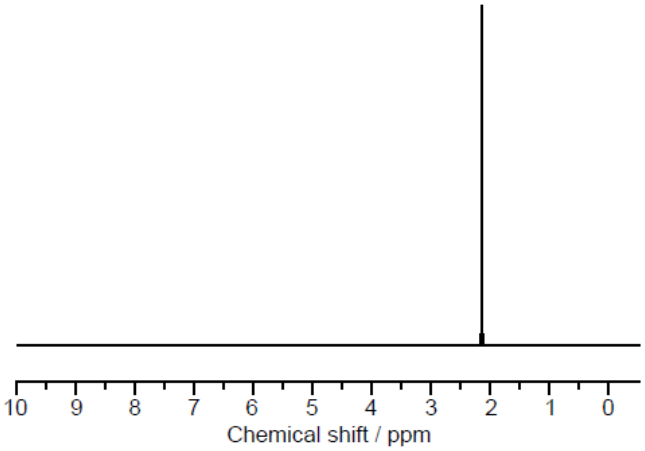
Practice Topic 11 questions *[55 marks]*

1. What can be deduced from the following ^{1}H NMR spectrum? *[1 mark]*



A. There is only one hydrogen atom in the molecule.

B. There is only one hydrogen environment in the molecule.

C. The molecule is a hydrocarbon.

D. There is only one isotope in the element.

2. What information is provided by ^{1}H NMR, MS and IR for an organic compound? *[1 mark]*

I. ^{1}H NMR: chemical environment(s) of protons
II. MS: fragmentation pattern
III. IR: types of functional group

A. I and II only

B. I and III only

C. II and III only

D. I, II and III

3. What can be determined about a molecule from the number of signals in its ^{1}H NMR spectrum? *[1 mark]*

A. Bonds present

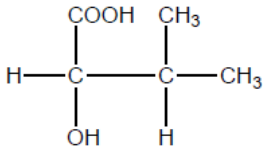
B. Molecular formula

C. Molecular mass

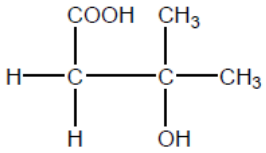
D. Number of hydrogen environments

The reactivity of organic compounds depends on the nature and positions of their functional groups.

The structural formulas of two organic compounds are shown below.



A



B

4a. Deduce the type of chemical reaction and the reagents used to distinguish between these compounds. *[1 mark]*

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4b. State the observation expected for each reaction giving your reasons. *[2 marks]*

Compound **A**:

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Compound **B**:

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4c. Deduce the number of signals and the ratio of areas under the signals in the ^{1}H NMR spectra of the two compounds. *[4 marks]*

Compound	Number of signals	Ratio of areas
A	. . . . .	. . . . .
B	. . . . .	. . . . .

4d. Explain, with the help of equations, the mechanism of the free-radical substitution reaction of ethane with bromine in presence of sunlight. *[4 marks]*

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This question is about carbon and chlorine compounds.

5a. Ethane, C_2H_6, reacts with chlorine in sunlight. State the type of this reaction and the name of the mechanism by which it occurs. *[1 mark]*

Type of reaction:

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Mechanism:

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5b. Formulate equations for the two propagation steps and one termination step in the formation of chloroethane from ethane. *[3 marks]*

Two propagation steps:

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One termination step:

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5c. One possible product, **X**, of the reaction of ethane with chlorine has the following composition by mass: *[2 marks]*

carbon: 24.27%, hydrogen: 4.08%, chlorine: 71.65%

Determine the empirical formula of the product.

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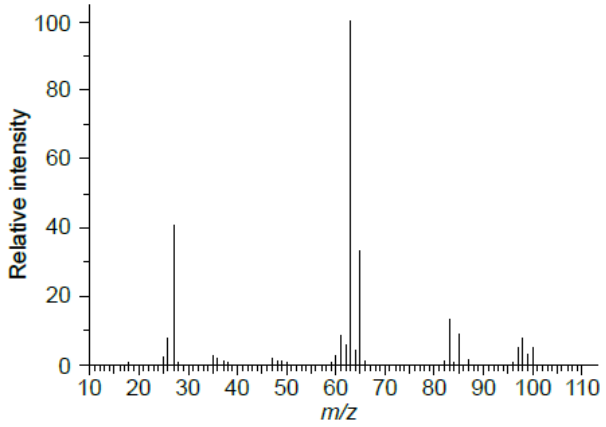
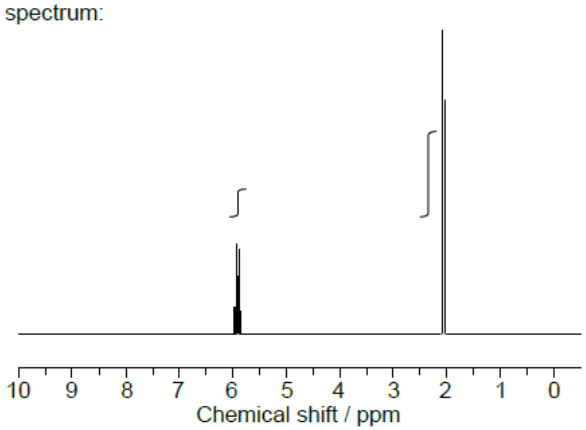
5d. The mass and ^{1}H NMR spectra of product **X** are shown below. Deduce, giving your reasons, its structural formula and hence the name of the compound. *[3 marks]*

Mass spectrum:



^{1}H NMR spectrum:



[Source: http://sdbs.db.aist.go.jp]

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5e. Chloroethene, C_2H_3Cl, can undergo polymerization. Draw a section of the polymer with three repeating units. *[1 mark]*

This question is about carbon and chlorine compounds.

6a. Ethane, C_2H_6, reacts with chlorine in sunlight. State the type of this reaction and the name of the mechanism by which it occurs. *[1 mark]*

Type of reaction:

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Mechanism:

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6b. Formulate equations for the two propagation steps and one termination step in the formation of chloroethane from ethane. *[3 marks]*

Two propagation steps:

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One termination step:

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6c. Deduce the splitting patterns in the ^{1}H NMR spectrum of C_2H_5Cl. *[1 mark]*

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6d. Explain why tetramethylsilane (TMS) is often used as a reference standard in ^{1}H NMR. *[2 marks]*

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6e. One possible product, **X**, of the reaction of ethane with chlorine has the following composition by mass: *[2 marks]*

carbon: 24.27%, hydrogen: 4.08%, chlorine: 71.65%

Determine the empirical formula of the product.

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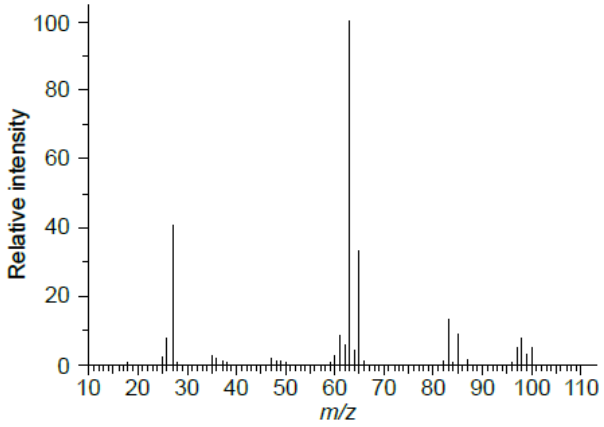
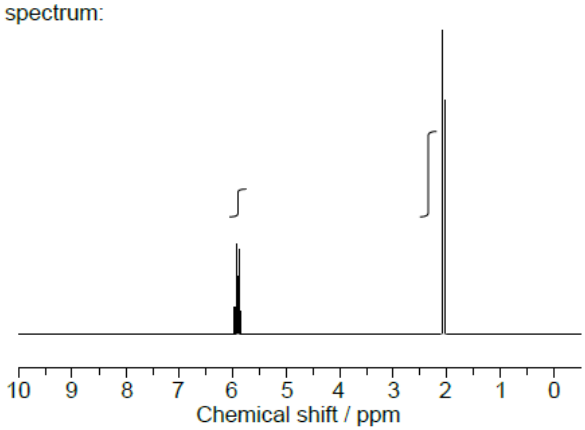
6f. The mass and ^{1}H NMR spectra of product **X** are shown below. Deduce, giving your reasons, its structural formula and hence the name of the compound. *[3 marks]*

Mass spectrum:



^{1}H NMR spectrum:



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6g. When the product **X** is reacted with NaOH in a hot alcoholic solution, C_2H_3Cl is formed. State the role of the reactant NaOH other than as a nucleophile. *[1 mark]*

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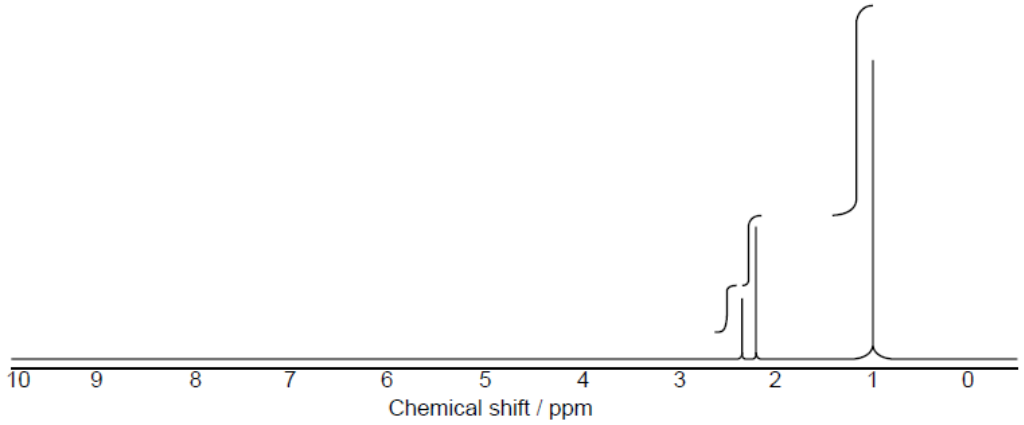
6h. Chloroethene, C_2H_3Cl, can undergo polymerization. Draw a section of the polymer with three repeating units. *[1 mark]*

A compound with a molecular formula $C_7H_{14}O$ produced the following high resolution ^1H NMR spectrum.



7a. Deduce what information can be obtained from the ^1H NMR spectrum. *[3 marks]*

Number of hydrogen environments:

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Ratio of hydrogen environments:

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Splitting patterns:

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7b. Identify the functional group that shows stretching at 1710 cm^{-1} in the infrared spectrum of this compound using section 26 of the data booklet and the ^1H NMR. *[1 mark]*

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7c. Suggest the structural formula of this compound. *[2 marks]*

7d. Bromine was added to hexane, hex-1-ene and benzene. Identify the compound(s) which will react with bromine in a well-lit laboratory. *[1 mark]*

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7e. Deduce the structural formula of the main organic product when hex-1-ene reacts with hydrogen bromide. *[1 mark]*

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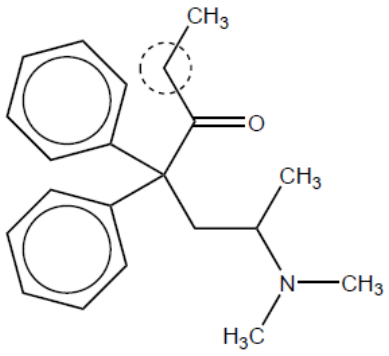
The structures of morphine, diamorphine and codeine are given in section 37 of the data booklet.

Methadone is used to treat heroin addiction. ^{1}H NMR spectroscopy can be used to study its structure.



8a. Predict the number of different hydrogen environments in the molecule ignoring the benzene rings. *[1 mark]*

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8b. Predict the chemical shift and the splitting pattern seen for the hydrogens on the carbon atom circled in the diagram. Use section 27*[2 marks]* of the data booklet.

Chemical shift:

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Splitting pattern:

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