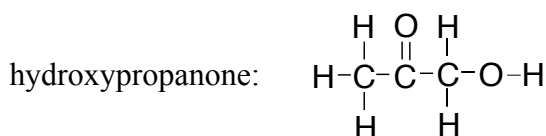
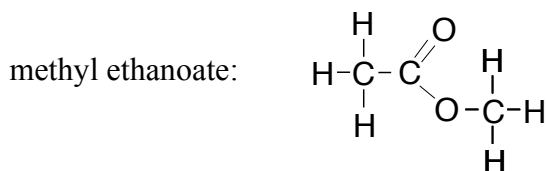
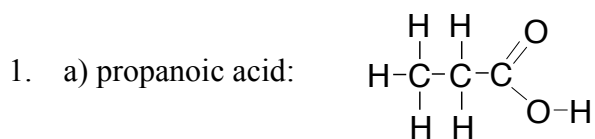


Chemguide – answers

INFRA-RED SPECTROSCOPY: INTERPRETING SPECTRA



b) Spectrum 1:

Notice that there isn't much of interest going on in the region around 3000 cm^{-1} , apart from the small troughs close to 3000 cm^{-1} which are due to C-H bonds. But there certainly isn't an O-H bond present either in an alcohol or an acid.

The only structure without an O-H bond is the ester, methyl ethanoate.

The spectrum shows the presence of the C=O bond by the trough at about 1750 cm^{-1} , and the two troughs in the region between 1000 and 1250 cm^{-1} will be due to C-O. The two C-O bonds in the molecule aren't quite the same because of the different bonding around the two carbon atoms (one is sp^3 hybridised and one sp^2), and so absorb at two different frequencies. But you don't really need this extra information to answer the question.

Spectrum 2:

This is showing an absorption due to an O-H bond at the left-hand side of the spectrum, but in an alcohol and not an acid. The trough for an acid O-H would be much wider, and slightly further to the right (see Spectrum 3).

The other important absorption is the one at just over 1700 cm^{-1} , showing a C=O bond.

So there is an O-H group and a separate C=O group. The molecule is hydroxypropanone.

You should also spot the trough due to C-H at about 2900 cm^{-1} , and one due to a C-O bond at about 1100 cm^{-1} , but again that isn't necessary for answering this particular question.

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Spectrum 3:

The key absorption here is very wide trough either side of 3000 cm^{-1} characteristic of the O-H group in a carboxylic acid.

So this has to be propanoic acid.

But you might also notice the absorption at about 1700 cm^{-1} due to the C=O bond in the acid. There is only one C-O bond in the acid, and that will cause a trough in the $1000 - 1300\text{ cm}^{-1}$ region, but we are in the fingerprint region here, and have to be cautious about which it is. But again, you don't need to worry about it for this question.