INFRA-RED SPECTROSCOPY: INTERPRETING SPECTRA

1. This question is going to give you three isomeric compounds and three IR spectra. What you have to do is to match each compound to its correct spectrum. You will find a list of useful infrared absorption data after the three spectra.

   The three compounds you are concerned with are

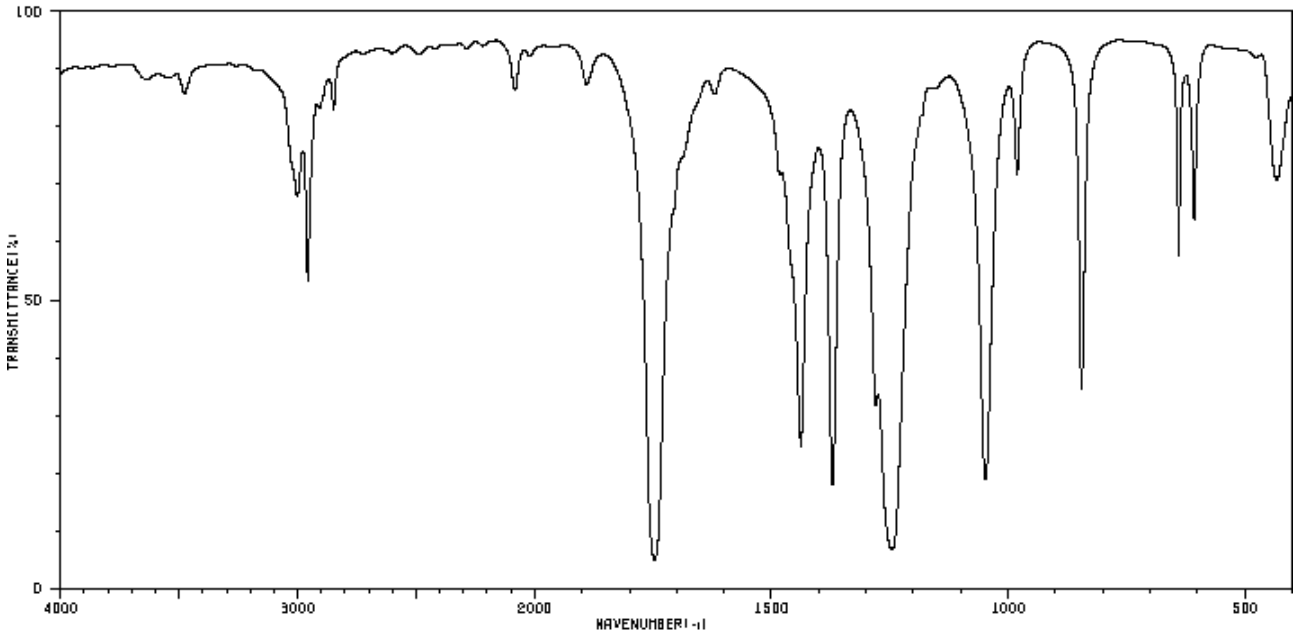
   - propanoic acid: CH_3CH_2COOH
   - methyl ethanoate: CH_3COOCH_3
   - hydroxypropanone: CH_3COCH_2OH

   a) Draw full structural formulae for the three compounds so that you can see exactly which bonds you need to think about.

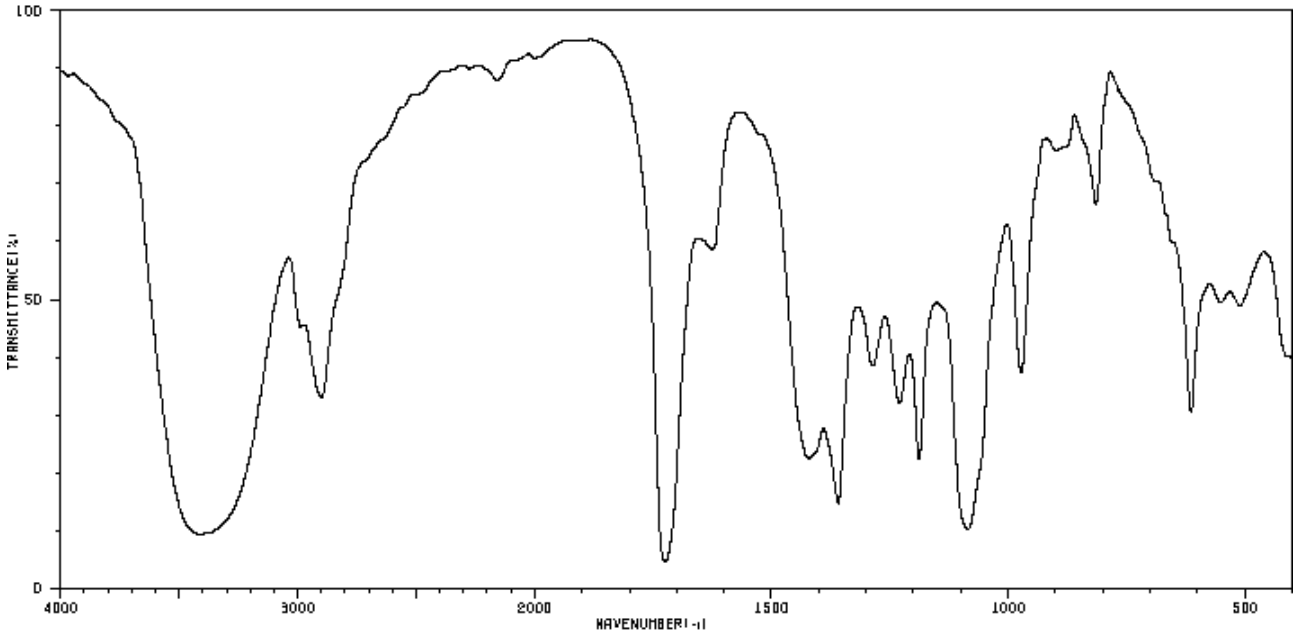
   b) Decide which compound corresponds to each of the spectra below, explaining how you made your decisions.

   The spectra are taken from the SDBS (SDBSWeb : http://sdbs.db.aist.go.jp (National Institute of Advanced Industrial Science and Technology, 14/8/2014). You may need to enlarge this page to read the numbers - I apologise for that, but it is a lot quicker than redrawing the spectra! Notice the change of scale either side of 2000 cm^{-1}.

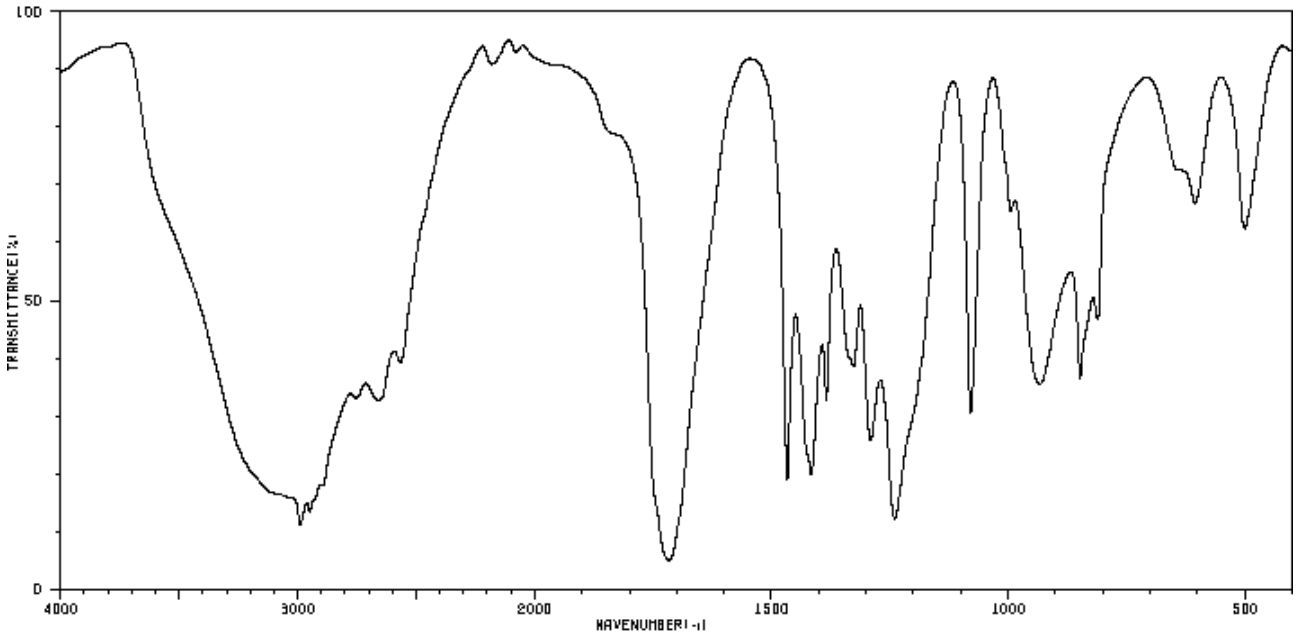
   Spectrum 1:



Spectrum 2:



Spectrum 3:



Infrared absorption data

Bond	Wavenumber / cm^{-1}
C-O	1000 - 1300
C=O	1680 - 1750
C-H	2850 - 2960
O-H (acids)	2500 - 3300
O-H (alcohols)	3200 - 3500

Note: These may not be exactly the same numbers that your examiners will use or expect. These are consistent with those on the Chemguide page, and with the spectra above. In an exam, use whatever numbers your examiners give you. They should always be consistent with the spectrum you are being asked to look at.

If you do an internet search for other similar tables, you will find some scarily big ones showing a lot more detail. Remember that this is only an introductory look at the topic suitable for 16 - 18 year old chemistry students.