

Revision of analytical chemistry.

1) An unknown compound was analysed and found to have an empirical formula C_2H_4O .

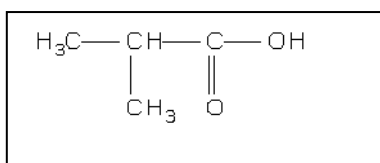
a) Consider the IR spectrum.

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

b) Determine the molecular formula of the compound

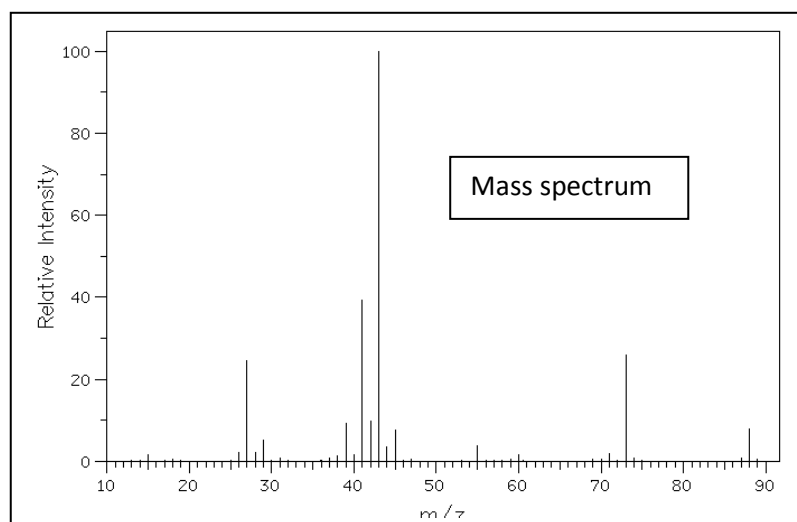
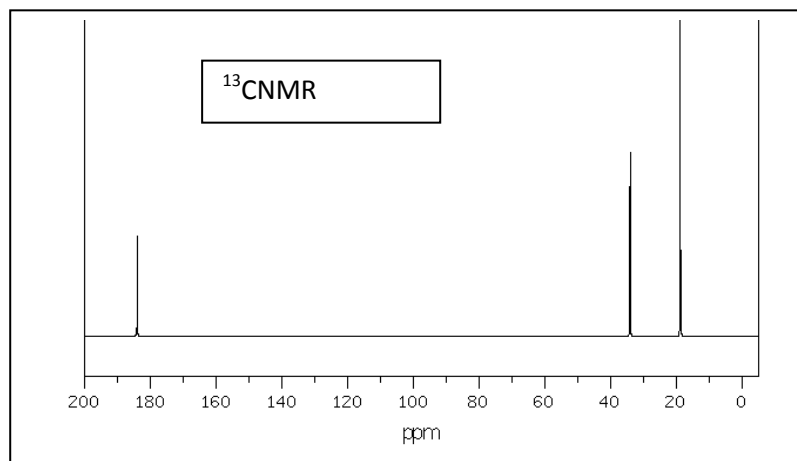
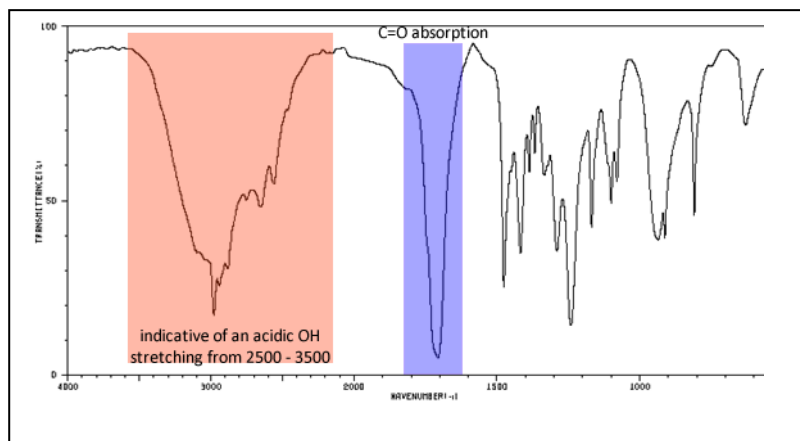
According to the mass spectrum the molar mass of the compound is 88 hence the molecular formula is $C_4H_8O_2$

c) Draw its structural formula



d) Consider the mass spectrum.

What fragment formed the base peak. *$(CH_3)_2CH^+$*

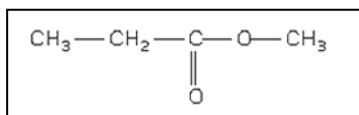


2) Another unknown compound was analysed and also found to have an empirical formula C_2H_4O .

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

b) Determine the molecular formula of the compound
The molar mass, as derived from the mass spectrum, is almost double the empirical formula mass (88). Hence the molecular formula is $C_4H_8O_2$

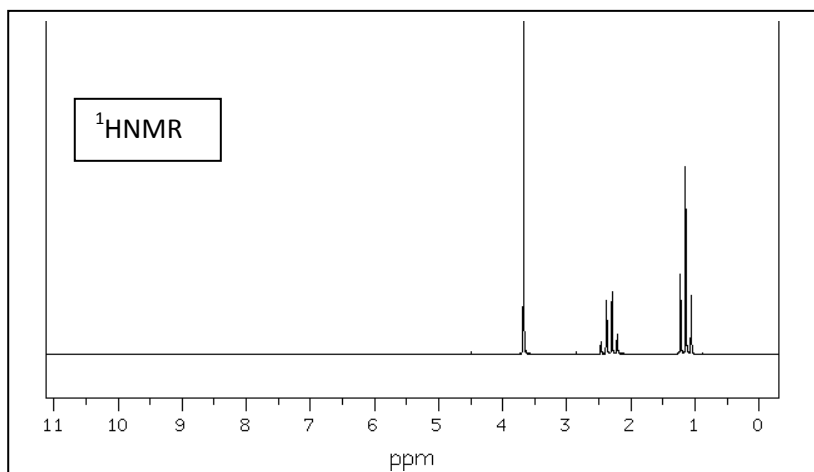
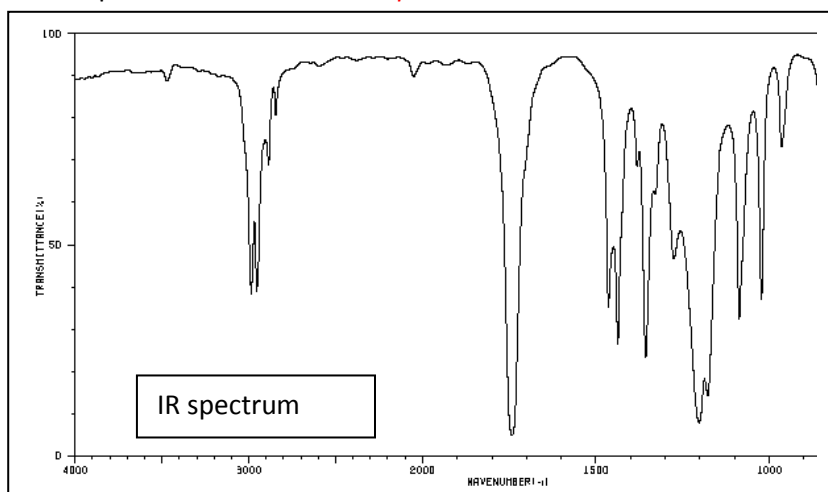
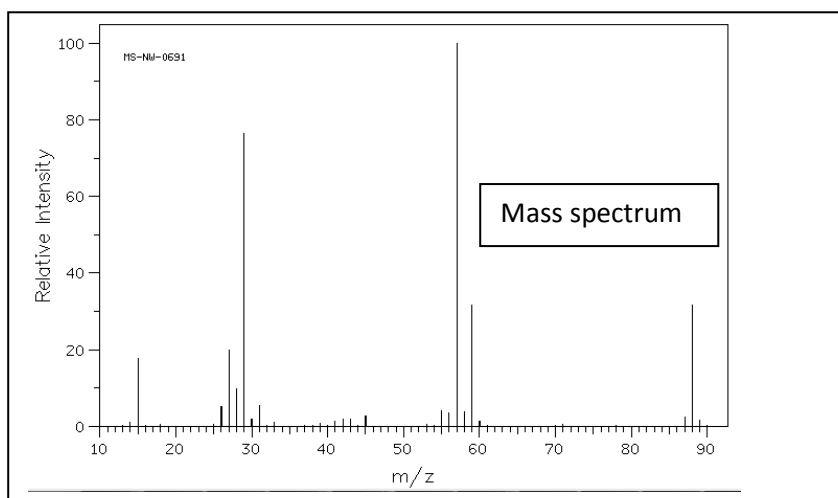
c) Draw its structural formula



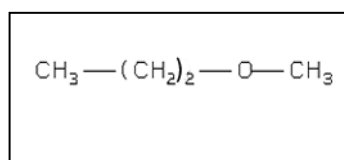
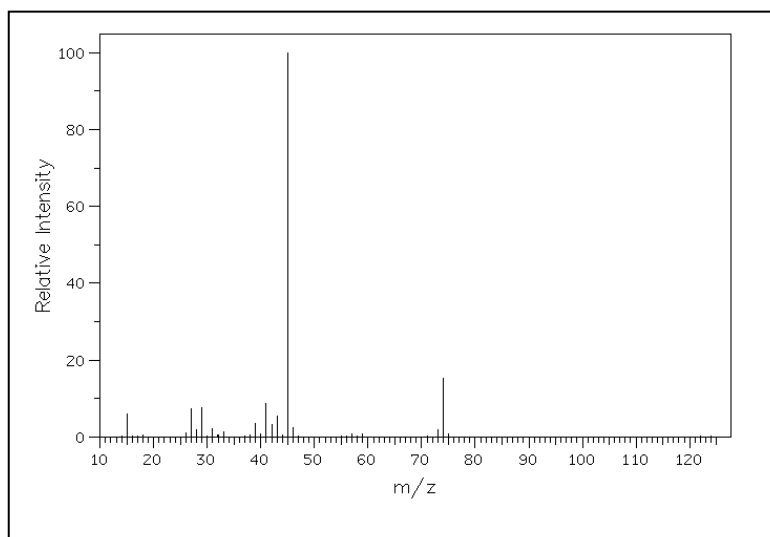
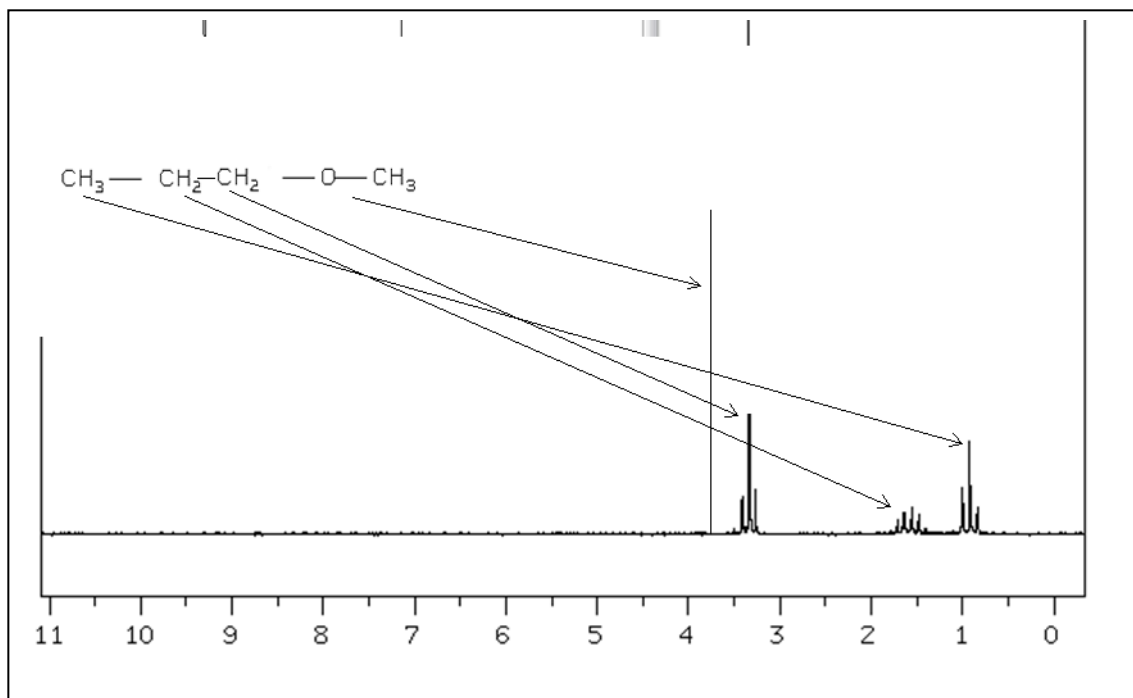
The fragment $CH_3CH_2CO^+$, from the mass spec below, should be used to identify the isomer as methyl propanoate rather than propyl methanoate.

d) What fragment produced the base peak in the IR spectrum? $CH_3CH_2CO^+$

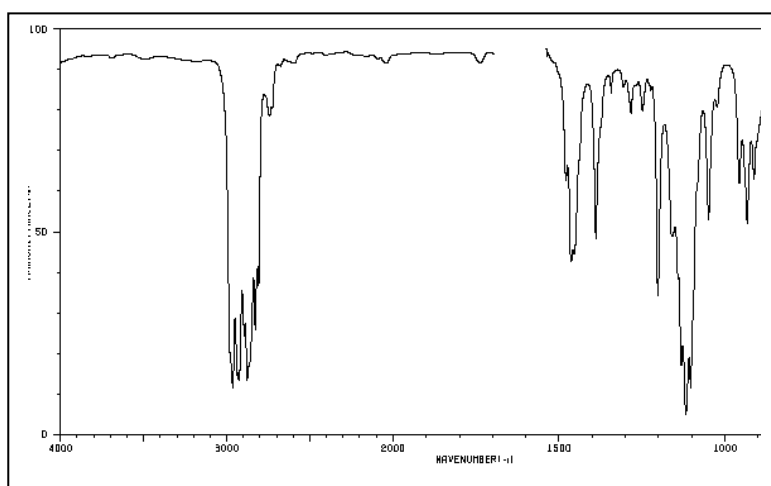
e) Explain the peak at m/z 89 in the mass spectrum. *Due to ^{13}C isotope.*



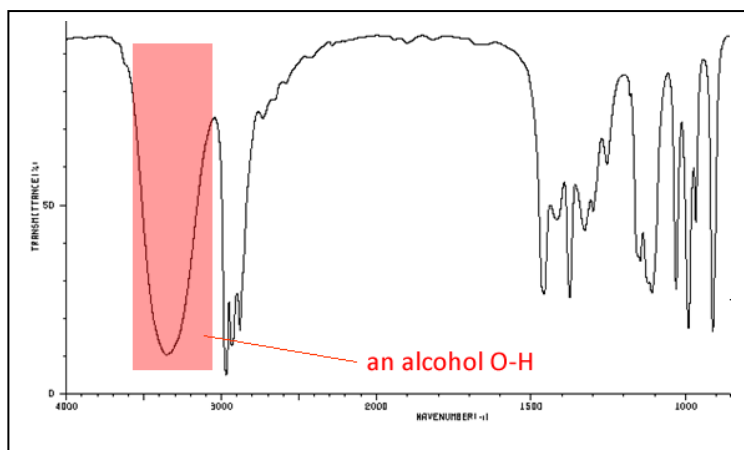
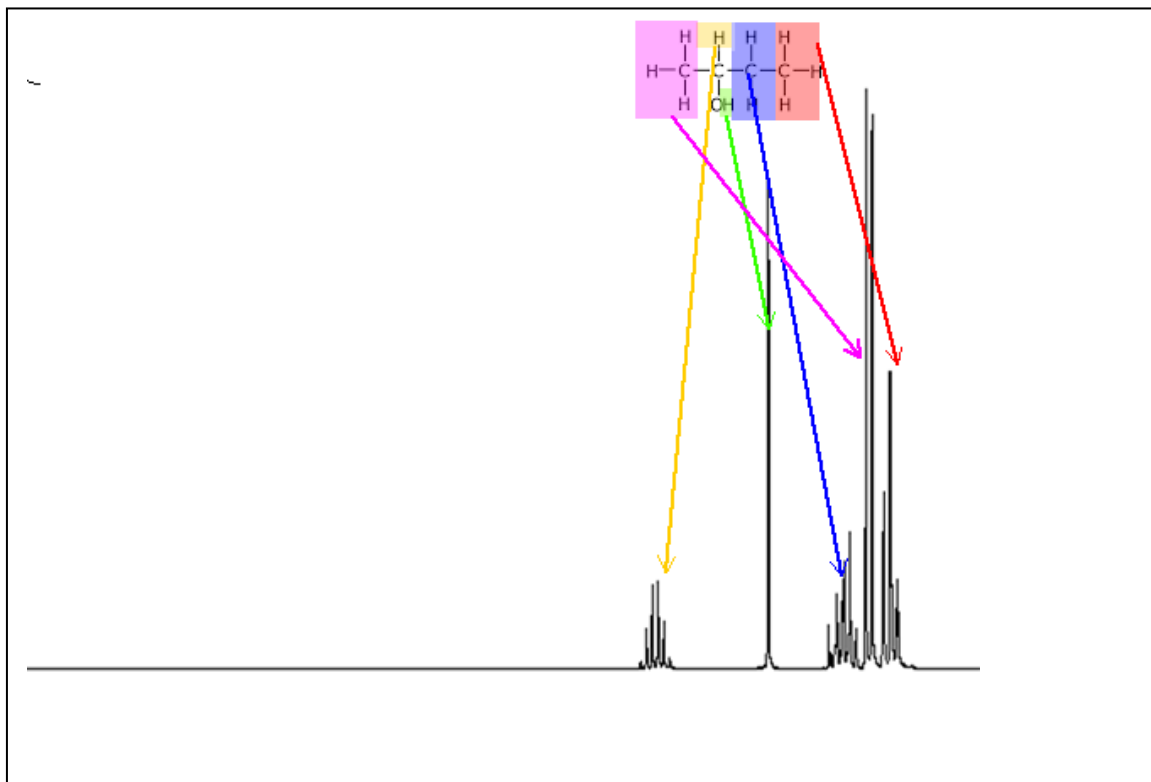
- 3) An unknown compound was analysed and found to have the molecular formula $C_4H_{10}O$. Draw the structural formula of the compound. Below are the compound's 1H NMR, IR and mass spectra



- The key indicators are:*
- The 1H NMR shows a match of the hydrogen pattern.*
 - The mass spec shows a base peak at m/z 45 that corresponds to the fragment $CH_2OCH_3^+$*
 - The IR spectrum shows strong absorption at 1100 that indicates a C-O bond.*



4) Another unknown compound was analysed and also found to have the molecular formula $C_4H_{10}O$. Name the compound. Below are the compound's 1H NMR, IR and mass spectra



Butan-2-ol

Key indicators from the spectra include:

- *The IR indicates an alcohol OH present*
- *The mass spec base peak at m/z 45 indicates the fragment CH_3CHOH^+ which is consistent with a secondary alcohol such as butan-2-ol*
- *The 1H NMR show a match.*

