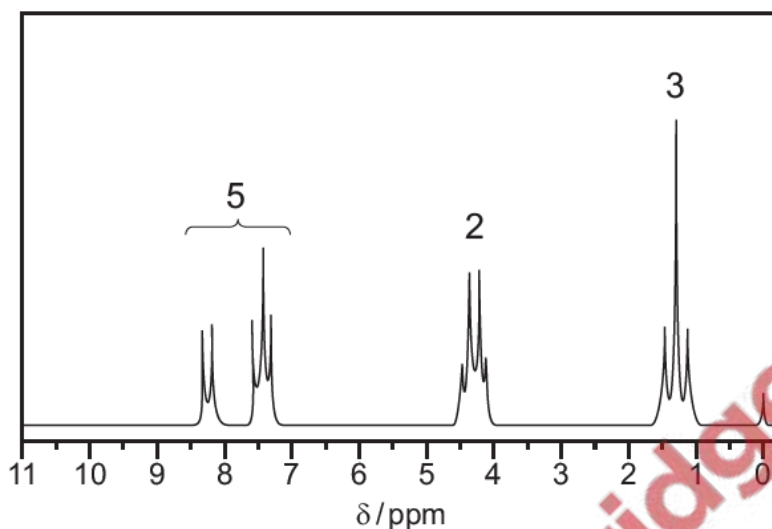


1. Nov/2020/Paper_41/No.9

The proton NMR spectrum of compound **E** in the solvent CDCl_3 is shown. The molecular formula of compound **E** is $\text{C}_9\text{H}_{10}\text{O}_2$.



(a) Explain why CDCl_3 is used as a solvent instead of CHCl_3 .
..... [1]

(b) Explain why TMS is added to give the small peak at chemical shift $\delta = 0$.
..... [1]

(c) Compound **E** is hydrolysed by hot $\text{NaOH}(\text{aq})$, giving two organic products only. One of these products is ethanol.
Name the functional group in compound **E** that is hydrolysed by hot $\text{NaOH}(\text{aq})$.
..... [1]

(d) (i) Describe and explain the splitting patterns of the peaks at $\delta = 1.4$ and $\delta = 4.3$.
splitting pattern at $\delta = 1.4$
reason for splitting pattern at $\delta = 1.4$
splitting pattern at $\delta = 4.3$
reason for splitting pattern at $\delta = 4.3$ [2]

- (ii) Each molecule of compound **E** contains five protons which give rise to the peaks between $\delta = 7.0$ and $\delta = 8.5$.

Identify the functional group in compound **E** which contains these protons.

..... [1]

- (iii) Give the structural formula of compound **E**.

[1]

- (e) The mass spectrum of compound **E** includes fragment ions with m/e values of 29 and 77.

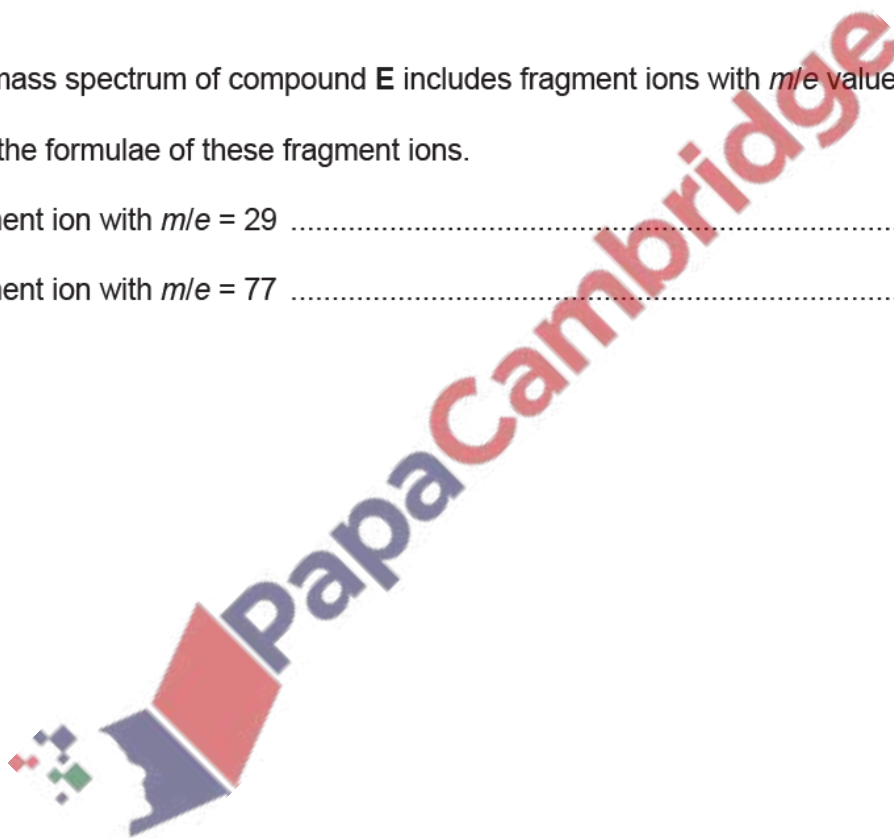
Give the formulae of these fragment ions.

fragment ion with $m/e = 29$

fragment ion with $m/e = 77$

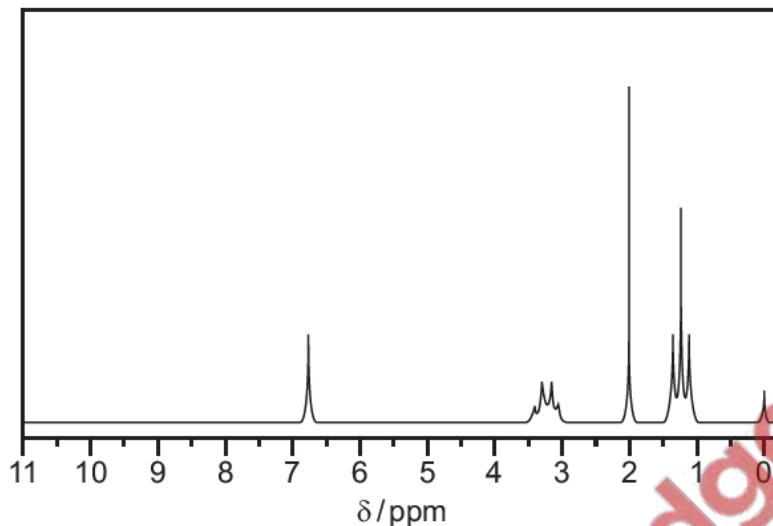
[2]

[Total: 9]



(d) Compound **A** can also be used to make the amide $\text{CH}_3\text{CONHC}_2\text{H}_5$.

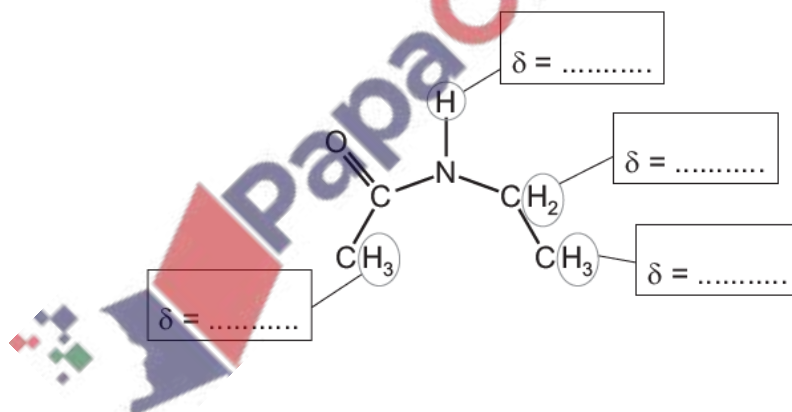
The proton NMR spectrum of the amide $\text{CH}_3\text{CONHC}_2\text{H}_5$ in the solvent CDCl_3 is shown.



(i) Explain why CDCl_3 is used as a solvent instead of CHCl_3 .

[1]

(ii) Complete the diagram with the chemical shifts, δ , of the protons labelled in the $\text{CH}_3\text{CONHC}_2\text{H}_5$ molecule.



[2]

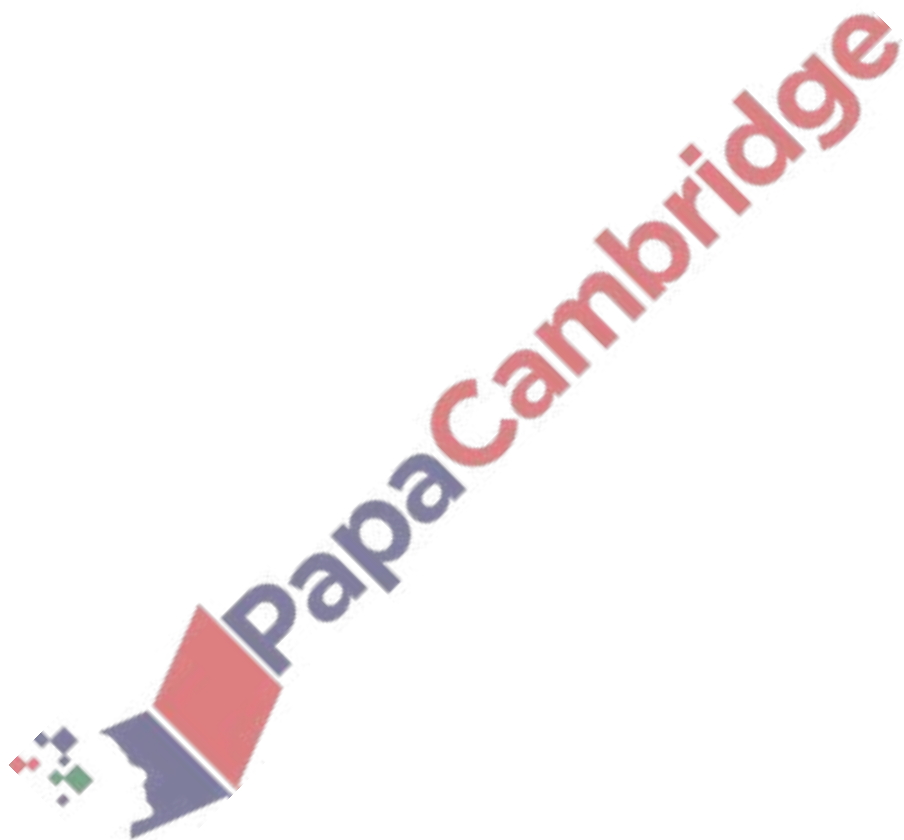
(iii) State and explain how the proton NMR spectrum of the amide $\text{CH}_3\text{CONHC}_2\text{H}_5$ differs when dissolved in D_2O rather than CDCl_3 .

[2]

(e) The mass spectrum of the amide $\text{CH}_3\text{CONHC}_2\text{H}_5$ includes a fragment ion with m/e value of 58.

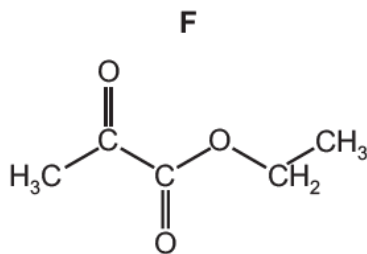
Give the molecular formula of this fragment ion.

fragment ion with m/e value of 58 is [1]

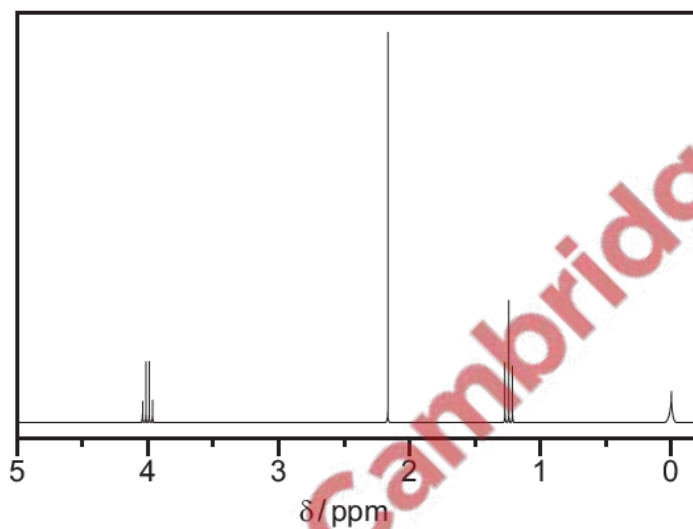


3. June/2020/Paper_41/No.6e,6f

(e) An ester of pyruvic acid, **F**, is dissolved in CDCl_3 and analysed by proton NMR spectroscopy.



The proton NMR spectrum of **F** is shown.

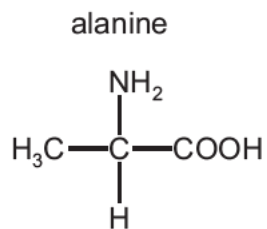


Use the proton NMR spectrum of **F** to complete the table.

chemical shift (δ)	group responsible for the peak	splitting pattern	number of ^1H atoms responsible for the peak
1.3			
2.2			
4.0			

[3]

- (f) Deuterium oxide, D_2O , where D is 2H , can be used as a solvent in proton NMR spectroscopy. The proton NMR spectrum of alanine in $CDCl_3$ has 4 peaks. The proton NMR spectrum of alanine in D_2O has 2 peaks.



On the diagram of alanine, circle the protons that show peaks in **both** NMR spectra. Explain your answer.

.....

.....

..... [2]

