Infra-red spectroscopy is used by organic chemists to help them identify compounds. The atoms joined by chemical bonds in molecules vibrate, (imagine two atoms joined by a spring). Strong bonds vibrate at a higher frequency (faster) and heavier atoms make the bond vibrate at a lower frequency (slower). Every bond has its own unique natural frequency which is in the infra-red region of the electromagnetic spectrum.

As well as stretching, bonds can also bend. Since the energies involved with the bending will be different for each kind of bond, each different bond will absorb a different frequency of infra-red radiation. This is why some groups can have different absorption peaks.
Infra-red Spectroscopy

What an infra-red spectrum looks like

A graph is produced showing how the percentage transmittance varies with the frequency of the infra-red radiation.

Be aware of the change in scale of the x axis. Some scales will all be even, others will look a little odd. Different machines will give different scales, but this does not matter as long as you read the scale correctly.
Infra-red Spectroscopy

<table>
<thead>
<tr>
<th>Bond</th>
<th>Location</th>
<th>Wavenumber / cm⁻¹</th>
</tr>
</thead>
<tbody>
<tr>
<td>C-O</td>
<td>Alcohols, esters</td>
<td>1000-1300</td>
</tr>
<tr>
<td>C=O</td>
<td>Aldehydes, ketones, carboxylic acids, esters</td>
<td>1680-1750</td>
</tr>
<tr>
<td>O-H</td>
<td>Hydrogen bonded in carboxylic acids</td>
<td>2500-3300 (broad)</td>
</tr>
<tr>
<td>N-H</td>
<td>Primary amines</td>
<td>3100-3500</td>
</tr>
<tr>
<td>O-H</td>
<td>Hydrogen bonded in alcohols, phenols</td>
<td>3230-3550</td>
</tr>
<tr>
<td>O-H</td>
<td>Free</td>
<td>3580-3670</td>
</tr>
</tbody>
</table>

Here are some common absorption peaks. One of the uses of infra-red can be to find out how a reaction is proceeding. Spectra can be taken at various intervals during the reaction, for example a primary alcohol being oxidised to an aldehyde, a spectra at the start would show a strong peak at around the 3300 region, and at the end show a strong peak at around the 1750 region. Often it is still very difficult to name a compound on IR spectra alone, and they are often used in tandem with other spectra, such as Mass Spectrometry and UV Spectroscopy.
Infra-red Spectra of Carboxylic Acids

The infra-red spectrum for a simple carboxylic acid Ethanoic acid

Ethanoic acid has the structure:

\[
\text{CH}_3\text{C} = \text{O} \quad \text{O-H}
\]

You will see that it contains the following bonds:

- carbon-oxygen double, C=O
- carbon-oxygen single, C-O
- oxygen-hydrogen, O-H
- carbon-hydrogen, C-H
- carbon-carbon single, C-C

The carbon-carbon bond has absorptions which occur over a wide range of wavenumbers in the fingerprint region - that makes it very difficult to pick out on an infra-red spectrum.
Acids

The C-H bond (where the hydrogen is attached to a carbon which is singly-bonded to everything else) absorbs somewhere in the range from 2853 - 2962 cm\(^{-1}\). Though this is not particularly useful because virtually all organic molecules contain these.

The other really useful bond is the O-H bond. This absorbs differently depending on its environment. It is easily recognised in an acid because it produces a very broad trough in the range 2500 - 3300 cm\(^{-1}\).

The carbon-oxygen double bond, C=O, is one of the really useful absorptions, found in the range 1680 - 1750 cm\(^{-1}\). Its position varies slightly depending on what sort of compound it is in.

The carbon-oxygen single bond also has an absorption in the fingerprint region, varying between 1000 and 1300 cm\(^{-1}\) depending on the molecule it is in. You have to be very wary about picking out a particular trough as being due to a C-O bond.

The carbon-carbon bond has absorptions which occur over a wide range of wavenumbers in the fingerprint region - that makes it very difficult to pick out on an infra-red spectrum.

The possible absorption due to the C-O single bond is queried because it lies in the fingerprint region. You couldn't be sure that this trough wasn't caused by something else.
Infra-red Spectra of an Alcohol

The O-H bond in an alcohol absorbs at a higher wavenumber than it does in an acid - somewhere between 3230 - 3550 cm$^{-1}$.

Notice the absorption due to the C-H bonds just under 3000 cm$^{-1}$, and also the troughs between 1000 and 1100 cm$^{-1}$ - one of which will be due to the C-O bond.

The O-H bond in an alcohol absorbs at a higher wavenumber than it does in an acid - somewhere between 3230 - 3550 cm$^{-1}$.
Infra-red Spectra of an Ester

This time the O-H absorption is missing completely. Don't confuse it with the C-H trough fractionally less than 3000 cm⁻¹. The presence of the C=O double bond is seen at about 1740 cm⁻¹.

The C-O single bond is the absorption at about 1240 cm⁻¹. This can be very tough to find, and depends on the data tables given in the exam, because C-O groups can be anywhere between 1000-1300 cm⁻¹, depending on the compound.
Infra-red Spectra of a Carboxylic Acid

- O-H bond in a carboxylic acid
- C=O bond
- C-O bond?
- Very broad trough
Infra-red Spectra of an Alcohol

Infra-red spectrum of ethanol, \( \text{CH}_3\text{CH}_2\text{OH} \)
Infra-red Spectra of an Ester

infra-red spectrum of ethyl ethanoate, $\text{CH}_3\text{C}O\text{OCH}_2\text{CH}_3$