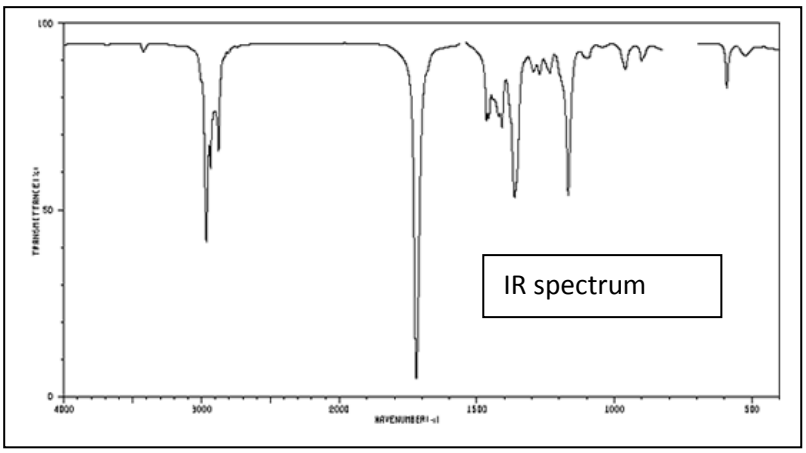
Revision 2 - analytical chemistry.

1) An unknown compound was analysed and found to have an empirical formula $C_5H_{10}O$. Consider the IR spectrum..

a) What information about the molecule can you derive from the spectrum ?

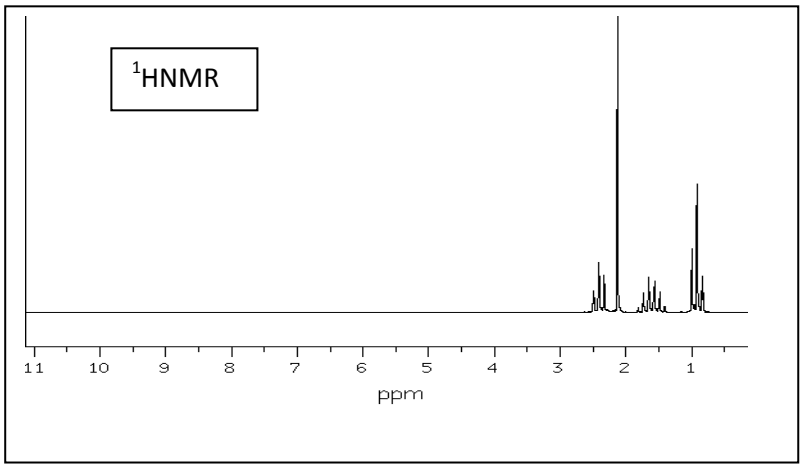
b) Determine the molecular formula of the compound

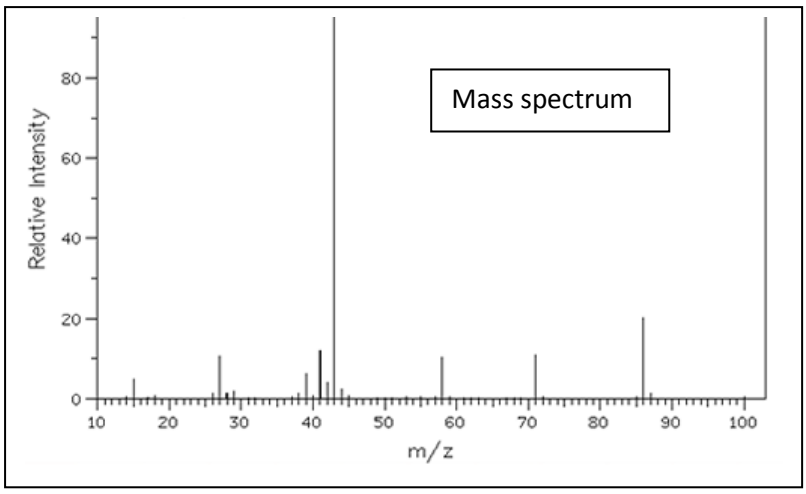
c) Draw its structural formula



d) Consider the mass spectrum. What fragment formed the base peak.

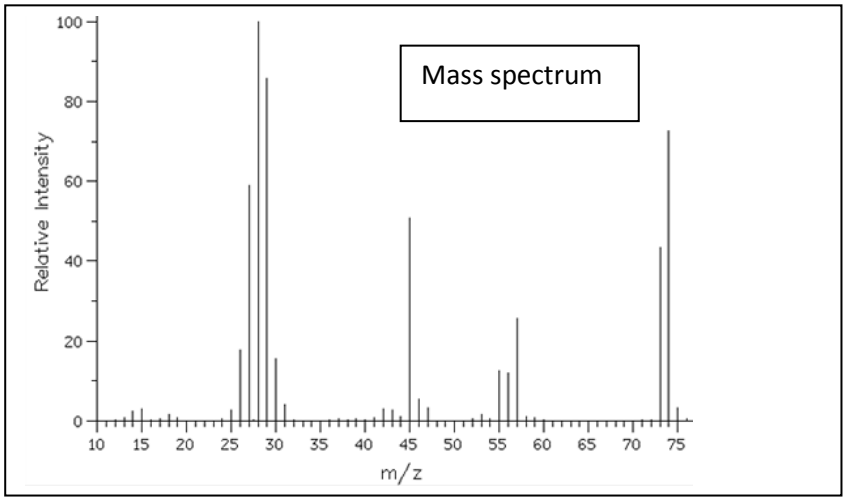
e) Explain the peak at m/z 87 in the mass spectrum.





2) Another unknown compound was analysed and also found to have the molecular formula $C_3H_6O_2$.

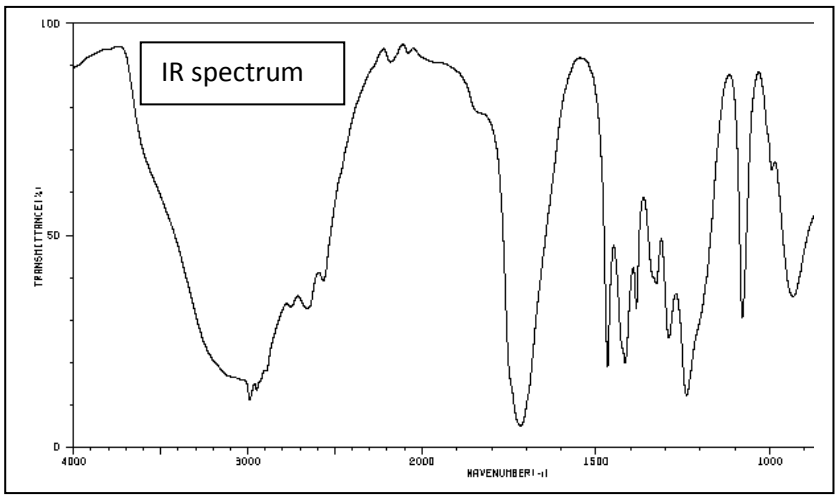
a) Consider the IR spectrum.
What information about the molecule can you derive from the spectrum?

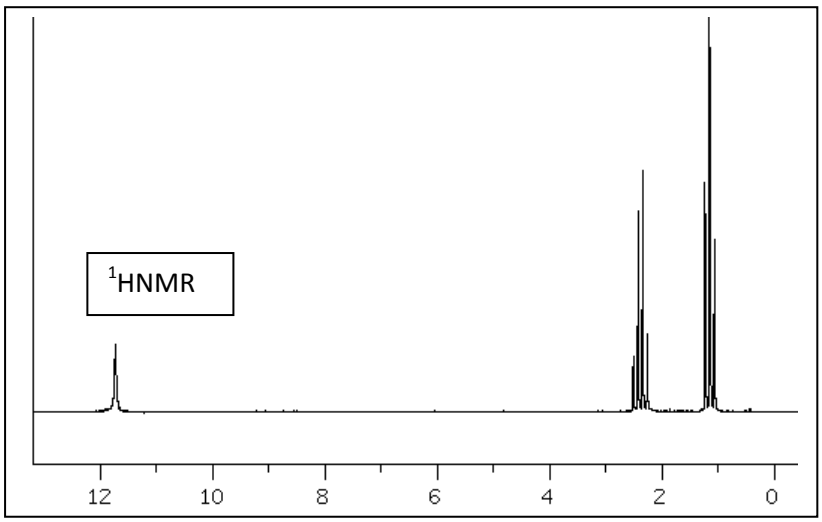


b) Draw its structural formula

c) What fragment produced the peak at:
- m/z 45 in the mass spectrum?

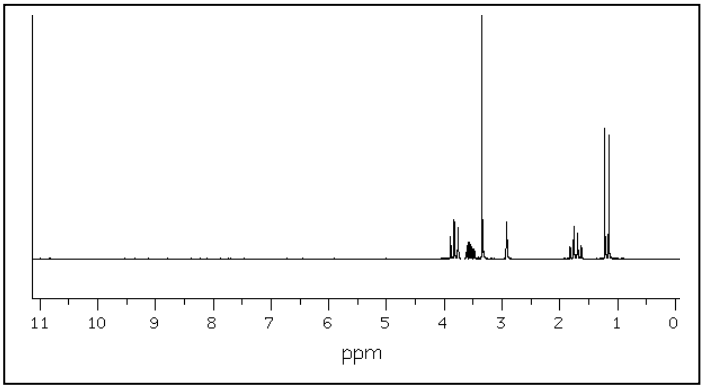
- m/z 74 in the mass spectrum?





3) An unknown compound was analysed and found to have the molecular formula $C_5H_{12}O_2$. The compound produces an aldehyde when oxidised. Below are the compound's ^{1}HNMR, IR and mass spectra

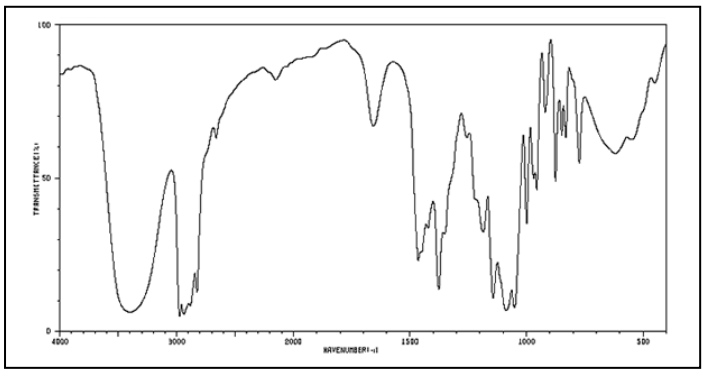
The ^{1}HNMR spectrum is shown on the right. The signal at 3.6 ppm is a sextet.



a) How many groups of chemically different hydrogens exist?

b) What group of equivalent hydrogens could have produced the singlet at 3.3 ppm?
Use the data sheet.

c) Identify one functional group obvious from the IR spectrum.



d) Draw the molecular structure

e) What fragment could have produced the peak at m/z 59?