GCE

Chemistry

User guide

Edexcel Advanced Subsidiary GCE in Chemistry (8CH01)

Edexcel Advanced GCE in Chemistry (9CH01)

Internal Assessment of Practical Skills

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This specification is Issue 2. Key changes are sidelined. We will inform centres of any changes to this issue. The latest issue can be found on the Edexcel website: www.edexcel.org.uk

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Contents

Introduction

This *User guide* has been written for students to help them in preparing for the tasks that are part of the internal assessment of practical skills. Teachers may also find this information helpful when preparing students for the assessment activities. The material contained in the booklet does not extend the specification content, but aims to help students to succeed in the assessment activities by:

- explaining in more depth what is required in carrying out the activities, making observations and measurements with appropriate precision and recording these methodically
- advising them how to interpret, explain, evaluate and communicate the results of the activities clearly and logically using the relevant chemical knowledge, understanding and appropriate specialist vocabulary.

1 — The scheme of assessment

1.1 Activities

At both AS and A2 Level the skills being assessed in the activities are:

a	General practical competence (GPC)	(verification)
b	Qualitative observation	(14 marks)
c	Quantitative measurement	(14 marks)
d	Preparation	(12 marks)

The maximum mark available at both AS and A2 Level is 40.

Students will have their practical skills assessed by carrying out the assessment activities on a number of occasions throughout the course. The assessment activities are set by Edexcel.

For activity **a,** the teacher is required to confirm that students have completed a range of practicals over the whole year and developed their laboratory skills. Students must have carried out at least five practicals in class. The practicals that the students complete must cover the three areas of physical, organic and inorganic chemistry. These five practicals can be either core practicals, or suitable alternatives.

The marks for activities **b**, **c** and **d** are awarded following the teacher's application of the mark schemes that accompany each assessed activity. Students need only carry out one exercise for each of activities **b**, **c** and **d**. However they may carry out more than one. In this case, only the highest mark for each activity will count towards the final mark out of 50.

At A2 there is the option of completing a **multi-stage** experiment at A2, which consists of activities **c** and **d** together in a longer practical, which is worth 26 marks.

Teachers have the option of marking these activities or having them marked by Edexcel.

1.2 Conditions under which assessments are to be carried out

The practical assessment activities must be carried out under controlled conditions that guarantee that students produce individual work. This includes those activities that involve the processing of results. Students must not consult with each other during the activities. Some activities can be completed in a laboratory session of approximately one hour. When an activity has to be carried over to a following session students must not remove any materials, including results and instruction sheets, from the laboratory. Instead, these must be collected by the teacher and reissued at the beginning of the next session when the activity is to be completed.

1.3 Materials allowed when carrying out assessment activities

Each activity has a cover sheet and a student brief giving full instructions for carrying out the activity and the questions based on it.

During the activity students **must not refer to books and notes** although the data booklet is required for some exercises. This *User guide* must **not** be used as a reference when carrying out the internal assessment tasks.

1.4 Health and safety

Students must follow the health and safety rules which normally operate in their chemistry laboratories, including the following:

- eye protection must always be worn
- laboratory coats must be worn when appropriate
- plastic gloves must be worn when supplied for a particular exercise
- all substances should be regarded as being potentially toxic and hazardous
- HazChem labels (eg flammable) should be read and appropriate precautions (eg keep liquid away from flame) taken
- all substances spilled on the skin should be rinsed off immediately
- chemicals must never be tasted
- gases and vapours should never be smelt unless the question instructs the students to do so, and then this should be done only with great care.

2 — Activity b: Qualitative observation

Activity **b** will be assessed by tasks that include a number of tests to be carried out, usually on a test tube scale. The instructions for each test will include details on quantities to be used, whether heat is required and whether excess reagent should be added. The reagents used for the tests will be limited to those included in the specification. Similarly, unknowns will be limited to compounds containing the ions, elements and organic compounds with the functional groups listed in the specification. As part of a task to identify an organic unknown, spectroscopic data may be included for students to analyse. Other physical data such as melting temperatures may also be given.

These qualitative observation tasks will change each year.

2.1 Recording observations

After a student has carried out each test, as instructed in the task, they must communicate the results by giving a brief description of what has been observed. Possible changes that can occur during tests are listed below, along with **examples** of what students should write in the observation boxes.

Possible change	Example of observation
a colour change in solution	yellow solution turns orange
the formation of a precipitate	white precipitate (ppte is allowed) is formed
a precipitate dissolves in excess reagent	precipitate dissolves in excess to form a green solution
a gas is evolved	bubbles of gas or effervescence
tests on a gas	the gas turned damp red litmus paper blue
flame tests	yellow flame
a solid dissolves	dissolves to give a blue solution
a reaction is exothermic	the mixture becomes hot
a reaction is endothermic	the mixture feels cold
a coloured solution loses its colour	the yellow solution turns colourless

There are a number of common mistakes which students make when recording their observations. The following should be avoided.

- Referring to ‘layers’ in test tubes. Almost certainly the presence of layers is due to inadequate mixing of the reagents. The exception to this is when an organic liquid is mixed with an aqueous solution, or with water, in which case ‘layers’ may be a valid observation.
- Describing colours with elaborate adjectives such as brown-black or blue-green. Marks are awarded for simple descriptions of the colours of solutions and precipitates, such as black or blue, even if there is a trace of a second colour.
- Stating that a gas is evolved without making an observation such as bubbles or effervescence.

- Using clear instead of colourless for a solution. All solutions are clear even if coloured, eg copper sulfate solution is clear but coloured blue, whereas sodium sulfate solution is colourless.

2.2 Making inferences from observations

The purpose of asking students to make inferences from their observations is to test their knowledge, understanding and evaluation of the chemistry which leads to the observations.

Activities include asking students to identify precipitates or gases formed in a test and which are recorded as an observation. Also, students could be asked to identify the unknown compound following a series of tests.

In some cases the test may be enough to enable students to suggest the identity of a particular ion or functional group, but in others a number of possibilities may exist as a result of a single test.

Example 1

The addition of aqueous ammonia to an inorganic compound produces a green precipitate. The inference from this test alone should be iron(II) hydroxide, chromium(III) hydroxide or nickel(II) hydroxide.

Example 2

In an organic analysis, a compound produces an orange precipitate with 2,4–dinitrophenylhydrazine. The expected inference would be that the unknown compound is an aldehyde, ketone or carbonyl compound. If a following test shows that the compound is an aldehyde then the inference still stands, as this was valid on the basis of the 2,4–dinitrophenylhydrazine test. If more is known about the compound, for example its molecular formula and the fact that it cannot be oxidised, then it may be that the compound can be identified as a result of the 2,4–dinitrophenylhydrazine test.

3 — Activity c: Quantitative measurement

Activity **c** will be assessed through tasks that involve using apparatus to make measurements and to process the results, to draw conclusions and evaluate the procedure.

Quantitative activities could involve:

- a volumetric analysis task
- a simple thermochemistry task
- a task to follow the rate of a reaction.

3.1 Accuracy

Unless an activity instructs students differently, they should assume that readings from equipment and apparatus should be made with the following precision.

Apparatus	Precision of reading
pipette	one volume only of 25.0 cm^3
burette	each volume to the nearest 0.05 cm^3 mean titre to 0.05 cm^3 or to the second decimal place
measuring cylinder	a 100 cm^3 size to 5 cm^3, a 10 cm^3 size to 1 cm^3
balance	readings should be made to 0.01 g or 0.001 g depending on the precision of the balance
timers	normally read to the nearest second.
thermometers	0 to 100°C thermometers should be read to the nearest 1.0°C 0 to 50°C thermometers to an accuracy of at least 0.5°C

The following points are important.

- When students record readings they should include the appropriate number of decimal places. For example a burette reading of exactly 24.7 cm^3 should be recorded in a results table as 24.70 cm^3.
- When titres have to be averaged, the mean should be expressed to either the nearest 0.05 cm^3 or to the second decimal place. Eg if a student records four titres as listed below the mean should be calculated as:

$$\frac{26.50 + 26.25 + 26.60 + 26.65}{4} = 26.5\ \text{cm}^3$$

- If the student decides to ignore the second titre and to average the remaining three:

$$\frac{26.50 + 26.60 + 26.65}{3} = 26.583$$

which should be recorded as 26.60 cm^3 or as 26.58 (to the second decimal place).

- Students should try to obtain **at least two** titres within 0.20 cm^3, or better, of each other and average these to obtain a mean titre. Students should make it clear which titres have been used to obtain a mean.
- A final result should only be given to the same number of significant figures as is suggested in the exercise. For example a task to find a ΔH value may involve a weighing of 1.56 g and a temperature rise of 7.5 °C. A student who calculates a value of ΔH from these figures may obtain a value of 195.6843 on a calculator but this should be finally recorded as 200 kJ mol^{-1}, although 196 kJ mol^{-1} may also be acceptable.
- Units should always be included with a quantitative result.

A significant proportion of the marks awarded for a quantitative measurement activity will be for **accuracy.** These marks will be awarded by comparing the student's results with an expected value.

3.2 Errors

Students should appreciate that any piece of equipment (burette, pipette, thermometer, balance) used in a quantitative exercise has an uncertainty associated with its use. Even if the equipment is used carefully, the uncertainty leads to an error in the reading and in the final result.

Eg a balance has an uncertainty of 0.01 g when read to the second decimal place. A reading of 2.64 g recorded in an experiment has an error of:

$$\frac{0.01}{2.64} \times 100\% = 0.38\%$$

The following points will apply.

1 The error in the reading = $\dfrac{\text{the uncertainty in the equipment}}{\text{the reading}} \times 100\%$

2 Students should:

- calculate the error involved in using a particular piece of equipment and state what effect this has on the overall accuracy of the activity
- understand that the percentage error would be affected by the magnitude of the quantity being measured. There will be a greater error in weighing a mass of 2.64 g than in weighing 8.64 g using the same balance.

3 Only a simple treatment of errors is needed and students will not be asked to combine errors.

3.3 Calculations

Usually calculations will be structured. Students will be taken/guided through a series of steps leading to a final answer. Since most of the marks for these steps will be for use of a correct method, rather than for the numerical answer, it is important that students include their workings even if these seem to be trivial. Marks cannot be awarded for an incorrect answer without workings, but a correct method followed by an incorrect answer can often receive credit. Units, if appropriate, should always be included with a quantitative result.

3.4 Graphs

For some activities students will need to treat their readings graphically.

The following are some useful points for students to consider when drawing graphs.

- Put the dependent variable, the quantity being measured (eg temperature), on the y–axis. And the pre-determined quantity (eg volume of solution) on the x–axis.
- Choose the scales so that the results are spread out as far apart as the size of the grid allows, but this should not be at the expense of using a sensible scale, eg using 1 cm on the axis to represent 3 or 4 units might spread the readings better than using 1 cm to represent 5 units, but the scale would be hard to read.
- The origin (0,0) does not need to be included on either scale if it is not relevant,
- For example if temperature readings between 21.0°C and 39.0°C are to be plotted there is no need to begin the y–axis at 0. Rather it could be scaled from 20.0°C to 40.0°C.
- Clearly label the axes with the quantity being plotted (eg time) and its units (eg minutes).
- Join the points plotted with a continuous straight line or smooth curve. Since the readings are all subject to experimental error the line drawn may not necessarily pass through every point. Points should never be joined by a series of short, straight lines.

3.5 Assumed laboratory skills

The instructions for carrying out a quantitative measurement activity will include the essential points for the particular task. For example:

- which chemicals to use
- the quantities needed
- the sequence of steps in the method
- the readings to be taken.

The assessment activities will assume that students have developed a range of routine practical skills in their course leading up to the exercise. Instructions may not, therefore, include every step needed to gain accurate readings.

Examples of normal laboratory procedures which may **not** be referred to in the instructions include:

- burettes, pipettes and measuring cylinders should be rinsed with the solution they are to contain
- a pipette filler should always be used with a pipette
- conical flasks and volumetric flasks should be rinsed out with distilled water
- a burette should be read at eye level
- a thermometer bulb must be held in the centre of a solution when temperature readings are taken
- care should be taken not to lose drops of a solution when thermometers or stirring rods are removed from it

- containers may need to be labelled if this has not already been done
- care should be taken as to where apparatus is placed on the bench, eg temperature measurements should not be taken in apparatus standing next to a Bunsen burner, in a patch of sunlight or in a strong draught.

4 — Activity d: Preparation

Activity **d** is assessed through tasks in which students follow a procedure to prepare and, in some cases, purify an inorganic or organic compound. Marks are awarded for the student's ability to follow laboratory procedures and to use apparatus competently and safely.

Preparations can include some of the following laboratory procedures:

- distillation
- heating under reflux
- filtration, including under reduced pressure
- purification by washing in a separating funnel
- solvent extraction
- drying
- boiling and melting temperature determination
- crystallization and recrystallization.

Following some preparations students will be asked to calculate the maximum mass of product and a percentage yield.

5 — Activity c+d: Multi-stage experiment

Instead of completing activities c and d separately, students could complete a multi-stage experiment, which combines the two. This would be a longer practical which covers all of the same aspects of c and d mentioned above. This would most likely be completed in two laboratory sessions and students would have to hand in their notes and results at the end on one session, and receive these back when they complete the practical in the second session.

Reference section

A — Inorganic compounds and elements

1 Appearance

- Coloured crystalline substances are usually hydrated salts of transition metals. The colour of the solid substance may provide evidence for its identity.

Colour	Possible transition metal ions in salt
blue	copper(II)
pale green	iron(II)
green	copper(II), chromium(III), nickel(II)
purple	manganate(VII)
brown	iron(III)
pink	manganese(II)
yellow	chromate(VI)
orange	dichromate(VI)

- The colours of transition metal ions in dilute, aqueous solution are shown in the table below.

Colour	Possible identity
blue	copper(II)
green	iron(II), chromium(III), nickel(II)
brown / yellow	iron(III)
pale pink	manganese(II)
yellow	chromate(VI)
orange	dichromate(VI)
purple	manganate(VII)
colourless	zinc(II)

2 Flame tests

- To carry out a flame test, a clean nichrome wire is used to mix a sample of a solid with one drop of concentrated hydrochloric acid. The wire is held in progressively hotter parts of a non-luminous Bunsen flame.

Flame colour	Inference
yellow	sodium ion
lilac	potassium ion
yellow-red*	calcium ion
red*	lithium or strontium ion
pale green	barium ion

* Further tests would be needed to distinguish these ions.

3 Heating

- Gases or vapours may be evolved on **heating** a solid compound.

Gas or vapour	Possible source
carbon dioxide	carbonates of metals other than group 1
oxygen	group 1 nitrates (other than Li)
oxygen and nitrogen dioxide	nitrates (other than Na or K)
water	hydrated salts

4 Recognition and identification of common gases

Gas	Observations
oxygen	colourless gas which relights a glowing splint
carbon dioxide	colourless gas which gives a white precipitate with limewater (calcium hydroxide solution)
ammonia	colourless gas which turns moist red litmus paper blue and forms white smoke with hydrogen chloride
nitrogen dioxide	brown gas*
hydrogen	colourless gas which ignites with a 'pop'
hydrogen chloride	steamy fumes on exposure to moist air, acidic and forms white smoke with ammonia
chlorine	pale green gas which bleaches moist litmus paper
bromine	brown gas*
iodine	purple vapour
water vapour	turns blue cobalt chloride paper pink

* Bromine dissolves in organic solvents to form a brown solution whereas nitrogen dioxide is insoluble.

5 Action of dilute acids

- When dilute sulfuric or hydrochloric acid is added to a substance a gas may be evolved or there may be a colour change in the solution.

Action of acid	Possible source
carbon dioxide evolved	carbonate
hydrogen evolved	a metal
yellow solution turns orange	chromate(VI) to dichromate(VI)
sulfur dioxide evolved and pale yellow precipitate formed	thiosulfate

6 Tests for oxidizing and reducing agents

Reducing agents usually:

decolourise aqueous acidified potassium manganate(VII) and

may also turn aqueous, acidified potassium dichromate(VI) from orange to green.

Reducing agents include:

iron(II) ions

iodide ions

hydrogen peroxide.

Oxidizing agents usually:

liberate iodine as a brown solution or black solid from aqueous potassium iodide. Iodine solution gives a blue-black coloration with starch.

Oxidizing agents include:

acidified manganate(VII) ions

acidified dichromate(VI) ions

hydrogen peroxide

copper(II)ions

aqueous chlorine

aqueous bromine.

7 Hydrogen peroxide solution

Aqueous hydrogen peroxide (H_2O_2) can act as both an oxidizing and a reducing agent often with the evolution of oxygen, although this may be unreliable.

Observation on adding H_2O_2	Inference
brown precipitate	manganate(VII), brown precipitate is MnO_2
purple solution is decolourised	manganate(VII) in acid solution
pale green solution turns yellow	iron(II) to iron(III) in acid solution
green precipitate turns brown	iron(II) hydroxide to iron(III) hydroxide
green alkaline solution goes yellow	chromium(III) to chromate(VI)
brown solution or black precipitate	iodine from iodide in acid solution

B — Precipitates

When two aqueous solutions are mixed together and an insoluble compound is formed this is known as a **precipitate** not a suspension. The observation that a precipitate is formed should always be accompanied by the colour of the precipitate, even if this is white. Some reagents should be added until they are in excess. This may result in a precipitate forming then dissolving in excess reagent.

1 Sodium hydroxide solution

- When dilute sodium hydroxide (NaOH) solution is added to a solution containing a metal ion a precipitate of the insoluble hydroxide, eg $Mn(OH)_2$, is usually formed. Precipitates which are amphoteric hydroxides will dissolve in excess sodium hydroxide to give a solution containing a complex ion, eg $[Cr(OH)_6]^{3-}$.
- Students should assume that aqueous sodium hydroxide should be added until it is **in excess** even if this is not explicitly stated in the instructions.

Observation on adding dilute NaOH	Observation on adding excess dilute NaOH	Likely ion
green precipitate	precipitate dissolves to a green solution	chromium(III)
off-white precipitate which darkens on exposure to air	precipitate is insoluble	manganese(II)
green precipitate which turns brown on exposure to air	precipitate is insoluble	iron(II)
brown precipitate	precipitate is insoluble	iron(III)
green precipitate	precipitate is insoluble	nickel(II)
blue precipitate	precipitate is insoluble	copper(II)
white precipitate	precipitate dissolves to a colourless solution	zinc(II)
white precipitate	precipitate is insoluble	magnesium, barium, strontium, calcium
no precipitate		sodium, potassium
no precipitate but ammonia evolved on warming		ammonium

2 Ammonia solution

- Dilute aqueous ammonia (NH_3), when added to a solution containing a cation, will form the same hydroxide precipitate as dilute sodium hydroxide solution, eg $Mn(OH)_2$. Excess aqueous ammonia may dissolve the precipitate to form a complex ion, eg $[Cu(NH_3)_4(H_2O)_2]^{2+}$.
- Students should assume that aqueous ammonia must be added until it is **in excess**.

Observation on adding dilute aqueous NH_3	Observation on adding excess dilute aqueous NH_3	Likely ion
green precipitate	precipitate is soluble to give green solution	chromium(III)
off-white precipitate	precipitate is insoluble	manganese(II)
green precipitate turning brown	precipitate insoluble	iron(II)
brown precipitate	precipitate insoluble	iron(III)
green precipitate	precipitate dissolves to give blue solution	nickel(II)
blue precipitate	precipitate dissolves to give deep blue solution	copper(II)
white precipitate	precipitate dissolves to give colourless solution	zinc(II)
white precipitate	precipitate is insoluble	magnesium

3 Barium chloride solution

- Aqueous barium chloride forms precipitates of insoluble barium salts with a number of anions but is usually used as the test for the sulfate, SO_4^{2-}, ion. Aqueous barium chloride is usually used with dilute hydrochloric acid.

Anion	Precipitate		Addition of dilute HCl
	colour	formula	
sulfate	white	$BaSO_4$	precipitate is insoluble
sulfite	white	$BaSO_3$	precipitate dissolves
carbonate	white	$BaCO_3$	precipitate dissolves with effervescence

If dilute hydrochloric acid is added to the anion solution before aqueous barium chloride then only the sulfate will form as a precipitate.

4 Silver nitrate solution

- Aqueous silver nitrate is commonly used to test for the presence of halide ions in solution. Anions which would interfere with the test (eg carbonate) are removed by adding dilute nitric acid before the aqueous silver nitrate.
- The identity of a halide may be confirmed by the addition of aqueous ammonia, (NH_3), both dilute and concentrated.
- Silver halides which dissolve in ammonia do so to form a colourless solution of the complex ion, $[Ag(NH_3)_2]^+$.

Anion	**Precipitate**		**Addition of aqueous NH_3**	
	colour	**formula**	**dilute**	**concentrated**
chloride	white	AgCl	soluble	
bromide	cream	AgBr	soluble in excess	soluble
iodide	yellow	AgI	insoluble	insoluble

5 Concentrated sulfuric acid

- When a few drops of concentrated sulfuric acid (H_2SO_4) are added to a solid halide the observed reaction products may be used to identify the particular halide ion present. **This is a potentially hazardous reaction.**
- **It must be carried out on a small scale and in a fume cupboard.**
- The products in brackets will not be observed since they are colourless gases. The halide ion may be identified without the need to test for these gases. **No attempt should ever be made to detect these gases by smell.**

Halide	**Observations on adding concentrated H_2SO_4**	**Observed reaction products**
chloride	steamy fumes, vigorous reaction	HCl
bromide	steamy fumes, brown vapour, vigorous reaction	HBr, Br_2 (SO_2)
iodide	steamy fumes, black solid, purple vapour, yellow solid, vigorous reaction	HI, I_2, S, (H_2S)

C — Organic compounds

Students will always be told if a compound, or mixture of compounds, to be identified is organic. Often the molecular formula, or the number of carbon atoms in a molecule, of a compound will be given. Chemical tests may be followed by spectroscopic information.

1 Appearance

Simple organic compounds are usually colourless liquids or white solids. It is unlikely that appearance alone will provide firm evidence for identification.

2 Solubility

Solubility of compound	Possible identity	pH of solution	Possible identity
dissolve in water	simple alcohols, simple carboxylic acids, propanone, simple aldehydes, simple amines and their salts	above 7	amines
		below 7	carboxylic acids, phenols
dissolve in dilute acid but may not dissolve in water	amines		
dissolve in aqueous alkali but may not dissolve in water	carboxylic acids, phenols		

3 Ignition

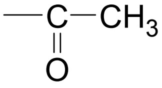
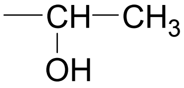
Igniting an organic unknown on a crucible lid may help in identifying it.

Observation	Possible inferences
burns with a smoky flame	aromatic, unsaturated eg alkene
burns with a clean flame	saturated low molar mass compound
no residue	most lower molar mass compounds

4 Chemical tests

The details of how these tests are to be carried out will be included in the instructions to students in the assessment activities.

Test	Observation	Inference
warm with acidified potassium dichromate(VI)	orange to green solution	primary or secondary alcohol, aldehyde
shake with bromine water	yellow solution is decolorised	alkene
	if white precipitate also formed	phenol
warm with aqueous sodium/potassium hydroxide, acidify with dilute nitric acid then add aqueous silver nitrate	precipitate: white cream yellow	halogenoalkanes: C–Cl C–Br C–I
phosphorus(V) chloride	steamy fumes of HCl that turn damp blue litmus paper red	OH group in alcohols and carboxylic acids
2,4–dinitrophenylhydrazine solution	orange precipitate	$C=O$ group in aldehydes and ketones
boil with Fehling's or Benedict's solution	blue solution gives red precipitate	aldehyde
warm with ammoniacal silver nitrate (Tollens' reagent)	silver mirror	aldehyde
sodium or potassium carbonate or hydrogencarbonate solution	effervescence	carboxylic acid
add a small piece of sodium	effervescence (bubbles), sodium dissolves, white solid formed	alcohol, phenol or carboxylic acid
warm with carboxylic acid and a few drops of concentrated sulfuric acid	ester smell, eg glue-like	alcohol

Test	Observation	Inference
sodium nitrite and dilute hydrochloric acid followed by an alkaline solution of phenol in ice-cold conditions	orange precipitate	aromatic amine
iodine in alkaline solution	pale yellow precipitate	methyl ketone or ethanal,  $-\underset{\underset{O}{\|}}{C}-CH_3$ methyl secondary alcohol or ethanol  $-\underset{\underset{OH}{\mid}}{CH}-CH_3$

D — Spectroscopy

Modern instrumentation plays a vital role in the characterisation and identification of molecules and ions. The sections which follow will enable interpretation of the data likely to be presented to students.

1 Mass spectrometry

Simplified mass spectra will be given which may be interpreted in two main ways.

1 The value of the compound's relative molar mass may be obtained from the *m*/*e* value of M^+, the molecular ion. This will have the highest value of *m*/*e*. This need not necessarily be the 'base' peak, which is simply the most abundant ion. Questions will be set in such a way that students will not be confused by the presence of a line due to the (M + 1) ion.

2 The fragmentation pattern of the spectrum gives useful information about the structure of the molecule. For example, a peak at *m*/*e* 29 is likely to be due to the presence of a C_2H_5 group in the molecule. Students are reminded that, when asked, they should give displayed structures for fragments, which must carry a positive charge also.

2 Infrared spectroscopy

This is a very powerful non-destructive technique which provides information regarding the nature of covalent bonds within the molecule.

Students should look at the most intense absorptions to quickly gain structural clues. Table 1 provides sufficient details to enable the principal bands to be assigned. Students should remember that absorption frequency is affected by the chemical environment and that absorption may take place outside the range given.

The connection between structures should be recognised. For instance, an alcohol [O-H] stretch will be accompanied by a [C-O] stretch.

Please see the *Data booklet* for specific IR spectroscopy data.

3 Nuclear magnetic resonance (nmr)

Nuclear magnetic resonance spectra may be included as part of an investigation into structure. Spectra will be high resolution with possible spin–spin coupling displayed.

Please see the *Data booklet* for specific nmr data.

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