

AS 91388 Spectroscopy

Here is a possible “plan of attack” when faced with 3 spectra for one molecule.

Find molar mass from highest m/z value to get M^+ , apply N rule, find or eliminate Cl on 3:1 peaks and Br on 1:1 peaks. Ignore rest of peaks for the moment.

Go into IR and look for presence AND absence of the "top 4" of N-H, O-H (2 differently located O-H peaks depending on alcohol or carboxylic acid O-H), C-H and C=O. Ignore the rest for the moment.

Go to the C NMR to find # of C environments and hence minimum # of C atoms, spotting any downfield shift for $\underline{C}=\underline{O}$ while there.

Then suggest a formula that fits the functional groups and the molar mass. Then draw the isomers - identifying those that fit the number of C environments and explaining why the others do not.

Then go back and look for at least 3 mass spec fragments that back up the molecule you think it is.

Then go back to IR to find a few more peaks due to bond stretch like a C-O found in c. acids or peaks due to C-H bend from the fingerprint region for their structure.

Try and assign at least some of the C NMR peaks.

Little hints

Learn the names of functional groups and how to draw them!

Alcohols often show a peak at $M^+ - 18$ due to a loss of water molecule – state this – don't try to draw the remaining fragment.

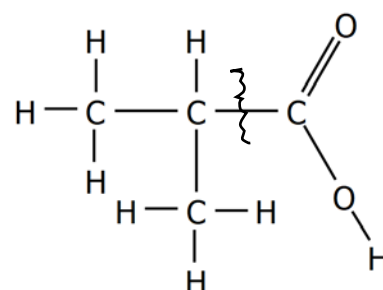
Peak at 28 m/z often due to loss of CO^+ from an aldehyde, ketone, ester, carboxylic acid or amide – state this – don't try to draw the remaining fragment.

Molecule has 2 x O but is not a carboxylic acid? Carboxylic acids and esters are isomers.

Aldehydes and ketones are isomers – check downfield C NMR peak and those 2 peaks an aldehyde has in IR (just to the right of the peaks C-H stretch) but the ketone does not.

Molecules often fragment at the C-C bond adjacent to a functional group – a good place to start looking for fragments when assigning mass spec peaks.

Don't stress if you can't identify a prominent looking peak in the mass spec – it could be due to a rearrangement – say that – but don't try and create the rearrangement for yourself.



Believe in yourself!