WORKBOOK

J. D. Coyle, E. J. Haws, K. Miller
and K. Norton

Consultants: M. E. A. Cudby and H. A. Willis

INTERPRETATION OF NMR SPECTRA

An Introductory Audiovisual Programme

A Wiley Heyden Publication
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SECTION A

Proton Spectra: The Chemical Shift

LEARNING OBJECTIVES

On completing this section you should be able to:

1. List the desirable properties of an internal reference compound.
2. Define chemical shift in terms of the delta (δ) scale, and list chemical shift values of signals in ppm.
3. Explain the following terms: upfield, downfield, offset, integration trace, shielding, deshielding.
4. Identify the protons in a simple structure which are deshielded, and estimate a chemical shift range where their pmr signals may occur.
5. Use an integration trace to estimate the numbers of protons giving rise to given pmr signals.
6. State the approximate chemical shift ranges for alkane, alkene and alkyne proton signals.
7. List the problems associated with the identification of OH and NH signals.
8. Explain how OH signals can be identified using D_2O.
9. Use a correlation table to predict the chemical shift values of protons in a particular environment, and hence interpret simple nmr spectra which do not exhibit spin-spin splitting.

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The chemical shift of the protons of acetone on the δ scale is:

1 On a 60 MHz instrument

$$\frac{10^6 \times (\qquad)}{(\qquad)} = \qquad \text{ppm}$$

2 On a 100 MHz instrument

$$\frac{10^6 \times (\qquad)}{(\qquad)} = \qquad \text{ppm}$$

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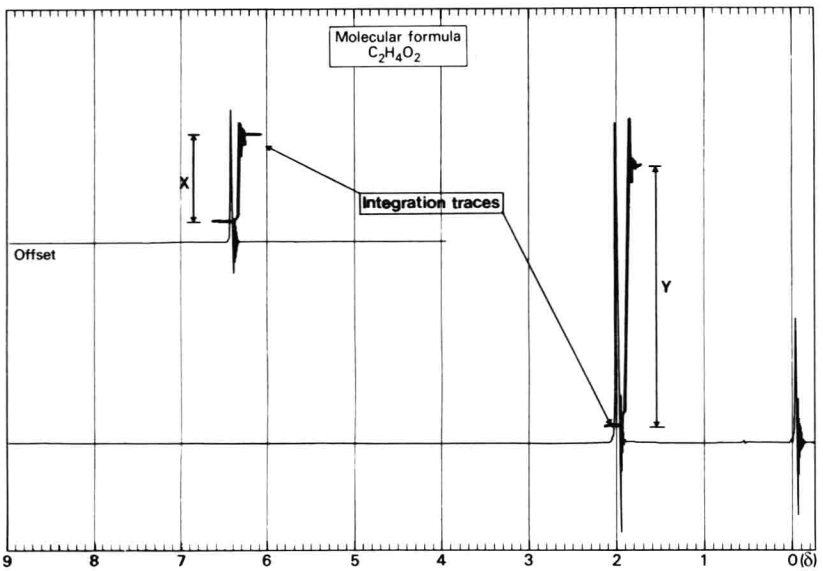

Height of X =

Height of Y =

Ratio of chemically different protons (Y : X) is .....

Possible structures of $C_2H_4O_2$ are

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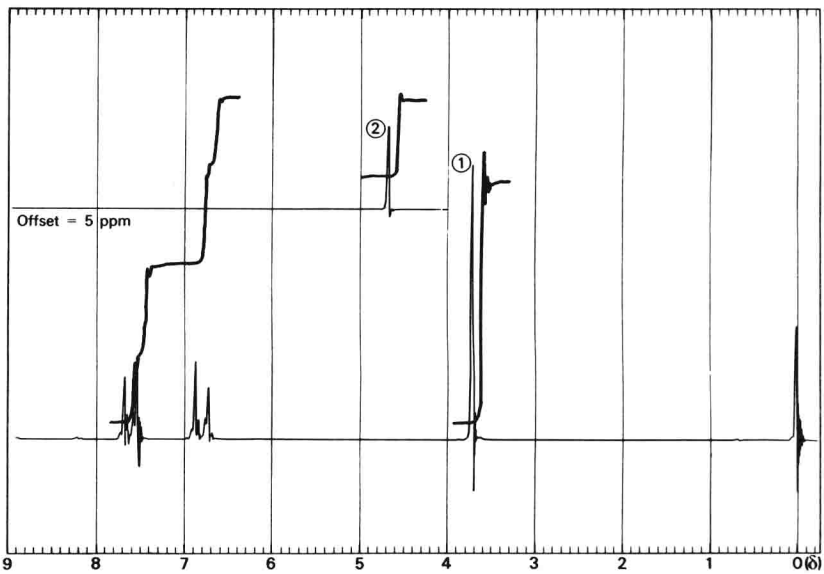

The chemical shift value of

1 The TMS signal is ..... ppm

2 Signal 1 is ..... ppm

3 Signal 2 is ..... ppm

If the integration step for signal number 2 corresponds to 1 proton, then the number of protons giving rise to signal number 1 is .....

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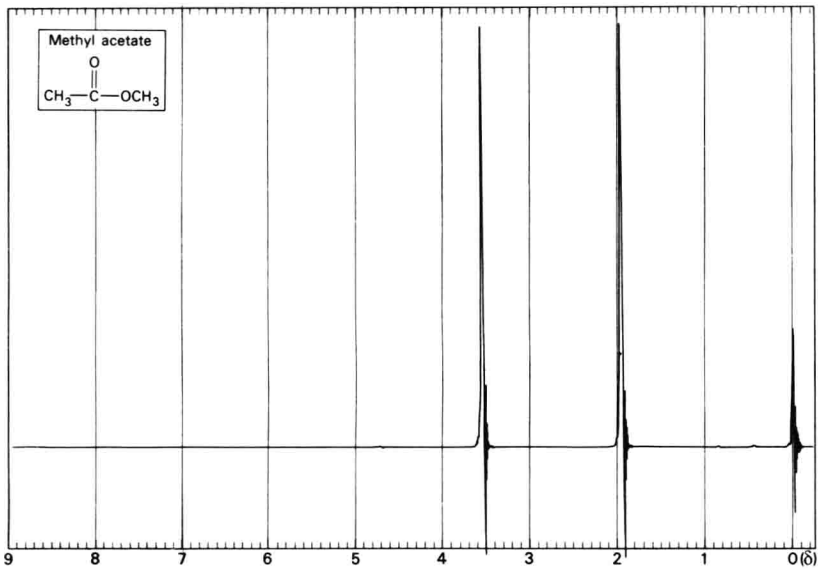

The signal arising from the protons of the methyl group attached to carbon has δ = ... ppm

The signal arising from the protons of the methyl group attached to oxygen has δ = ... ppm

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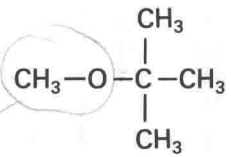
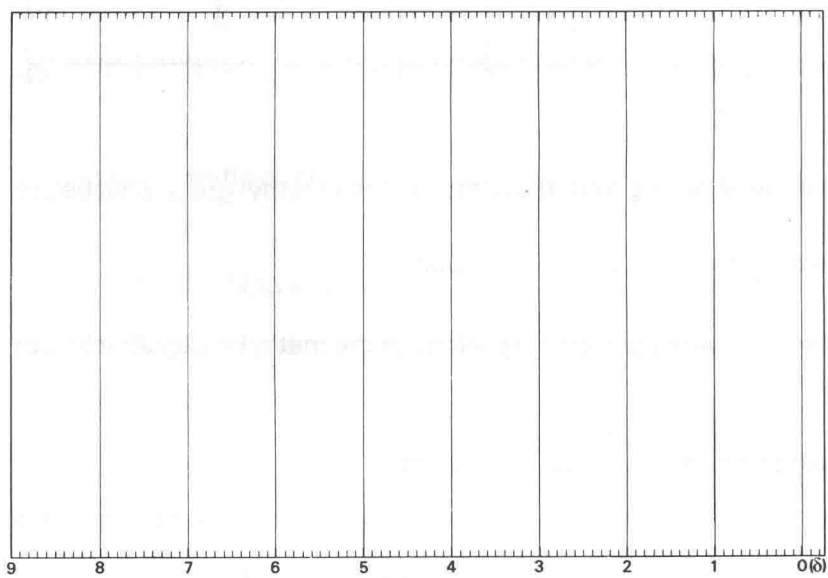


2-methoxy-2-methylpropane

The least shielded protons belong to the group .....



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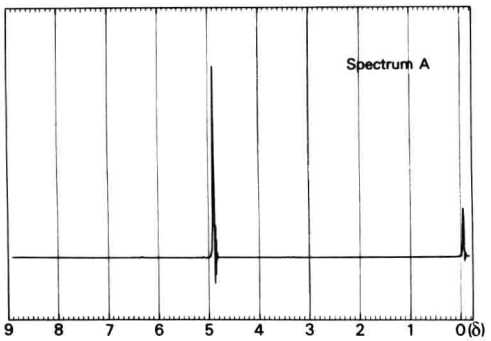

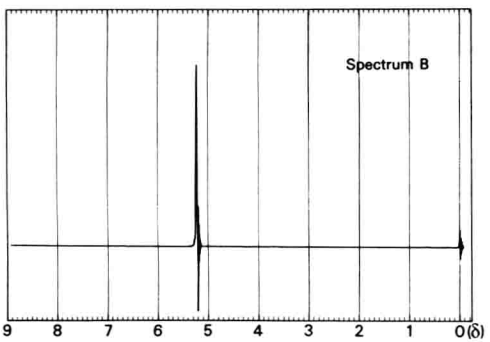

Spectrum ..... is that of dibromomethane

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	Chemical shift values (ppm)		
	CH_3Cl	CH_2Cl_2	$CHCl_3$
(a)	5.30	3.05	7.27
(b)	3.05	5.30	7.27
(c)	7.27	5.30	3.05

Series ..... gives the correct δ values for the series chloromethane, dichloromethane, and trichloromethane.

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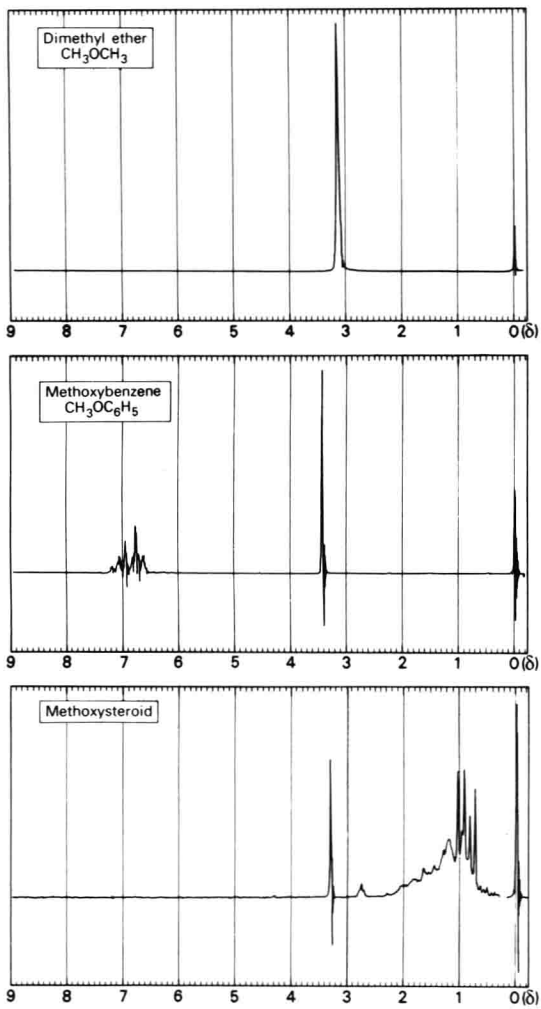

The methoxy signal for dimethyl ether has δ = ... ppm

The methoxy signal for methoxybenzene has δ = ... ppm

The methoxy signal for the methoxysteroid has δ = ... ppm

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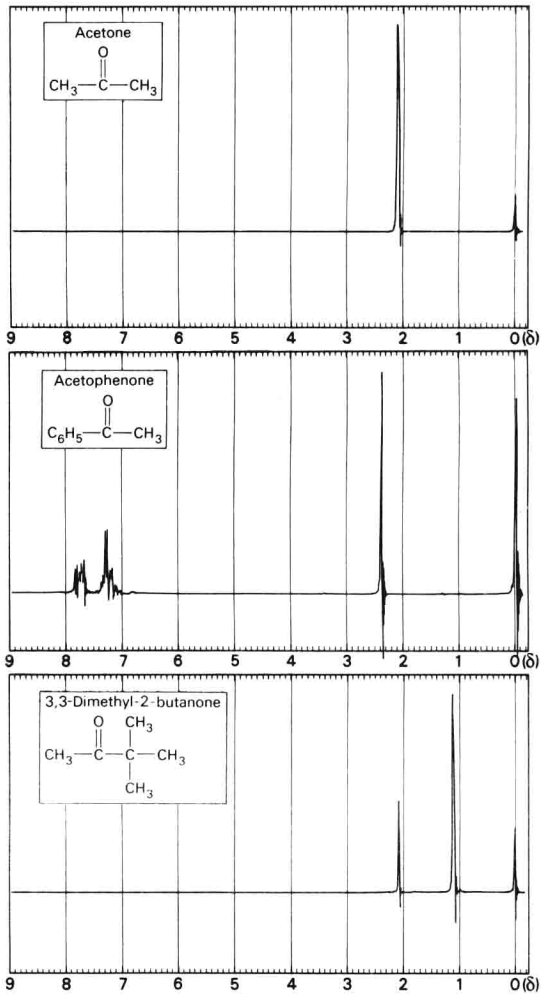

The protons in the methyl group next to the carbonyl group give signals at

for acetone, $\delta =$ ..... ppm

for acetophenone, $\delta =$ ..... ppm

for 3,3-dimethyl-2-butanone, $\delta =$ ..... ppm

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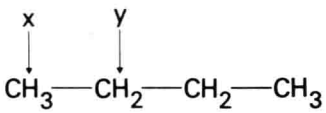
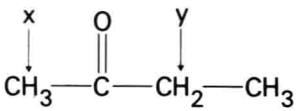


Alkane

δ_x = _____ to _____ ppm

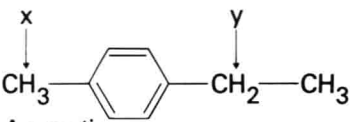
δ_y = _____ to _____ ppm



Ketone

δ_x = _____ to _____ ppm

δ_y = _____ to _____ ppm



Aromatic

δ_x = _____ to _____ ppm

δ_y = _____ to _____ ppm

Using a correlation table, write down the appropriate chemical shift ranges for the protons labelled X and Y.

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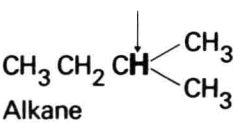
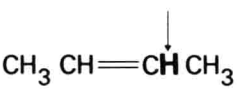


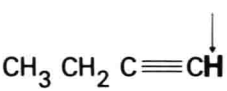
Alkane

δ = ____ to ____ ppm



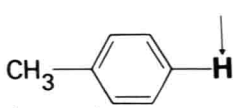
Alkene

δ = ____ to ____ ppm



Alkyne

δ = ____ to ____ ppm



Aromatic

δ = ____ to ____ ppm

Using a correlation table, write down the appropriate chemical shift ranges for the protons indicated by an arrow.

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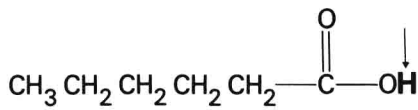
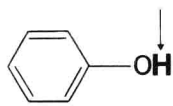
Alcohol

$\delta =$ ____ to ____ ppm



Carboxylic acid

$\delta =$ ____ to ____ ppm



Phenol

$\delta =$ ____ to ____ ppm

Using a correlation table, write down the chemical shift ranges for the protons indicated by an arrow in the alcohol, carboxylic acid and phenol.

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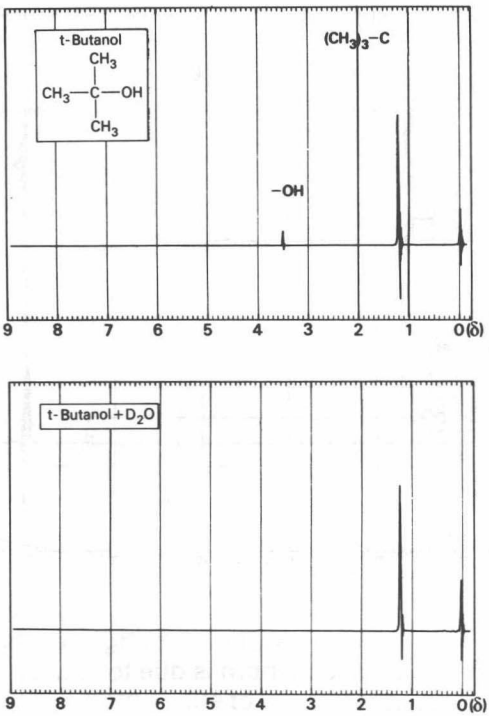

The spectrum of t-butanol with D_2O differs from that of t-butanol alone as follows:

.....

.....

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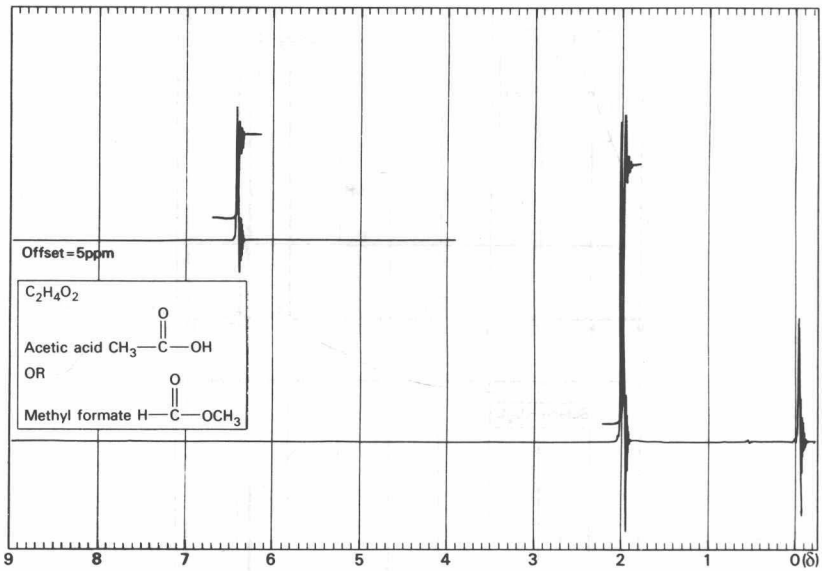

The signal at δ = ... ppm is due to .....

The signal at δ = ... ppm is due to .....

The compound which gives rise to this spectrum is therefore: