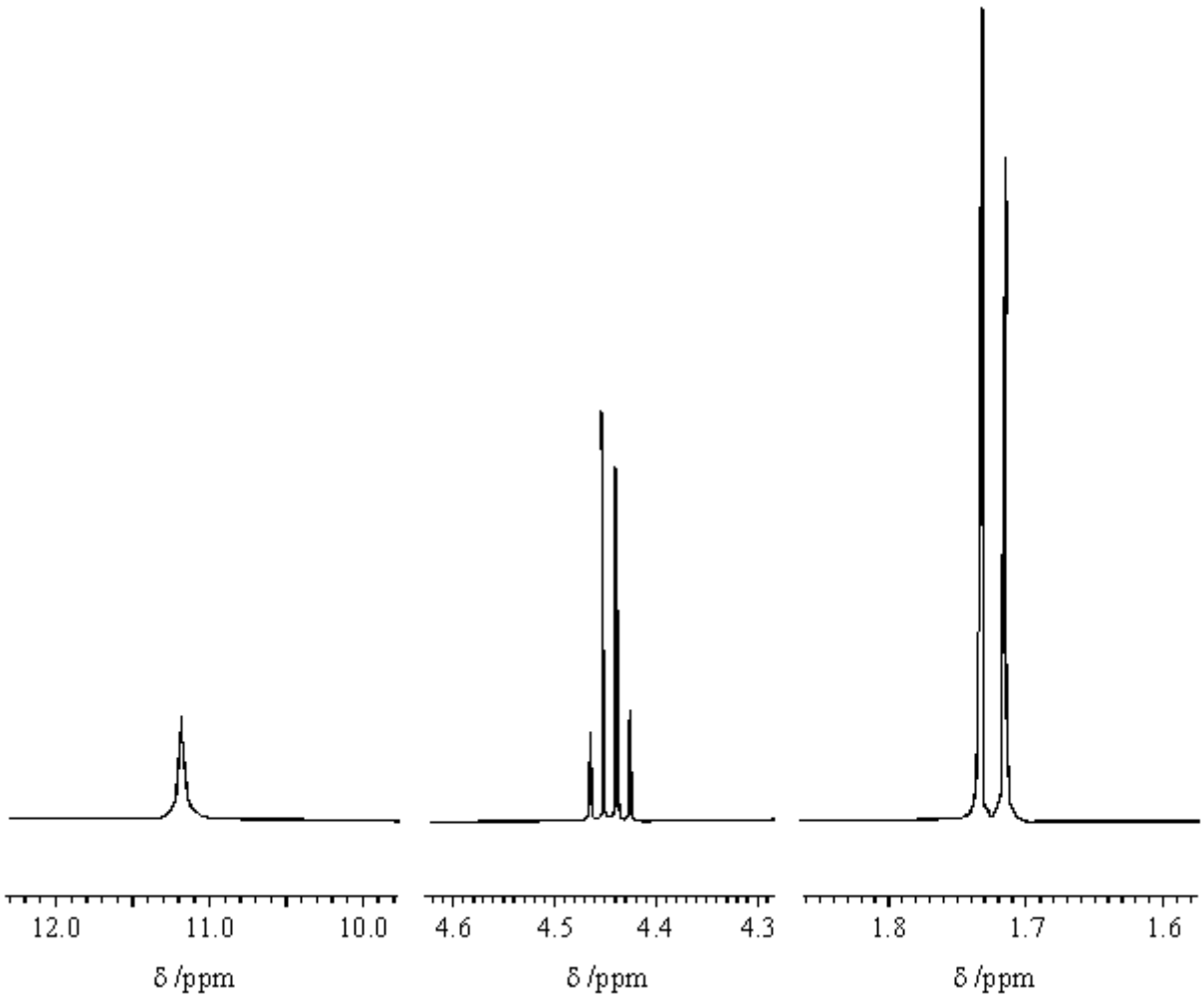
Q1. Three sections of the proton n.m.r. spectrum of $CH_3CHClCOOH$ are shown below.



(a) Name the compound $CH_3CHClCOOH$

.....

(1)

(b) Explain the splitting patterns in the peaks at δ 1.72 and δ 4.44

.....

.....

.....

(2)

(c) Predict the splitting pattern that would be seen in the proton n.m.r. spectrum of the isomeric compound $ClCH_2CH_2COOH$

.....

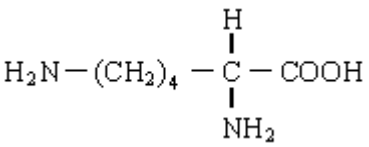
.....

(1)

(d) The amino acid *alanine* is formed by the reaction of $CH_3CHClCOOH$ with an excess of ammonia. The mechanism is nucleophilic substitution. Outline this mechanism, showing clearly the structure of *alanine*.

(5)

(e) The amino acid *lysine* has the structure



Draw structures to show the product formed in each case when lysine reacts with

(i) an excess of aqueous HCl,

(ii) an excess of aqueous NaOH,

(iii) another molecule of lysine.

(3)
(Total 12 marks)

Q2. Use the data given on the back of the Periodic Table (PT) to help you answer this question.
Compounds **A** to **G** are all isomers with the molecular formula $C_6H_{12}O_2$

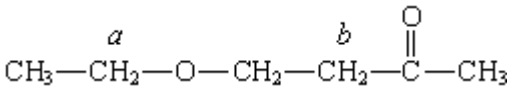
(a) Isomer **A**, $C_6H_{12}O_2$, is a neutral compound and is formed by the reaction between compounds **X** and **Y** in the presence of a small amount of concentrated sulphuric acid.
X and **Y** can both be formed from propanal by different redox reactions.
X has an absorption in its infra-red spectrum at 1750 cm^{-1}.
Deduce the structural formulae of **A**, **X** and **Y**. Give suitable reagents, in each case, for the formation of **X** and **Y** from propanal and state the role of concentrated sulphuric acid in the formation of **A**.

(7)

(b) Isomers **B**, **C**, **D** and **E** all react with aqueous sodium carbonate to produce carbon dioxide.
Deduce the structural formulae of the three isomers that contain an asymmetric carbon atom.
The fourth isomer has only three singlet peaks in its proton n.m.r. spectrum. Deduce the structural formula of this isomer and label it **E**.

(4)

(c) Isomer **F**, $C_6H_{12}O_2$, has the structural formula shown below, on which some of the protons have been labelled.



A proton n.m.r. spectrum is obtained for **F**. Using Table 1 at the back of the Periodic Table (PT), predict a value of δ for the protons labelled *a* and also for those labelled *b*. State and account for the splitting patterns of the peaks assigned to the protons *a* and *b*.

(6)

(d) Isomer **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)
(Total 19 marks)

Q3. Which one of the following has a singlet peak in its proton n.m.r. spectrum?

A ethyl propanoate

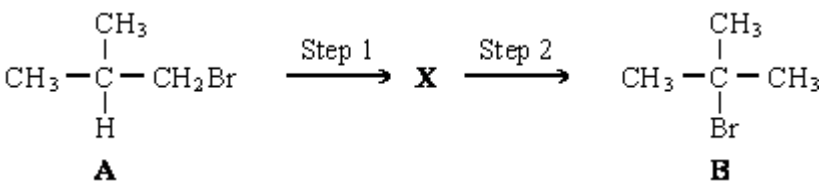
B propyl methanoate

C hexan-3-one

D 2-chlorobutane

(Total 1 mark)

Q4. The conversion of compound **A** into compound **B** can be achieved in two steps as shown below.



A **B**

The intermediate compound, **X,** has an absorption at 1650 cm^{-1} in its infra-red spectrum.

(a) Identify compound **X**. Explain your answer.

(2)

(b) For each step in this conversion, give the reagents and essential conditions required and outline a mechanism.

(11)

(c) Show how the number of peaks in their proton n.m.r. spectra would enable you to distinguish between compounds **A** and **B**.

(2)

(Total 15 marks)