

Spectroscopy

Three activities that could be used to teach spectroscopy are presented within this resource. A good introduction to spectroscopy is to do the Cold light practical or to demonstrate that many objects absorb UV light and then emit light of a different wavelength/frequency. Explain that the same thing happens with infrared radiation (and many other types of electromagnetic radiation) except that we cannot see it. Instead, a detector is used to read which wavelengths of infrared are being absorbed (or transmitted). Every substance has its own unique infrared (IR) spectrum. A spectrum obtained during an experiment can be matched against a data bank of sample spectra to identify a substance. It is also possible to interpret certain individual peaks on the spectrum using a data book/sheet.

When IR radiation interacts with matter and is absorbed, it causes the bonds in the substance to vibrate. They can either bend or stretch – this is the basis of the activity Chemical aerobics, which is another good introduction to the topic of spectroscopy. Two problem-solving activities relating to IR spectroscopy are given in the student sheet entitled Spectroscopy.

For further examples of spectra and for video clips showing how an IR spectrometer is operated, see the RSC CDRom Spectroscopy for schools and colleges or the website <http://www.chemsoc.org/networks/learnnet/spectra/index2.htm>.

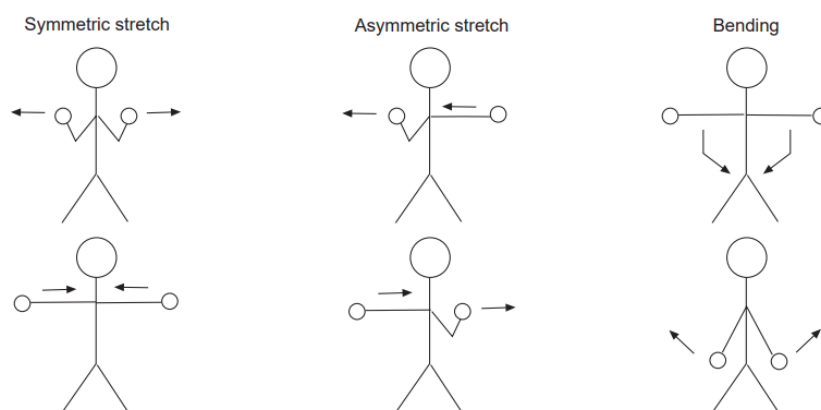
Chemical aerobics

When infrared radiation interacts with a substance, certain wavelengths cause particular bonds in that substance to vibrate. Only certain wavelengths will do this and each different type of bend or stretch of a bond will require a different wavelength of radiation.

Get the class to stand up and pretend that they are each a water molecule. Their heads are the oxygen atoms, their hands the hydrogen atoms and their arms the bonds. If you want to make this really clear, you can make large labels for the heads and hands. Ask the students to try to work out which bends or stretches are possible.

They should be able to work out that there are three possible kinds of vibration, although they almost certainly will not get the names for them. The three vibrations are:

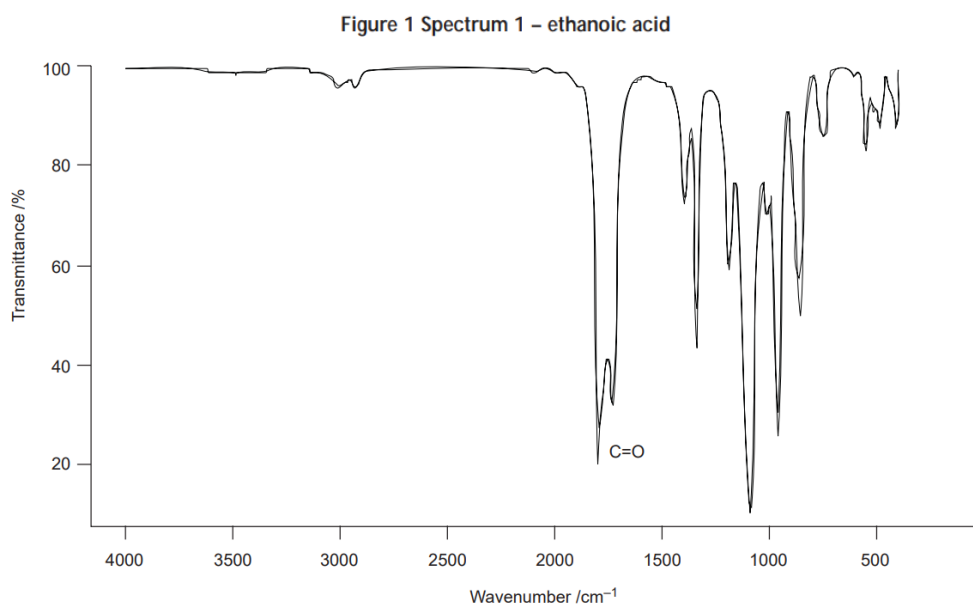
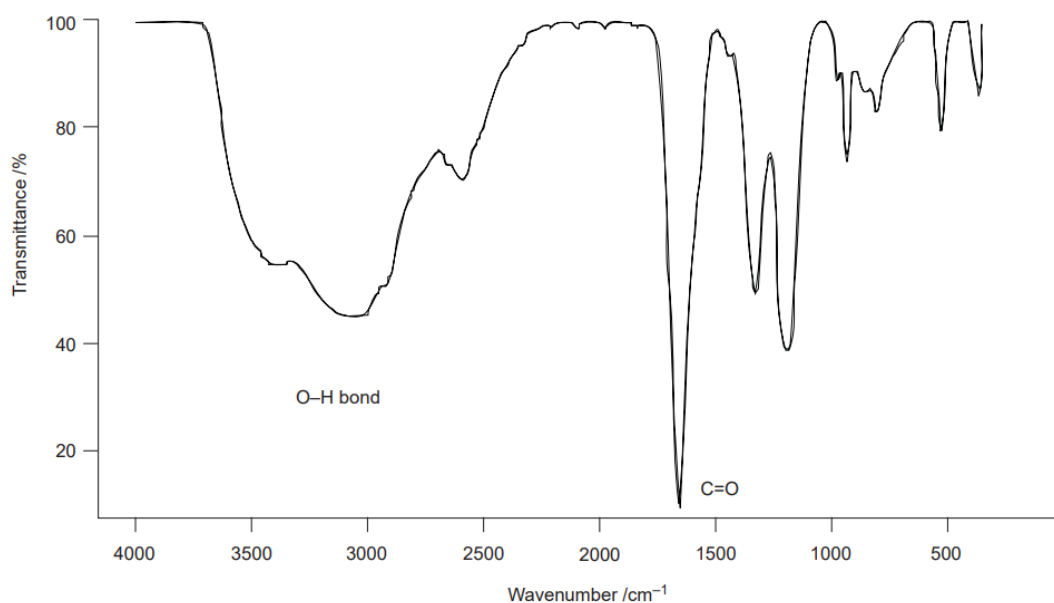
- symmetric stretch (both hands moving back and forth away from the body together and both arms bending together)
- asymmetric stretch (one hand moves forward as the other moves back towards the body, or one arm bending as the other straightens)
- bending (hands moving towards each other in front of the body and back again with arms staying straight).



If you wish to make this exercise more fun, you could have some music clips prepared on a tape or CD. Assign a different singer/group/song to each movement. When the students hear the singer they have to make the correct move – if there is a singer with no movement assigned then they stay still. You can be as cheesy or up-to-date as you like but the singers do need to be well known by the vast majority of the class and the clips need to be short.

Solutions to spectroscopy problems

1. Spectrum 1 is ethanoic acid; 2 is ethanoic anhydride and 3 is ethanol. Labelled spectra are given below



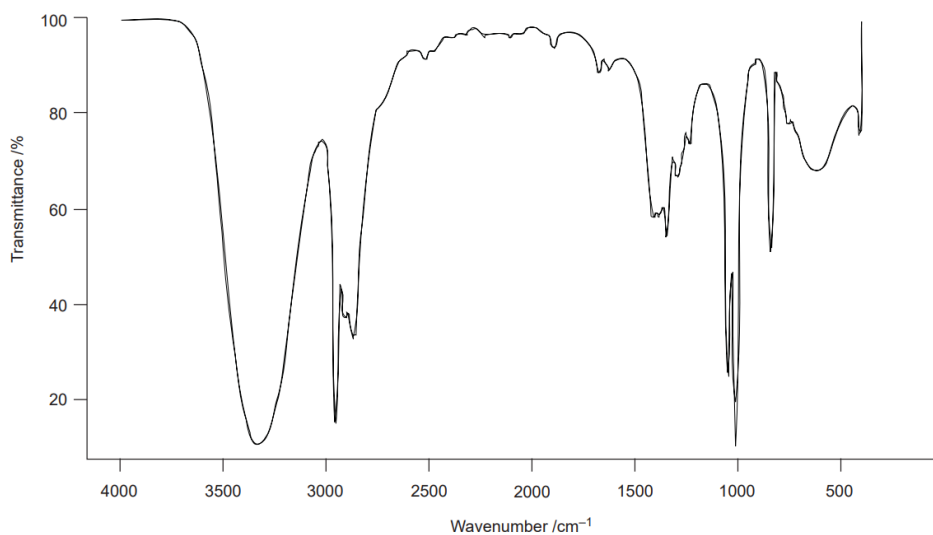


Figure 3 Spectrum 3 – ethanol

2. Smell Fresh deodorant contains chloroethane and Jaguar contains butane. Labelled spectra are given below:

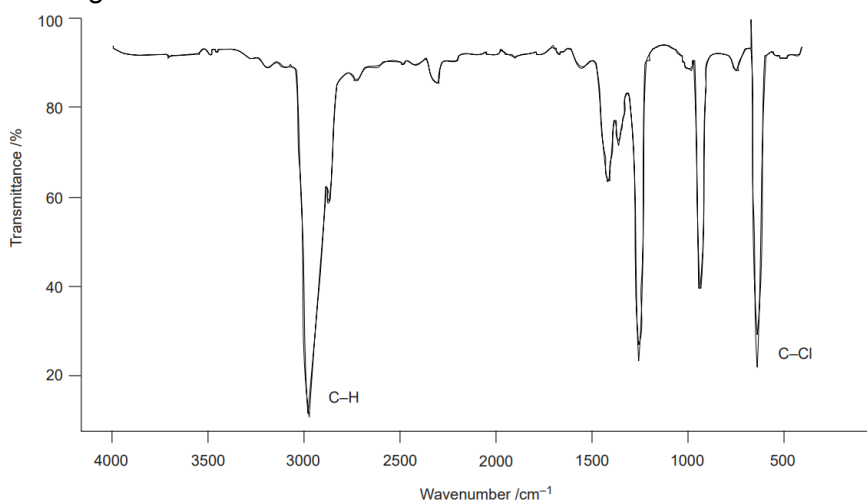


Figure 4 Smell Fresh deodorant – chloroethane

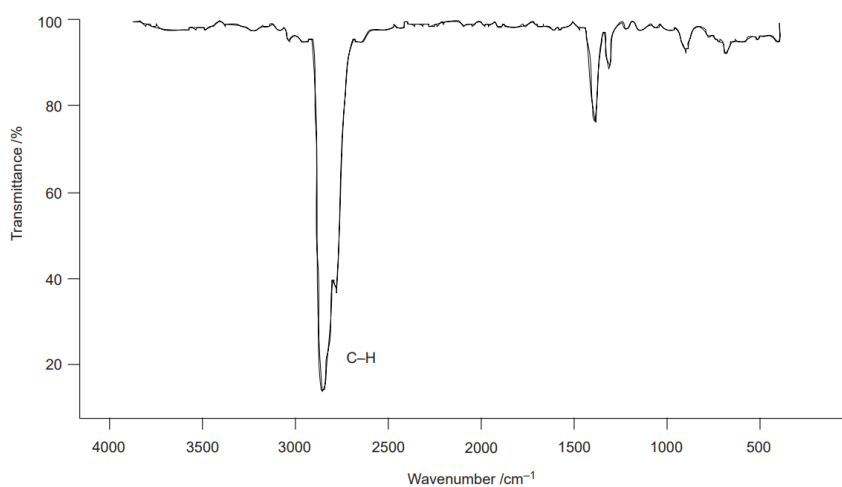


Figure 5 Jaguar deodorant – butane

3. Yes, they have obtained the product they wanted. The annotated spectrum is shown below. There is no O-H stretch at around $3200\text{--}3400\text{ cm}^{-1}$ but a peak corresponding to a C=O stretch can be seen.

Note: This reaction is reversible and in reality it would not go to completion.

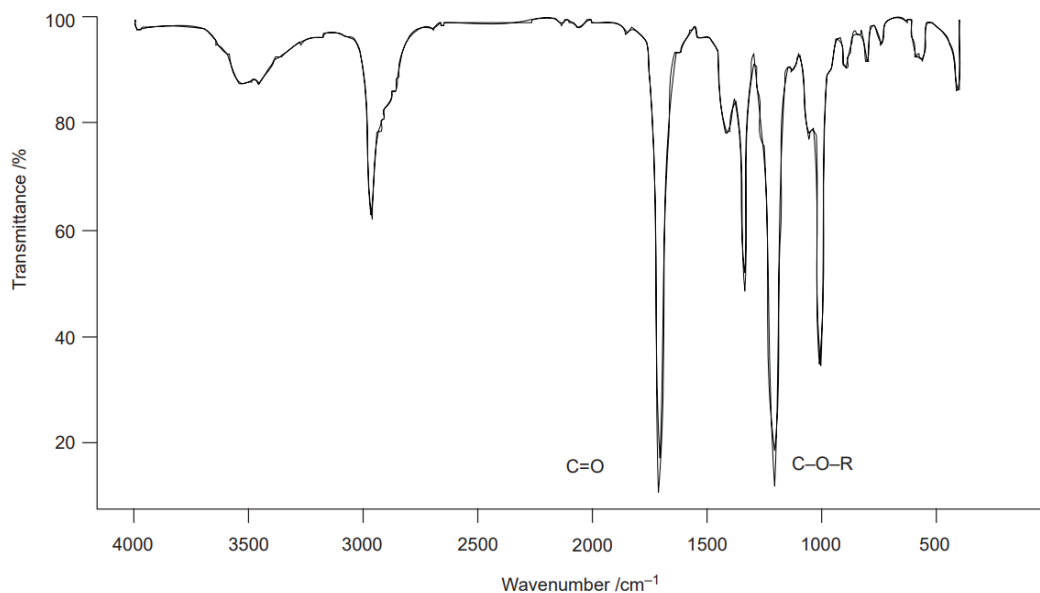


Figure 6 Spectrum of ethyl ethanoate

Spectroscopy

Introduction

Many substances absorb light at one wavelength and emit it at another. We make use of this in many ways, for example in glow-in-the-dark stickers. Compounds can also absorb and emit radiation that we cannot see, such as infrared, microwave and ultraviolet radiation.

Finding out which radiation is absorbed and emitted can tell us a lot of useful information about a compound. This branch of chemistry is called 'spectroscopy'. It is used in a very wide variety of applications, from helping chemists to work out the structure of a new molecule they have made to testing for drugs, forensics testing and quality control.

Spectroscopy can even be used to help museum conservators assess what damage has occurred to an object.

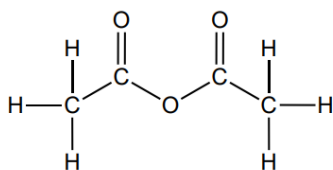
Infrared (IR) spectroscopy involves firing infrared radiation at a substance and measuring the radiation that is absorbed by the molecules. It is particularly useful for studying organic (carbon-containing) chemicals. The spectra that result look quite complex – each one is a line with a series of 'bumps' called peaks at the particular wavelengths where radiation is absorbed by the sample. However, it is often not necessary to decide what each peak represents in order to get useful information from a spectrum.

Different bonds cause peaks (we call them peaks, even though they are actually troughs) in particular places in a spectrum. Charts like the one below are used to decide what certain peaks tell us.

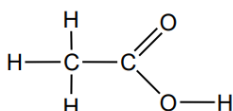
Bond	What is it?	Where is it? (cm ⁻¹)
O-H	Alcohols, carboxylic acids	3600–3000
N-H	Amines and amides	3600–3100
C-H	In non-aromatic compounds	3000–2850
C-H	In the CHO group in aldehydes	2830–2720
C≡C	Alkynes	2250–2070
C=O	Various	1815–1640
	Ketones	1725–1700
	Aldehydes	1740–1720
	Carboxylic acids	1725–1700
	Esters	1750–1730
	Amides	1680–1640
	Acid chlorides	1815–1790
C=C	Alkenes	1680–1610
C-O-R	Various	1300–1060
C-Cl	Various	800–700

Problems

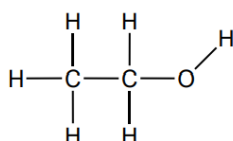
1. The following three compounds have got muddled up. Chemists have run IR spectra on samples of each to find out which is which. Which spectra belongs to which compound?



Ethanoic anhydride

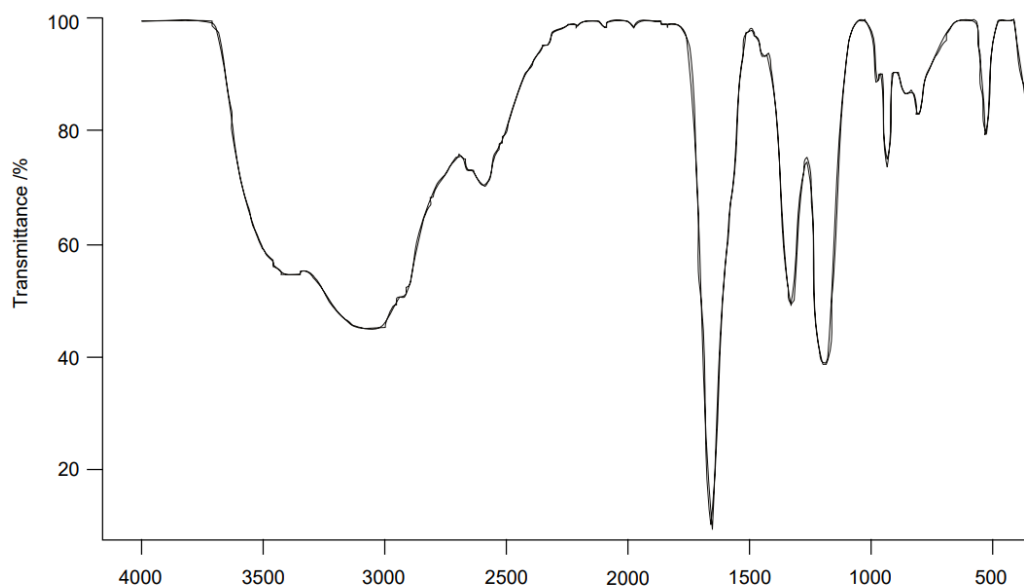


Ethanoic acid

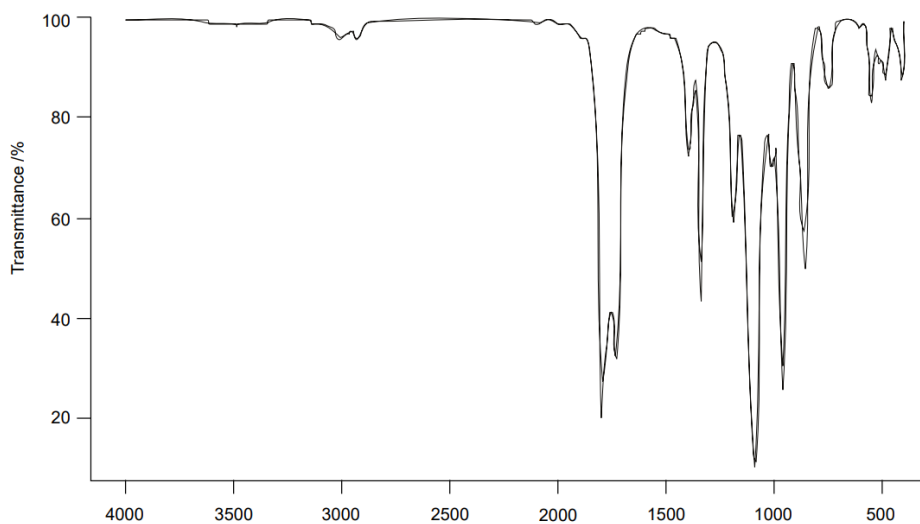


Ethanol

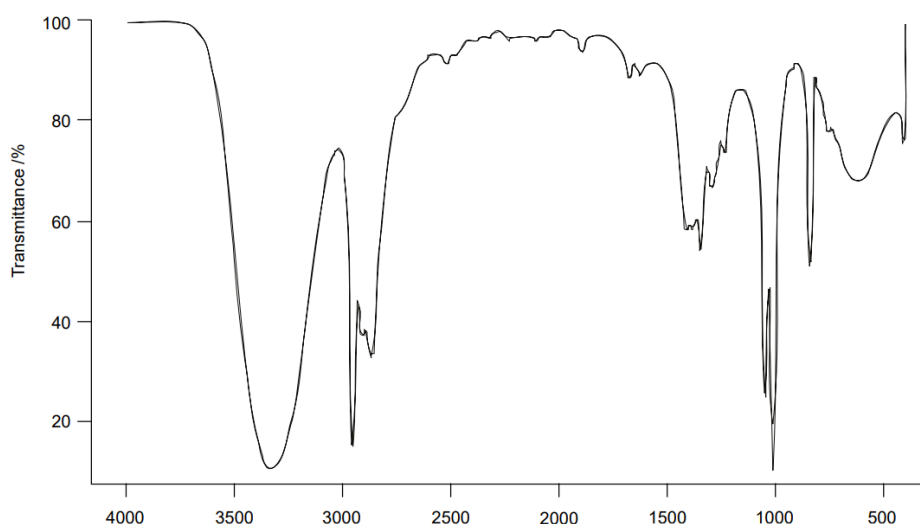
- Ignoring the C-H and C-O single bonds, write down which bonds each molecule contains. The numbers of each do not matter.
- Look at the chart above and decide where you would expect to find the peak for each of these bonds.
- Decide which of the spectra below belongs to each of the molecules above.



Spectrum 1

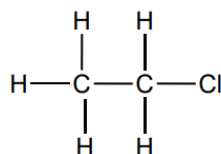


Spectrum 2

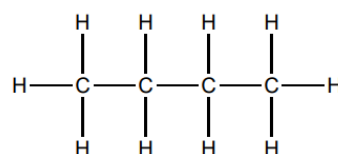


Spectrum 3

2. Butane and chloroethane are both used as propellants in aerosols.



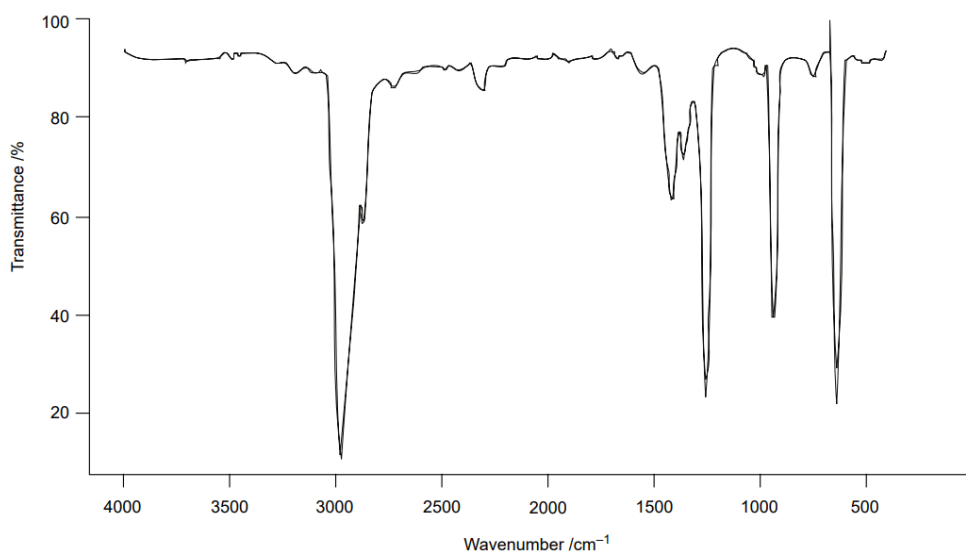
Chloroethane



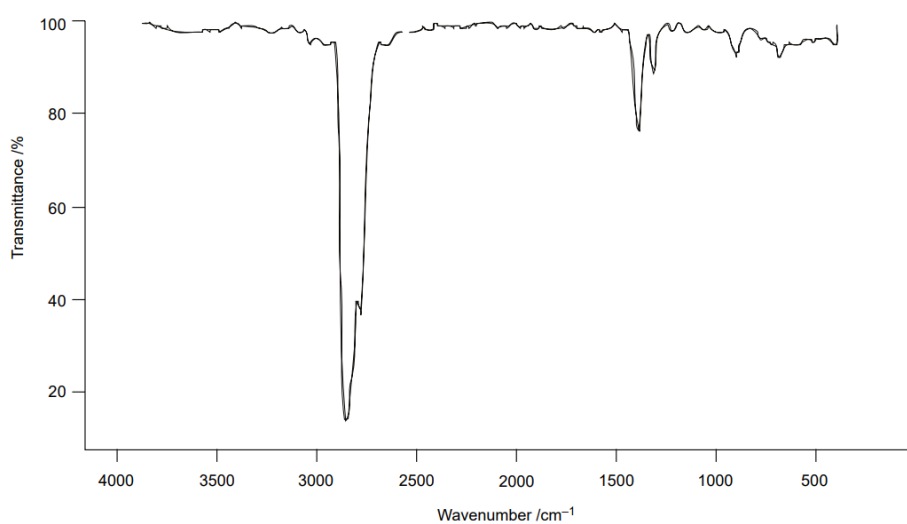
Butane

A chemist wished to find out which propellant was used in each of two deodorants. She ran IR spectra of the deodorants and the results are shown below. Which propellant does each deodorant contain?

Hint: Think about how the bonds in the two compounds differ and where you might expect to find the peaks corresponding to the different bonds.



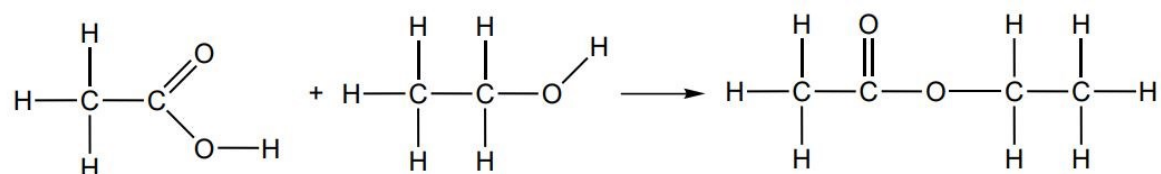
Smell Fresh deodorant



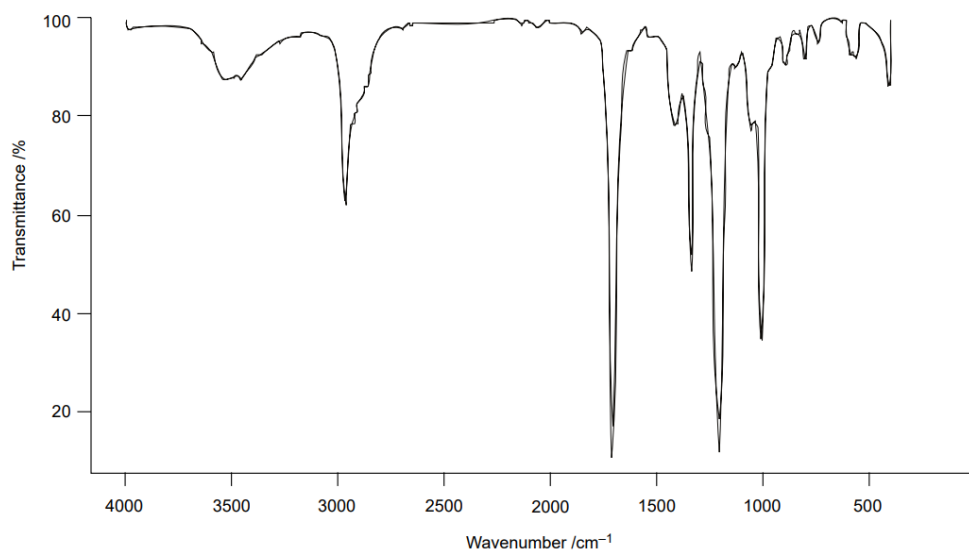
Jaguar deodorant

3. Some chemists were making esters, which are often used in perfumes. They reacted ethanoic acid with ethanol and hoped to make ethyl ethanoate.

This is the equation showing the reaction the chemists hoped would occur:



They ran an IR spectrum to find out if their reaction was a success. The spectrum is shown below. Have they made the product they wanted? Explain how you used the spectrum to help you answer this question.



Product spectrum