ChemFactsheet

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Organic Analysis I : Infrared Spectroscopy

Before working through this Factsheet you should:

- Have a good knowledge of the organic chemistry covered at AS and A2 level.
- Understand covalent bonding.
- Be able to recognise functional groups within organic structures.

After working through this Factsheet you will:

- Be able to interpret simple Infrared spectra.
- Have a basic understanding of how an infrared spectrometer works.

The A2 syllabus requires candidates to be able to interpret simple infrared spectra. At first glance this can appear to be a daunting task - the spectra themselves look complex, and background reading about how the spectra are produced can sometimes be confusing.

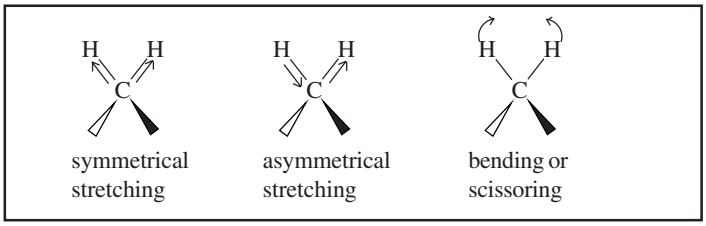
Do not fear infrared spectra - they are a tool to help chemists determine the structure of organic chemicals. With a little experience and use of any data supplied in an exam paper, scoring marks on questions involving IR spectra is not as difficult as it may seem.

In this Factsheet the workings of the infrared spectrometer will be briefly outlined - look to a textbook for a more detailed description if you are interested. The main focus of the Factsheet is to give candidates the necessary experience of IR spectra, and the expertise to pick up some valuable exam marks.

Introduction

Infra-red spectroscopy depends on the fact that infrared radiation is **absorbed** by certain molecular bonds and causes them to vibrate vigorously. These vibrations involve stretching or bending (Fig 1).

Fig 1. Symmetrical, asymmetrical, bending effects

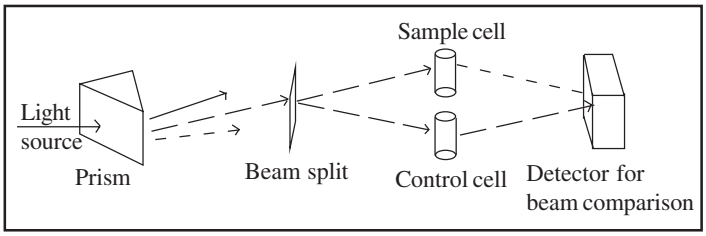


Different bonds absorb IR of different wavelengths and frequencies, e.g. C=O absorbs IR of a different wavelength to O-H.

By looking at the frequencies at which a substance absorbs IR radiation, we can therefore gain an idea of the bonds in it.

The apparatus used in this form of analysis, an infrared spectrometer, is based on a split-beam mechanism (Fig 2).

Fig 2. Infrared spectrometer



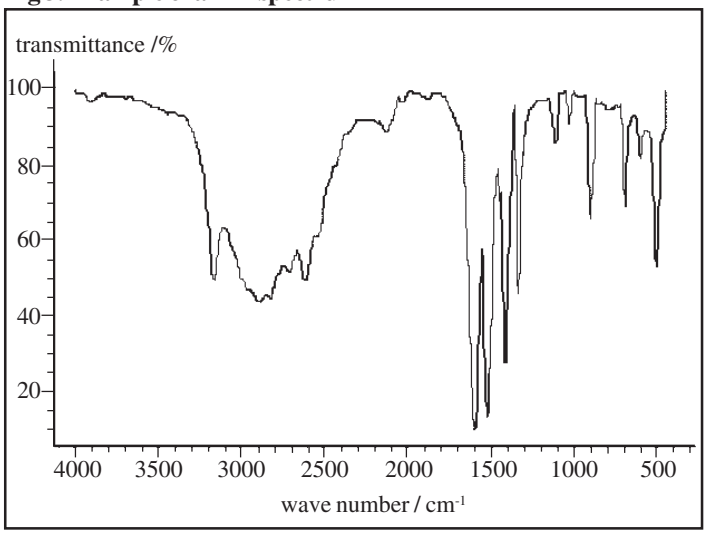
The amount of IR radiation absorbed at different wavelengths by the sample chemical is compared with a blank sample cell and quoted as a percentage.

If a sample absorbs IR at a certain frequency and wavelength, the IR will not pass through the compound to the detector, so a low transmittance % will be recorded.

Spectra

An example of an IR spectrum is shown below (fig 3).

Fig 3. Example of an IR spectrum



Note the axis labels:

- wavenumber (cm^{-1}) (x-axis)
- transmittance (a percentage) (y-axis)

The wavenumber is related to the wavelength of the IR absorbed:

$$\text{Wavenumber} = \frac{1}{\text{Wavelength}}$$

The transmittance shows the percentage of the IR that passes through the sample cell - so the lower it is, the more is absorbed.

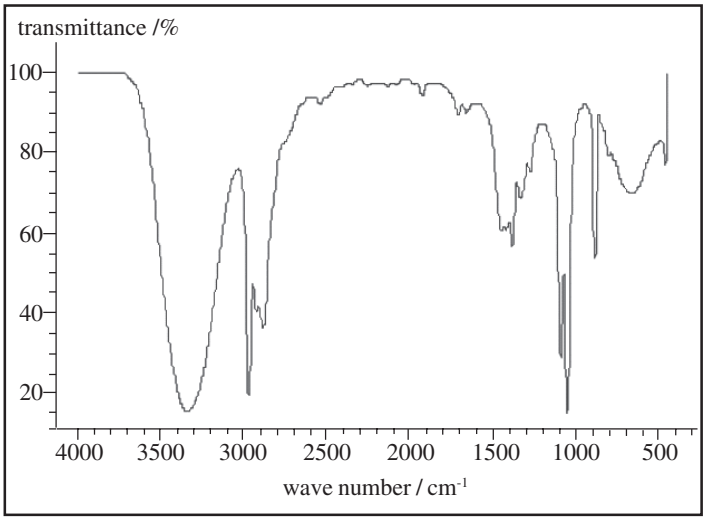
Here is a data table showing some different IR absorption ranges of different bonds:

Bond	Wavenumber Range (cm^{-1})	
C-O	1000 - 1300	
C=O	1650 - 1750	
C-H (alkanes)	2850 - 3000	
C-H (alkenes)	3000 - 3100	
O-H	2500 - 3500	broad peaks due to H-bonding
N-H	3300 - 3500	

Such data was compiled by comparing the IR spectra of related compounds. Note that bonds (such as C-H) will absorb slightly different wavelengths depending on the surrounding atoms. This means that it is impossible to assign a precise wavenumber to a bond. Nevertheless, we can identify bands or ranges corresponding to specific bonds, as shown in the data table.

For the following IR spectrum of an 'unknown' organic compound, we can assign different absorption peaks to particular bonds (using the data table) and gain some information about the content and structure of the sample compound (Fig 4).

Fig 4. IR spectrum of unknown organic compound



Peak	Assigned Bond
3100 - 3500 cm^{-1}	O-H
2800 - 3000 cm^{-1}	C-H
1050 - 1100 cm^{-1}	C-O

Note that this information alone does not tell us what the unknown chemical is, but helps to build a picture. We now know the following about the sample:

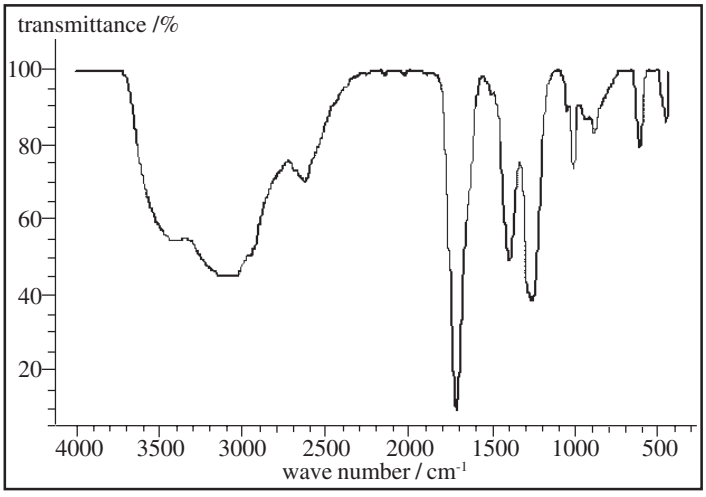
- Not a carbonyl or carboxylic acid (no C=O).
- Not an amine, amide or amino acid (no N-H).
- O-H, C-O and C-H bonds are present.

The spectrum is actually that of ethanol, so all of the above-deduced information is correct.

***Exam Hint**: Look at the shape of the broad O-H absorption peak - it is very distinctive and easy to spot (now you know what you are looking for!).*

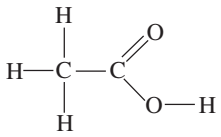
The peaks given by O-H and N-H are usually broad owing to hydrogen bonding.

Now look at this next spectrum and 'assign' the major peaks:



Peak	Assigned Bond
2500 - 3500 cm^{-1}	Broad O-H peak, characteristic shape
1700 - 1750	C=O
1250 - 1300	C-O

The spectrum is in fact that of ethanoic acid, so the above bonds are present:

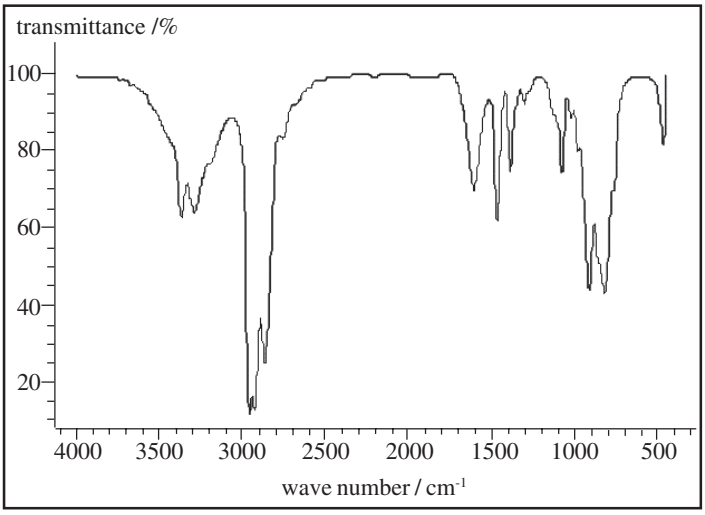


***Remember** that assigning peaks in IR spectra is not an 'exact science', instead careful use of a data table and common sense is required.*

***Exam Hint**: Ignore 'interference peaks', or 'weak absorption peaks', and focus on strong peaks where transmittance drops to below 70%.*

Assign peaks for the following spectrum (Fig 7):

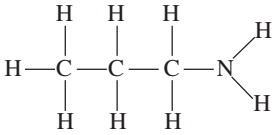
Fig 7.



Peak	Assigned bond
3300 - 3500 cm^{-1}	Broad N-H peak, 'double pronged' shape
2800 - 3000 cm^{-1}	C-H

There are no other **significant** peaks that **correlate with the data table**.

The spectrum is that of **propyl amine**



As mentioned above, the shapes of N-H peaks and O-H peaks are different, so usually can be told apart despite them being in the same region of the spectra. The O-H peaks are broader, whilst the N-H peaks are often 'double-pronged' in shape.

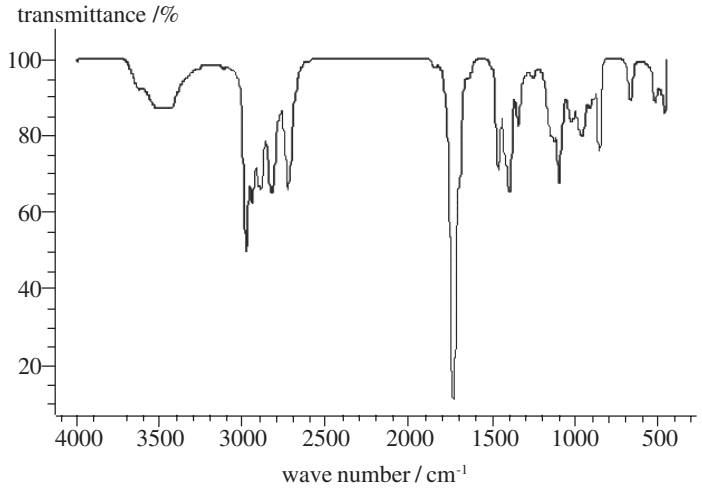
***Exam Hint**: IR spectra are commonly used in conjunction with other organic analysis techniques, such as UV spectrometry, mass spectrometry and NMR, to identify unknown compounds.*

The interpretation of simple IR spectra often forms part of an exam question, as knowledge of these other forms of organic analysis are also required - see later Factsheets.

Questions

Assign the peaks to bonds in the following spectra. In the answers you will simply be given the structure of the compound from which the spectrum was generated, but with a little thought you can check to see if you have assigned the correct bonds!

1.



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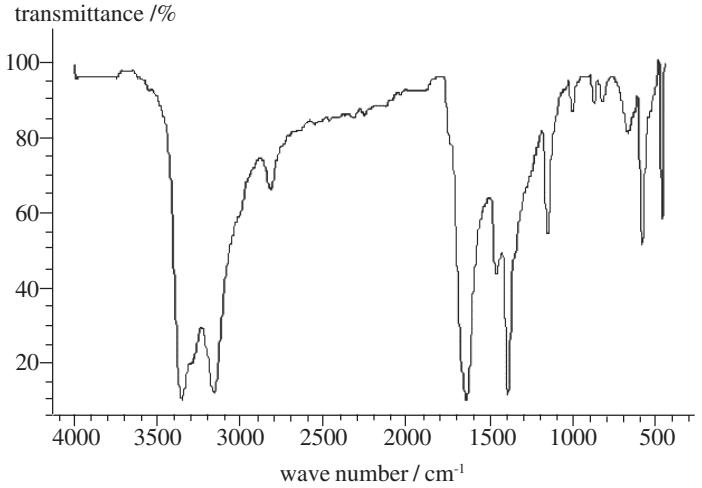

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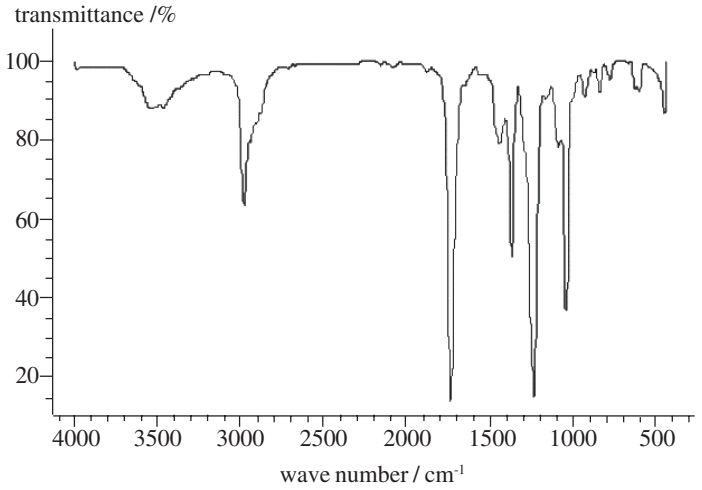
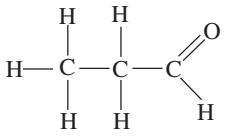


Answers

1.



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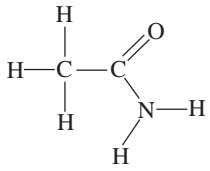

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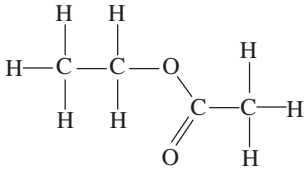

Acknowledgements:
This Factsheet was researched and written by Kieron Heath
Curriculum Press, Unit 305B, The Big Peg, 120 Vyse Street, Birmingham, B18 6NF