IR SPECTROSCOPY

a analyse an infra-red spectrum of a simple molecule to identify functional groups (see the Data Booklet for functional groups required in the syllabus) ☐

IR SPECTROSCOPY

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22 Analytical techniques

Analytical techniques are important tools for investigating organic compounds.

	Learning outcomes Candidates should be able to:
22.2 Infra-red spectroscopy	a) analyse an infra-red spectrum of a simple molecule to identify functional groups (see the *Data Booklet* for functional groups required in the syllabus)

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INFRA-RED (IR) SPECTROSCOPY

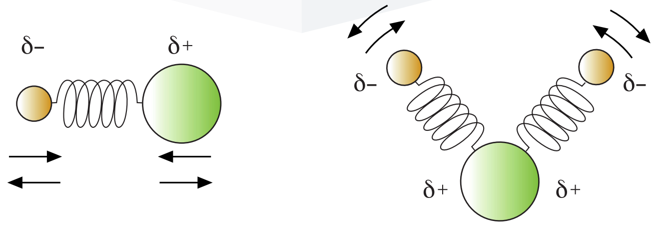
IR ABSORPTION

Infrared spectroscopy is used to identify functional groups in organic molecules.

Most compounds absorb infrared radiation.

The wavelengths of the radiation they absorb correspond to the natural frequencies at which vibrating bonds in the molecules bend and stretch.

However, it is only molecules that change their polarity as they vibrate that interact with infrared radiation.



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IR ABSORPTION

Bonds vibrate in particular ways and absorb radiation at specific wavelengths. This means that it is possible to look at an infrared spectrum and identify functional groups.

As a result, the infrared spectrum gives valuable clues to the presence of functional groups in organic molecules.

An 'IR spectrum' can be read to analyze the structure of an organic molecule - most importantly the functional groups present. These are analysed in an instrument called the spectrophotometer.

Only molecules that are polar (and hence have dipole moments) can absorb IR radiation.

SKILL CHECK

Which of these molecules will absorb IR radiation?

A. O_2

B. HCN

C. H_2S

D. N_2

E. CCl_4

F. CO_2

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IR ABSORPTION

The major use of infrared spectroscopy is in determining the structures of organic compounds. In an infrared spectrometer, infrared radiation in the range 400–4000cm^{-1} is passed through a sample.

The printout of the spectrum then shows which frequencies (wavenumbers) are absorbed.

Infrared spectra are always looked at with the baseline (representing 100% transmittance, i.e. zero absorbance) at the top.

The troughs (usually called ‘bands’) thus represent wavenumbers at which radiation is absorbed.

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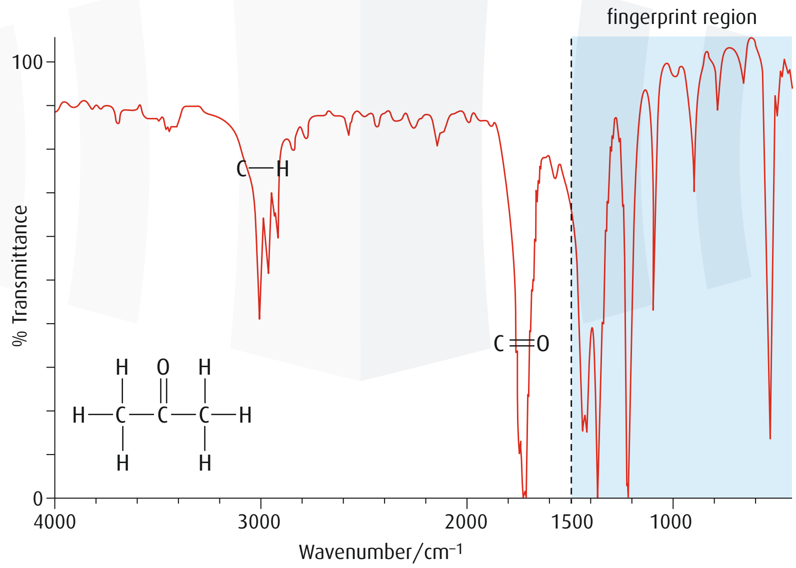
IR SPECTRUM OF PROPANONE



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IR SPECTRUM OF PROPANONE

The infrared spectrum can be used to determine the bonds present in a molecule.

Thus, in the region above 1500 cm^{-1} in the infrared spectrum of propanone there are two bands, corresponding to the C–H stretch and the C=O stretch.

The region below 1500 cm^{-1} is called the 'fingerprint region' and is characteristic of the molecule as a whole. Comparison of the spectrum in the fingerprint region with spectra in databases of infrared spectra can be used to identify the molecule.

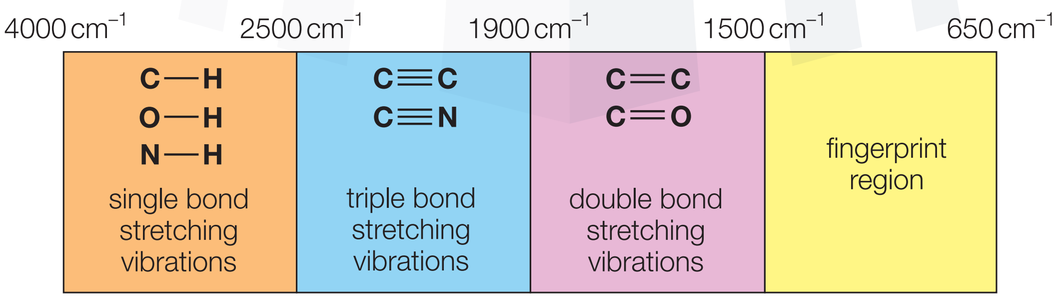
For example, the infrared spectra of butanone and propanone can be distinguished using the fingerprint region. They both show very similar bands in the region above 1500cm^{-1} because they have the same functional group, but they have different fingerprint regions.

IR SPECTRUM OF PROPANONE

We are interested in identifying the bonds/functional groups in an organic molecule.

To a good approximation the various bonds in a molecule can be considered to vibrate independently of each other.

The wavenumbers at which some bonds vibrate are shown below.



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WAVENUMBERS

So how do we connect molecular features to wavenumbers absorbed? **Take a look at this table:**

Bond	Functional group	Characteristic range of wavenumber / cm^{-1}
C–Cl	chloroalkane	600–800
C–O	alcohol, ether, ester, carboxylic acid	1000–1300
C=C	alkene	1610–1680
C=O	aldehyde, ketone, carboxylic acids, ester	1700–1750
C≡C	alkyne	2100–2260
O–H	hydrogen bonded in carboxylic acids	2400–3400
C–H	alkane, alkene, arene	2840–3100
O–H	hydrogen bonded in alcohols, phenols	3200–3600
N–H	primary amine	3300–3500

WAVENUMBERS

Note: These values are a very close approximation to the actual wavenumbers absorbed by different parts of the molecule. The surrounding environment of each type of bond determines the exact wavenumber absorbed.

We can use an infrared spectrum to identify the bonds present in a molecule but cannot always distinguish between functional groups. For example, we could identify the presence of C=O in a molecule but would not be able to distinguish between an aldehyde and a ketone.

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SKILL CHECK

Which of the following molecules will have an infrared band in the 1700 to 1750cm^{-1} region?

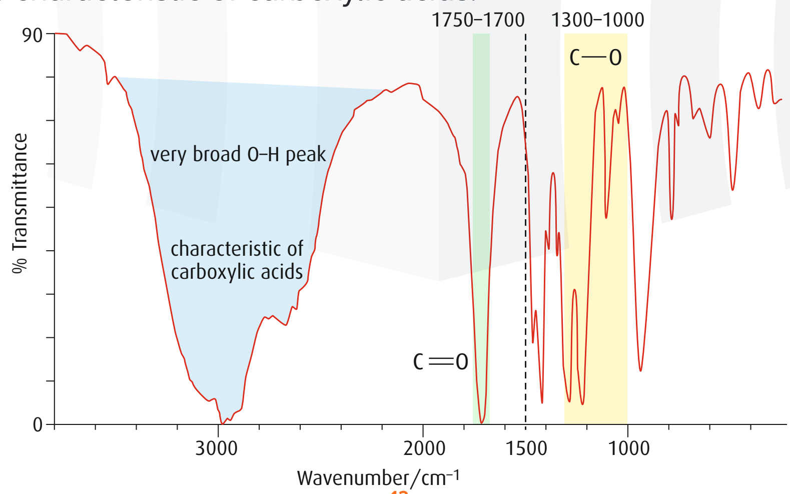
A. but-2-ene

B. propanal

C. $CH_3CH_2CH(OH)CH_3$

BUTANOIC ACID

This is the IR spectrum for butanoic acid. The 'broad band' absorption around 3000 cm^{-1} is characteristic of carboxylic acids:



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BUTANOIC ACID

We first of all look at the region above 1500 cm^{-1}.

We can identify the C=O stretch, as this absorption band occurs in the 1700–1750 cm^{-1} region.

The very broad absorption band between about 2400 and 3400cm^{-1} is due to the O–H stretch in carboxylic acids and is very characteristic of those molecules.

The functional group of a carboxylic acid contains a C–O bond, and therefore we should now look in the ngerprint region to con rm the presence of an absorption in the region 1000–1300cm^{-1} which is, indeed, the case.

If there were no band in this region, we would have to review our hypothesis that the molecule is a carboxylic acid.

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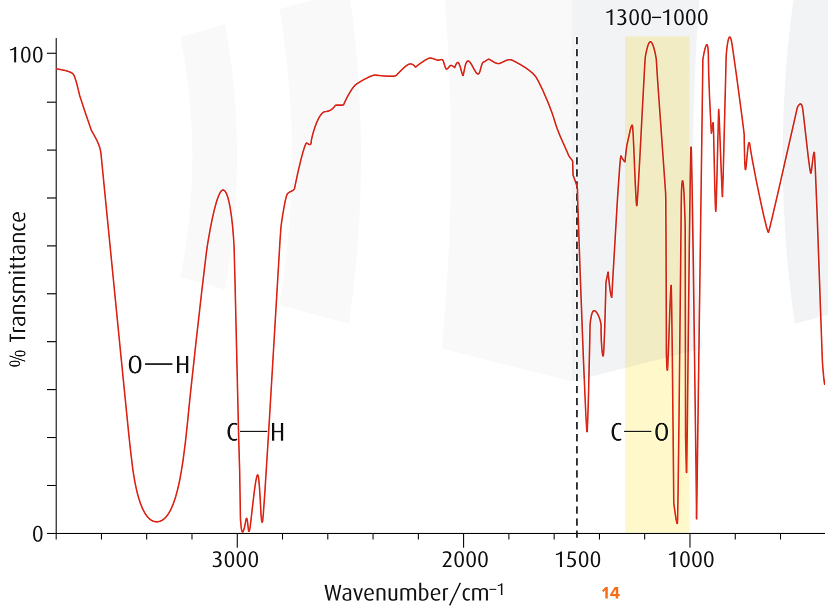
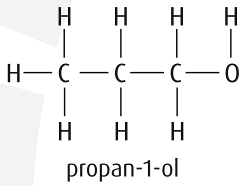
PROPAN-1-OL





We can identify

O–H (about 3350cm^{-1}) and

C–H (about 2900–3000cm^{-1}) bonds.

A C–O bond should also be present, and we can see that there is a band in the region 1000–1300cm^{-1}.

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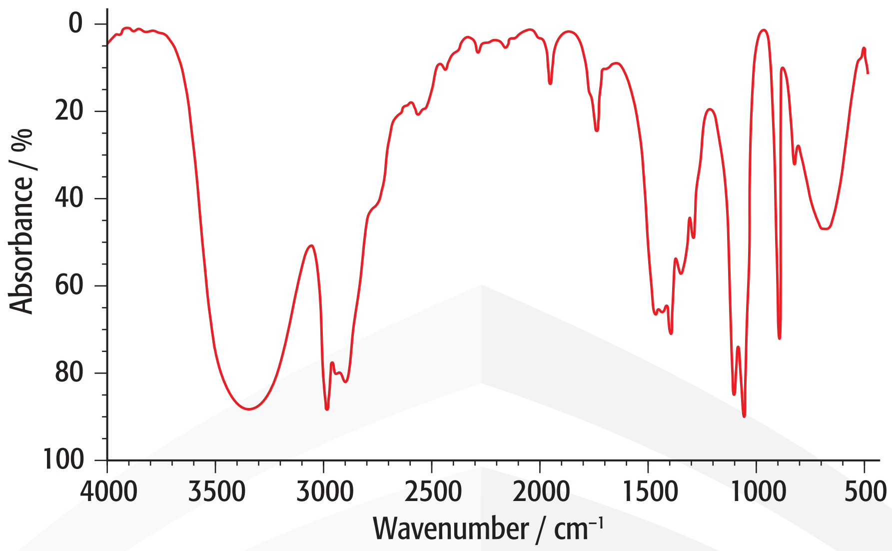
ETHANOL



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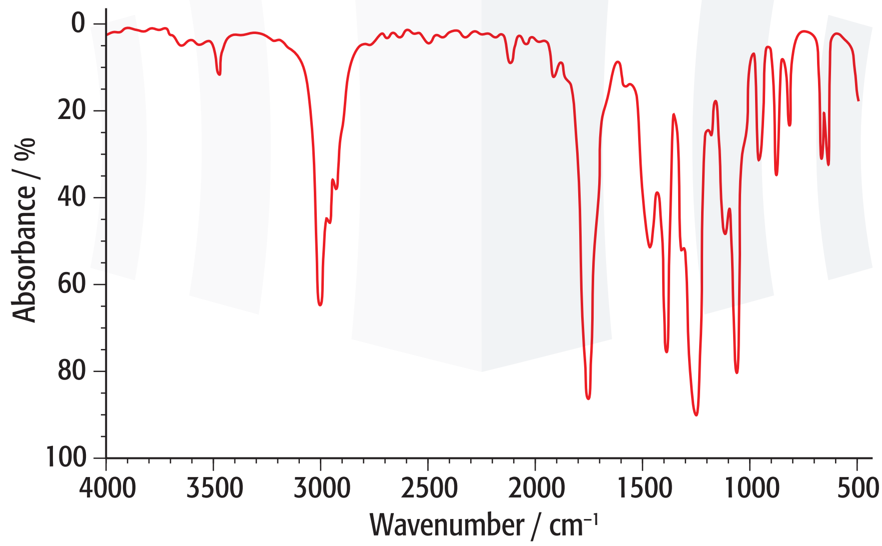
ETHYL ETHANOATE



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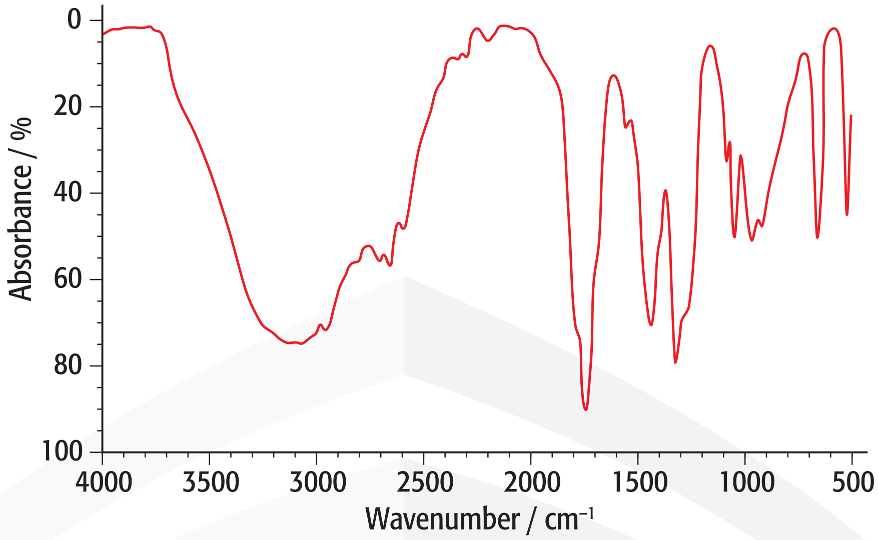
ETHANOIC ACID



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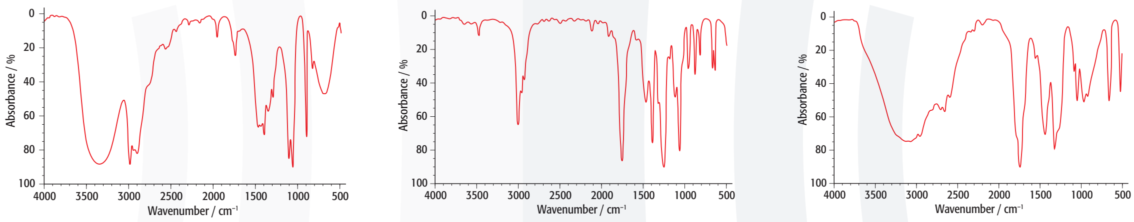
COMPARING IR SPECTRUMS



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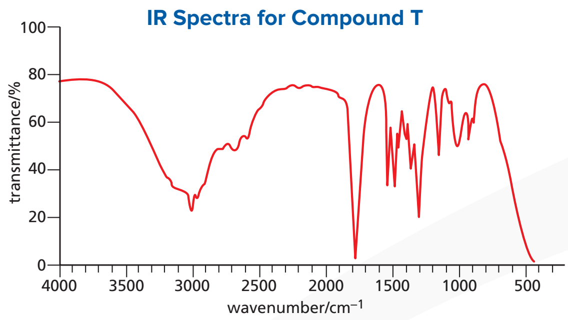
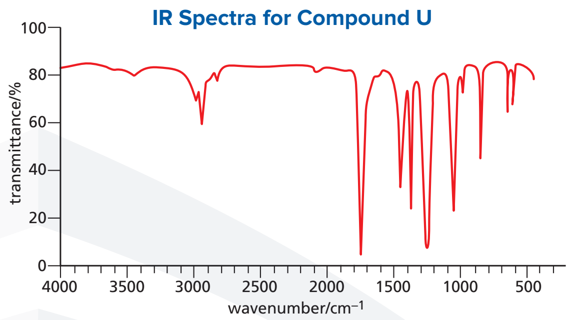
SKILL CHECK

Compounds T and U are isomers with the molecular formula $C_3H_6O_2$.

Suggest their structures based on the spectra shown below:



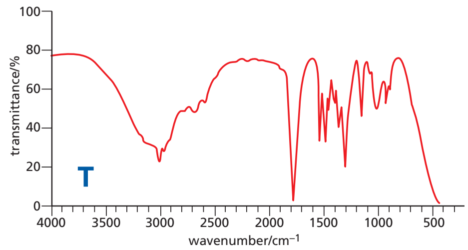


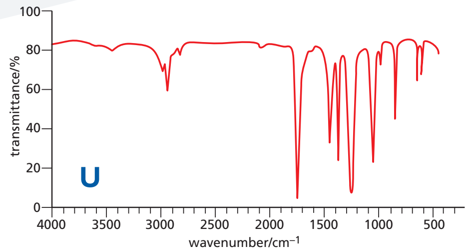
SKILL CHECK

Both T and U show a C=O absorption in their spectrum at 1700-1800 cm^{-1}, and a C—O absorption at about 1250cm^{-1}.

T shows 'broad band' absorption around 3000 cm^{-1}, indicating the presence of an O-H bond, while U shows no O-H band.

So, T is **$CH_3CH_2CO_2H$** (propanoic acid) and U could either be the ester **$CH_3CO_2CH_3$** (methyl ethanoate) or the ester **$HCO_2CH_2CH_3$** (ethyl ethanoate).





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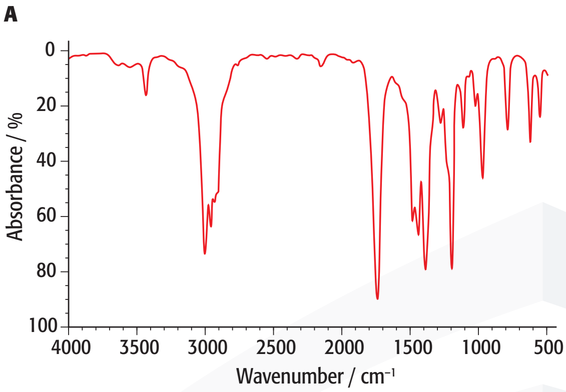
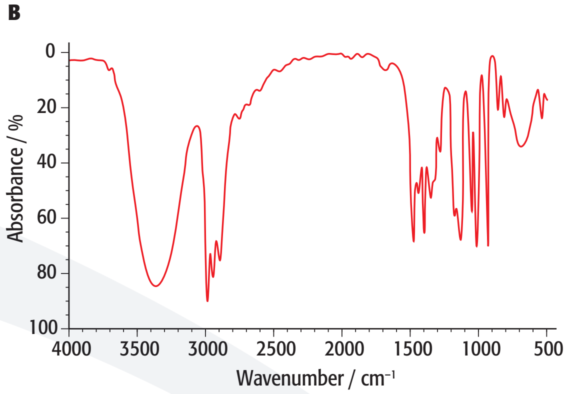
SKILL CHECK

Which one of the infra-red spectra is that of butanone and which one is of butan-2-ol?





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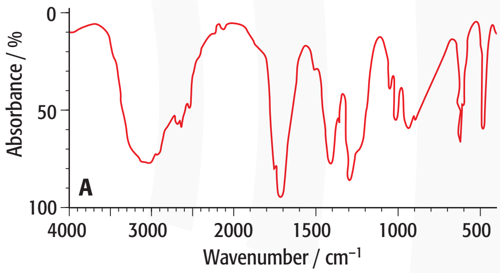
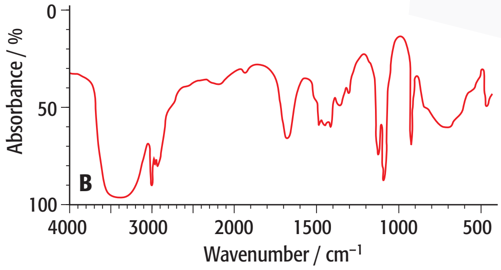
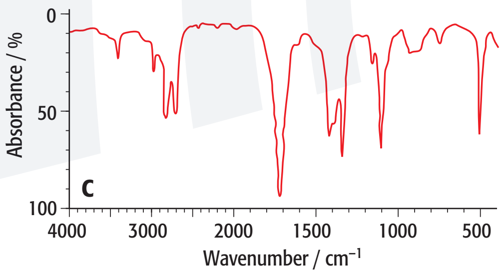
SKILL CHECK

Which one of the infra-red spectra is that of ethanal? Give three reasons.







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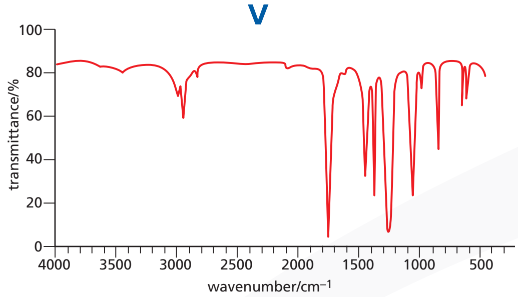
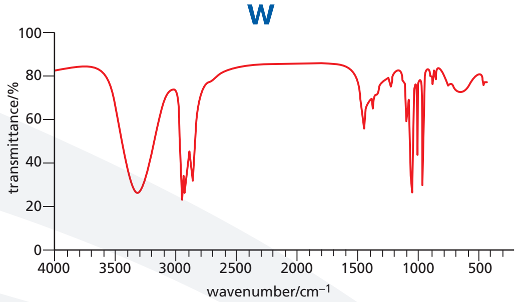
SKILL CHECK

Compound **V** (C_3H_6O) gives a silver mirror when warmed with Tollens' reagent. It can be converted to compound **W** by reagent **X**. Use the spectra below to identify the functional groups present in **V** and **W**, and suggest the identity of reagent **X.**

V



W



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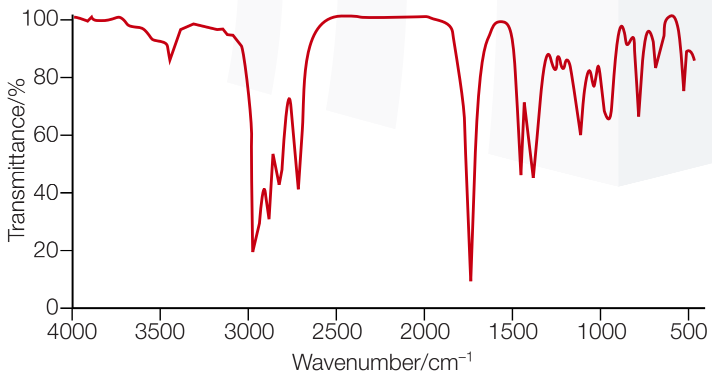
SKILL CHECK

Oxidation of butan-1-ol gives a product with the infrared spectrum shown below. Use the data sheet to interpret the spectrum. State the reagents and conditions that were used to carry out the oxidation of the alcohol and give your reasons.



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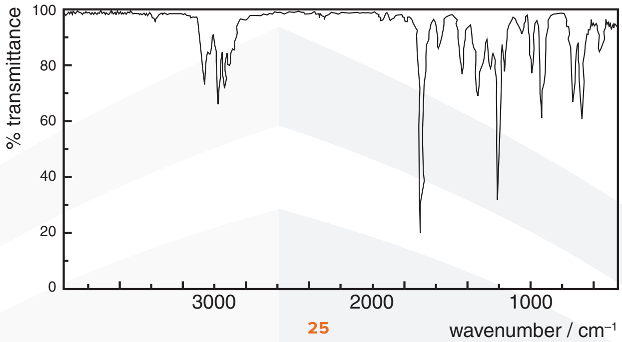
SKILL CHECK

The infra-red spectrum of compound A is shown below.

(a) What information does the absorption at 1690 cm^{-1} give about compound A?

(b) There is a sharp absorption at 2950 cm^{-1}. What could this be due to?

(c) The infra-red spectrum of compound A does not show a broad absorption at about 3300 cm^{-1}. What information does give about compound A?



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SKILL CHECK

Q. Infrared spectroscopy is a powerful tool for identifying organic compounds. List the absorption regions expected for:

(i) ethanoic acid.

(ii)methylmethanoate.

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SKILL CHECK

Q. Identify the absorption listed in (a) which could be used to distinguish between these two compounds. Explain why the other absorptions could not be used.

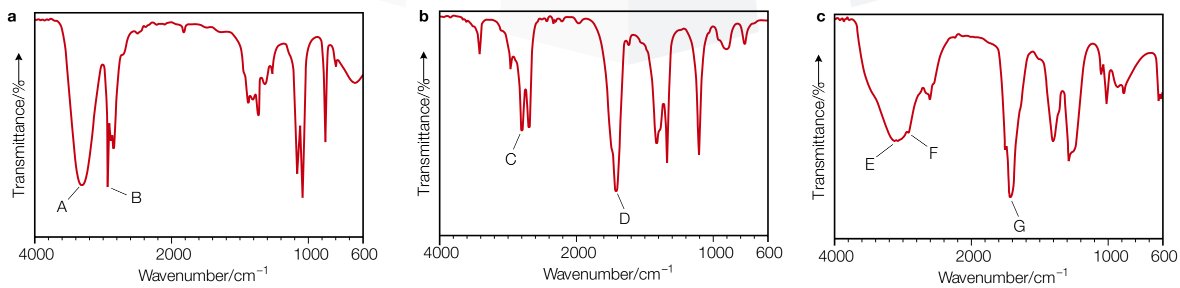
SKILL CHECK

The following are the infrared spectra of ethanol, ethanal and ethanoic acid.

(a) Which spectrum belongs to which compound?

(b) Why do all three spectra have a peak at around 3000 cm^{-1}?

(c) Why do two of the spectra have broad peaks at wavenumbers between 3000 and 3500cm^{-1}?



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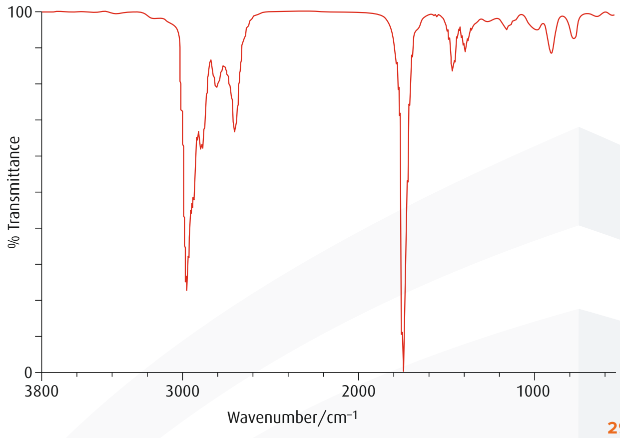
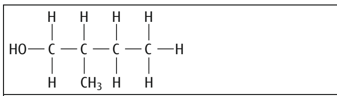
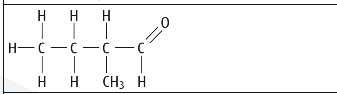
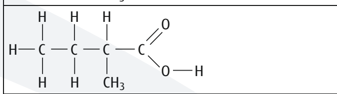
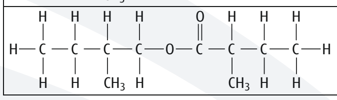
SKILL CHECK

A student recorded the IR spectrum of a compound, X. He knew that X was one of the following compounds. Deduce which of the molecules is X and explain your choice by reference to the spectrum.



	I
	II
	III
	IV

ENVIRONMENTAL CONCERNS

Small molecules in the atmosphere (especially CO_2, CH_4, H_2O and CFCs) are responsible for the **greenhouse effect**: they absorb infrared radiation that is emitted from the surface of the Earth, preventing it from being lost to space.

Consequently, the amount of heat lost is less than that gained from solar radiation, and the Earth warms up.

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ENVIRONMENTAL CONCERNS

- IR spectroscopy works quickly and accurately to monitor pollutants, including nitrogen dioxide, sulfur dioxide, carbon monoxide and carbon dioxide, as well as more than a hundred VOCs (volatile organic compounds) and low-level ozone.
- Scientists can use the characteristic wavelengths of infrared radiation absorbed by the molecules of the pollutants to identify them. They can also analyse the intensity of the absorptions to find the concentration of each pollutant present in a sample.
- Monitored over a period of time, this data provides useful information on the effectiveness of pollution control measures introduced locally and on a global level.

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