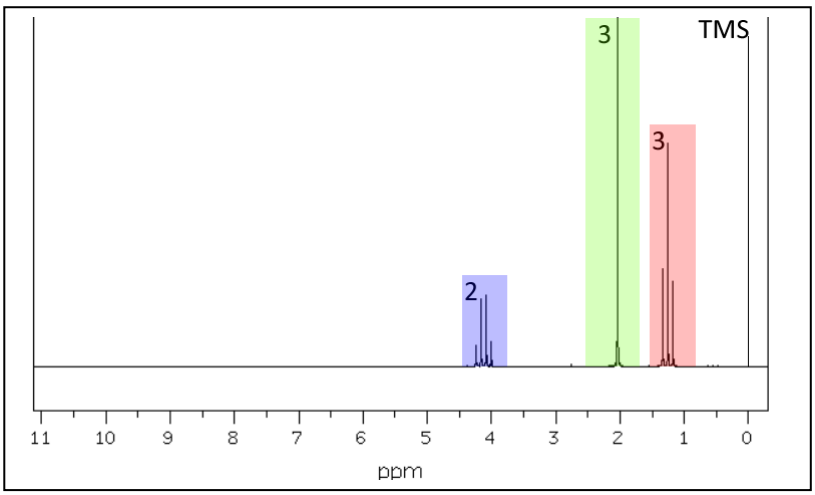
Lesson 4 $^{1}$HNMR

When interpreting HNMR spectra don't forget>

- Each signal represents a non-equivalent hydrogen
- The integration tells us about the relative number of hydrogens that caused the signal
- The splitting pattern tells us something about the neighbouring non-equivalent hydrogens

A compound has the molecular formula $C_4H_8O_2$. Its $^{1}$HNMR spectrum is shown on the right.



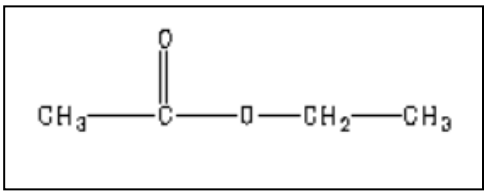

What can be deduced from the spectrum.

i. There are three equivalent sets of hydrogens

ii. Most likely there is a:

- $CH_3$ next to a $CH_2$ group of hydrogens as indicated by the red shaded signal. Its integration is 3 so it represents, most likely 3 hydrogens being split by a neighbouring $CH_2$ according to the n+1 rule.
- $CH_3$ on its own represented by the green shaded hydrogens.
- $CH_2$ next to a $CH_3$ as indicated by the blue shaded hydrogens. It is most likely close to a electronegative atom, such as oxygen, as indicated by its chemical shift.

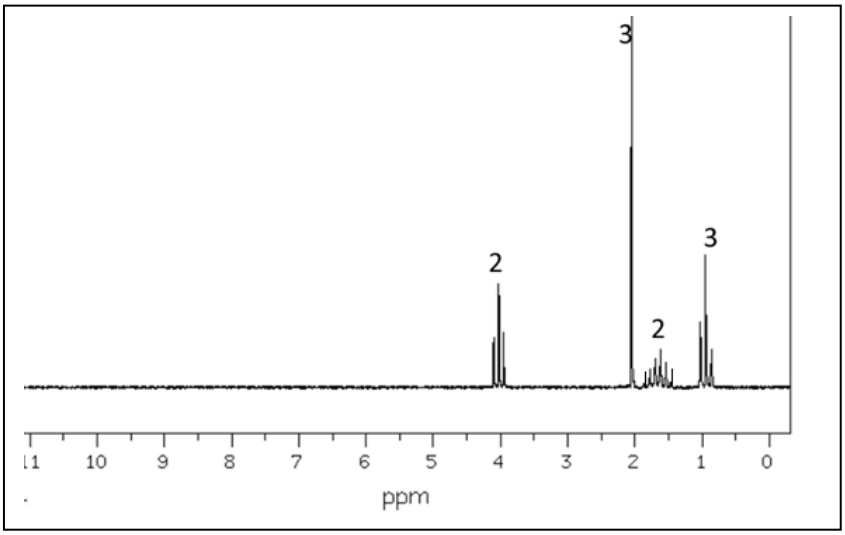
The most likely structure is shown on the right.




1) A compound has the molecular formula $C_5H_{10}O_2$. Below is its HNMR spectrum

a) Draw its structural formula, you may refer to the information given in the data sheet.

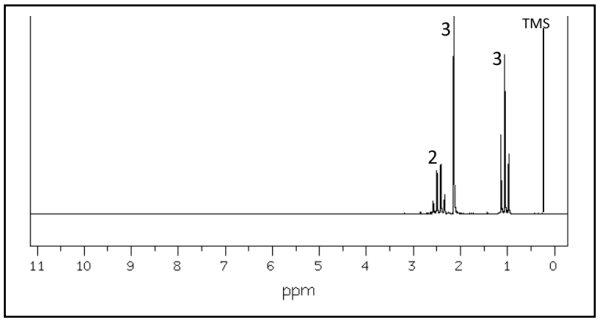
b) Name the compound.



c) An unknown compound has the molecular formula $C_4H_8O$.

i. What can you say about the equivalent hydrogens that formed the signals at:

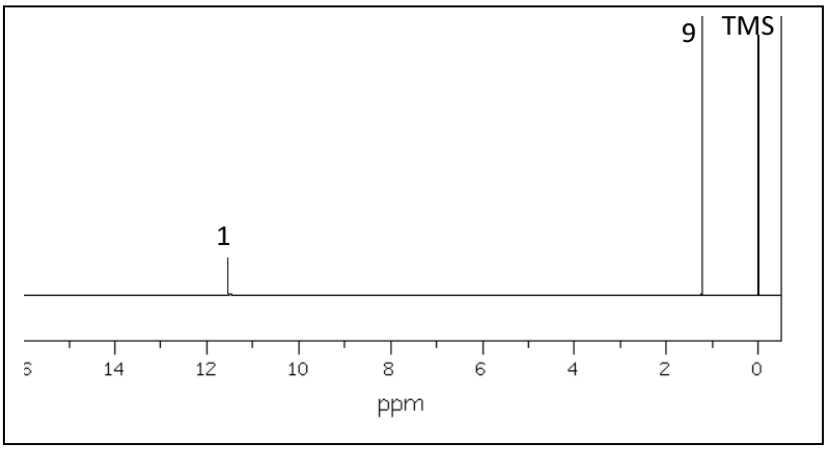
- 2.5 ppm
- 2.1 ppm
- 1.0 ppm




2) A compound has the molecular formula $C_5H_{10}O_2$. Its HNMR spectrum is shown below.

a) Draw its structural formula

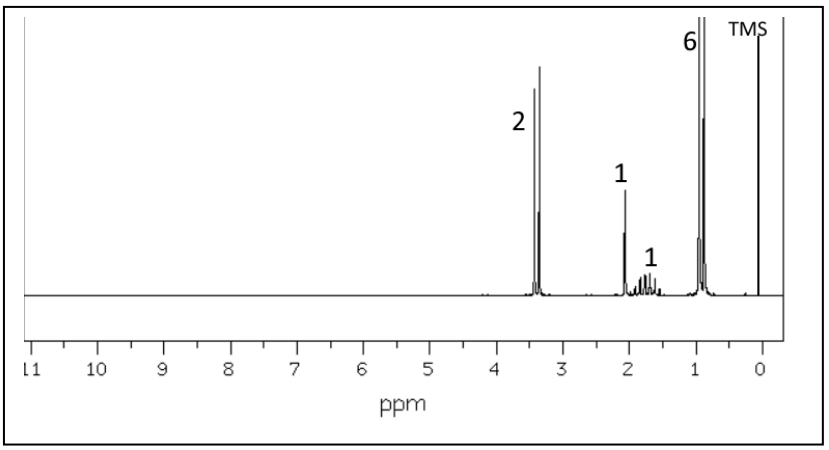
b) Name the compound.




3) A compound has the molecular formula $C_4H_{10}O$. Its HNMR spectrum is shown below. The peak signal at 1.75 ppm is split into a nonet (9).

a) Draw its structural formula

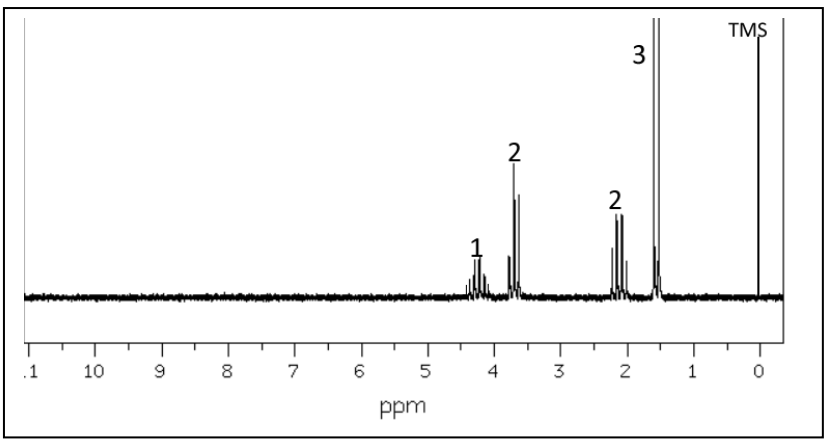
b) Name the compound.




4) A compound has the molecular formula $C_4H_8Cl_2$. Its HNMR spectrum is shown below.

a) Draw its structural formula

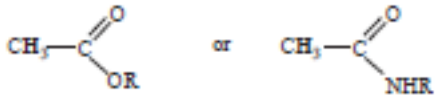
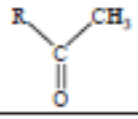
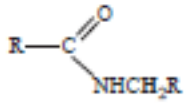
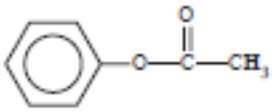
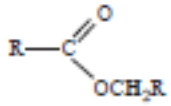
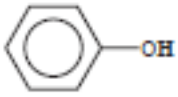
b) Name the compound.



## 16. $^1$H NMR data

Typical proton shift values relative to TMS = 0

These can differ slightly in different solvents. The shift refers to the proton environment that is indicated in bold letters in the formula.

| Type of proton | Chemical shift (ppm) |
|---|---|
| R–$CH_3$ | 0.9–1.0 |
| R–$CH_2$–R | 1.3–1.4 |
| RCH=CH–$CH_3$ | 1.6–1.9 |
| $R_3$–CH | 1.5 |
|  | 2.0 |
|  | 2.1–2.7 |
| R–$CH_2$–X (X = F, Cl, Br or I) | 3.0–4.5 |
| R–$CH_2$–OH, $R_2$–CH–OH | 3.3–4.5 |
|  | 3.2 |
| R—O—$CH_3$ or R—O—$CH_2$R | 3.3–3.7 |
|  | 2.3 |
|  | 3.7–4.8 |
| R–O–H | 1–6<br>(varies considerably under different conditions) |
| R–$NH_2$ | 1–5 |
| RHC ═ CHR | 4.5–7.0 |
|  | 4.0–12.0 |