

Note that in high resolution spectrum the broad peaks appear as groups of separate sharp peaks, called the splitting pattern. The reason for this is that the precise frequency at which absorption occurs is influenced by the direction of the magnetic field of any hydrogens attached to the **neighbouring** carbon atom as the hydrogen producing the signal (not the same carbon atom). If therefore there was one hydrogen on the neighbouring carbon, as would be the case in the signal for the methyl groups in $(\text{CH}_3)_3\text{CH}$, then the peak would be split into two (a doublet) corresponding to the single hydrogen on the central carbon having a \uparrow spin or a \downarrow spin. Similarly the signal of the CH_3- group in ethanol ($d = 1.1$) is affected by the alignment of the hydrogens of the $-\text{CH}_2-$ group. There are three combinations for this ($+2 - \uparrow\uparrow$, $0 - \uparrow\downarrow$ and $\downarrow\downarrow$, or $-2 - \downarrow\downarrow$) so the signal is split into three (a triplet) with an intensity ratio of 1:2:1 (the same as the probabilities of the three states of the CH_2 hydrogens). Similarly the signal of the $-\text{CH}_2-$ group ($d = 3.8$) is split into four peaks (a quartet) by the possible alignments of the hydrogens in the CH_3- group

($\uparrow\uparrow\uparrow$; $\uparrow\uparrow\downarrow$, $\uparrow\downarrow\uparrow$ & $\downarrow\uparrow\uparrow$; $\uparrow\downarrow\downarrow$, $\downarrow\uparrow\downarrow$ & $\downarrow\downarrow\uparrow$; $\downarrow\downarrow\downarrow$; hence a 1:3:3:1 ratio). The general rule is that the number of peaks is equal to the number of hydrogens on the neighbouring carbon plus one. The O-H signal is not split because the rapid exchange of this atom between ethanol molecules averages out the different possible spins.

Combining various data

Often the different spectra and elemental analysis can be combined to reinforce each other in the elucidation of the structure of an unknown substance. Consider an example – Compound X. The empirical formula of X was determined as $\text{C}_2\text{H}_4\text{O}$ from the fact that 1.000 g of X, on complete combustion, yielded 2.000 g of carbon dioxide and 0.818 g of water (doing the calculation would be good practice!). The various spectra of X are given in Figure 11-13.

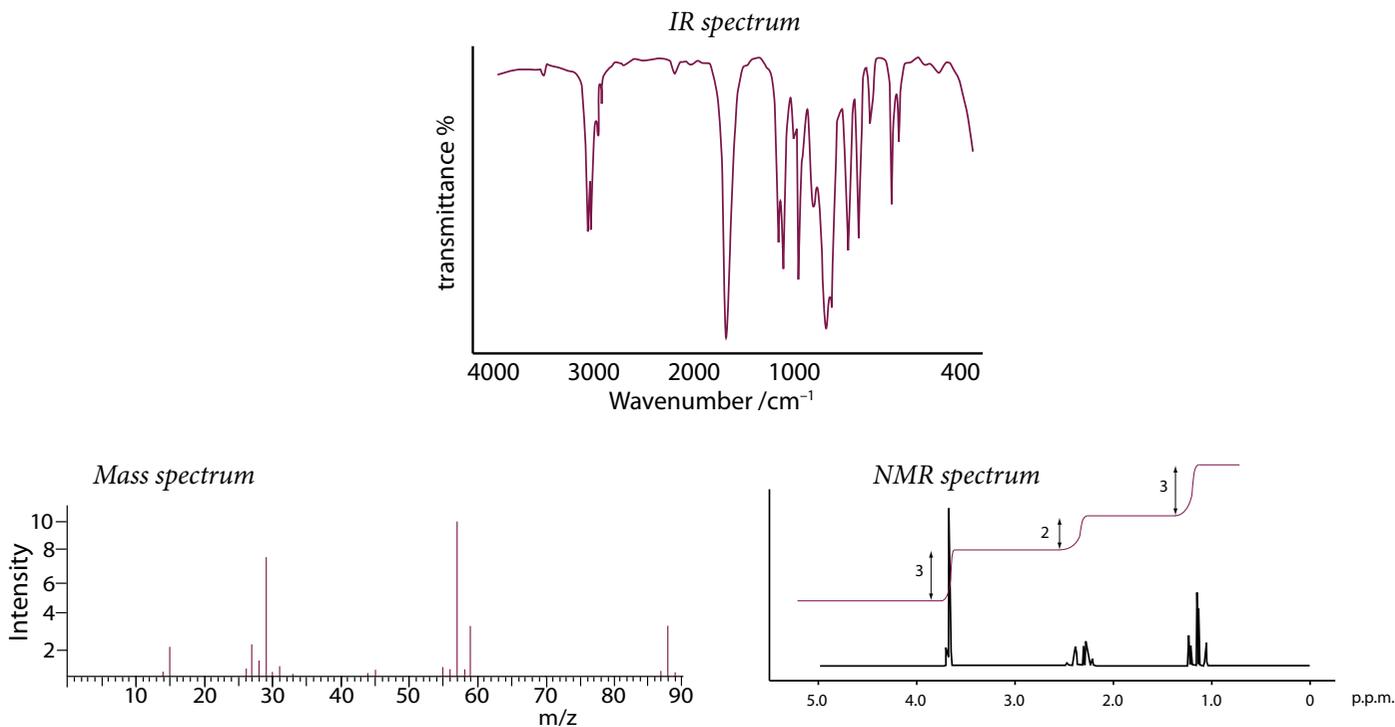


Figure 11-13 Spectra of Compound X

- From the mass spectrum the molecular ion peak is at $m/z = 88$, so that the molecular formula of the compound must be $\text{C}_4\text{H}_8\text{O}_2$, twice the empirical formula.
- The compound has an IHD of 2 (C_4H_8 not C_4H_{10} , remembering O has no effect), so it must have a ring or a double bond.
- The IR spectrum gives us two important pieces of information:
 - There is a strong peak at $\sim 1750 \text{ cm}^{-1}$ so the molecule clearly contains a carbonyl ($>\text{C}=\text{O}$) group.
 - There is no broad peak $\sim 3000 \text{ cm}^{-1}$ so the molecule does not contain a hydroxyl ($-\text{OH}$) group, nor is there a peak at $\sim 1650 \text{ cm}^{-1}$ so it does not contain a carbon-carbon double bond ($>\text{C}=\text{C}<$). Note that the absence of peaks is often just as informative as their presence!