IB 11 HL EQ From 2009 Analytical Chemistry option for the 2016 Topics 11&21 246marks

2016 Syllabus details

Core

Topic 11: Measurement and data processing — 10 hours

Essential idea: Analytical techniques can be used to determine the structure of a compound, analyse the composition of a substance or determine the purity of a compound. Spectroscopic techniques are used in the structural identification of organic and inorganic compounds.

11.3 Spectroscopic identification of organic compounds

Nature of science:

Improvements in instrumentation—mass spectrometry, proton nuclear magnetic resonance and infrared spectroscopy have made identification and structural determination of compounds routine. (1.8)

Models are developed to explain certain phenomena that may not be observable—for example, spectra are based on the bond vibration model. (1.10)

Understandings:

- The degree of unsaturation or index of hydrogen deficiency (IHD) can be used to determine from a molecular formula the number of rings or multiple bonds in a molecule.
- Mass spectrometry (MS), proton nuclear magnetic resonance spectroscopy (^{1}H NMR) and infrared spectroscopy (IR) are techniques that can be used to help identify compounds and to determine their structure.

Applications and skills:

- Determination of the IHD from a molecular formula.
- Deduction of information about the structural features of a compound from percentage composition data, MS, ^{1}H NMR or IR.

Guidance:

- The electromagnetic spectrum (EMS) is given in the data booklet in section 3. The regions employed for each technique should be understood.
- The operating principles are not required for any of these methods.

International-mindedness:

- Monitoring and analysis of toxins and xenobiotics in the environment is a continuous endeavour that involves collaboration between scientists in different countries.

Theory of knowledge:

- Electromagnetic waves can transmit information beyond that of our sense perceptions. What are the limitations of sense perception as a way of knowing?

Utilization:

- IR spectroscopy is used in heat sensors and remote sensing in physics.
- Protons in water molecules within human cells can be detected by magnetic resonance imaging (MRI), giving a three-dimensional view of organs in the human body.

Syllabus and cross-curricular links:
Topic 1.2—determination of the empirical formula from percentage composition data or from other experimental data and determination of the molecular formula from both the empirical formula and experimental data.

11.3 Spectroscopic identification of organic compounds

- The data booklet contains characteristic ranges for IR absorptions (section 26), ^{1}H NMR data (section 27) and specific MS fragments (section 28). For ^{1}H NMR, only the ability to deduce the number of different hydrogen (proton) environments and the relative numbers of hydrogen atoms in each environment is required. Integration traces should be covered but splitting patterns are not required.

Topic 2.1—the nuclear atom
Topic 5.3—bond enthalpies

Aims:

- **Aim 7**: Spectral databases could be used here.
- **Aim 8**: The effects of the various greenhouse gases depend on their abundance and their ability to absorb heat radiation.

Additional higher level

Topic 21: Measurement and analysis — 2 hours

Essential idea: Although spectroscopic characterization techniques form the backbone of structural identification of compounds, typically no one technique results in a full structural identification of a molecule.

21.1 Spectroscopic identification of organic compounds

Nature of science:

Improvements in modern instrumentation—advances in spectroscopic techniques (IR, ^{1}H NMR and MS) have resulted in detailed knowledge of the structure of compounds. (1.8)

Understandings:

- Structural identification of compounds involves several different analytical techniques including IR, ^{1}H NMR and MS.
- In a high resolution ^{1}H NMR spectrum, single peaks present in low resolution can split into further clusters of peaks.
- The structural technique of single crystal X-ray crystallography can be used to identify the bond lengths and bond angles of crystalline compounds.

Applications and skills:

- Explanation of the use of tetramethylsilane (TMS) as the reference standard.
- Deduction of the structure of a compound given information from a range of analytical characterization techniques (X-ray crystallography, IR, ^{1}H NMR and MS).

Guidance:

- Students should be able to interpret the following from ^{1}H NMR spectra: number of peaks, area under each peak, chemical shift and splitting patterns. Treatment of spin-spin coupling constants will not be assessed but students should be familiar with singlets, doublets, triplets and quartets.
- High resolution ^{1}H NMR should be covered.

International-mindedness:

- The chemical community often shares chemical structural information on the international stage. The Cambridge Crystallographic Database, ChemSpider developed by the *Royal Society of Chemistry* and the *Protein Data Bank (RCSB PDB)* (at Brookhaven National Laboratory, USA) are examples which highlight the international nature of the scientific community.

Theory of knowledge:

- The intensity ratio of the lines in the high resolution NMR spectrum is given by the numbers in Pascal's triangle, a mathematical pattern known independently over a thousand years ago by a number of different cultures. Why is mathematics such an effective tool in science? Is mathematics the science of patterns?

Utilization:

- Protons in water molecules within human cells can be detected by magnetic resonance imaging (MRI), giving a three-dimensional view of organs in the human body. Why is MRI replacing computerized tomography (CT) scans for some applications but is used as a complementary technique for others?
- MS (and other techniques such as TLC, GC, GC-MS and HPLC) can be used in forensic investigations at crime scenes.
- Analytical techniques can be used to test for drug abuse by high-performance athletes.

21.1 Spectroscopic identification of organic compounds	
• The precise details of single crystal X-ray crystallography need not be known in detail, but students should be aware of the existence of this structural technique in the wider context of structural identification of both inorganic and organic compounds. • The operating principles are not required for any of these methods.	Syllabus and cross-curricular links: Topic 11.3—spectroscopic identification of compounds Option B.2—chromatography and protein separation Option B.9—chromatography and pigments Option D.7—chiral auxiliaries **Aims:** • **Aim 7**: Spectral databases can be used here.

A note on mass spectrometry from the previous syllabus (Analytical Chemistry option) because the meaning in new syllabus is vague:

A.4.2	Analyse fragmentation patterns in a mass spectrum to find the structure of a compound.	3	Examples of fragments should include: • $(M_r - 15)^+$ loss of CH_3 • $(M_r - 17)^+$ loss of OH • $(M_r - 29)^+$ loss of C_2H_5 or CHO • $(M_r - 31)^+$ loss of CH_3O • $(M_r - 45)^+$ loss of COOH.

Topic:**11:IB P32 An Chem HL 10s**

A1. State two reasons for the use of analytical techniques in today's society. *[2]*

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Topic:**11:IB P31 An Chem HL 10w**

A1. There is a wide range of analytical techniques available to chemists.

(a) State two reasons why the use of analytical chemistry techniques is important in society today. *[1]*

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Topic:**11:IB P31 An Chem HL 09s**

A1. (a) State two reasons for using analytical techniques. *[2]*

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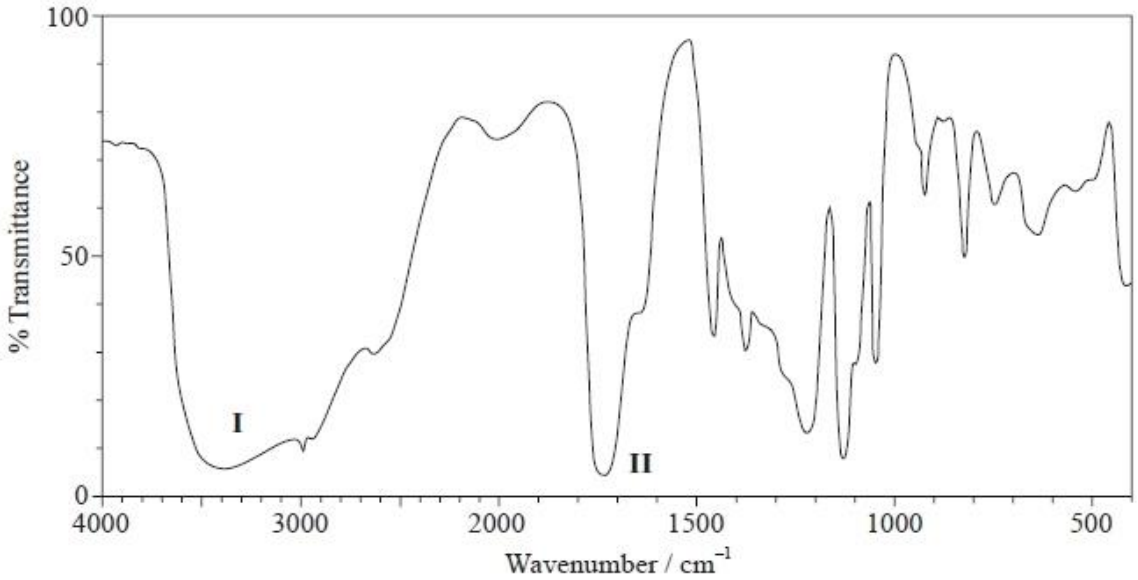
Topic:**11:IB P32 An Chem HL 14s**

3. Compound **X** has the molecular formula $C_3H_6O_3$ and is found in human perspiration.

(a) Its infrared (IR) spectrum is represented below.



[Source: SDBS web: www.sdbs.riodb.aist.go.jp (National Institute of Advanced Industrial Science and Technology, 2013)]

Deduce the bonds responsible for the absorptions labelled **I** and **II**. *[1]*

I:

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II:

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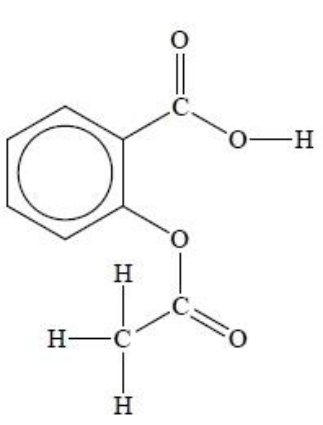
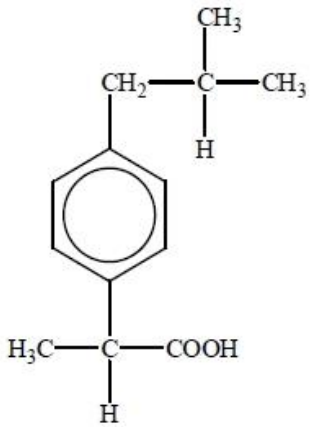
Topic:**11:IB P32 An Chem HL 13s Q A4**

(b) Another painkiller is aspirin. The structures of aspirin and ibuprofen are:



Aspirin



Ibuprofen

(iii) State how the infrared spectra of aspirin and ibuprofen will differ in the region 1700–1750 cm^{-1}. *[2]*

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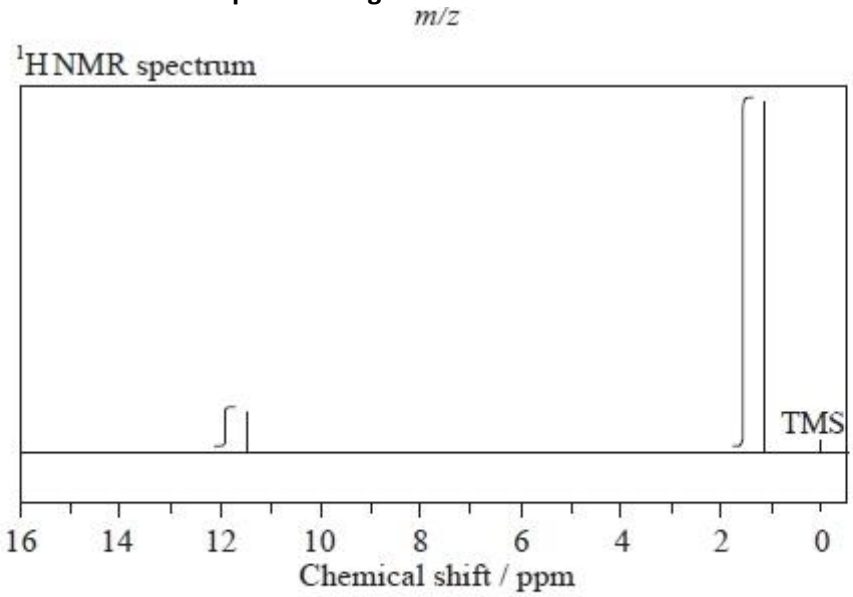
Topic:**11:IB P32 An Chem HL 11s Q A2**

The ^{1}HNMR spectrum of an unknown compound A is given below:



[Source: SDBSWeb:http://riod01.ibase.aist.go.jp/sdbs/(National Institute of Advanced Industrial Science and Technology)]

(This question continues on the following page)

The following information is necessary to answer these questions, X has a molecular mass of 102 and contains a C=O bond and a $(CH_3)_3C$ group

(iii) Identify the peak at 11.5 ppm in the ^{1}HNMR spectrum. *[1]*

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(iv) State what information can be obtained from the integration traces in the ^{1}HNMR spectrum about the hydrogen atoms responsible for the peak at 1.2 ppm. *[1]*

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(v) Deduce the structure of **X**. *[1]*

Topic:**11:IB P32 An Chem HL 11s**

A2. Infrared spectroscopy is commonly used as an analytical technique by inorganic, physical and organic chemists.

(a) Explain why hydrogen bromide is IR active whereas bromine is IR inactive. *[1]*

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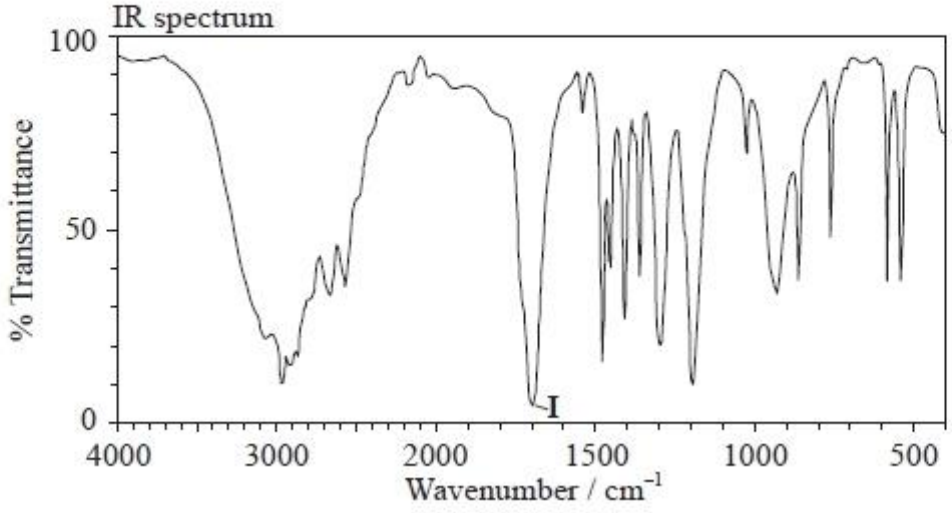
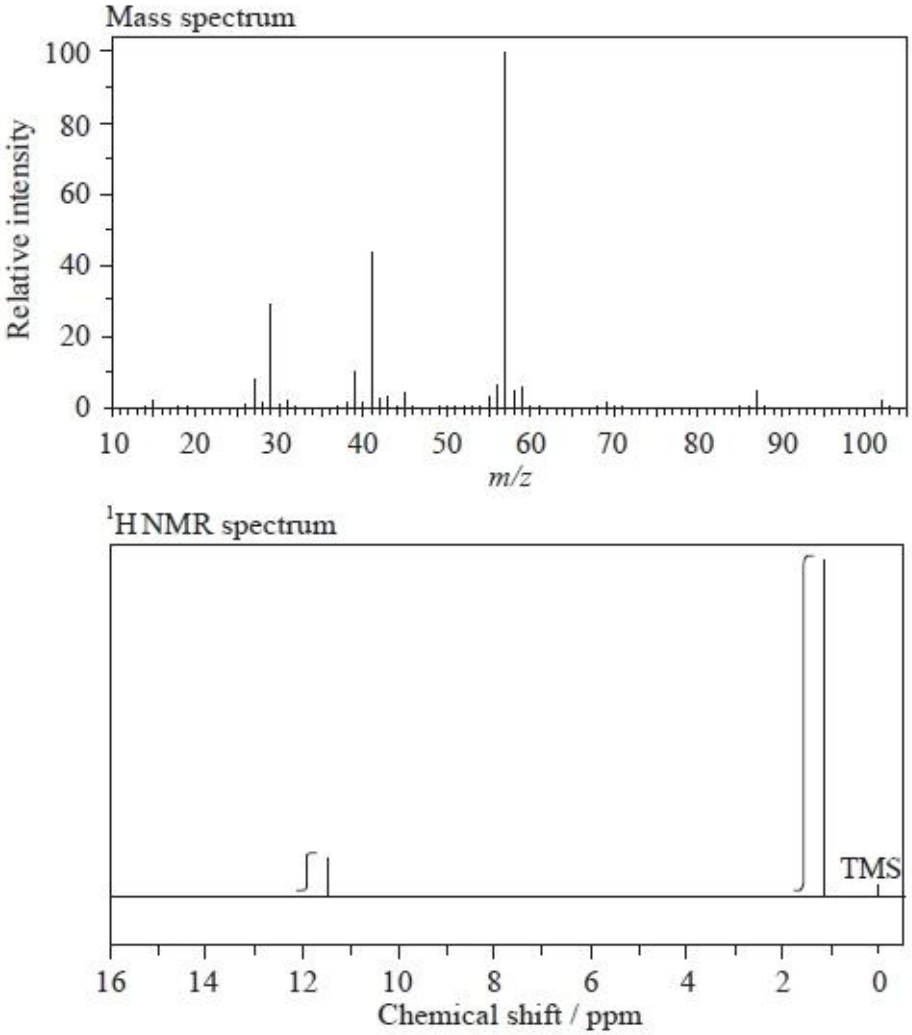
(b) The IR spectrum, mass spectrum and ^{1}HNMR spectrum of an unknown compound, **X**, of molecular formula $C_5H_{10}O_2$, are as follows.





[Source: SDBSWeb:http://riod01.ibase.aist.go.jp/sdbs/(National Institute of Advanced Industrial Science and Technology)]

(This question continues on the following page)

(i) In the IR spectrum, identify the bond responsible for the absorption labelled **I**. *[1]*

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Topic:**11:IB P32 An Chem HL 10s**

A3. (a) Explain why the nitrogen molecule, N_2, does not absorb infrared radiation. *[2]*

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(b) Describe two vibrations in the water molecule that absorb infrared radiation. *[2]*

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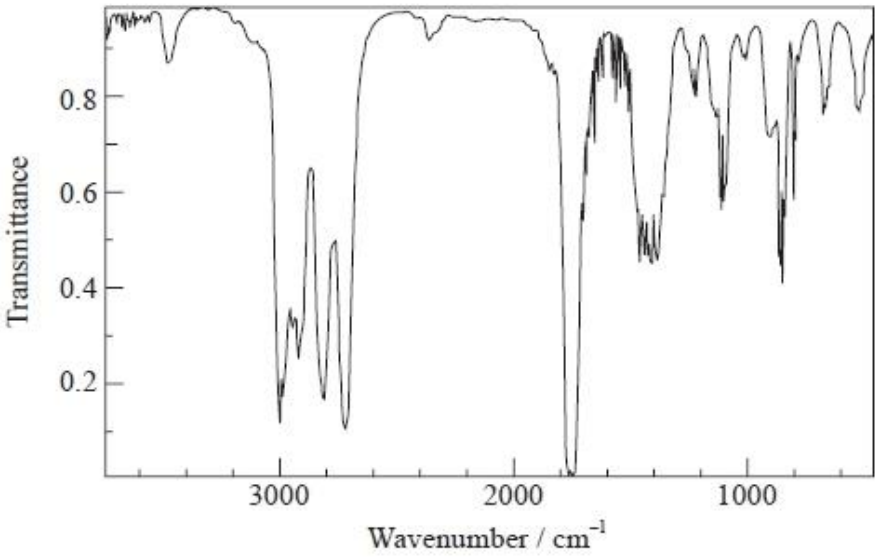
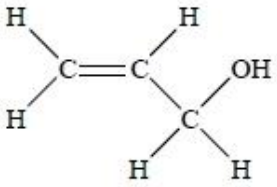
Topic:**11:IB P32 An Chem HL 09s Q A3**

(b) The infrared spectrum of a substance, X, with empirical formula C_3H_6O is given below.



[Source: NIST http://webbook.nist.gov/chemistry]

(i) Explain why the structural formula of X **cannot** be: *[2]*



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Topic:**11:IB P32 An Chem HL 08s**

G1. (a) Identify an analytical technique that is suitable for each of the following.

(ii) Measuring the degree of unsaturation of an oil. *[1]*

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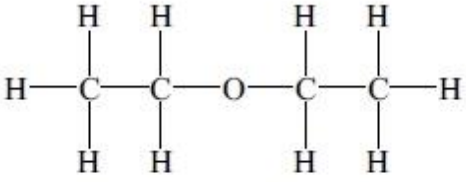
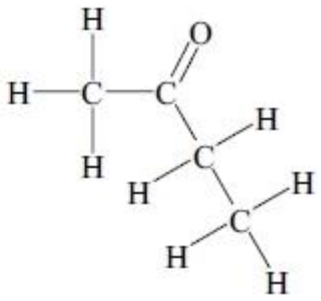
Topic:**11:IB P32 An Chem HL 08s**

G2. A student was asked to predict the ^{1}H NMR spectrum of ethoxyethane, whose structure is shown below.



The structure of butanone is shown below.



(e) Identify and account for two differences in the infrared spectra of ethoxyethane and butanone. *[2]*

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Topic:**11:IB P32 An Chem HL 08s**

G3. (a) Using the water molecule as an example and including diagrams, describe what occurs at a molecular level during the absorption of infrared radiation. *[4]*

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(b) State the mathematical relationship between wavenumber and wavelength. *[1]*

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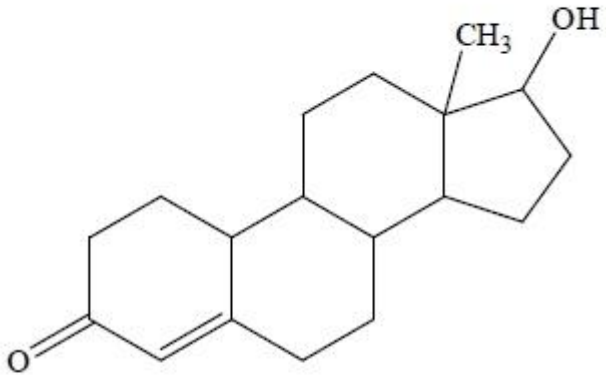
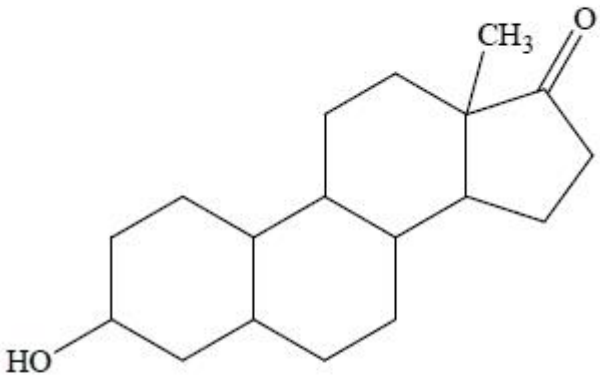
3. Some famous athletes have been banned from competing after failing tests for the drug nandrolone. The molecule changes in the body and is excreted as norandrosterone, which can be detected in urine samples.



Nandrolone



Norandrosterone

(a) The characteristic ranges for infrared absorptions are shown in Table 17 of the Data Booklet. Identify **two** ranges in which the infrared spectra of nandrolone and norandrosterone would be similar and **one** range in which they would differ. *[3]*

Two similarities:

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One difference:

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A1. Compound P contains a carbonyl group (C=O) and has the molecular formula C_3H_6O.

(a) Draw the two possible structures of compound P. *[1]*

(b) Explain why the infrared spectra of the structures in (a) are very similar. *[1]*

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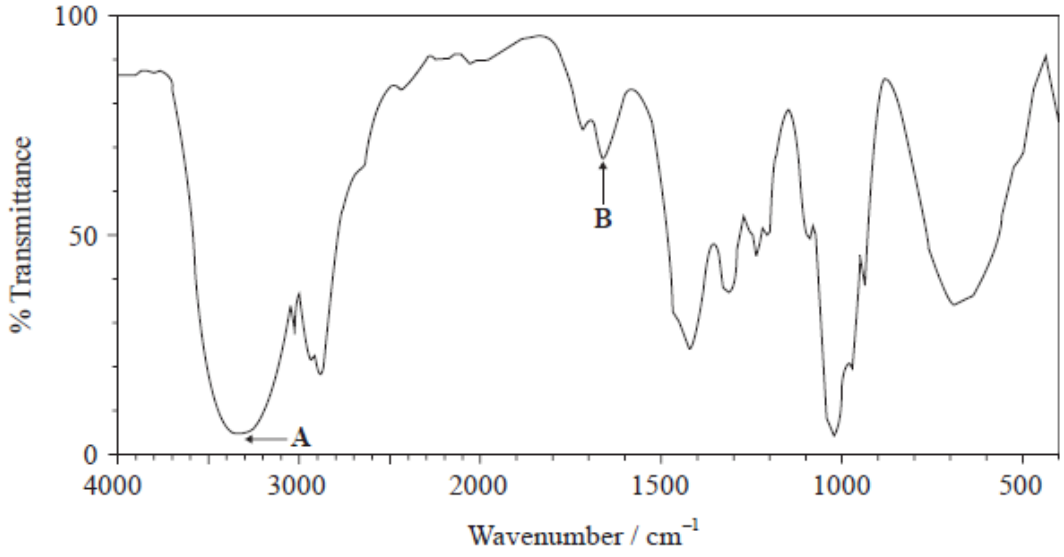
Topic:**11:IB P31 An Chem HL 12s**

A1. Analytical techniques are very useful in determining molecular structures. A compound, **X**, has the empirical formula C_2H_4O.

(b) The molecular formula of **X** is $C_4H_8O_2$. The information in the IR spectrum below can be used to help determine the structure of **X**.



(i) Deduce the information obtained from absorptions **A** and **B**. *[2]*

A: .....

B: .....

(ii) Comment on the absence of any major absorption in the region 1700–1750 cm^{-1}. *[1]*

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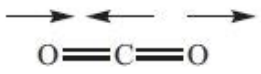
Topic:**11:IB P31 An Chem HL 11w**

A2. (a) One type of molecular vibration that occurs when CO_2 molecules are exposed to IR radiation is illustrated in the diagram below.



asymmetric stretching

Identify **two** other types of molecular vibrations that occur when CO_2 molecules are exposed to IR radiation. Illustrate your answer with appropriate diagrams. *[2]*

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(b) Explain which molecular vibration of CO_2 in (a) above is IR **active** and which is IR **inactive**. *[3]*

Topic:**11:IB P31 An Chem HL 11s Q A2** **NOT WITH Q A2 (a)**

Compound X is CH_3COCH_3.

(c) The infrared and mass spectra for **X** were also recorded.

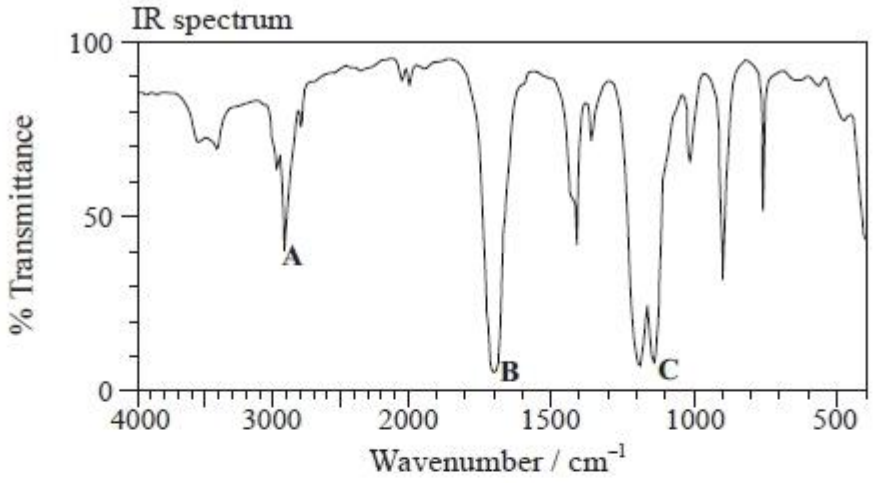
(i) Apart from absorptions due to C–C and C–H bonds, suggest **one** absorption, in wavenumbers, that would be present in the infrared spectrum. *[1]*

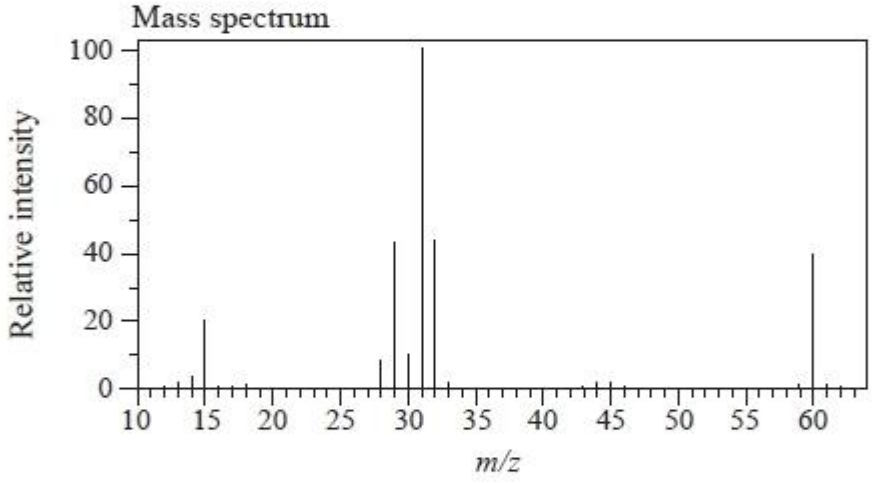
(ii) Apart from absorptions due to C–C and C–H bonds, suggest **one** absorption, in wavenumbers, absent in this infrared spectrum but present in one of the other compounds shown in part (a). *[1]*

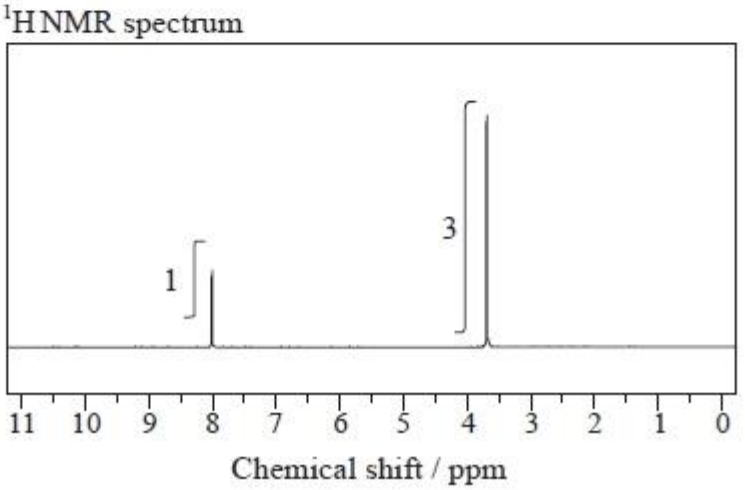
Topic:**11:IB P31 An Chem HL 10w Q A2**

(b) Explain what happens at a molecular level during the absorption of IR radiation by carbon dioxide, CO_2. *[3]*

(c) The IR spectrum, mass spectrum and ^{1}H NMR spectrum of an unknown compound, **Y**, of molecular formula $C_2H_4O_2$ are as follows.







[Source: SDBSWeb: http://riodb01.ibase.aist.go.jp/sdbs/ (National Institute of Advanced Industrial Science and Technology)]

(i) Identify the bonds responsible for the peaks **A**, **B** and **C** in the IR spectrum of **Y**. *[2]*

A: .....

B: .....

C: .....

Topic:**11:IB P31 An Chem HL 10s**

A1. Butan-1-ol, butan-2-ol, 2-methylpropan-1-ol and 2-methylpropan-2-ol are four structural isomers with the molecular formula $C_4H_{10}O$.

(c) Explain why the infrared spectra of all four alcohols are very similar. *[2]*

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Topic:**11:IB P31 An Chem HL 09w Q A1**

(b) Identify which of the following molecules absorbs IR radiation and explain your choice. *[2]*

H_2 O_2 HCl

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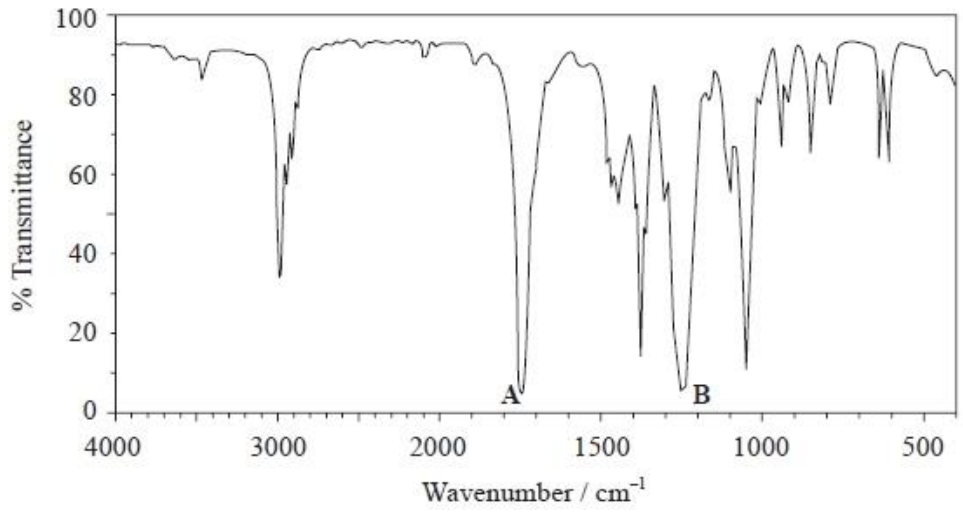
Topic:**11:IB P31 An Chem HL 09w**

A2. (a) The mass spectrum of an unknown compound, **X**, of empirical formula C_2H_4O is shown below.

(b) The IR spectrum of **X** is shown below.



(i) Use Table 17 of the Data Booklet to identify the bonds which correspond to the absorptions **A** and **B**. *[1]*

A: .....

B: .....

(ii) Deduce the name of the functional group present in **X**. *[1]*

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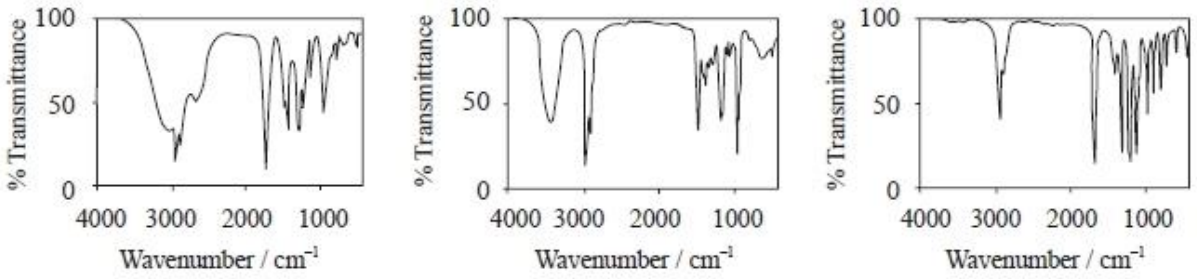
Topic:**11:IB P31 An Chem HL 09s Q A1**

(d) Consider the IR spectra of the following three compounds.

$A = CH_3(CH_2)_3COOH$

$B = CH_3COOC(CH_3)_3$

$C = (CH_3CH_2)_3COH$



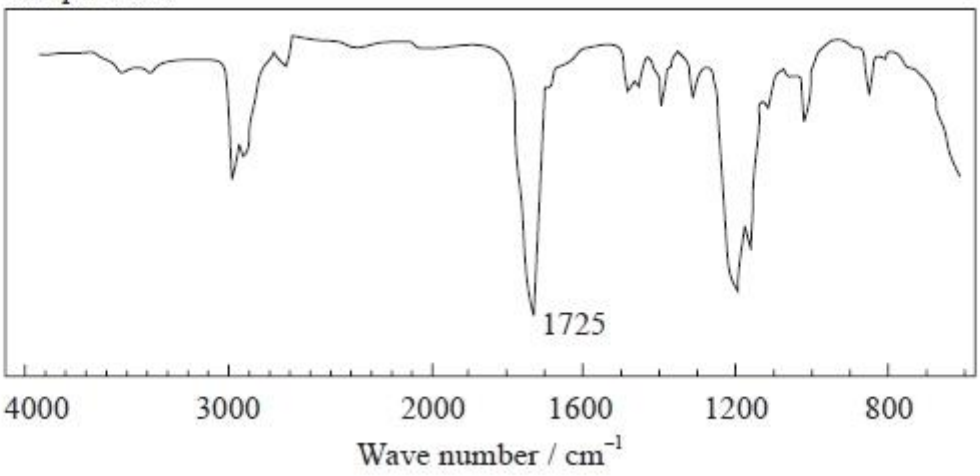
Determine which IR spectrum corresponds to each compound A, B and C. Explain your reasoning. IR data can be found in Table 17 of the Data Booklet. *[5]*

Compound	Spectrum	Reason
A	....	.....
B	....	.....
C	....	.....

G1. Compounds can be identified using information from their mass spectra, infrared spectra and ^1H NMR spectra.

The spectra below are for ethyl methanoate, $HCOOC_2H_5$.

IR spectrum



(b) Chemical bonds vibrate at particular frequencies. Explain why some vibrations of chemical bonds absorb in the infrared region of the spectrum but others do not. *[1]*

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(c) The absorption at 1725 cm^{-1} in the infrared spectrum on the previous page is due to the stretching vibration of the C=O bond in ethyl methanoate. Explain why other compounds containing a C=O bond do not absorb at exactly 1725 cm^{-1} in the infrared region of the spectrum. *[1]*

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(h) Propanoic acid is an isomer of both esters in (g). Describe **two** ways in which its infrared spectrum differs from that of the two esters, other than the exact position of the C=O absorption. *[2]*

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Topic:**11:IB P31 An Chem HL 08s Q G1**

(c) (i) The absorption of infrared radiation causes bonds in a molecule to stretch. Explain why a molecule of hydrogen bromide is IR active but a molecule of oxygen is not. *[2]*

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(ii) Describe a different way, other than stretching, in which a molecule of water can absorb infrared radiation. *[1]*

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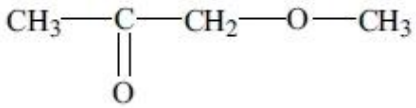
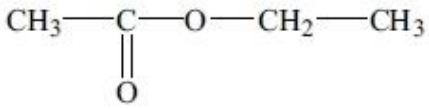
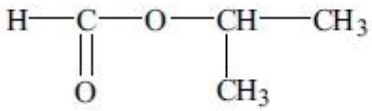
Topic:**11:IB P31 An Chem HL 08s**

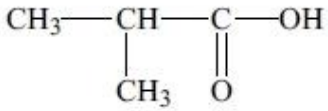
G2. Use information from Table 18 in the Data Booklet to help answer this question.

There are several isomers with the molecular formula $C_4H_8O_2$. The structural formulas of some of them are shown below.

A. 

B. 

C. 

D. 

(a) (i) Identify **two** wavenumber ranges, other than 2840–3095 cm^{-1}, of absorptions that are present in the infrared spectra of all four isomers. *[1]*

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(ii) Identify **one** wavenumber range of an absorption that is present in the infrared spectrum of only one isomer. *[1]*

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(iii) Suggest a structural formula for another isomer of $C_4H_8O_2$ that has an absorption close to 1650 cm^{-1}. *[1]*

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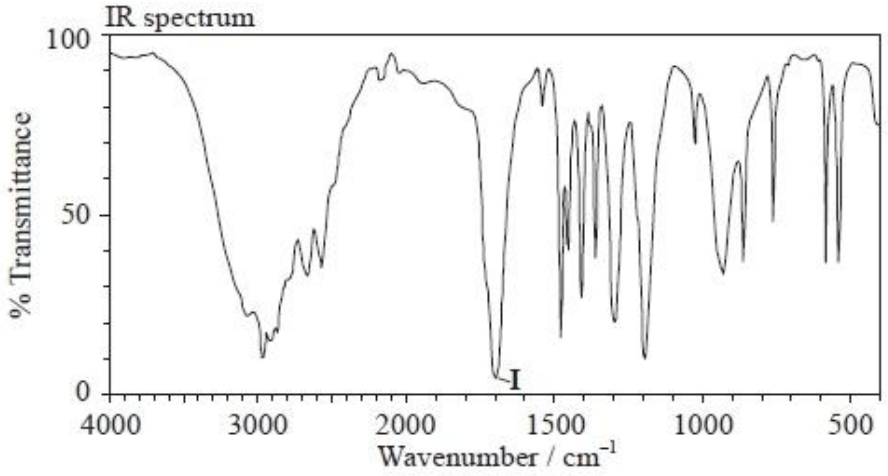
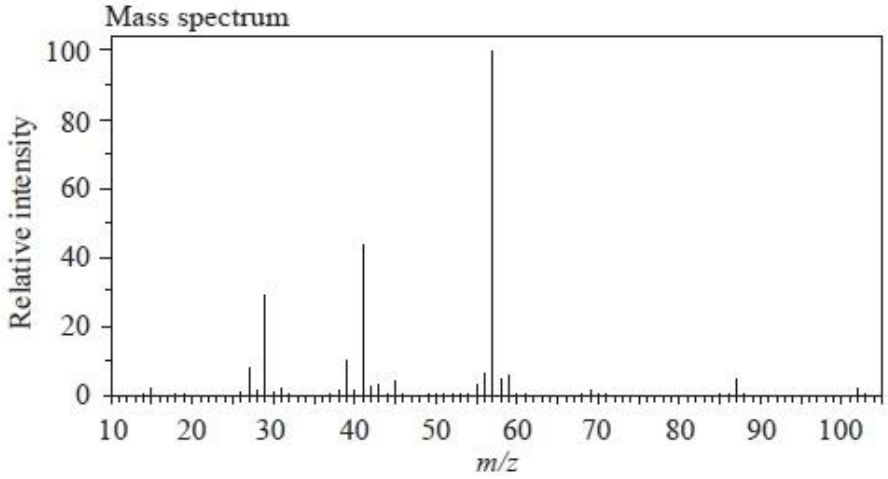
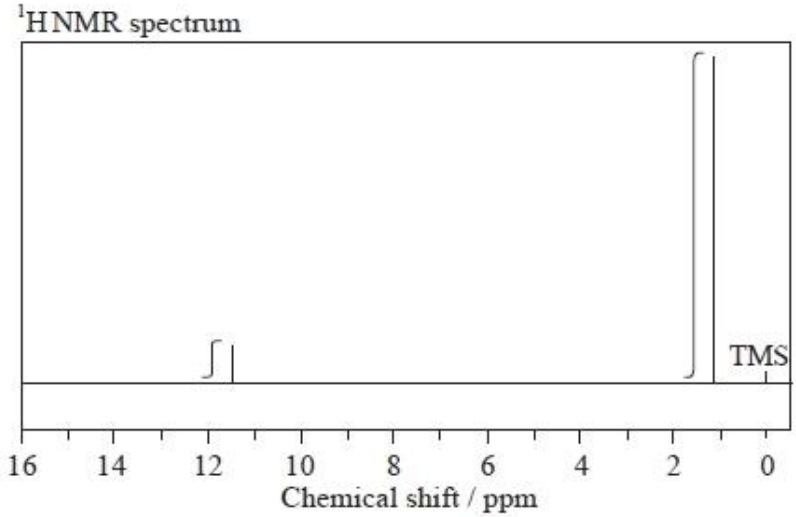
Topic:**11:IB P32 An Chem HL 11s Q A2**

(b) The IR spectrum, mass spectrum and ^1H NMR spectrum of an unknown compound, **X**, of molecular formula $C_5H_{10}O_2$, are as follows.







[Source: SDBSWeb:http://riod01.ibase.aist.go.jp/sdbs/(National Institute of Advanced Industrial Science and Technology)]

(This question continues on the following page)

(ii) In the mass spectrum, deduce which fragments the *m/z* values at 102 and 57 correspond to. *[2]*

m/z = 102: .....

m/z = 57: .....

Topic:**11:IB P31 An Chem HL 12s**

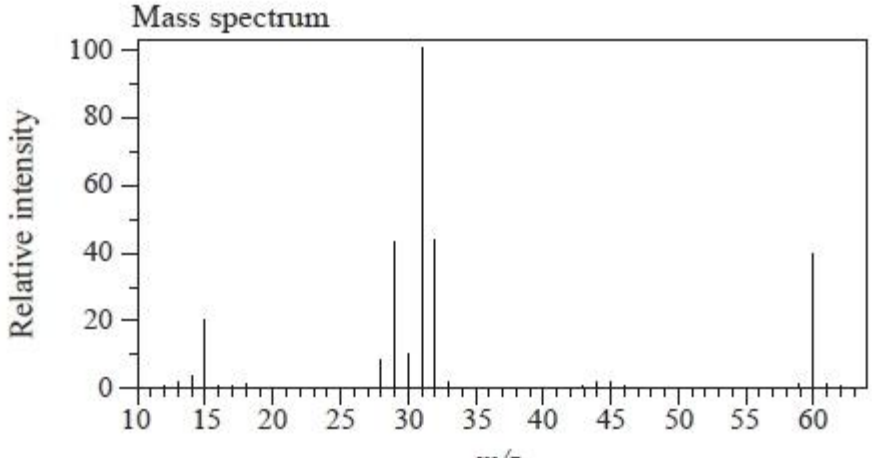
A1. Analytical techniques are very useful in determining molecular structures. A compound, **X**, has the empirical formula C_2H_4O.

(a) Identify the analytical technique that would most readily provide the additional data required to calculate the molecular formula of **X**. *[1]*

.....

Topic:**11:IB P31 An Chem HL 10w Q A2**

(c) The IR spectrum, mass spectrum and ^{1}H NMR spectrum of an unknown compound, **Y**, of molecular formula $C_2H_4O_2$ are as follows.



(ii) In the mass spectrum of **Y**, deduce which ions the *m/z* values at 31 and 29 correspond to. *[2]*

m/z = 31: .....

m/z = 29: .....

Topic:**11:IB P31 An Chem HL 10s**

A1. Butan-1-ol, butan-2-ol, 2-methylpropan-1-ol and 2-methylpropan-2-ol are four structural isomers with the molecular formula $C_4H_{10}O$.

(b) The mass spectrum of one of the alcohols shows peaks at m/z values of 74, 59 and 45.

(i) Deduce which **two** of the alcohols could produce this spectrum and identify the species responsible for the three peaks. *[4]*

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(ii) The spectrum also shows a significant peak at $m/z = 31$. Suggest which alcohol is responsible for this spectrum and deduce the species responsible for the peak at $m/z = 31$. *[2]*

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Topic:**11:IB P31 An Chem HL 08s Q G1**

(b) Identify **one** analytical technique, not involving the absorption of energy from the electromagnetic spectrum, that is used to determine the structures of organic compounds and accurate values of relative atomic masses. *[1]*

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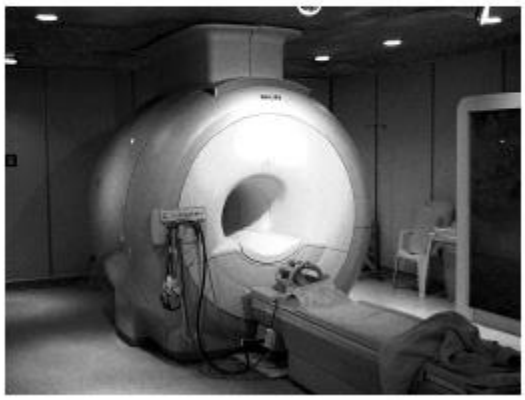
Topic:**11:IB P32 An Chem HL 11s**

A3. Nuclear magnetic resonance (NMR) spectroscopy is the basis of a diagnostic medical technique called magnetic resonance imaging (MRI). The instrument used in this technique in a hospital is shown below.



Explain the role of NMR in this technique which can be used to obtain a three-dimensional view of organs in the human body. *[2]*

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Topic:**11:IB P32 An Chem HL 09s Q A1**

(b) Identify the most suitable spectroscopic technique to

(i) distinguish between butan-1-ol and butan-2-ol. *[1]*

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Topic:**11:IB P32 An Chem HL 08s Q G1**

(b) Outline how ^{1}HNMR is used in body scanners to produce an image of a human body. *[2]*

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Topic:**11:IB P31 An Chem HL 13w**

1. Magnetic resonance imaging (MRI) is a diagnostic technique in which protons, in water and other molecules inside a patient, interact with a magnetic field.

(b) State **one** advantage, other than reducing health risks, of using MRI rather than X-ray radiography. *[1]*

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Topic:**11:IB P31 An Chem HL 12w**

A4. Magnetic resonance imaging (MRI) is a medical application of NMR spectroscopy.

(a) State **one** advantage of MRI over X-ray medical imaging with reference to the electromagnetic spectrum. *[1]*

. . . . . .

. . . . . .

(b) Outline how MRI is used to scan the human body. *[3]*

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Topic:**11:IB P31 An Chem HL 11w**

A3. Nuclear magnetic resonance (NMR) and mass spectrometry are diagnostic techniques often used in the identification of organic compounds.

(c) Outline how the technique of magnetic resonance imaging (MRI) is used in body scanners. *[2]*

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Topic:**11:IB P31 An Chem HL 10w Q A1**

(b) Identify which analytical technique is regularly used for

(iii) scanning of the human body to detect diseases such as cancer and multiple sclerosis. *[1]*

. . . . . .

Topic:**11:IB P31 An Chem HL 11s Q A2 NOT WITH Q A2 (a)**

Compound X is CH_3COCH_3.

(d) Suggest the formulas and m/z values of two species that would be detected in the mass spectrum. *[2]*

Species: . . . . . .
m/z: . . . . . .

Species: . . . . . .
m/z: . . . . . .

Topic:**11:IB P31 An Chem HL 09s Q A2**

(b) Outline how NMR is used in body scanners. *[2]*

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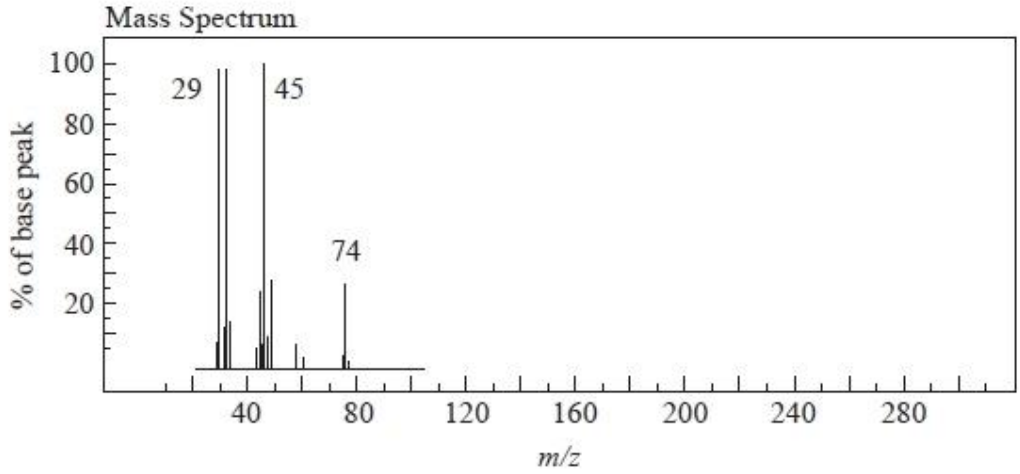
Topic:**12:IB P31 An Chem HL 08w**

G1. Compounds can be identified using information from their mass spectra, infrared spectra and ^{1}H NMR spectra.

The spectra below are for ethyl methanoate, $HCOOC_2H_5$.



(a) (i) Identify the species responsible for the peaks at *m/z* values of 74, 45 and 29 in the mass spectrum. *[3]*

74 . . . . . .

45 . . . . . .

29 . . . . . .

(ii) Explain why there is also a small peak with an *m/z* value of 75. *[1]*

. . . . . .

. . . . . .

(g) An isomer of ethyl methanoate is methyl ethanoate, CH_3COOCH_3. Describe how the following features of the spectra of methyl ethanoate will differ, if at all, from those of ethyl methanoate.

(i) The molecular ion peak in the mass spectrum. *[1]*

. . . . . .

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Topic:**21:IB P32 An Chem HL 14s**

1. Modern analytical techniques are used widely for different purposes in everyday life.

(a) State which analytical technique or combination of techniques would be most suitable for the following purposes. *[2]*

Purpose	Analytical technique(s)
Determining the level of ethanol in the breath of a driver of a vehicle	.....
Body scanning to diagnose the autoimmune disease, multiple sclerosis	.....
Testing for the presence of volatile performance-enhancing drugs such as nandrolone	.....

Topic:**21:IB P31 An Chem HL 08s**

G1. Several analytical techniques are based on the absorption of energy from different parts of the electromagnetic spectrum.
The following diagram shows part of the electromagnetic spectrum.

X-rays	P	visible	Q	microwaves

(a) (i) Identify the types of radiation labelled P and Q. *[1]*

P .....

Q .....

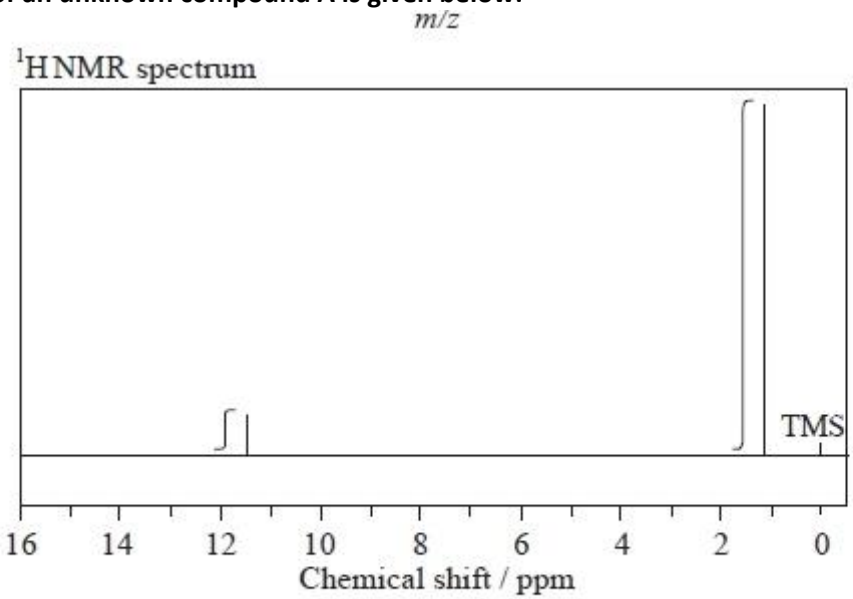
(ii) Identify which **one** of the five regions of the spectrum has radiation of the lowest frequency. *[1]*

.....

.....

Topic:**21:IB P32 An Chem HL 11s Q A2**

The ^{1}HNMR spectrum of an unknown compound A is given below:



[Source: SDBSWeb:http://riod01.ibase.aist.go.jp/sdbs/(National Institute of Advanced Industrial Science and Technology)]

(This question continues on the following page)

Topic:**21:IB P32 An Chem HL 14s**

3. Compound **X** has the molecular formula $C_3H_6O_3$ and is found in human perspiration.

Compound X has the flowing features:

- **O-H and C=O bonds**
- **One CH_3- group**
- **COOH, and OH groups**

(c) Deduce the fragments in the mass spectrum which correspond to the following *m/z* values. *[2]*

m/z = 45:

. . . . . .

m/z = 17 :

. . . . . .

m/z = 15 :

. . . . . .

(d) Deduce the structural formula of **X**. *[1]*

(e) **Y** is an isomer of **X**, which contains the same functional groups. Deduce the structural formula of **Y**. *[1]*

(f) (i) Like **X**, 3-methylbutanoic acid is also a source of body odour. Deduce the *m/z* value for the molecular ion peak on the mass spectrum of this compound. *[1]*

. . . . . .

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Topic:**21:IB P32 An Chem HL 09s**

A2. Mass spectrometry is a powerful analytical technique used in the identification of organic compounds. The mass spectrum of a compound with empirical formula CH_2O displays peaks at *m/z* 15, 45 and 60.

(a) Determine the molecular formula of the compound. *[1]*

. . . . . .

. . . . . .

(b) Identify the fragments responsible for the peaks at *[2]*

m/z = 15 . . . . . .

m/z = 45 . . . . . .

(c) Identify a compound that could produce this spectrum. *[1]*

. . . . . .

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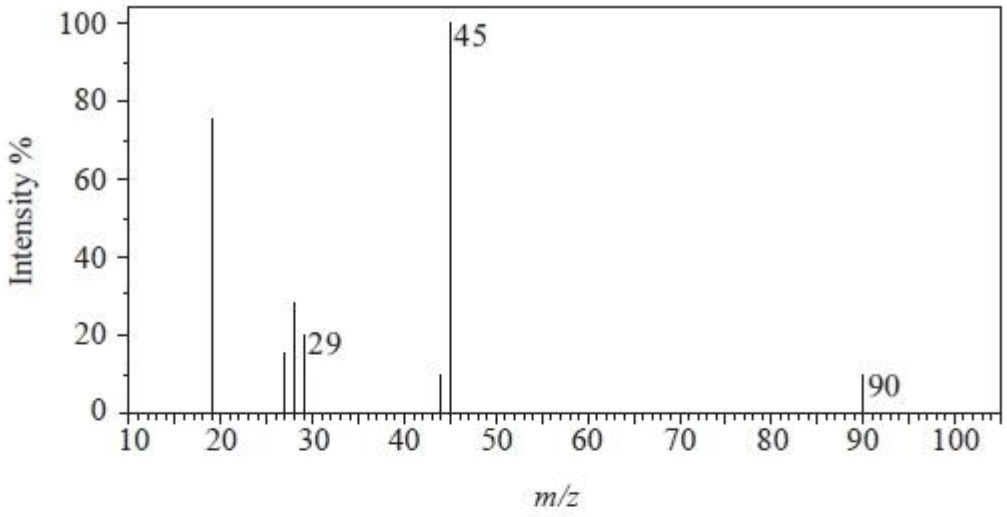
2. (a) The mass spectrum of an unknown acidic compound, **X**, with empirical formula CH_2O, is shown below.



(i) Determine the relative molecular mass, to the nearest integer, of the compound from the mass spectrum and deduce the formula of the molecular ion. *[2]*

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(ii) Deduce the formula of the fragment responsible for the peak at 45. *[1]*

. . . . . .

. . . . . .

(iii) Deduce the formula of the fragment responsible for the peak at 29. *[1]*

. . . . . .

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A1. (a) CH_3COCH_3 **and** CH_3CH_2CHO;

The two structures above are needed to answer the following question:

(c) Explain how the mass spectra of the structures in (a) can be used to distinguish between them. *[2]*

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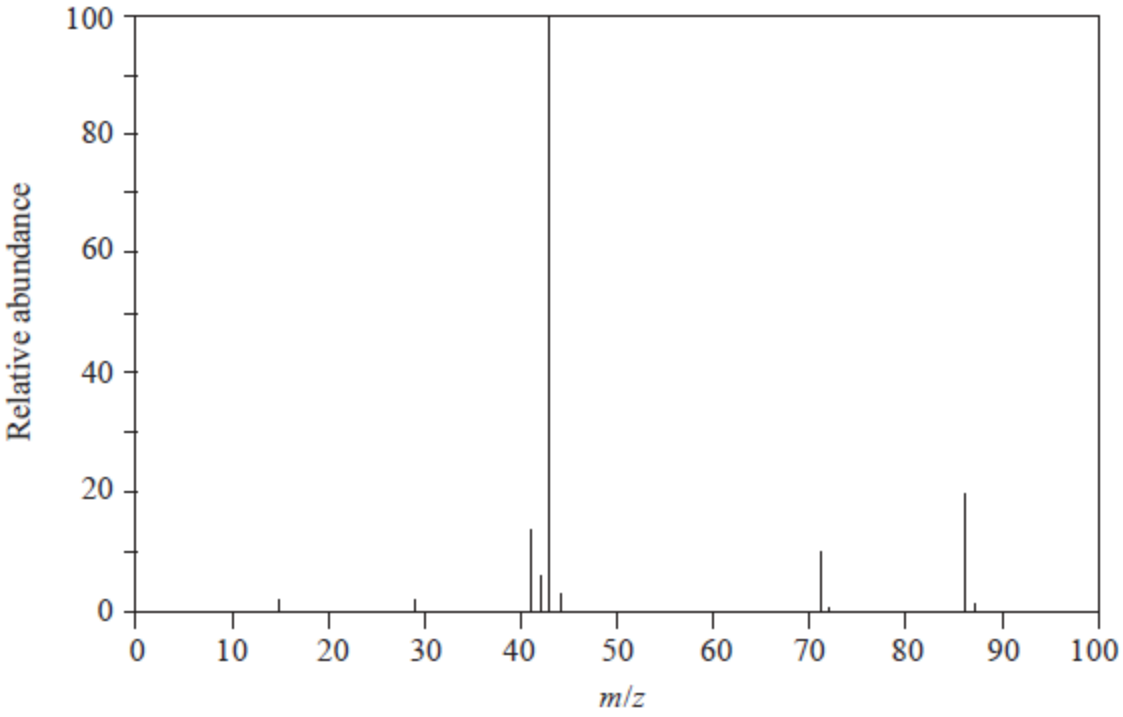
(d) Pentan-2-one has the following mass spectrum.



Deduce the formulas of the species with the m/z values at 71 and 43. *[2]*

$m/z = 71$: . . . . . .

$m/z = 43$: . . . . . .

Topic:**21:IB P31 An Chem HL 11w**

A3. Nuclear magnetic resonance (NMR) and mass spectrometry are diagnostic techniques often used in the identification of organic compounds.

Two isomers relevant to this question are:

isomers CH_3COOH, a carboxylic acid, and $HCOOCH_3$, an ester.

(b) The mass spectrum of one of the two isomers above has significant peaks at mass to charge ratios of 15, 45 and 60, while the other isomer has peaks at 15, 29, 31 and 60. Analyse these fragmentation patterns in the two mass spectra in order to distinguish between the two isomers. *[2]*

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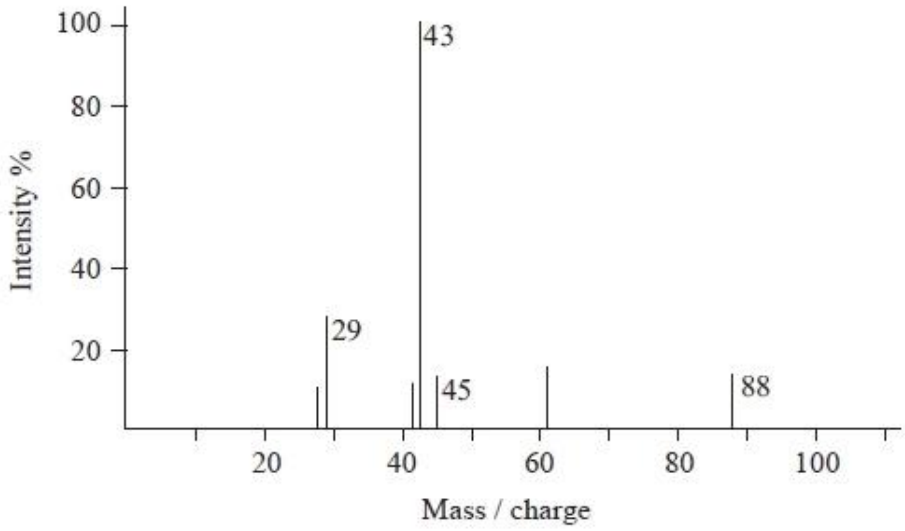
Topic:**21:IB P31 An Chem HL 09w**

A2. (a) The mass spectrum of an unknown compound, **X**, of empirical formula C_2H_4O is shown below.



[Source: Cleapss Guides: L202 Spectra (Cleapss School Science Service), Sept 2000.]

(i) Determine the relative molecular mass of **X** from the mass spectrum and deduce the formula of the molecular ion. *[2]*

. . . . . .

. . . . . .

(ii) Identify a fragment which gives rise to the peak at $m/z = 29$. *[1]*

. . . . . .

(iii) Comment on the absence of a peak at $m/z = 59$. *[1]*

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Topic:**21:IB P31 An Chem HL 12s NOT with A1 (b)**

A1. Analytical techniques are very useful in determining molecular structures. A compound, **X**, has the empirical formula C_2H_4O.

The following information about compound X is needed to answer the next question. It contains an OH (hydroxyl) group and a C=C carbon double bond, but it does not contain a C=O (carbonyl) group)

(c) The ^{1}HNMR spectrum of **X** shows three peaks with relative areas of 2:1:1.

(i) Deduce what information can be obtained from these data. *[2]*

. . . . . .

. . . . . .

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. . . . . .

(ii) Deduce the structure of **X**. *[2]*

Topic:**21:IB P32 An Chem HL 14s**

3. Compound **X** has the molecular formula $C_3H_6O_3$ and is found in human perspiration.

(b) The ^{1}HNMR spectrum recorded showed four peaks with the following chemical shift values (in ppm):

Peaks	Chemical shift / ppm
A	12.4
B	4.0
C	3.4
D	1.2

The integration trace for A:B:C:D was found to be 1:1:1:3.

Deduce what information can be obtained about the hydrogen atoms responsible for peak D at 1.2 ppm from the integration trace in the ^{1}HNMR spectrum of **X**. *[1]*

.....

.....

.....

(f)

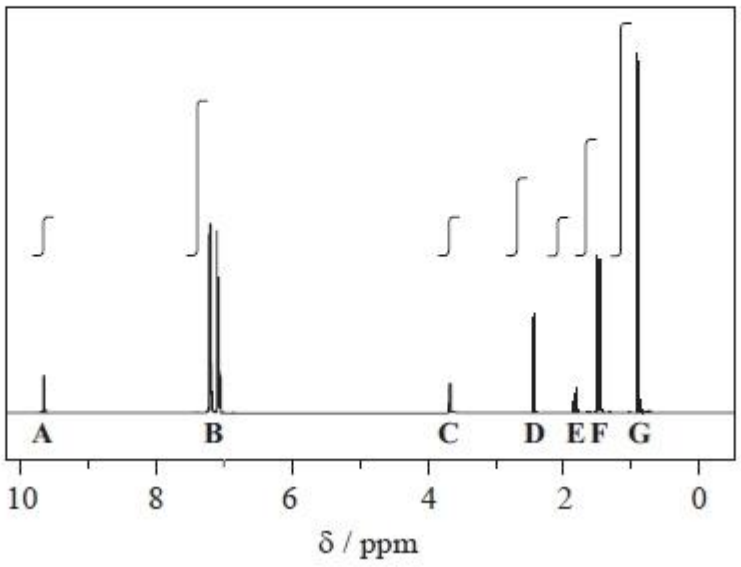
(ii) Ethyl propanoate (ethyl propionate) is an isomer of 3-methylbutanoic acid. Its ^{1}HNMR spectrum consists of four peaks.

Deduce the ratios of the areas under each peak in the ^{1}HNMR spectrum of ethyl propanoate. For each peak, deduce the range of chemical shift values (in ppm), using Table 18 of the Data Booklet, and predict the splitting pattern. *[3]*

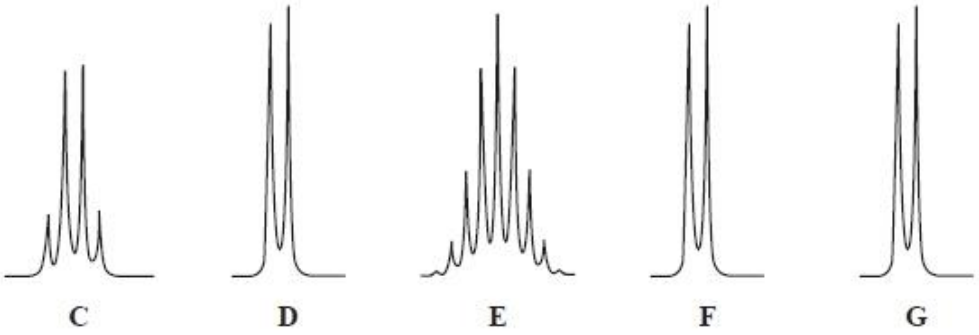
Ratio under each peak	Range of chemical shift values / ppm	Splitting pattern

Topic:**21:IB P32 An Chem HL 13s**

A4. (a) The ^{1}HNMR spectrum of one of the intermediate compounds formed during the synthesis of the painkiller ibuprofen is shown below. The peaks labelled **A** to **G** are not fully expanded to show the splitting but the integration trace for each peak is included.

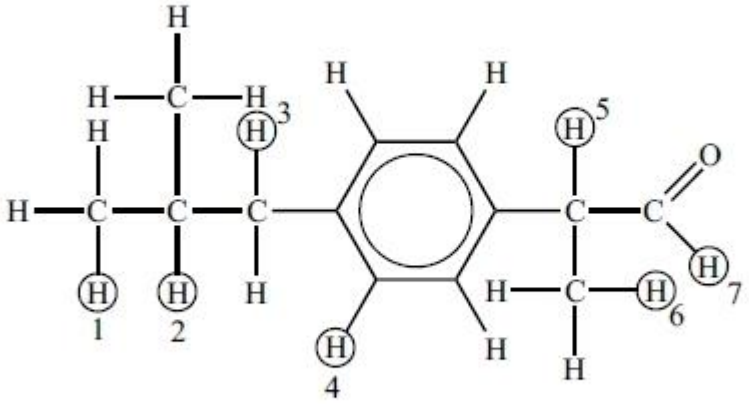


The peak labelled **A** is a singlet. The two peaks labelled **B** centred at 7.1 ppm are due to the four hydrogen atoms on the benzene ring. The expansions to show the splitting for the other five peaks are shown below.



C **D** **E** **F** **G**

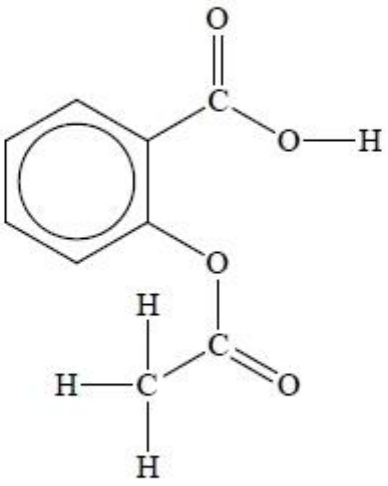
The structure of the intermediate compound is given below, with seven of the hydrogen atoms labelled.



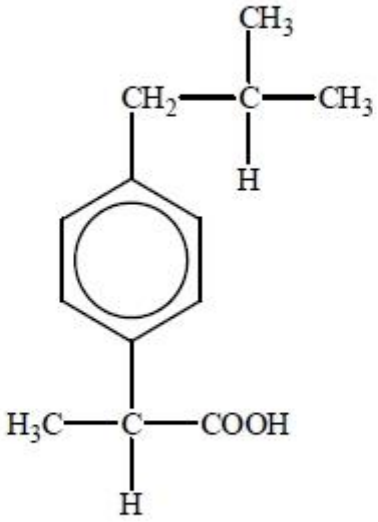
Deduce which labelled hydrogen atoms are responsible (wholly or in part) for each of the peaks and complete the table. *[6]*

Peak	Hydrogen atom responsible
A	
B	4
C	
D	
E	
F	
G	

(b) Another painkiller is aspirin. The structures of aspirin and ibuprofen are:



Aspirin



Ibuprofen

(i) State the number of peaks in the ^{1}HNMR spectrum of aspirin (**ignore** the peaks due to the hydrogen atoms on the benzene ring and the reference sample). *[1]*

. . . . . .

(ii) Describe the splitting pattern for each of the peaks given in (b) (i). *[1]*

. . . . . .

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(iii) State how the infrared spectra of aspirin and ibuprofen will differ in the region 1700–1750 cm^{-1}. *[2]*

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A3. (a) Deduce the number of peaks in the ^{1}HNMR spectra of 1-bromobutane and 2-bromobutane. Explain how the integration trace can be used to distinguish between the two compounds. *[3]*

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(b) Another structural isomer of C_4H_9Br is 2-bromo-2-methylpropane. Deduce the number of peaks and the splitting pattern in the ^{1}HNMR spectrum of this isomer. *[2]*

Number of peaks:

. . . . . .

. . . . . .

Splitting pattern:

. . . . . .

. . . . . .

(c) Outline the principle behind magnetic resonance imaging (MRI) used to diagnose and monitor conditions such as cancer in humans. *[3]*

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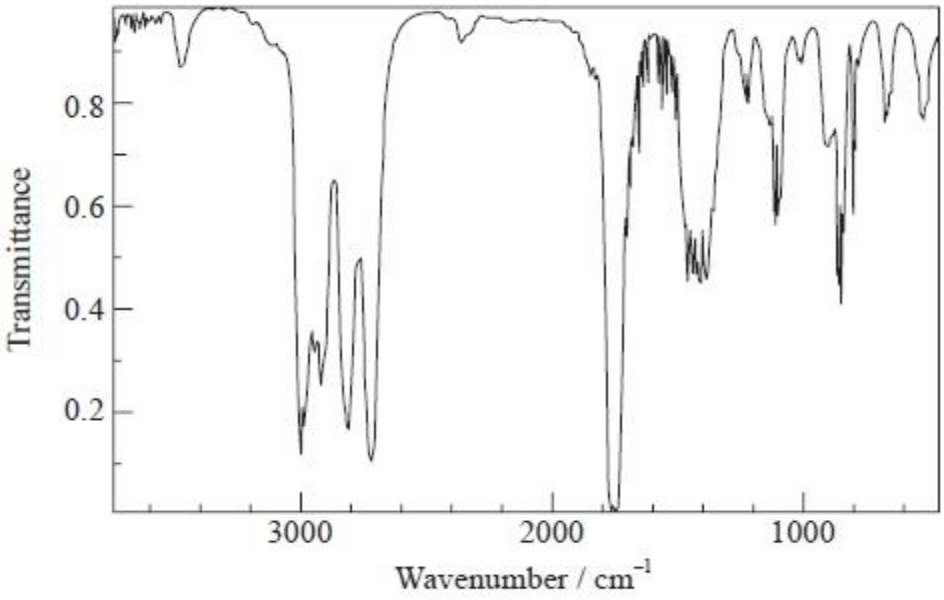
(b) The infrared spectrum of a substance, X, with empirical formula C_3H_6O is given below.



[Source: NIST http://webbook.nist.gov/chemistry]

From this information we can see that there are the following bonds:

1. **O-H**
2. **C=O**
3. **C=C**

(ii) The ^{1}H NMR spectrum of X consists of three peaks. Deduce the structural formula of X and the relative areas under each peak. *[2]*

. . . . . .

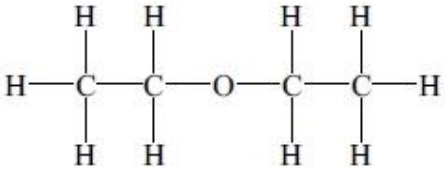
. . . . . .

(iii) Predict the splitting pattern of the peak with the biggest area. *[1]*

. . . . . .

. . . . . .

G2. A student was asked to predict the ^{1}H NMR spectrum of ethoxyethane, whose structure is shown below.



(a) Deduce the number of different environments for hydrogen atoms in ethoxyethane. *[1]*

. . . . . .

(b) Using Table 19 of the Data Booklet and the structure given for ethoxyethane, predict for each environment:

(i) the chemical shift in ppm; *[2]*

CH_3 . . . . . .

CH_2 . . . . . .

(ii) the ratio of the areas under each peak; *[1]*

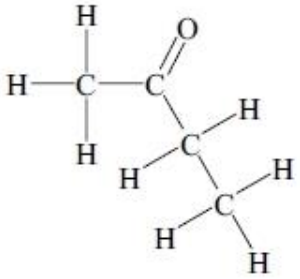
. . . . . .

(iii) the splitting pattern. *[2]*

CH_3 . . . . . .

CH_2 . . . . . .

(c) The structure of butanone is shown below. State **one** feature of the ^{1}H NMR spectrum of butanone that differs from the ^{1}H NMR spectrum of ethoxyethane. *[1]*



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(d) All ^{1}H NMR spectra have a peak at 0 ppm. Identify the substance that produces this peak and state its function. *[2]*

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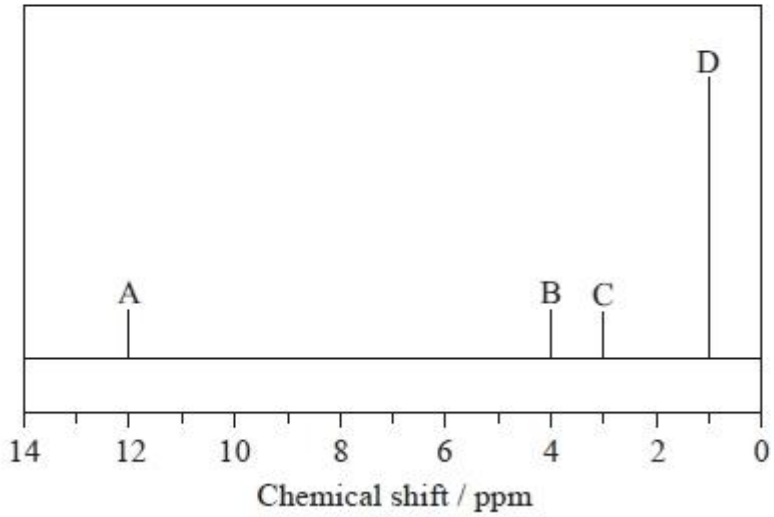
Topic:**21:IB P31 An Chem HL 13w**

2. (a) The mass spectrum of an unknown acidic compound, **X**, with empirical formula CH_2O, is shown below.

(b) The low-resolution ^{1}HNMR spectrum of **X** shows four peaks. A simplified representation is shown alongside a table with relative peak areas.



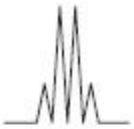
Peak	Relative peak area
A	1
B	1
C	1
D	3

(i) Identify the group responsible for the peak at **D**. *[1]*

. . . . . .

(ii) Suggest a possible structure for **X**. *[1]*

(c) Peak **B** shows the following splitting pattern in the high-resolution spectrum.



Explain the splitting pattern, indicating the hydrogen responsible for peak **B**. *[3]*

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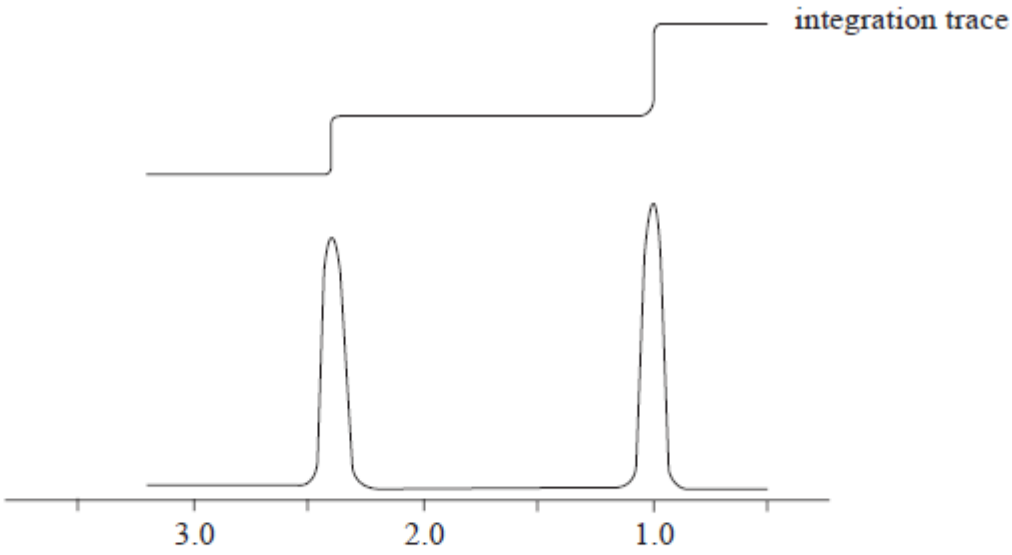
A3. The low resolution ^{1}H NMR spectrum of compound **Q** is shown.



(a) Identify what information from the spectrum allows the determination of the relative numbers of hydrogen atoms producing each peak. *[1]*

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(b) Deduce which of the following compounds is **Q**. *[1]*

$CH_3CH_2CH_3$ $CH_3CH_2COCH_2CH_3$ CH_3CH_2OH

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(c) Predict the splitting pattern for the peak at a chemical shift of 2.4 ppm. *[1]*

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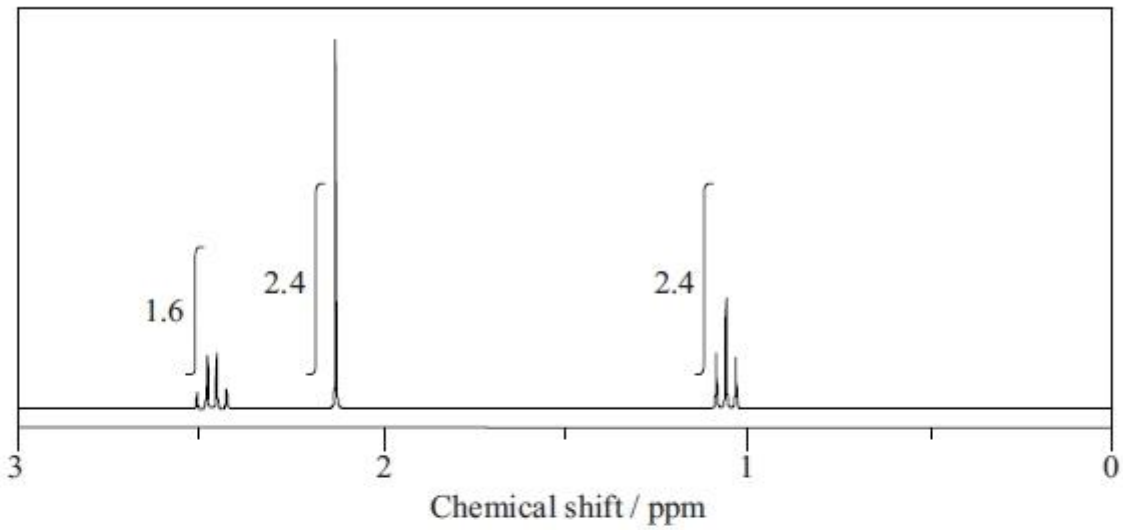
A3. The molecule of an unknown straight-chain compound consists of 4 carbon, 8 hydrogen, and 1 oxygen atoms. The ^{1}H NMR spectrum of the compound is given below (the numbers next to integration traces correspond to areas under each peak).



(a) Calculate the number of hydrogen atoms for peaks with chemical shifts of 2.15 and 2.4–2.5 ppm. An example for the peak at 1.0–1.1 ppm is given. *[2]*

Chemical shift / ppm	Number of hydrogen atoms
1.0–1.1	3
2.15	
2.4–2.5	

(b) Analyse the splitting pattern of each peak and determine the relative positions of hydrogen atoms in the molecule. One example is given. *[2]*

Chemical shift / ppm	Splitting pattern	Number of adjacent hydrogen atoms
1.0–1.1	triplet	2
2.15		
2.4–2.5		

(c) Using the information from (a) and (b), deduce the structural formula of the organic compound. *[1]*

Topic:**21:IB P31 An Chem HL 12s**

A1. Analytical techniques are very useful in determining molecular structures. A compound, **X**, has the empirical formula C_2H_4O.

(d) Peaks in a ^{1}HNMR spectrum are measured relative to a reference standard. State the name of a substance used and identify **one** property that makes it particularly suitable for this application. *[2]*

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Topic:**21:IB P31 An Chem HL 11w**

A3. Nuclear magnetic resonance (NMR) and mass spectrometry are diagnostic techniques often used in the identification of organic compounds.

(a) Deduce **two similarities** and **one difference** in the ^{1}HNMR spectra of the two isomers CH_3COOH, a carboxylic acid, and $HCOOCH_3$, an ester. ^{1}HNMR data are given in Table 18 of the Data Booklet. *[3]*

Similarities:

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Difference:

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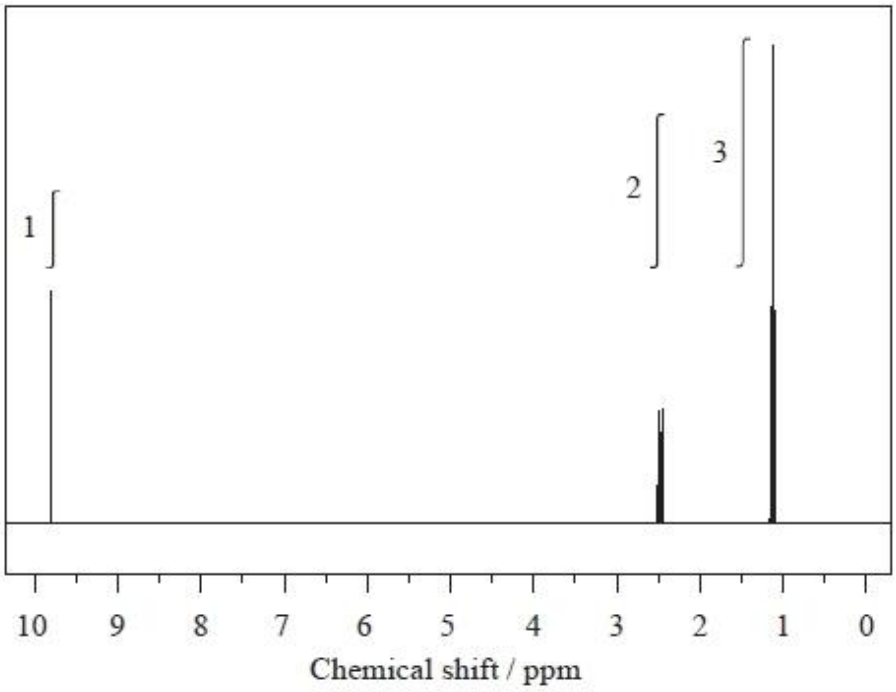
A2. The ^{1}H NMR spectrum of **X** with molecular formula C_3H_6O is shown below.



(a) Deduce which of the following compounds is **X** and explain your answer. *[2]*

$CH_3–CO–CH_3$ $CH_3–CH_2–CHO$ $CH_2=CH–CH_2OH$

Compound:

. . . . . .

Explanation:

. . . . . .

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(b) State and explain the splitting pattern you would expect in a high resolution spectrum for the peak at 1.1 ppm. *[2]*

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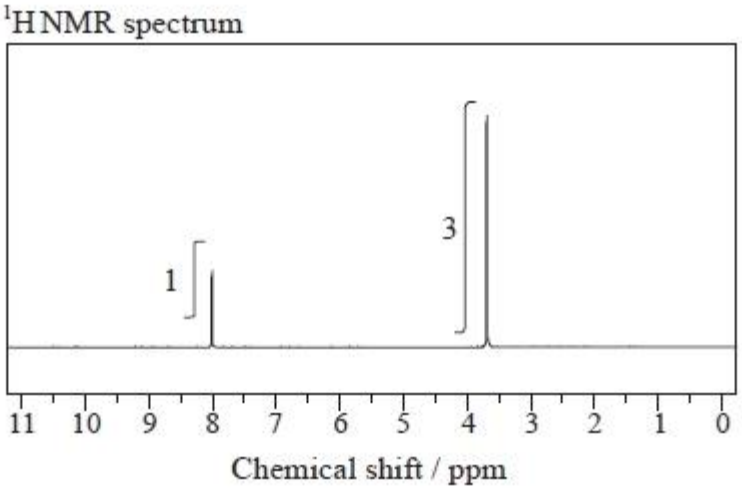
Topic:**21:IB P31 An Chem HL 10w Q A2**

(c) The IR spectrum, mass spectrum and ^{1}HNMR spectrum of an unknown compound, **Y**, of molecular formula $C_2H_4O_2$ are as follows.



[Source: SDBSWeb: http://riodb01.ibase.aist.go.jp/sdbs/ (National Institute of Advanced Industrial Science and Technology)]

Compound Y is known to have the following bonds: C-H, C=O, C-O
And produce the following mass spec fragment ions: CH_3O^+ and HCO^+.

(iii) Identify the peaks at 3.76 and 8.07 ppm in the ^{1}HNMR spectrum. *[1]*

3.76 ppm: . . . . . .

8.07 ppm: . . . . . .

(iv) State what information can be obtained from the integration trace about the hydrogen atoms responsible for the peak at 3.76 ppm in the ^{1}HNMR spectrum. *[1]*

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(v) Deduce the structure of **Y**. *[1]*

(vi) Explain why tetramethylsilane (TMS) is suitable as a reference standard. *[2]*

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Topic:**21:IB P31 An Chem HL 10s**

A1. Butan-1-ol, butan-2-ol, 2-methylpropan-1-ol and 2-methylpropan-2-ol are four structural isomers with the molecular formula $C_4H_{10}O$.

(a) Details of the ^1H NMR spectra of two of these alcohols are given below.

Spectrum 1

Two peaks: A singlet at 1.3 ppm (relative to the TMS reference) with an integration trace of nine units, and another singlet at 2.0 ppm with an integration trace of one unit.

Spectrum 2

Four peaks: A doublet at 0.9 ppm with an integration trace of six units.
A complex pattern at 1.7 ppm with an integration trace of one unit.
A singlet at 2.1 ppm with an integration trace of one unit.
A doublet at 3.4 ppm with an integration trace of two units.

Consider the proton environments present in each of the alcohol molecules when answering the following questions.

(i) Identify which alcohol gives spectrum 1 and explain your answer by stating which hydrogen atoms in the molecule are responsible for each of the two peaks. *[3]*

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(ii) Deduce which alcohol gives spectrum 2. Explain which hydrogen atoms are responsible for the peaks at 0.9 ppm and 3.4 ppm and explain why both of these peaks are split into doublets. *[4]*

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Topic:**21:IB P31 An Chem HL 09w NOT with QA2 (a) or (b)**

A2. (a) The mass spectrum of an unknown compound, **X**, of empirical formula C_2H_4O is shown below.

The molecular ion for this compound is $C_4H_8O_2^2$ and it contains an ester functional group.

(c) Typical proton chemical shift values are given in Table 18 of the Data Booklet. The ^{1}HNMR spectrum of **X** contains three peaks. Details of two of these are shown in the table below.

Peak	Chemical shift / ppm	Relative peak area	Splitting pattern
First	2.0	3	Singlet
Second	4.1	2	Quartet
Third			

(i) Deduce a possible structure for **X** that is consistent with the mass, IR and ^{1}HNMR spectra. *[1]*

(ii) Complete the table above by suggesting the chemical shift of the third peak, and state its relative peak area and splitting pattern. *[3]*

(iii) Explain the splitting pattern of the peak at chemical shift **4.1** ppm. *[2]*

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Topic:**21:IB P31 An Chem HL 09w**

A1. ^{1}H NMR and IR spectroscopy both involve the absorption of electromagnetic radiation.

(a) (i) Identify the region of the electromagnetic spectrum used in ^{1}H NMR spectroscopy. *[1]*

. . . . . .

(ii) Explain why tetramethylsilane (TMS) is used as a reference standard in ^{1}H NMR spectroscopy. *[1]*

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Topic:**21:IB P31 An Chem HL 09s**
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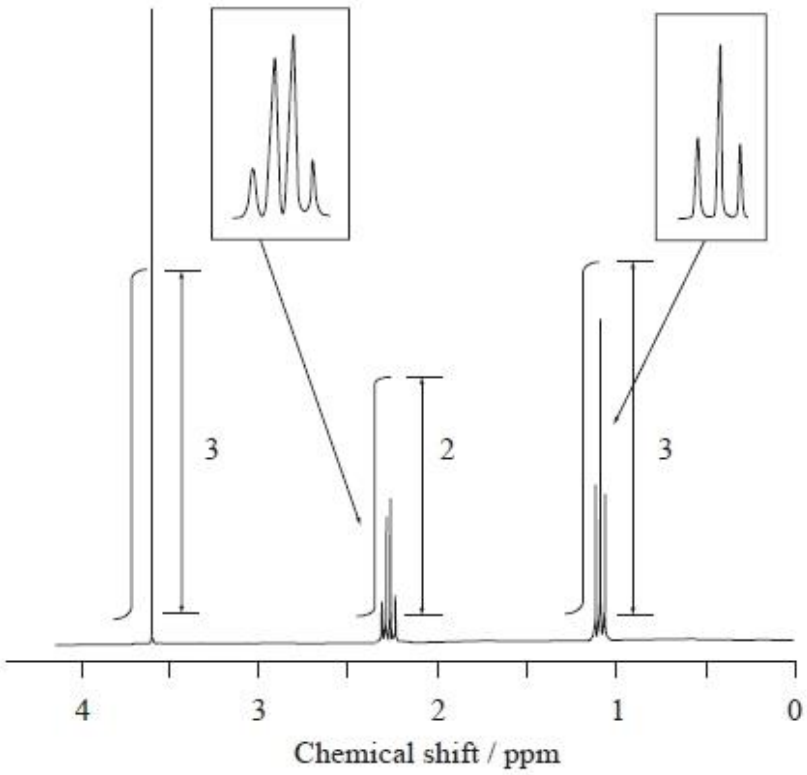
A2. (a) A feature of some ^{1}H NMR spectra is the electron-withdrawing effect of electronegative atoms. These atoms cause nearby protons to produce peaks at higher chemical shift values, often in the range 2.5 to 4.5 ppm.
Consider the ^{1}H NMR spectrum of an unknown compound, D, which has a molecular formula $C_4H_8O_2$ and is known to have an absorption in its IR spectrum corresponding to a C=O absorption.



Use this information and the values in Table 18 of the Data Booklet to deduce the structure of D. *[4]*

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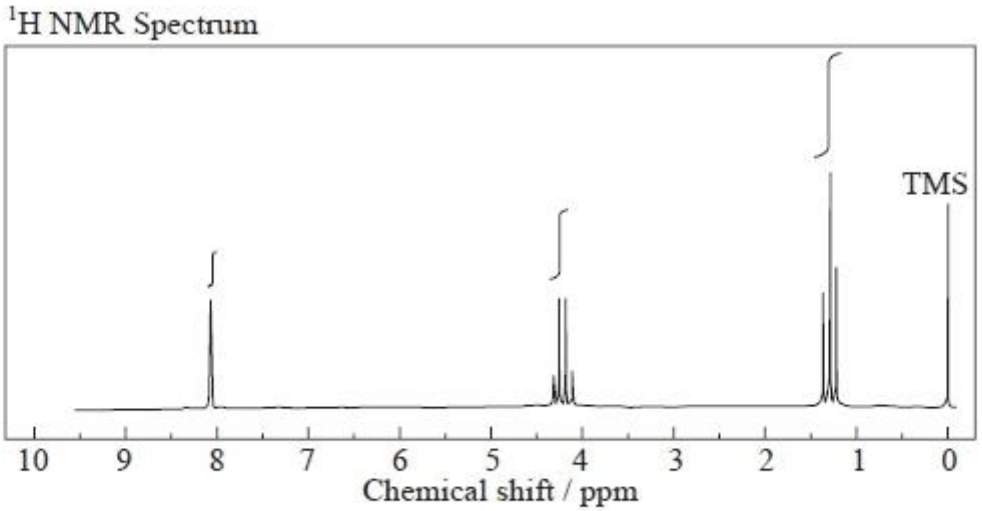
Topic:**21:IB P31 An Chem HL 08w**

G1. Compounds can be identified using information from their mass spectra, infrared spectra and ^{1}H NMR spectra.

The spectra below are for ethyl methanoate, $HCOOC_2H_5$.



[Source: Spectra taken from: L.Field, S. Sternhell & J. Kalman, *Organic Stuctures from Spectra*, John Wiley and Sons, 1995]

(d) The ^{1}H NMR spectrum for ethyl methanoate shows three separate peaks. Use the integration trace to determine which hydrogen atom(s) is/are responsible for the peak with a shift of 1.3 ppm. *[1]*

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. . . . . .

(e) Explain why the peak at 1.3 ppm in the ^{1}H NMR spectrum is split into a triplet. *[1]*

. . . . . .

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(f) The chemical shifts of protons are influenced by several factors including the solvent. The values given in the Data Booklet are not always precise. Explain how information from the integration trace and the splitting pattern can be used to identify which hydrogen atom(s) is/are responsible for the peak with a shift of 8.1 ppm. *[3]*

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(g) An isomer of ethyl methanoate is methyl ethanoate, CH_3COOCH_3. Describe how the following features of the spectra of methyl ethanoate will differ, if at all, from those of ethyl methanoate.

(ii) The number of peaks and the integration trace in the ^1H NMR spectrum. *[2]*

. . . . . .

. . . . . .

(iii) The splitting patterns in the ^1H NMR spectrum. *[1]*

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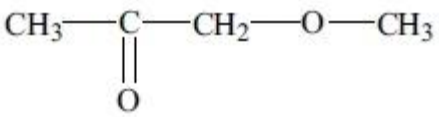
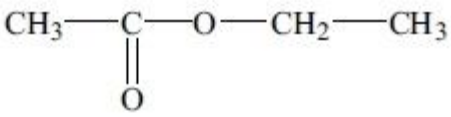
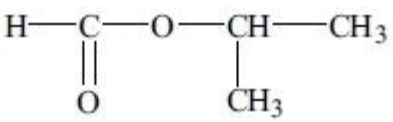
Topic:**21:IB P31 An Chem HL 08s**

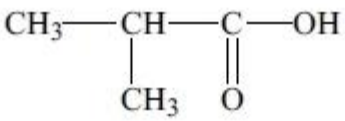
G2. Use information from Table 18 in the Data Booklet to help answer this question.

There are several isomers with the molecular formula $C_4H_8O_2$. The structural formulas of some of them are shown below.

A. 

B. 

C. 

D. 

(b) The technique of ^1H NMR spectroscopy can also be used to distinguish between different organic compounds. State what information can be obtained from: *[3]*

the number of peaks

. . . . . .

the ratio of areas under each peak

. . . . . .

the splitting pattern.

. . . . . .

(c) For isomers **B** and **C** deduce the ratio of peak areas and the splitting pattern. *[4]*

B ratio of peak areas

. . . . . .

B splitting pattern

. . . . . .

C ratio of peak areas

. . . . . .

C splitting pattern

. . . . . .

(d) The ratio of peak areas and the splitting pattern are the same for isomers **C** and **D**. State how their ^1H NMR spectra differ. *[1]*

. . . . . .

. . . . . .

(e) Suggest the structural formula of an isomer of $C_4H_8O_2$ that has the same ratio of peak areas and splitting pattern as isomer **B**. *[1]*

Mark Scheme

IB P32 An Chem HL 10s

A1. structure determination;
composition of substances;
determination of purity;
determination of amount/concentration of substance;
identification of substances; *[2 max]*

IB P31 An Chem HL 10w

A1. (a) determination of structure
determination of concentrations
identification of substances
Allow separation of substances.

analysis of (different) composition of substances/compounds/mixtures
determination of purity of substances
in medicine for body imaging
Do not allow just in medicine.

determining illegal drug use
forensic science for evidence in courts
monitoring of the environment
DNA testing
testing foods for levels of sugar/testing quality of food *[1]*
Accept other specific examples.
Do not award mark for repeating examples given in (b).
Award [1] for any two.

IB P31 An Chem HL 09s

A1. (a) determination of structure (of a substance/compound);
determination of the purity (of a substance/compound);
analysis of the composition (of a substance/compound);
separation of mixtures; *[2 max]*

IB P32 An Chem HL 14s

Penalize incorrect bond linkages (eg, CH_2–HO instead of CH_2–OH) and/or missing hydrogens once only in option at first occurrence.

3. (a) *I*: O–H **and** *II*: C=O; *[1]*
Do not allow CO for C=O.
Allow OH for O–H.

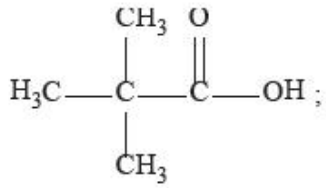
IB P32 An Chem HL 13s Q A4

(iii) aspirin will have two (sharp) peaks / wider/greater absorption (due to two C=O groups);
ibuprofen will have one (sharp) peak / narrower/less absorption (due to one C=O group); *[2]*

IB P32 An Chem HL 11s Q A2

(iii) (H of) COOH group; *[1]*

(iv) nine hydrogens in the same environment / $(CH_3)_3C-$(group); *[1]*

(v) $(CH_3)_3CCOOH$ / $(CH_3)_3CCO_2H$ /  ; *[1]*

IB P32 An Chem HL 11s

A2. (a) (stretches/vibrations in) HBr involve change in bond dipole / (stretches/vibrations in) Br_2 do not involve change in bond dipole; *[1]*

(b) (i) C=O / carbonyl; *[1]*

IB P32 An Chem HL 10s

A3. (a) no change in dipole moment/bond polarity;
as vibration/stretching occurs; *[2]*
Ignore bending if included.

(b) symmetrical stretching;
asymmetrical stretching;
bending/change in bond angle; *[2 max]*
Accept diagrams of the water molecules which illustrate the bending and stretching.
Allow [1] for stretching alone.

IB P32 An Chem HL 09s Q A3

(b) (i) absence of peak between 3200–3600 cm^{-1} /above 3000 cm^{-1}/peak for OH;
presence of peak between 1700–1750 cm^{-1} /peak for C=O;
absence of peak between 1610–1680 cm^{-1}/peak for C=C; *[2 max]*

IB P32 An Chem HL 08s Q G1

(ii) IR spectroscopy / iodine titration; *[1]*

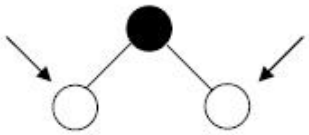
IB P32 An Chem HL 08s Q G2

(e) ethoxyethane will have an absorption between 1000 to 1300 cm^{-1} for the C–O–C;
butan-2-one will have an absorption between 1680 to 1750 cm^{-1} for the C=O; *[2]*

IB P32 An Chem HL 08s

G3. (a) bending and stretching of bonds;
for absorption to occur there must be a change in dipole moment / polarity of the molecule;
diagram of H_2O demonstrating asymmetric / symmetric stretching;
e.g.

diagram of H_2O demonstrating bending; *[4]*
e.g.



(b) inverse/reciprocal relationship / inversely proportional / wavelength $= \frac{1}{\text{wavenumber}}$; *[1]*

IB P31 An Chem HL 13w

3. (a) *Similarities [2 max]:*
$1050-1410\,cm^{-1}$ (due to C–O);
$1700-1750\,cm^{-1}$ (due to C=O);
$2850-3100\,cm^{-1}$ (due to C–H);
$3200-3600\,cm^{-1}$ (due to O–H);

Differences:
$1610-1680\,cm^{-1}$ (due to C=C only in nandrolone); *[3]*

IB P31 An Chem HL 13s

A1. (a) CH_3COCH_3 **and** CH_3CH_2CHO; *[1]*
Accept full or condensed structural formulas.
Ignore incorrect names as long as structures are correct.

(b) same/similar (types of) bonds / both contain the carbonyl group/C=O; *[1]*
Do not accept same functional group.

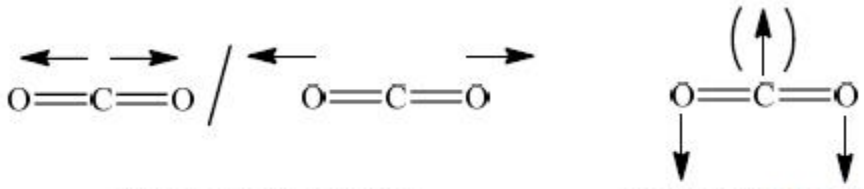
IB P31 An Chem HL 12s Q A1

(b) (i) *A:* O–H/hydroxyl;
B: C=C/carbon-carbon double bond; *[2]*

(ii) no C=O/carbonyl present; *[1]*

IB P31 An Chem HL 11w

A2. (a)



(symmetric) stretching (symmetric) bending *[2]*

Award [1] for stretching and bending without diagrams.
Award [1] for clearly illustrated diagrams without mention of stretching and bending.
Do not penalize if single lines drawn between atoms.

(b) change in dipole moment/(molecular) polarity leads to IR absorption / *OWTTE*;
symmetric stretching is IR inactive;
asymmetric stretching/(symmetric) bending is IR active; *[3]*

IB P31 An Chem HL 11s Q A2

(c) (i) $1700–1750\ cm^{-1}$ (>C=O); *[1]*

(ii) $1610–1680\ cm^{-1}$ (>C=C<) / $3200–3600\ cm^{-1}$ (–O–H); *[1]*

IB P31 An Chem HL 10w

(b) change in bond length / bond stretching / asymmetric stretch;
change in bond angle / bending (of molecule);
Allow [1 max] for only stating vibrations.

induces molecular polarity/dipole moment / *OWTTE*; *[3]*

(c) (i) **A**: C–H
B: C=O
C: C–O *[2]*
Award [2] for three correct, [1] for two correct.

IB P31 An Chem HL 10s Q A1

(c) they all contain O–H;
they all contain C–H;
they all contain C–O; *[2 max]*
Award [1max] for the same functional groups/bonds.

IB P31 An Chem HL 09w Q A1

(b) HCl;
vibration/stretching of bond/molecule produces a change in dipole moment/polarity; *[2]*
Do not accept contains a polar bond.
Ignore reference to bending.
M2 cannot be awarded for incorrect choice of molecule.
Accept explanation of why O_2 and H_2 do not absorb IR.

IB P31 An Chem HL 09w Q A2

(b) (i) *A*: C=O **and** *B*: C–O; *[1]*
No mark if two bonds are given for A or B.
Ignore names if incorrect.

(ii) ester; *[1]*
Do not accept COO.

IB P31 An Chem HL 09s Q A1

(d) A is Spectrum I **and** B is Spectrum III **and** C is Spectrum II;

A Spectrum I:
only spectrum with a (broad) peak in the range 2500–3300 (cm^{-1}) corresponding to the carboxylic acid functional group / –OH in carboxylic acid / H-bonding in carboxylic acid (so must be a carboxylic acid);

B Spectrum III:
peak in the range 1700–1750 (cm^{-1})corresponding to the carbonyl/C=O group;
but no peak for O–H/no peak at 2500–3300 (cm^{-1}) or 3200–3600 (cm^{-1});

C Spectrum II:
peak in the range 3200–3600 (cm^{-1}) corresponding to the alcohol functional group/OH / the only one without a peak at 1700–1750 (cm^{-1}) corresponding to an alcohol; *[5]*

IB P31 An Chem HL 08w Q G1

(b) The vibration must involve a change in dipole moment/bond polarity; *[1]*

(c) The precise value of the absorption depends on the groups/atoms attached to the C=O / *OWTTE*; *[1]*

(h) a different fingerprint region;
a (broad) absorption in range 2500–3300 cm^{-1}; *[2]*

IB P31 An Chem HL 08s

(c) (i) (only) HBr has (atoms with) different electronegativities / (only) H–Br is polar / O_2 is non-polar;
No credit just for saying atoms are different.

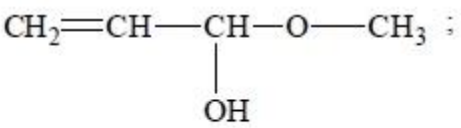
(only) HBr changes dipole moment/bond polarity; *[2]*

(ii) molecule can bend/change shape / deform / change its bond angle; *[1]*

IB P31 An Chem HL 08s

G2. (a) (i) 1000-1300 (cm^{-1}) **and** 1680-1750 (cm^{-1}); *[1]*

(ii) 2500-3300 (cm^{-1}); *[1]*

(iii)  ;

Accept any correct structure of $C_4H_8O_2$ with $C=C$. *[1]*

IB P32 An Chem HL 11s Q A2

(b) (i) C=O / carbonyl; *[1]*

(ii) *m/z = 102:* molecular parent ion / $(CH_3)_3CCOOH^+$ / $C_5H_{10}O_2^+$ / M^+;

m/z = 57: $(CH_3)_3C^+$ / $(M-COOH)^+$ / $C_4H_9^+$; *[2]*
Penalize missing + once only.

IB P31 An Chem HL 12s

A1. (a) mass spectrometry/spectroscopy / MS; *[1]*

IB P31 An Chem HL 10w Q A2

(ii) $m/z = 31: CH_3O^+$;
$m/z = 29: HCO^+$; *[2]*
Penalize missing + charge once only.
Elements can be given in any order (i.e. OCH_3^+, COH^+, CHO^+).

IB P31 An Chem HL 10s Q A1

(b) (i) butan-1-ol and butan-2-ol;

74: M^+ / $C_4H_{10}O^+$ / $CH_3CH_2CH_2CH_2OH^+$ **and** $CH_3CH_2CH(OH)CH_3^+$;

59: $C_3H_7O^+$ / $(M-CH_3)^+$ / $CH_2CH_2CH_2OH^+$ **and** $CH_2CH(OH)CH_3^+$/$CH_3CH_2CH(OH)^+$;

45: $C_2H_5O^+$ / $(M-C_2H_5)^+$ / $CH_2CH_2OH^+$ **and** $CH(OH)CH_3^+$; *[4]*
Accept explained answers instead of formula

(ii) butan-1-ol;
CH_2OH^+ / $(M-C_3H_7)^+$; *[2]*
Penalize missing + signs once only in parts (b) (i) and (ii).

IB P31 An Chem HL 08s Q G1

(b) mass spectrometry/spectroscopy; *[1]*

IB P32 An Chem HL 11s

A3. human body consists of 70 %/mostly/a lot of water;
protons in water molecules/in carbohydrates, proteins and fats can be detected by MRI;
water in different environments;
organs have different water to lipid ratios;
so that protons have different environments so produce different effects; *[2 max]*

IB P32 An Chem HL 09s Q A1

(b) (i) (^{1}H /proton) NMR/nuclear magnetic resonance; *[1]*

IB P32 An Chem HL 08s Q G1

(b) *Any two of the following.*
protons/hydrogen atoms in water, lipids (etc) in body can be detected by magnetic resonance imaging/MRI;
different water-lipid ratios / hydrogen atoms in different chemical environments absorb different (radio) frequencies;
giving a two/three dimensional view of body organs; *[2 max]*

IB P31 An Chem HL 13w

(b) MRI can detect soft tissues/body organs / different properties of (soft) tissue (and bone);
Accept "contrast can be a problem in X-ray". *[1]*
Accept three-dimensional image.

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A4. (a) uses no ionizing radiation / uses low-energy radio waves / radio waves safer than x-rays / *OWTTE*; *[1]*
Accept "does not damage body tissue".

(b) MRI is (usually) a proton NMR/^{1}H NMR;
(the states of) protons/hydrogen atoms in water/lipids/carbohydrates/proteins/ different (chemical) environments are detected;
different organs have different water concentration;
(strong) magnetic field **and** radio waves/frequency are used;
(by focusing the scanner on different parts of the body) three-dimensional/3-D images of (organs in) the body are produced / *OWTTE*; *[3 max]*

IB P31 An Chem HL 11w Q A3

(c) protons in water/lipid/carbohydrates (within cells) can be detected by MRI / cells have different water to lipid ratios / protons in water have different chemical environments/give different signals;
Accept protons detected by MRI.

gives a (3D) view/image of organs (in body) / *OWTTE*; *[2]*

IB P31 An Chem HL 10w Q A1

(iii) (^{1}H/proton) NMR/nuclear magnetic resonance / MRI/magnetic resonance imaging; *[1]*

IB P31 An Chem HL 11s Q A2

(d) $C_3H_6O^+$ **and** m/z = 58;
$C_2H_5^+$ **and** m/z = 29;
CHO^+ **and** m/z = 29;
CH_3^+ **and** m/z = 15; *[2 max]*
Penalize missing + sign once only.

IB P31 An Chem HL 09s Q A2

(b) magnetic resonance imaging (MRI) gives a three-dimensional view of organs in the human body / *OWTTE*;
because protons in water molecules/lipids/carbohydrates in human cells give different signals, depending upon their environment / *OWTTE*; *[2]*

IB P31 An Chem HL 08w

G1. (a) (i) 74: M^+ / molecular ion / $HCOOC_2H_5^+$;
45: $HCOO^+$ / $C_2H_5O^+$;
29: $C_2H_5^+$ / HCO^+; *[3]*
[2 max] if positive sign missing.

(ii) (peak at 75) due to presence of carbon-13; *[1]*

(g) (i) no change / still at *m/z* of 74; *[1]*

IB P32 An Chem HL 14s

Penalize incorrect bond linkages (eg, CH_2–HO instead of CH_2–OH) and/or missing hydrogens once only in option at first occurrence.

1. (a)

Purpose	*Analytical Technique*
Determining the level of ethanol in the breath of a driver of a vehicle	infrared (spectroscopy)/IR *Allow gas (liquid) chromatography/GLC.*
Determining the concentration of chromium in seawater	atomic absorption (spectroscopy)/AA/AAS
Body scanning to diagnose the autoimmune disease, multiple sclerosis	(^{1}H/proton) nuclear magnetic resonance/NMR / magnetic resonance imaging/MRI *Allow PET.*
Testing for the presence volatile performance of volatile performance-enhancing drugs, such as nandrolone	gas-liquid chromatography/GLC / gas chromatography-mass spectrometry/GCMS *Allow HPLC / IR (spectroscopy).*

[2]

Award [2] for all four correct, [1] for two or three correct.

IB P31 An Chem HL 08s

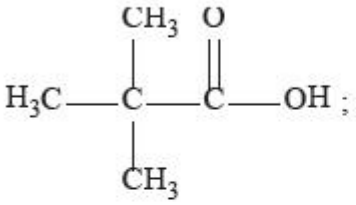
G1. (a) (i) (P) ultraviolet/uv **and** (Q) infrared/ir; *[1]*

(ii) microwaves; *[1]*

IB P32 An Chem HL 11s Q A2

(iii) (H of) COOH group; *[1]*

(iv) nine hydrogens in the same environment / $(CH_3)_3C-$(group); *[1]*

(v) $(CH_3)_3CCOOH$ / $(CH_3)_3CCO_2H$ /  ; *[1]*

(vi) *Number of peaks:* 2;
Ratio of peak areas: 1:9 / 9:1;
Splitting patterns: two singlets / no splitting; *[3]*

(vii) *Number of peaks:* 4;
Ratio of peak areas: 3:2:2:3;
Accept in any order.

Splitting patterns: two triplets **and** two quartets; *[3]*

IB P32 An Chem HL 14s Q A3

Penalize incorrect bond linkages (eg, CH_2–HO instead of CH_2–OH) and/or missing hydrogens once only in option at first occurrence.

(c) *Award [2] for all three correct, [1] for any two correct.*
m/z = 45 :
$COOH^+$/CO_2H^+ / $C_2H_5O^+$;

m/z = 17 :
OH^+;

m/z = 15 :
CH_3^+; *[2]*
Penalize missing + once only.

(d) $CH_3CH(OH)COOH$ / $CH_3CH(OH)CO_2H$; *[1]*
Allow full or condensed structural formula.

(e) $CH_2(OH)CH_2COOH$ / $HO(CH_2)_2CO_2H$; *[1]*
Allow full or condensed structural formula.

(f) (i) 102; *[1]*

IB P32 An Chem HL 09s

A2. (a) $C_2H_4O_2$; *[1]*

No mark for $(CH_2O)_2$.

(b) *m/z = 15*

CH_3^+;

m/z = 45

$COOH^+/CO_2H^+/HCOO^+/OCOH^+$; *[2]*

Penalize once if charges are missing.

(c) ethanoic acid/CH_3COOH / methyl methanoate/ $HCOOCH_3$; *[1]*

Accept acetic acid.

IB P31 An Chem HL 13w

2. (a) (i) 90;

$C_3H_6O_3^+$; *[2]*

Penalize missing positive charge of ion only once in (a).

(ii) $COOH^+$;

Accept $C_2H_5O^+$. *[1]*

Penalize missing positive charge of ion only once in (a).

(iii) CHO^+ / COH^+; *[1]*

Accept $C_2H_5^+/CH_3CH_2^+$.

Penalize missing positive charge of ion only once in (a).

IB P31 An Chem HL 13s Q A1

(c) (mass spectrum of) CH_3CH_2CHO contains peak at *m/z* = 29 / CH_3COCH_3 does **not** contain peak at *m/z* = 29;

(corresponding to) loss of C_2H_5 / $M_r - C_2H_5$ / CHO^+ / loss of CHO / M_r – CHO / $C_2H_5^+$;

OR

(mass spectrum of) CH_3CH_2CHO contains a (strong) peak at *m/z* = 57 / CH_3COCH_3 does **not** contain a (strong) peak at *m/z* = 57;

(corresponding to) loss of H / $M_r - H$ / $CH_3CH_2CO^+$; *[2]*

Penalize missing + once only in A1.

(d) *m/z = 71:* $CH_3CH_2CH_2CO^+$ / $C_3H_7CO^+$ / $C_4H_7O^+$;

Accept $CH_3COCH_2CH_2^+$.

m/z = 43: $CH_3CH_2CH_2^+$ / CH_3CO^+ / $C_3H_7^+$ / $C_2H_3O^+$; *[2]*

Penalize missing + once only in A1.

IB P31 An Chem HL 11w Q A3

(b) CH_3COOH :

peak at 45 due to $(COOH)^+$ / $(M_r - 15)^+$ due to loss of CH_3 ;

$HCOOCH_3$:

peak at 31 due to $(OCH_3)^+$ / $(M_r - 29)^+$ due to loss of HCO/CHO / peak at 29 due to $(HCO)^+$/$(CHO)^+$ / $(M_r - 31)^+$ due to loss of OCH_3 ; *[2]*

Penalize missing + sign once only.
Brackets not required around fragments for marks.

IB P31 An Chem HL 09w

A2. (a) (i) 88;
Do not award mark if units are given.

$C_4H_8O_2^+$; *[2]*

(ii) $CH_3CH_2^+$/$C_2H_5^+$ / CHO^+; *[1]*
Only penalize once for missing charge in (a) (i) and (ii).

(iii) $C_2H_3O_2$ produced has no charge / fragment produced after loss of C_2H_5 from molecular ion has no charge; *[1]*
Accept fragment(s) too unstable, fragment breaks up etc.
Do not accept answers with reference to $^{13}C/^{14}C$ isotopes and peak at m/z = 61.
Do not accept $C_2H_3O_2^-$ / $C_3H_7O^-$ does not exist.

IB P31 An Chem HL 12s Q A1

(c) (i) protons/H's in three different chemical environments / *OWTTE*;
2:1:1 ratio of protons/H's (in these environments) / *OWTTE*; *[2]*
Accept 4:2:2.

(ii) $HO–CH_2–CH=CH–CH_2–OH$ / $CH_2=C(CH_2OH)_2$;; *[2]*

IB P32 An Chem HL 14s Q A3

(b) three hydrogens in same (chemical) environment / CH_3/methyl (group); *[1]*

(f) (i) 102; *[1]*

(ii)

Ratio under each peak	*Range of chemical shift values / ppm*	*Splitting pattern*
3	0.9–1.0 (CH_3)	(3H) triplet
2	2.0–2.5 (CH_2)	(2H) quartet
2	3.8–4.1 (OCH_2)	(2H) quartet
3	0.9–1.0 (CH_3)	(3H) triplet

[3 max]

Award [3 max] for four correct rows.
Award [2 max] for any two or three correct rows and [1 max] for any correct row.

IB P32 An Chem HL 13s

A4. (a)

Peak	Hydrogen atom responsible
A	7;
B	4
C	5;
D	3;
E	2;
F	6;
G	1;

[6]

(b) (i) two/2; *[1]*

(ii) both are singlets / *OWTTE*; *[1]*

(iii) aspirin will have two (sharp) peaks / wider/greater absorption (due to two C=O groups);
ibuprofen will have one (sharp) peak / narrower/less absorption (due to one C=O group); *[2]*

IB P32 An Chem HL 12s

A3. (a) both 1-bromobutane and 2-bromobutane have four peaks;
(ratio of areas in) 1-bromobutane: 3:2:2:2;
(ratio of areas in) 2-bromobutane: 3:1:2:3; *[3]*
For second and third points accept correct ratios given in a different order.
Accept correct number of hydrogen atoms for each peak instead of area.

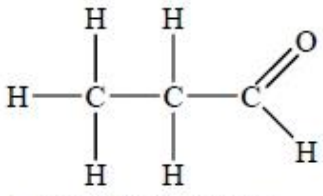
(b) *Number of peaks*:
1;

Splitting pattern:
singlet / it is not split; *[2]*

IB P32 An Chem HL 09s A3

(b) (i) absence of peak between 3200–3600 cm^{-1} /above 3000 cm^{-1}/peak for OH;
presence of peak between 1700–1750 cm^{-1} /peak for C=O;
absence of peak between 1610–1680 cm^{-1}/peak for C=C; *[2 max]*

(ii)



;

Accept CH_3CH_2CHO.

3:2:1; *[2]*
Ignore order
ECF if structure is incorrect only if its NMR spectrum contains three peaks.

(iii) triplet/1:2:1; *[1]*
ECF if structure is incorrect.

IB P32 An Chem HL 08s

G2. (a) 2; *[1]*

(b) (i) CH_3 0.9 (ppm);
CH_2 3.8 (ppm); *[2]*
Units are not required for mark.

(ii) 3 : 2 / 6 : 4; *[1]*

(iii) CH_3 triplet;
CH_2 quartet/quadruplet; *[2]*

(c) ^{1}H NMR of butan-2-one will have 3 peaks (whereas ethoxyethane has 2);
ratio of peaks for butan-2-one 3 : 2 : 3 (ethoxyethane 3 : 2 / 6 : 4);
butan-2-one has a singlet peak;
butan-2-one has a peak at $\delta = 2.1$ ppm; *[1 max]*
Award [1] for any above.

(d) tetramethylsilane / TMS;
to calibrate the instrument / as a reference / standard; *[2]*

IB P31 An Chem HL 13w

(b) (i) CH_3/methyl; *[1]*

(ii) $CH_3CH(OH)COOH$; *[1]*
Allow full or condensed structural formula.

(c) quartet means next C has 3 H atoms / is CH_3;
due to the CH group;
due to relative orientation of spinning nuclei/protons;
with relative probabilities of 1,3,3,1;
OH group results in no splitting (due to rapid proton exchange); *[3 max]*

IB P31 An Chem HL 13s

A3. (a) (ratio of) area under each peak / integration trace; *[1]*
Accept size of peak but not height of peak.

(b) $CH_3CH_2COCH_2CH_3$; *[1]*

(c) quartet / 1:3:3:1; *[1]*

IB P31 An Chem HL 12w

A3. (a)

Chemical shift / ppm	Number of hydrogen atoms
1.0–1.1	3
2.15	3;
2.4–2.5	2;

[2]

(b)

Chemical shift / ppm	Splitting pattern	Number of adjacent hydrogen atoms
1.0–1.1	triplet	2
2.15	singlet	0
2.4–2.5	quartet	3

[2]

Award [1] for both splitting patterns correct.
Award [1] for both number of adjacent hydrogen atoms correct.

(c) $CH_3COCH_2CH_3$; *[1]*

Accept more detailed formula.

IB P31 An Chem HL 12s Q A1

(d) tetramethylsilane/TMS;

Any of these for second mark:
strong single peak (as there are 12 protons in identical chemical environment);
absorbs upfield/away from most other protons/H's;
low boiling point/bp / volatile (so easily removed from sample);
not toxic / unreactive / does not interfere with sample; *[2 max]*

IB P31 An Chem HL 11w

A3. (a) *Similarities*: *[2 max]*
both have two peaks;
in the same/1:3 ratio;
both have only singlet peaks;

Difference:
CH_3COOH will have an absorption/chemical shift/δ in the range 2.0–2.5, ($HCOOCH_3$ will not) / $HCOOCH_3$ will have an absorption in the range 3.8–4.1, (CH_3COOH will not) / CH_3COOH will have an absorption in the range 9.0–13.0, ($HCOOCH_3$ will not); *[3]*

IB P31 An Chem HL 11s

A2. (a) *Compound:*
$CH_3–CH_2–CHO$;

Explanation: [1 max]
only this compound would give 3 peaks / *OWTTE*;
only this compound has H–atoms in 3 different chemical environments / *OWTTE*;
only this compound has protons in ratio 3:2:1 in each environment / *OWTTE*
only this compound would give a peak in the 9.4–10 ppm region / *OWTTE*; *[2]*

(b) triplet;
next to a carbon atom that is attached to two hydrogen atoms; *[2]*
Apply ECF.
CH_3COCH_3: singlet; no neighbouring H–atoms
CH_2=CH–CH_2OH: correct multiplicity and explanation for any peak.

IB P31 An Chem HL 10w Q A2

(iii) 3.76 ppm : CH_3O **and** 8.07 ppm : HCO ; *[1]*
Allow CH_3 for CH_3O.
Allow $RCOOCH_2$ and $RCOOCH_3$ for 3.76 ppm and RCHO for 8.07 ppm.

(iv) three hydrogens in same environment; *[1]*
Allow three times as many hydrogens in this environment as for the other peak.

(v) HCO_2CH_3 / $HCOOCH_3$; *[1]*

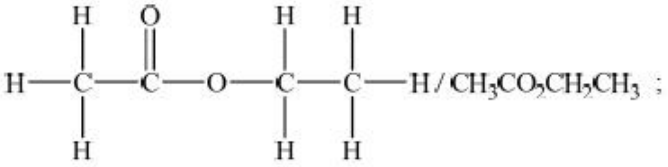
(vi) all (12) protons/hydrogens in same chemical environment (and hence gives 1 peak);
absorbs upfield/away from most other protons/H's;
low boiling point/bp / volatile / easily removed from sample;
not toxic;
highly unreactive (and hence does not interfere with sample) / inert; *[2 max]*

IB P31 An Chem HL 10s

A1. (a) (i) (2-)methylpropan-2-ol;
the (H atoms in the three) $–CH_3$ groups are responsible for the peak at 1.3 ppm;
the –O**H** hydrogen atom is responsible for the peak at 2.0 ppm; *[3]*
Accept explanation with suitable diagram.

(ii) (2-)methylpropan-1-ol;
the first peak (at 0.9 ppm) is due to the (H atoms in the) two $–CH_3$ groups (bonded to the second carbon atom) / $(C\mathbf{H}_3)_2CHCH_2OH$;
the peak at 3.4 ppm is due to the (H atoms in the) $–CH_2–$ group / $(CH_3)_2CHC\mathbf{H}_2OH$;
both of the peaks are split into a doublet as there is one H atom bonded on the adjacent carbon atom / *OWTTE*; *[4]*
Accept explanations with suitable diagram.

IB P31 An Chem HL 09w Q A2

(c) (i)  / $CH_3CO_2CH_2CH_3$; *[1]*

(ii)

Peak	Chemical shift / ppm	Relative peak	Splitting pattern
First	20	3	Singlet
Second	4.1	2	Quartet
Third	0.9 –1.0;	3;	Triplet;

ECF from structure in (c)(i). *[3]*

(iii) (quartet means) neighbouring C;
has 3 H atoms/protons; *[2]*
Award [1] for stating CH_3CH_2.
Award [2] for stating CH_3CH_2 group and indicating number of protons.

IB P31 An Chem HL 09w

A1. (a) (i) radiowaves; *[1]*

(ii) strong single peak as there are 12 protons in identical chemical environment;
absorbs upfield/away from most other protons/H's;
low boiling point/bp / volatile (so easily removed from sample);
not toxic / unreactive / does not interfere with sample; *[1 max]*

IB P31 An Chem HL 09s

A2. (a) D could be $CH_3CH_2COOCH_3$ or $CH_3COOCH_2CH_3$;
this is because there are 3 peaks / 3:2:3 ratio;
explanation of splitting into a singlet a triplet and a quartet;
methyl propanoate/$CH_3CH_2COOCH_3$ is correct isomer because of higher chemical shift value of singlet (3.6 instead of 2.0–2.5); *[4]*

IB P31 An Chem HL 08w Q G1

(d) $-CH_3$ (of the ethyl group – CH_2CH_3); *[1]*

(e) (the three hydrogen atoms of the methyl group are) split by/spin spin coupling with the two hydrogen atoms on the adjacent $-CH_2-$ group; *[1]*

(f) integration pattern: only one hydrogen atom in that environment;
splitting: not split so no H atoms on adjacent carbon atoms;
the absorption is due to the H of $HCOOC_2H_5$; *[3]*

IB P31 An Chem HL 08w Q G1

(d) $-CH_3$ (of the ethyl group – CH_2CH_3); *[1]*

(e) (the three hydrogen atoms of the methyl group are) split by/spin spin coupling with the two hydrogen atoms on the adjacent $-CH_2-$ group; *[1]*

(f) integration pattern: only one hydrogen atom in that environment;
splitting: not split so no H atoms on adjacent carbon atoms;
the absorption is due to the H of $HCOOC_2H_5$; *[3]*

(ii) only two absorptions (not three);
two equal areas/heights (three protons for each absorption); *[2]*

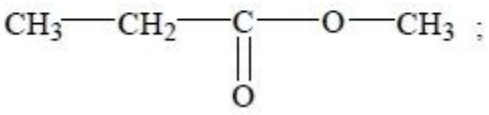
(iii) there will just be two singlets / there is no splitting; *[1]*

IB P31 An Chem HL 08s Q G2

(c) (B ratio) 3:3:2 *(any order)*;
(B splitting pattern) 1 singlet + 1 triplet + 1 quartet;
(C ratio) 6:1:1 *(any order)*;
(C splitting pattern) 1 singlet + 1 doublet + 1 quartet/septet; *[4]*

If B splitting pattern given as 1,3,4 (any order) do not award mark but use ECF and award mark for C splitting pattern if given as 1,2,7/4 (any order).

(d) (peaks with) different δ values/chemical shifts / different shielding; *[1]*
Do not accept 'different ppm values'

(e)  ; *[1]*