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CHEMISTRY

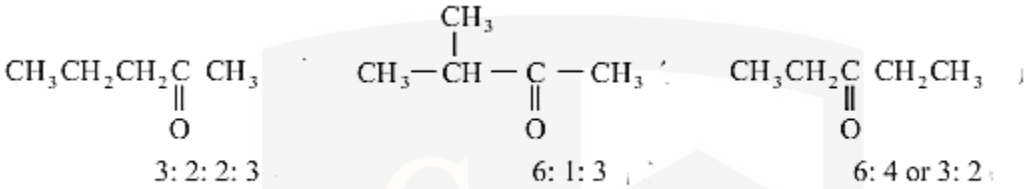
ORGANIC CHEMISTRY II

Level & Board	AQA (A-LEVEL)
TOPIC:	NMR SPECTROSCOPY
PAPER TYPE:	SOLUTION - 3
TOTAL QUESTIONS	10
TOTAL MARKS	/48

NMR Spectroscopy – 3

1.

3 Ketones and the ratio of the areas under each peak in its low-resolution proton n.m.r. spectrum:



(6)

2.

(a)

A suitable solvent for dissolving compound J before obtaining its ^1H NMR spectrum is **deuterated chloroform ($CDCl_3$)**.

(1)

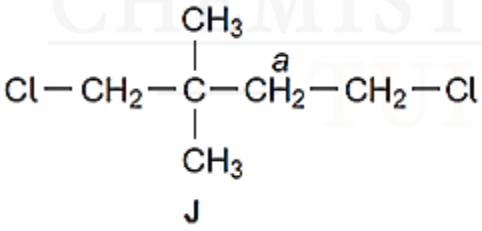
(b)

There are four peaks in the ^1H n.m.r. spectrum of J.

(1)

(c)

The protons labeled "a" in compound J have two equivalent neighboring protons.



J

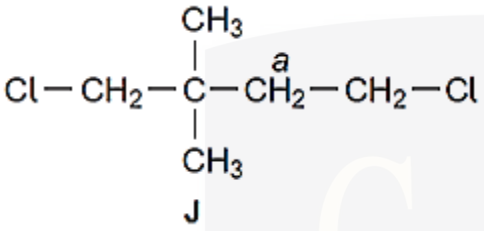
According to the n+1 rule in ^1H NMR spectroscopy, the splitting pattern can be determined as follows:

As the proton labeled "a" is adjacent to two equivalent protons (n=2), the splitting pattern will be n+1=2+1=3.

Therefore, the splitting pattern of the protons labeled "a" will be a **triplet**.

(1)

(d)



J

The IUPAC name of J is :

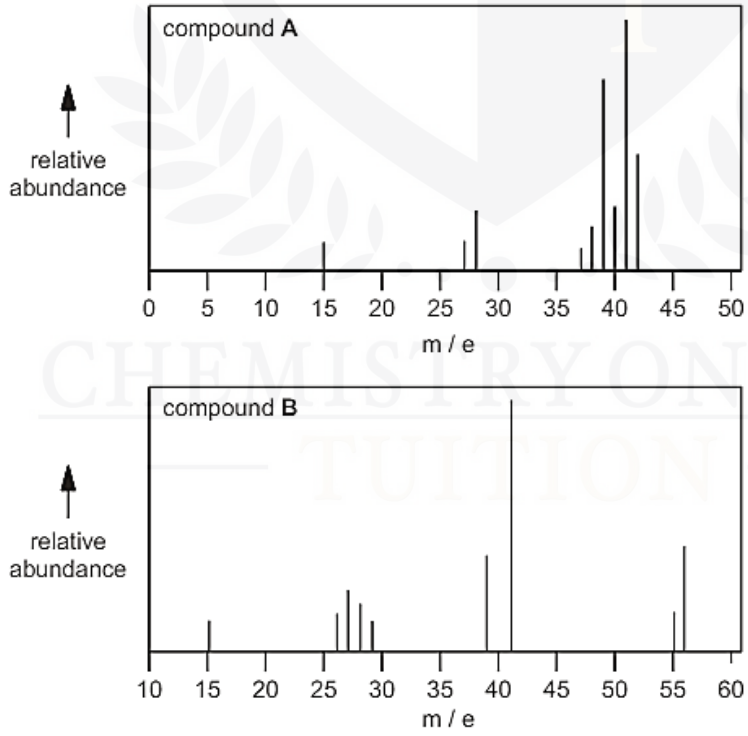
1,4-dichloro-2,2-dimethylbutane.

(1)

3.

(a)

The molecular formula of each compound.



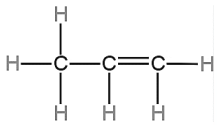
Compound A: C_3H_6

Compound **B**: C_4H_8

(2)

(b)

The structural formula of compound A.



$CH_3CH=CH_2$

(1)

(c)

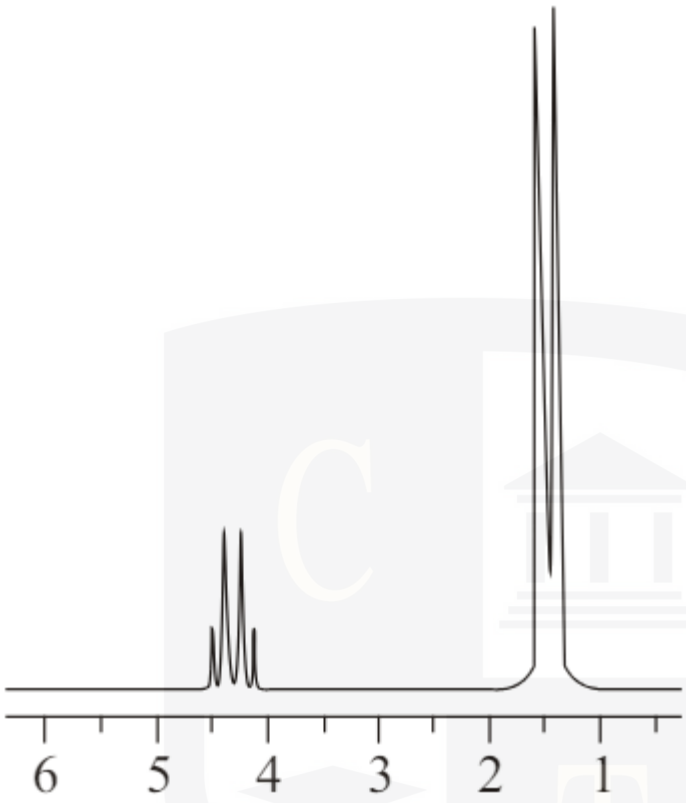
$C_3H_5^+$ is responsible for the peak at m/e 41 in the spectrum of compound B.

(1)

4.

(a)

The high resolution n.m.r. spectrum of lactic acid in D_2O.



Splitting:

Doublet peak is at 1.4

Quartet peak is at 4.3

(4)

(b)

Four peaks:

Methyl Group (CH_3):
A doublet due to coupling with the adjacent methine hydrogen.

Methine Group (CH):
A quartet due to coupling with the three hydrogens in the methyl group.

Hydroxyl Group (OH): A broad singlet.

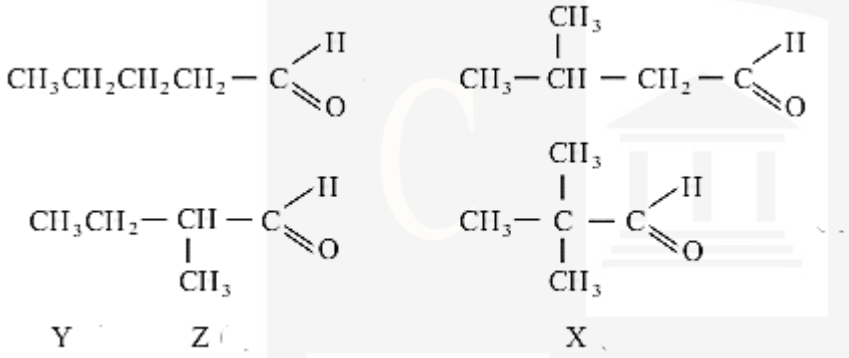
Carboxyl Group (COOH): A broad singlet.

The labile protons (OH and COOH) are now visible, appearing as singlets since they are not exchanged out as they would be in D_2O.

(2)

5.

4 aldehydes with structure having the molecular formula $C_5H_{10}O$



Y Z X

Z is the compound showing optical isomerism

Y is the compound which has five peaks with the ratios of the areas under each peak 3:3:2:1:1

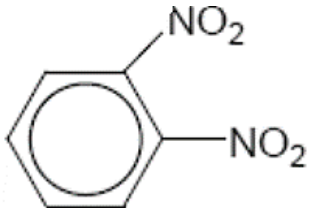
(7)

6.

(a)

A has two peaks in its ^{13}C n.m.r. spectrum.

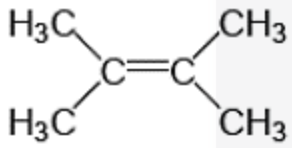
B has three peaks in its ^{13}C n.m.r. spectrum.



(2)

(b)

Compound C



Compound D

(2)

7.

(a)

Single, intense peak:

TMS produces a single, intense peak in both 1H and 13C NMR spectra because all hydrogen atoms (12 equivalent H) and all carbon atoms (4 equivalent C) are in the same chemical environment.

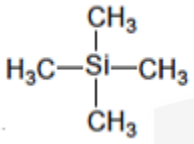
Upfield reference:

The peak for TMS appears upfield (to the right) of most other peaks in the spectrum.
This positioning ensures that the TMS peak does not interfere with the peaks of the sample being analyzed.

(2)

(b)

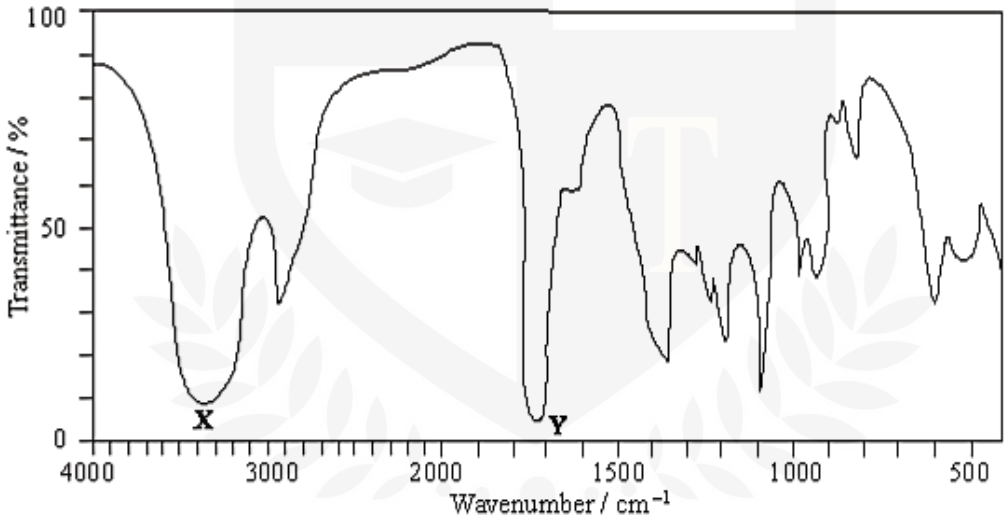
Structural formula of TMS.



$C_4H_{12}Si$

(1)

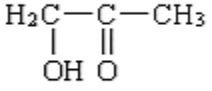
8.

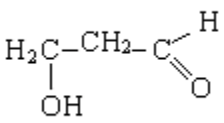


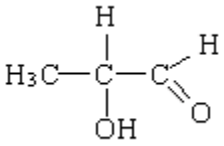
Functional groups labelled X: (O-H) (alcohols)

Functional groups labelled Y: C=O (carbonyl)

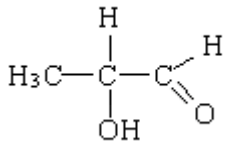
Structures of the three possible structural isomers for A:







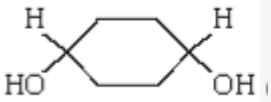
Structure which represents a pair of optical isomers.



(6)

9.

Structural formula for G.



As 3269 cm^{-1} (OH alcohol)

(2)

10.

(a)

In the 1H NMR spectrum of 2,3-dichlorobutane ($C_4 H_8 Cl_2$):

Number of Peaks: There are **2 peaks**.

Integration Ratio:

The integration ratio of the peaks will be **6:2** (or simplified to 3:1).

Splitting Patterns:

- The peak corresponding to the methyl groups (6 hydrogens) will be a **doublet**.
- The peak corresponding to the methine hydrogens (2 hydrogens) will be a **quartet**.

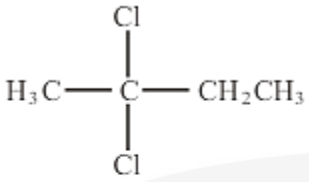
So, the 1H NMR spectrum of 2,3-dichlorobutane will show two peaks, with an integration ratio of 6:2, where the doublet is due to the methyl groups and the quartet is due to the methine groups.

(2)

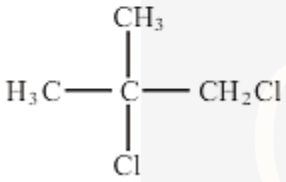
(b)

Structures of S and T are:

S



T



(4)

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