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CHEMISTRY

INORGANIC CHEMISTRY II

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

NMR Spectroscopy - 3

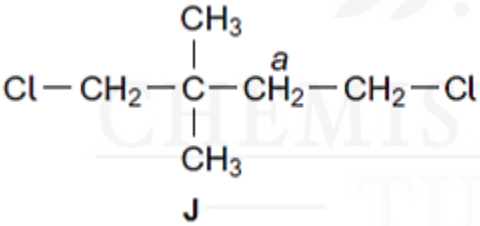
1. Draw the structure of each of the three ketones which have the molecular formula $C_5H_{10}O$.

For each compound give the ratio of the areas under each peak in its low-resolution proton n.m.r. spectrum.

(6)

2. N.m.r. spectroscopy can be used to study the structures of organic compounds.

Compound J was studied using ^1H n.m.r. spectroscopy.



J

(a) Identify a solvent in which J can be dissolved before obtaining its ^1H n.m.r. spectrum.

I am Sorry !!!!!

(1)

(b) Give the number of peaks in the ^{1}H n.m.r. spectrum of J.

(1)

(c) Give the splitting pattern of the protons labelled a.

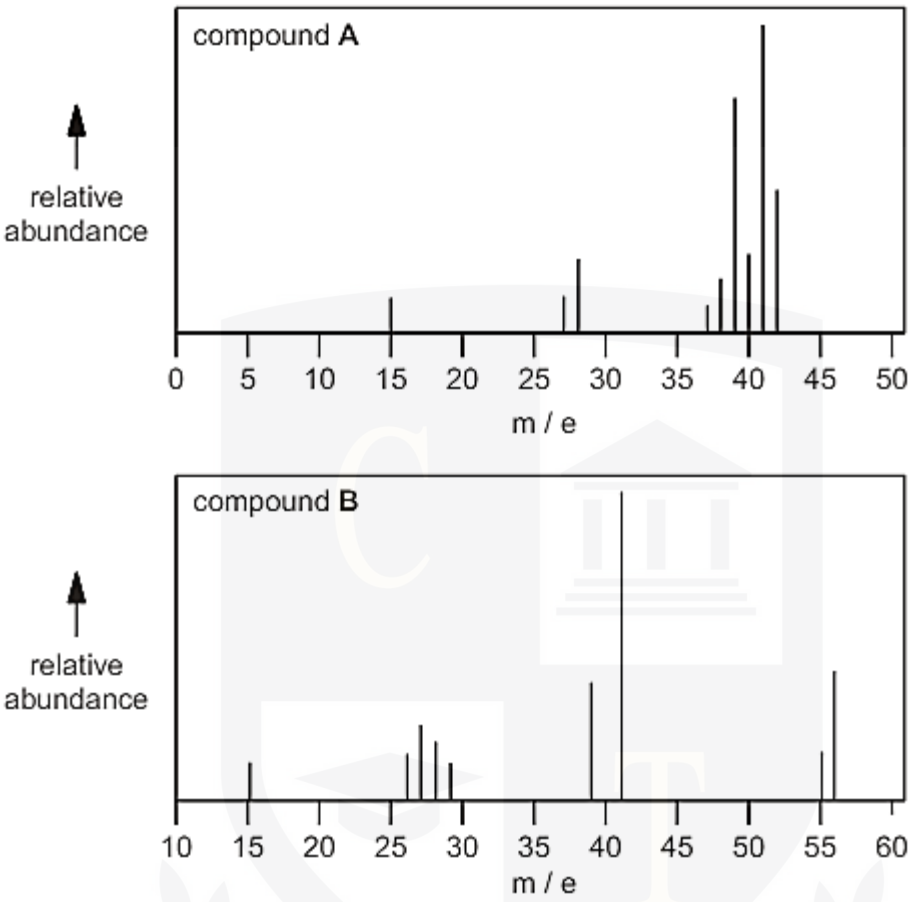
(1)

(d) Give the IUPAC name of J.

(1)

3. This question is about the use of spectrometry in helping to gain information about the structure of organic molecules.

The major peaks in the mass spectra of two hydrocarbons A and B are shown below.



Compounds A and B have the same empirical formula.

(a) Deduce the molecular formula of each compound.

(2)

(b) Draw the structural formula of compound A.

(1)

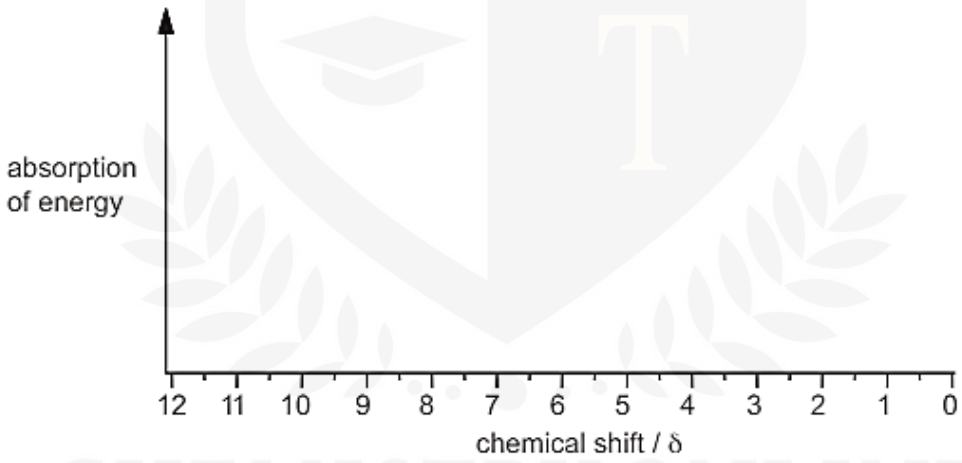
(c) Suggest the species responsible for the peak at m/e 41 in the spectrum of compound B.

(1)

4. Lactic acid produces an n.m.r. spectrum in D_2O with peaks at chemical shift values of 1.4 ppm and 4.3 ppm.

(a) On the axes below, sketch the high resolution n.m.r. spectrum of lactic acid in D_2O.

Show any splitting patterns and state the relative areas of the two peaks**.**



(4)

(b) How many peaks would you expect if the n.m.r. spectrum of lactic acid was run in an inert solvent rather than in D_2O?
Explain your answer.

(2)

5. Draw the structure of each of the four aldehydes which also have the molecular formula $C_5H_{10}O$.

Label with the letter X the compound which has only two peaks in its low-resolution proton n.m.r. spectrum.

Label with the letter Y the compound which has five peaks with the ratios of the areas under each peak 3:3:2:1:1 in its low-resolution proton n.m.r. spectrum.

Label with the letter Z the compound which shows optical isomerism.

(7)

6. When the molecular formula of a compound is known, spectroscopic and other analytical techniques can be used to distinguish between possible structural isomers.

Draw one possible structure for each of the compounds.

(a) Compounds A and B have the molecular formula $C_6H_4N_2O_4$ and both are dinitrobenzenes.

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) Compounds C and D have the molecular formula C_6H_{12}.

Both have only one peak in their ^{1}H n.m.r. spectra.
C reacts with aqueous bromine but D does not.

(2)

7. The non-toxic, inert substance TMS is used as a standard in recording both ^{1}H and ^{13}C n.m.r. spectra.

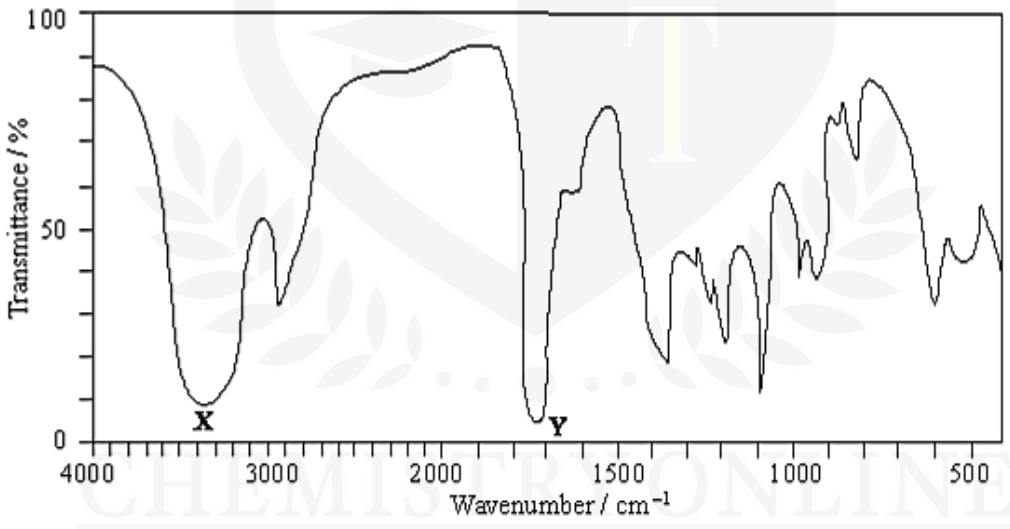
(a) Give two other reasons why TMS is used as a standard in recording n.m.r. spectra.

(2)

(b) Give the structural formula of TMS.

(1)

8. The infra-red spectrum of compound A, $C_3H_6O_2$, is shown below.



Identify the functional groups which cause the absorptions labelled X and Y.

Using this information draw the structures of the three possible structural isomers for A.

Label as A the structure which represents a pair of optical isomers.

(6)

9. A compound G, $C_6H_{12}O_2$, contains six carbon atoms in a ring.

It has an absorption in its infra-red spectrum at 3270 cm^{-1} and shows only three different proton environments in its proton n.m.r. spectrum.

Deduce a structural formula for G.

(2)

10. The reaction of but-2-ene with chlorine produces 2,3-dichlorobutane, $C_4H_8Cl_2$

(a) State the number of peaks, their integration ratio and any splitting of peaks in the proton n.m.r. spectrum of 2,3-dichlorobutane.

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(2)

(b) Compound S, an isomer of $C_4H_8Cl_2$, produces a proton n.m.r. spectrum which consists only of a singlet, a triplet and a quartet with an integration ratio of 3:3:2 respectively.

Compound T, also an isomer of $C_4H_8Cl_2$, produces a proton n.m.r. spectrum which consists only of two singlets with an integration ratio of 3:1 Draw the structures of S and of T.

(4)

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