

4.11 EXERCISE 2 – nmr spectra

1. A compound with molecular formula $C_3H_6O_2$ gives the following peaks in its proton nmr spectrum:

Chemical shift	Splitting	Integration factor
1.1	Triplet	3
2.2	Quartet	2
11.8	Singlet	1

Identify the molecule and account for the chemical shifts, splitting and integration factors of all three peaks.

2. A compound with molecular formula $C_5H_{10}O_2$ gives the following peaks in its proton nmr spectrum:

Chemical shift	Splitting	Integration factor
1.2	Triplet	3
1.3	Triplet	3
2.3	Quartet	2
4.1	Quartet	2

- a) Identify the molecule and account for the chemical shifts, splitting and integration factors of all four peaks.
- b) Explain why CH_3Cl is not used as a solvent in proton nmr spectroscopy.
- c) Give three reasons why T.M.S. is a good standard in proton nmr spectroscopy.
3. a) Suggest how propanal and propanone could be distinguished from their carbon-13 nmr spectra.
- b) Suggest how propan-2-ol and propanone could be distinguished from their carbon-13 nmr spectra.
- c) Predict the number of peaks in the carbon-13 nmr spectrum of:
- i) butanone
 - ii) pentan-2-one
 - iii) pentan-3-one