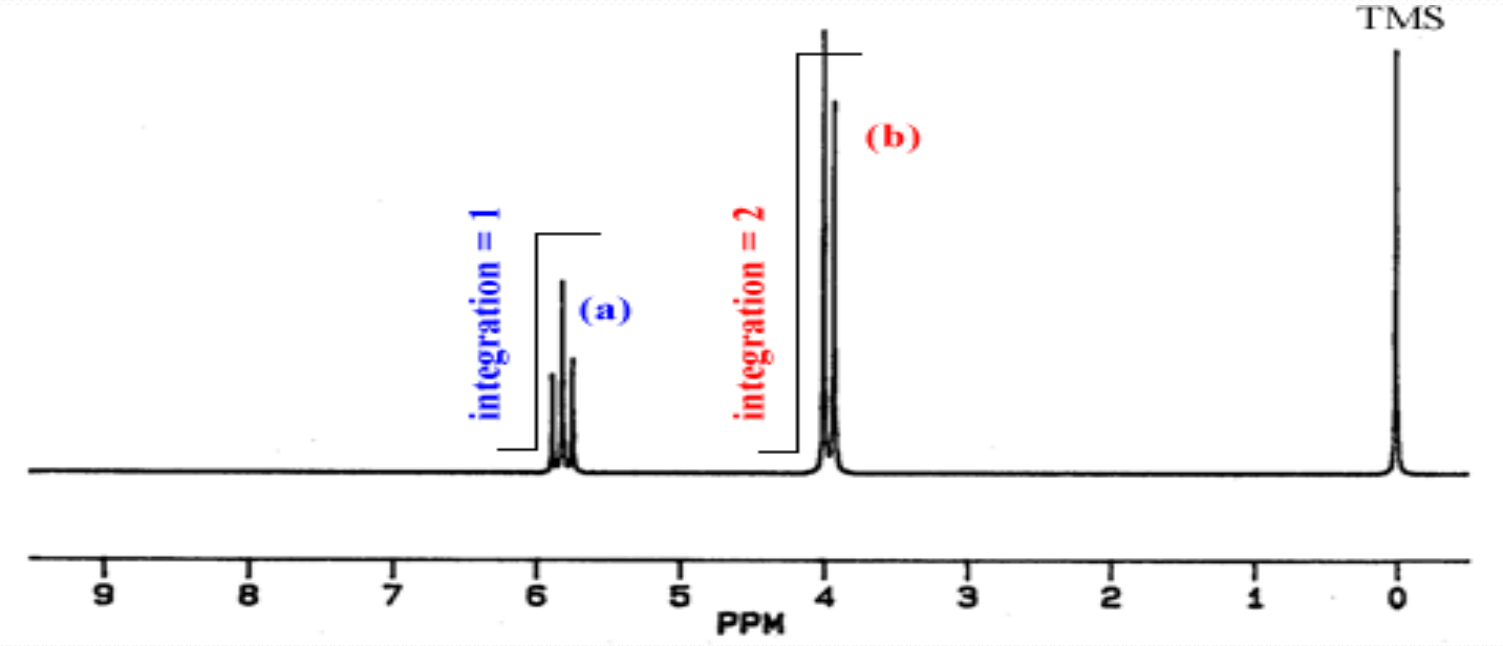
(a) This compound has four different kinds of protons, highlighted here. In each case, we apply the $n+1$ rule, giving the multiplicities shown:





The Intensity (Integration) of the signal

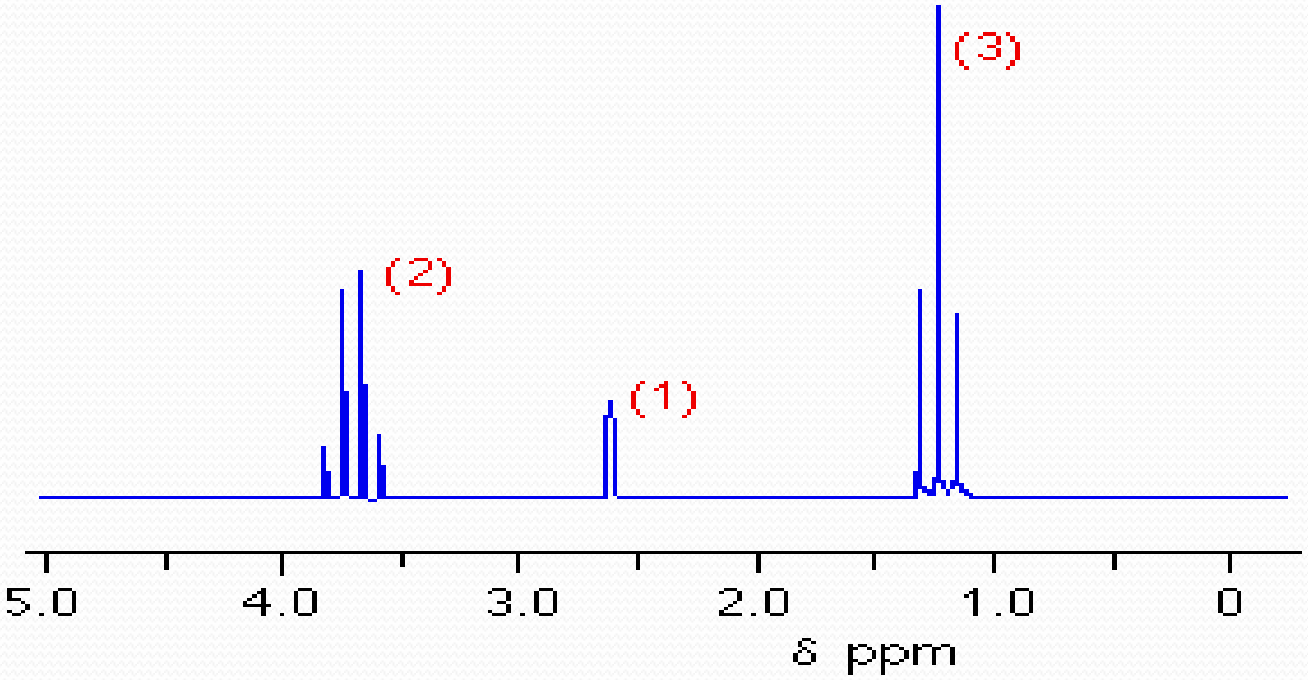
- show the number of protons of that type.
- The area under each signal is proportional to the number of hydrogen atoms producing that signal .



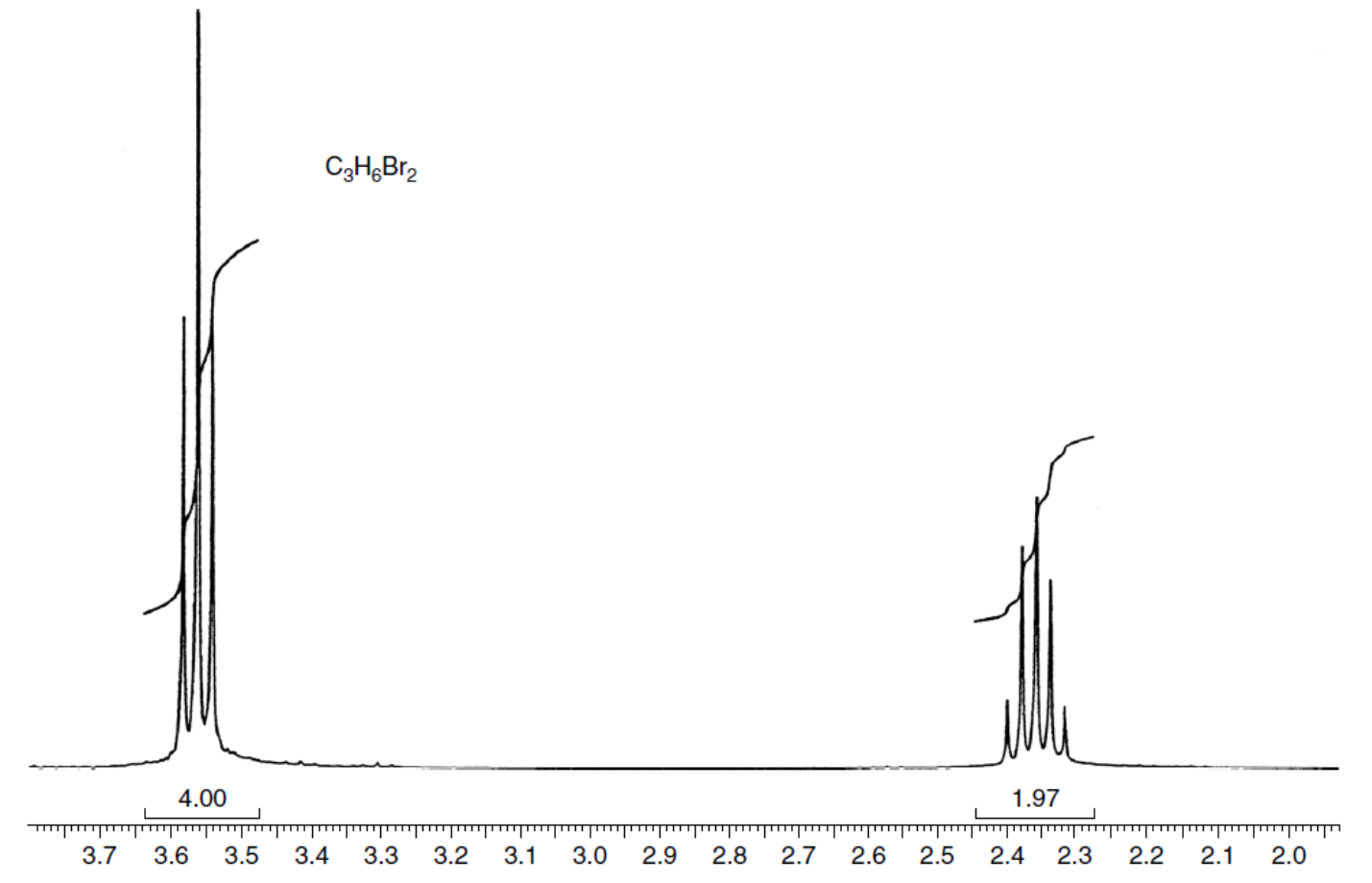
H-NMR Problems

- The compound that has the following NMR spectrum and the formula .....
- Draw it's structure

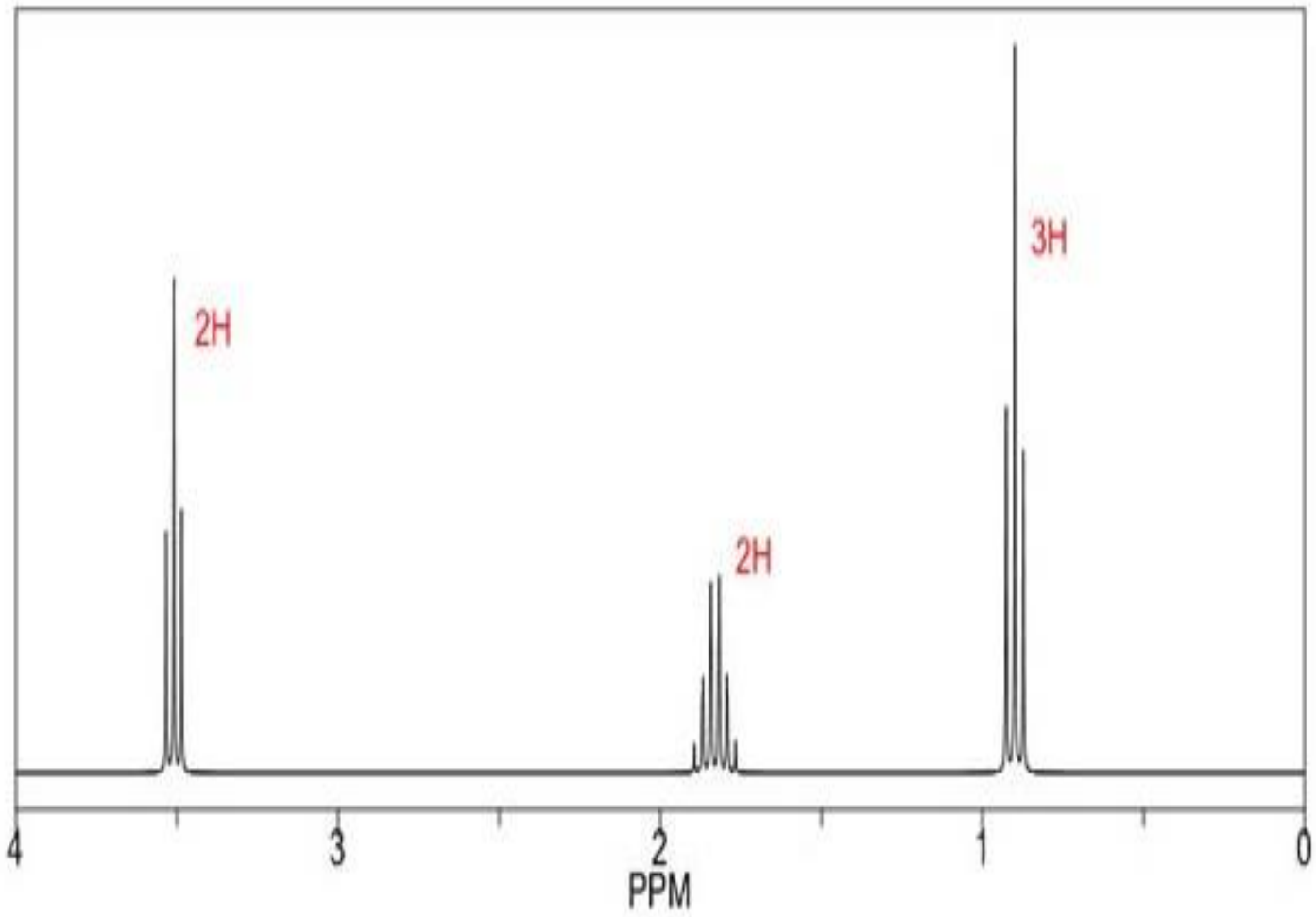
1-C_2H_6O



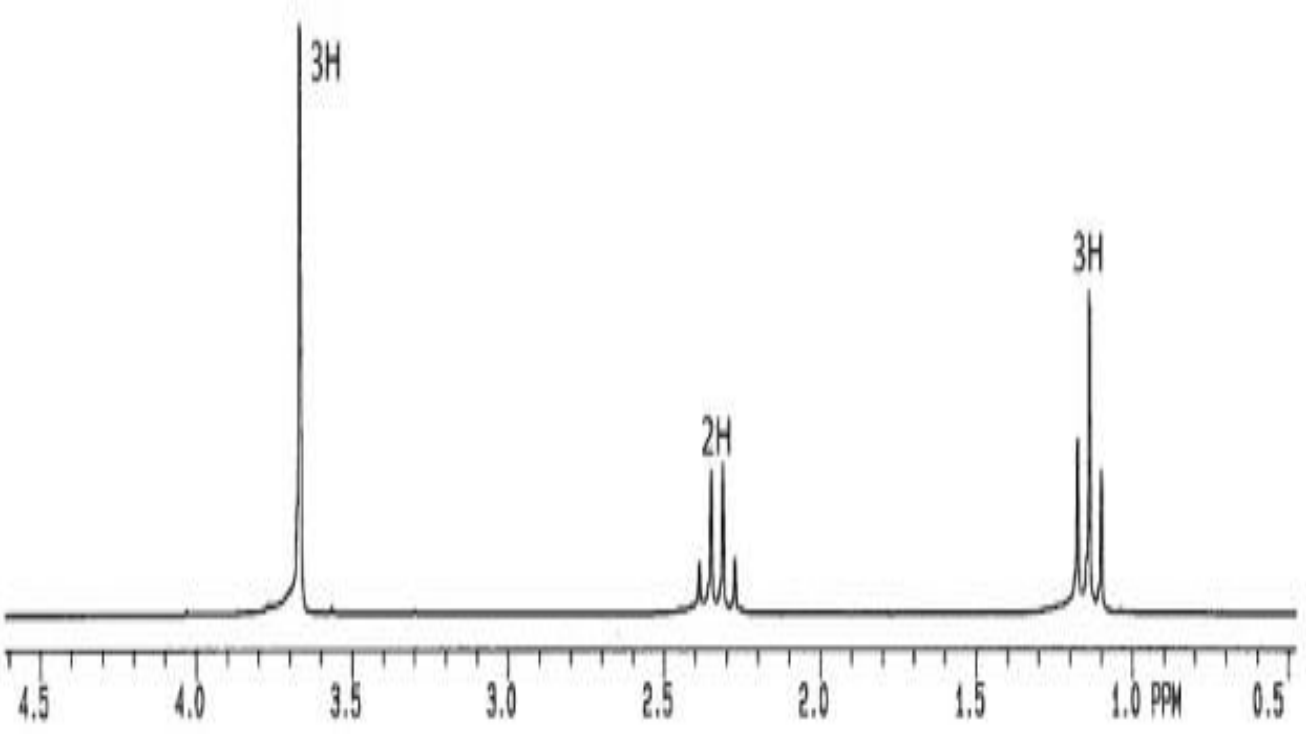
2-$C_3H_6Br_2$



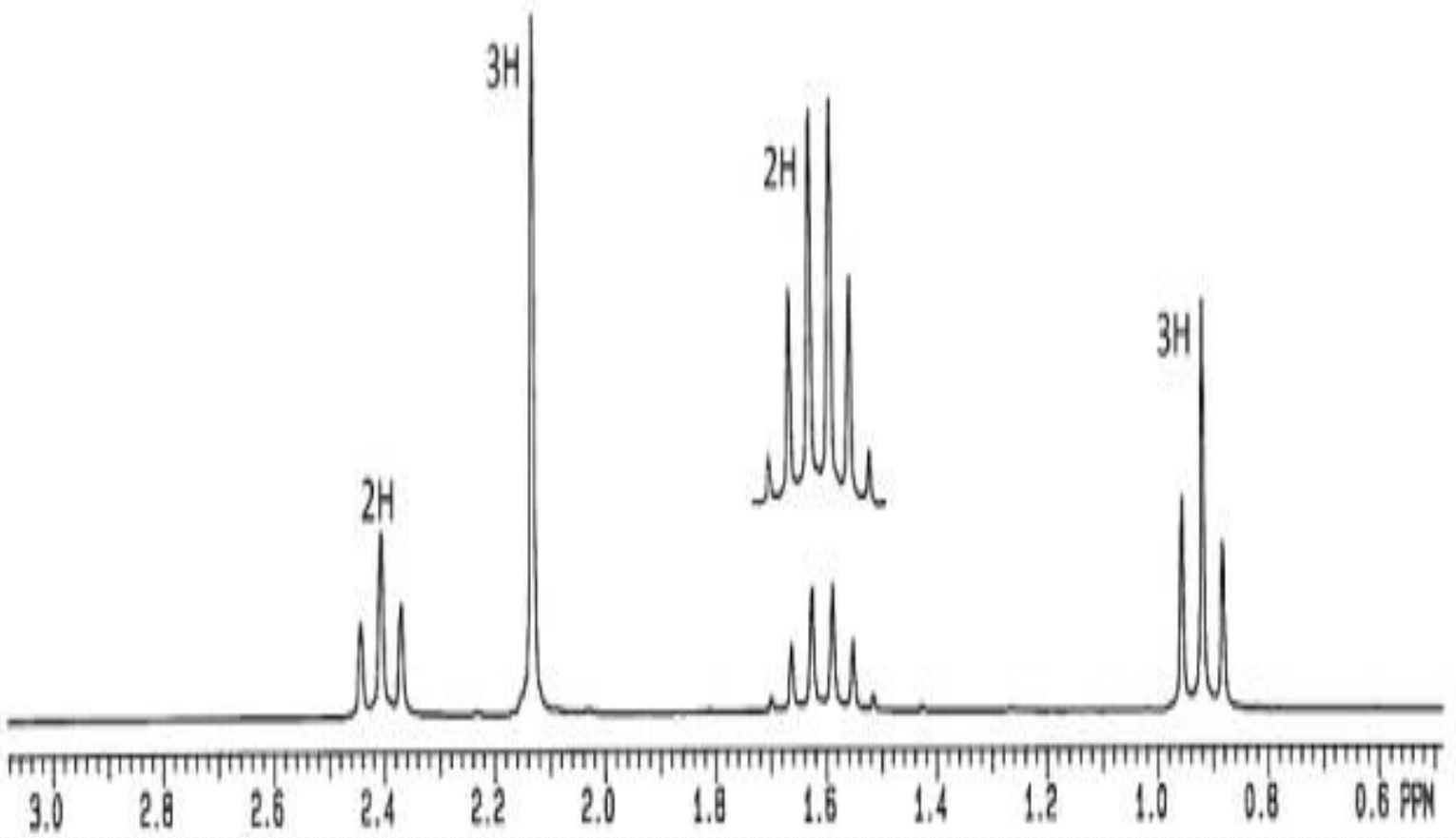
3-C_3H_7Br



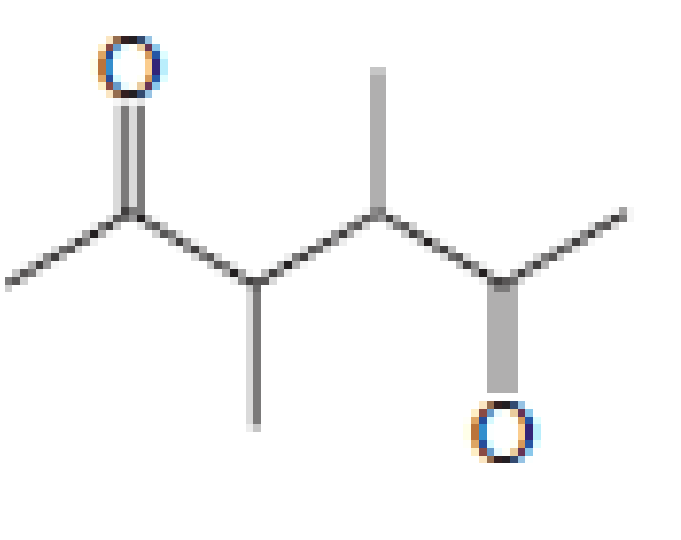
4- $C_4H_8O_2$

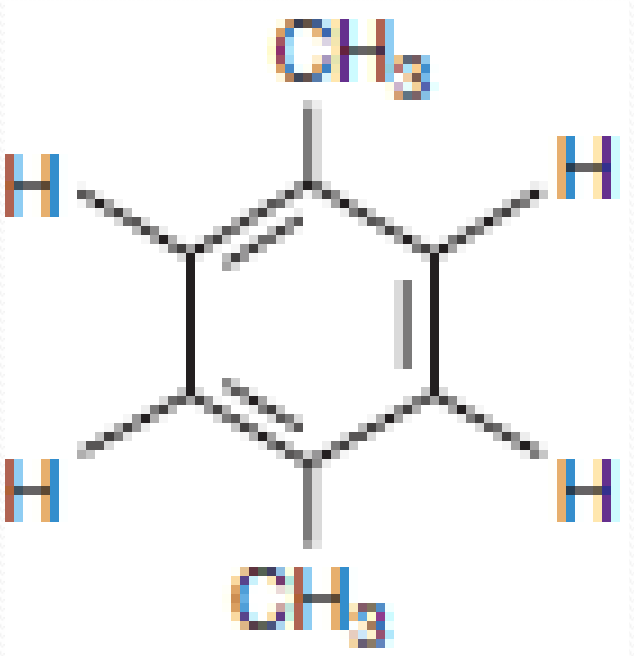


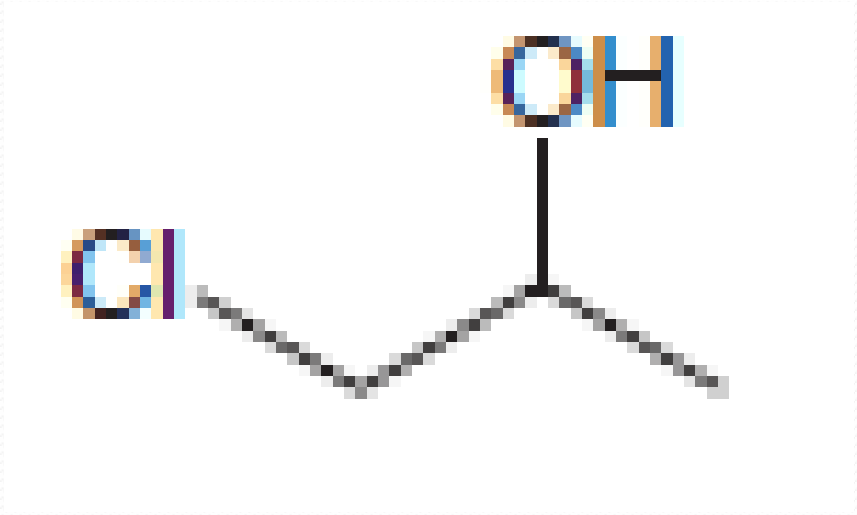
5-$C_5H_{10}O$



Predict the H- NMR for this compound




CH3
H
H
H
H
CH3


OH
Cl