TOPIC 20 EXERCISE 3 – PROTON 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.

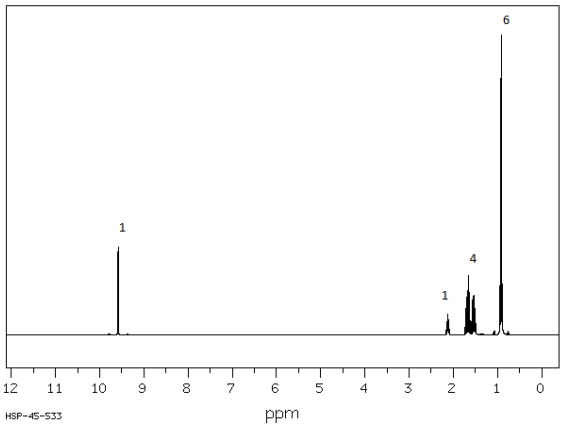
b) Explain why CH_3Cl is not used as a solvent in proton nmr spectroscopy.

c) Give three reasons why T.M.S. is a good standard in proton nmr spectroscopy.

3. Use the information in the table below to identify molecule A from its proton nmr spectrum:

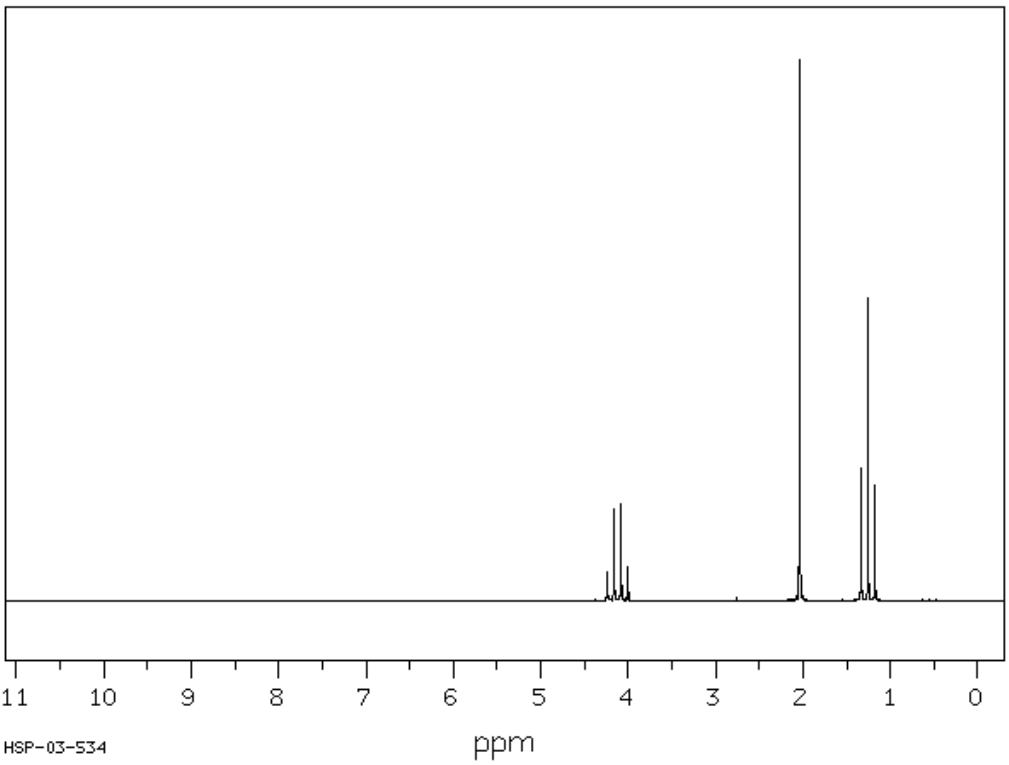
peak	chemical shift/ppm	relative intensity	peak type
a	2.4	1	multiplet
b	2.1	3	Singlet
c	1.5	2	multiplet
d	1.1	3	doublet
e	0.9	3	triplet

4. Identify the molecule responsible for the proton nmr spectrum below:



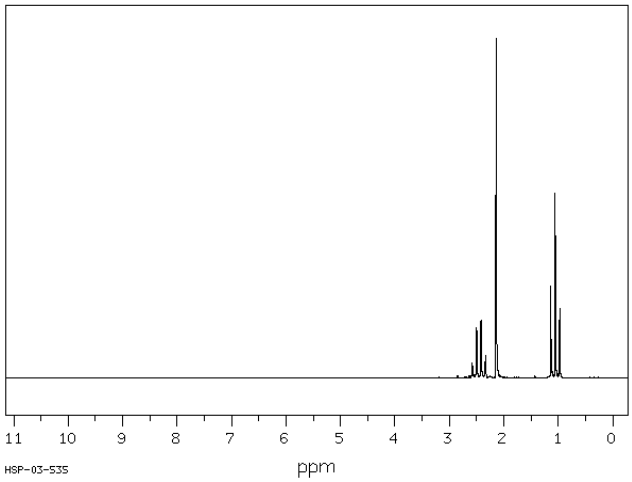
The peak at 9.6 is a doublet; the peak at 2.1 is a multiplet; the peak at 1.7 is a multiplet and the peak at 0.9 is a triplet

5. Identify this molecule:



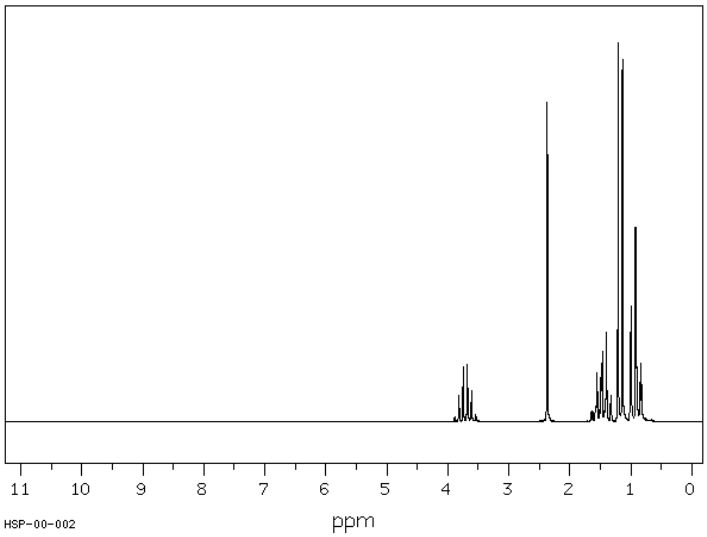
Shift	Relative peak intensity	Splitting
4.1	2	Quartet
2.1	3	Singlet
1.3	3	Triplet

6. Identify this molecule:



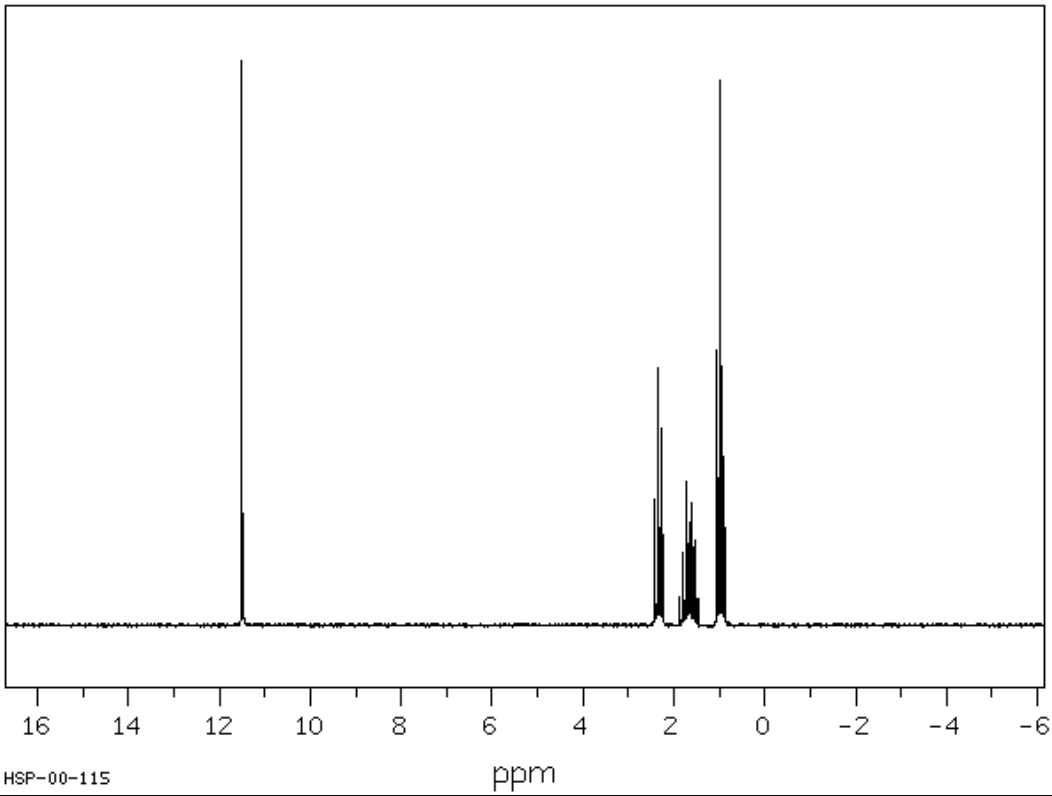
Shift	Relative peak intensity	Splitting
2.4	2	Quartet
2.2	3	Singlet
1.1	3	Triplet

7. Identify this molecule:



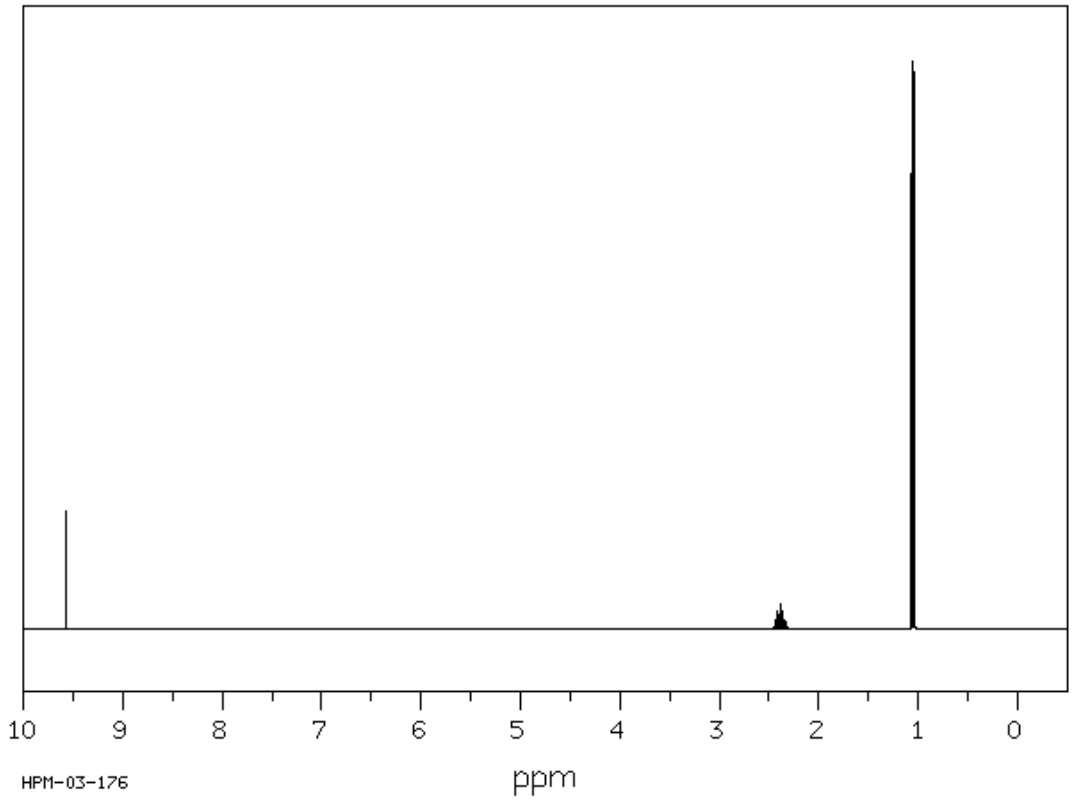
Shift	Relative peak intensity	Splitting
3.6	1	Multiplet
2.3	1	Singlet
1.4	2	Multiplet
1.2	3	Doublet
0.9	3	Triplet

8. Identify this molecule:



Shift	Relative peak intensity	Splitting
11.6	1	Singlet
2.2	2	Triplet
1.9	2	Multiplet
1.0	3	Triplet

9. Identify this molecule:



Shift	Relative peak intensity	Splitting
9.6	1	Doublet
2.3	1	Multiplet
1.1	6	Doublet

SOLUTIONS

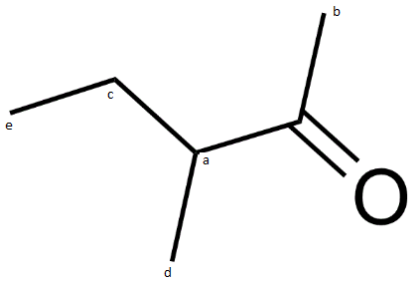
1. peak at 1.1 is CH_3- adjacent to -CH_2-
peak at 2.2 is -CH_2CO-, adjacent to CH_3-
peak at 11.8 is –COOH
so molecule is propanoic acid, CH_3CH_2COOH

2. a) peak at 1.2 is CH_3-, adjacent to -CH_2-
peak at 1.3 is also CH_3-, adjacent to -CH_2-
peak at 2.3 is -CH_2CO-, adjacent to CH_3-
peak at 4.1 is -CH_2O-, adjacent to CH_3-
so molecule is ethyl propanoate, $CH_3CH_2COOCH_2CH_3$

b) $CHCl_3$ is not used as a solvent because it contains a proton which will interfere with the spectrum of the substance being analysed.

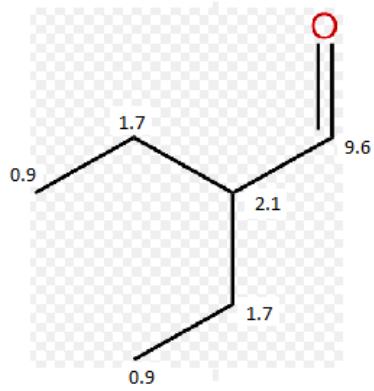
c) TMS is a good standard because
- it contains 12 identical protons, giving a single intense peak
- it contains highly shielded protons, which do not interfere with the spectrum
- it is cheap and non-toxic

3. e is -C<u>H</u>$_3$ adjacent to -C<u>H</u>$_2$- (c)
b is -C<u>H</u>$_3$ adjacent to -C=O
d is -C<u>H</u>$_3$ adjacent to -C<u>H</u>- (a)
a is -C<u>H</u>- adjacent to -C=O



3-methylpentan-2one

4. 9.6 is -C<u>H</u>O adjacent to -C<u>H</u>- (2.1)
2.1 is -C<u>H</u>- adjacent to -C<u>H</u>O (9.6)
0.9 is 2 x -C<u>H</u>$_3$ adjacent to -C<u>H</u>$_2$- (1.7)



ethylbutanal

5. 4.1 is O-C<u>H</u>$_2$- adjacent to -C<u>H</u>$_3$ (1.3)
   2.1 is C<u>H</u>$_3$C=O
   $CH_3COOCH_2CH_3$ (ethyl ethanoate)
   (2.1) (4.1)(1.3)
6. 2.4 is O=CC<u>H</u>$_2$ adjacent to C<u>H</u>$_3$ (1.1)
   2.2 is C<u>H</u>$_3$C=O
   $CH_3COCH_2CH_3$ (butanone)
   (2.2) (2.4)(1.1)

7. 0.9 is C<u>H</u>$_3$ adjacent to C<u>H</u>$_2$ (1.4)
   1.2 is C<u>H</u>$_3$ adjacent to C<u>H</u> (3.6)
   3.6 is O-C<u>H</u>-
   2.3 is -O<u>H</u>
   $CH_3CH_2CH(OH)CH_3$ (butan-2-ol)
   (0.9)(1.4)(3.6)(2.3)(1.2)

8. 11.6 is -COOH
   2.2 is O=CCH_2- adjacent to -CH_2- (1.9)
   1.0 is -CH_3 adjacent to -CH_2- (1.9)
   $CH_3CH_2CH_2COOH$ (butanoic acid)
   (1.0)(1.9)(2.2) (11.6)

9. 9.6 is -C<u>H</u>O adjacent to -C<u>H</u>- (2.3)
   2.3 is -C<u>H</u>C=O
   1.1 is 2 x CH_3 adjacent to -CH- (2.3)
   $(CH_3)_2CHCHO$ **(**methylpropanal)
   (1.1) (2.3)(9.6)