

NMR Spectroscopy

Answer key with worked solutions

A. Environments

1. Four kinds of information.

(1) **Number of signals:** number of H environments. (2) **Chemical shift δ :** the type of environment. (3) **Integration:** relative number of H in each environment. (4) **Splitting:** number of H on neighbouring carbons.

2. Signals.

(a) **1** (all 6 H equivalent) (b) **2**, ratio **6 : 2** (= 3 : 1) (c) **2**, ratio **9 : 1** (d) **1** (all 6 H equivalent)
(e) **3:** CH₃ of ethyl, CH₂, and O-CH₃, ratio **3 : 2 : 3**

B. Chemical shift

3. Shift calculations.

$$(a) \delta = \frac{2220 \text{ Hz}}{600 \text{ MHz}} = \mathbf{3.70 \text{ ppm}}$$

$$(b) 1.20 \text{ ppm} \times 300 \text{ MHz} = \mathbf{360 \text{ Hz}} \text{ from TMS}$$

C. Splitting and predicting spectra

4. Splitting.

(a) CH₂ (next to 3 H): **quartet**, about 3.6 ppm; CH₃ (next to 2 H): **triplet**, about 1.5 ppm.
(b) CH (next to 6 equivalent H): **septet** (7 peaks); each CH₃ (next to 1 H): **doublet**, area 6.

5. Propanoic acid.

Group	δ (ppm)	Area	Splitting
CH ₃	about 1.2	3	triplet
CH ₂ (next to C=O)	about 2.4	2	quartet
COOH	about 11–12	1	singlet

6. ^{13}C signals.

(a) 2 (the two CH_3 are equivalent; plus $\text{C}=\text{O}$) (b) 4 (CH_3 next to $\text{C}=\text{O}$, $\text{C}=\text{O}$, $\text{O}-\text{CH}_2$, CH_2-CH_3) (c) 1 (all six carbons equivalent)

D. Solving structures

7. $\text{C}_3\text{H}_8\text{O}$.

Propan-2-ol, $(\text{CH}_3)_2\text{CHOH}$. Doublet (6H) at 1.2 ppm: two equivalent CH_3 groups next to one H. Septet (1H) at 4.0 ppm: the CH on the carbon bonded to O, next to 6 H. Singlet (1H) at 2.2 ppm: the OH.

E. Challenge

8. $\text{C}_4\text{H}_8\text{O}$.

Butanone, $\text{CH}_3\text{COCH}_2\text{CH}_3$. IR 1715 cm^{-1} : $\text{C}=\text{O}$ (no O-H). MS m/z 72: molar mass of $\text{C}_4\text{H}_8\text{O}$. NMR: singlet (3H) at 2.1 ppm: CH_3 next to $\text{C}=\text{O}$ with no neighbouring H; quartet (2H) at 2.4 ppm: CH_2 next to $\text{C}=\text{O}$ and next to a CH_3 ; triplet (3H) at 1.1 ppm: the CH_3 of the ethyl group, next to CH_2 .