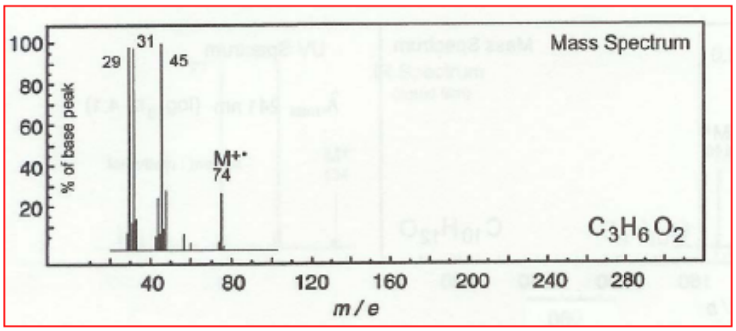
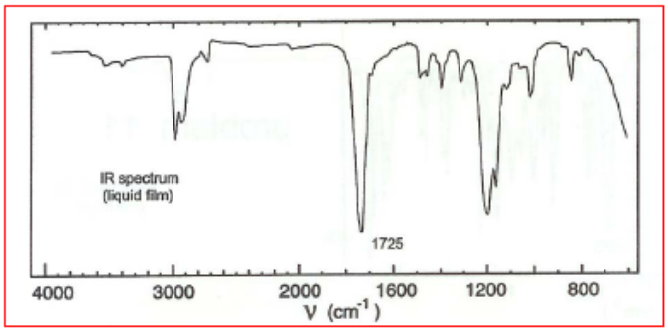
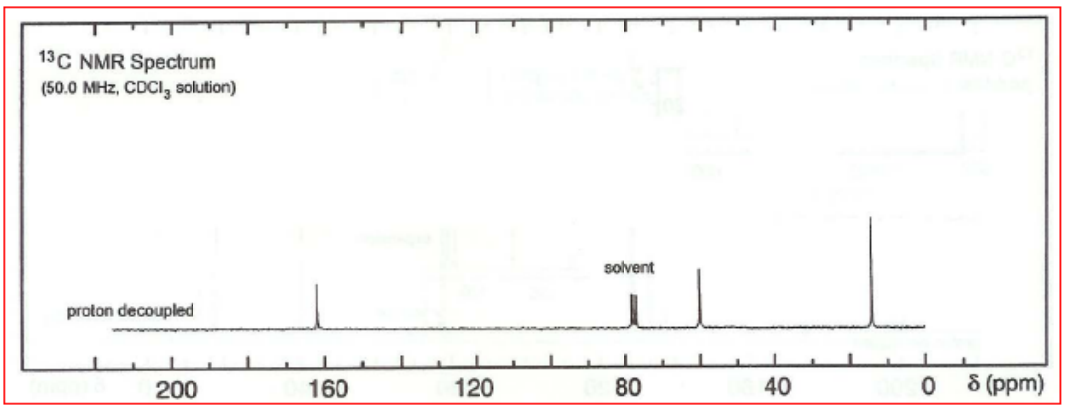
Identify the molecule …

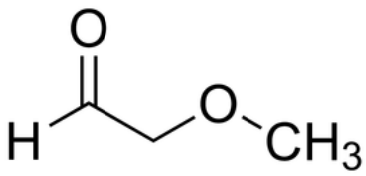






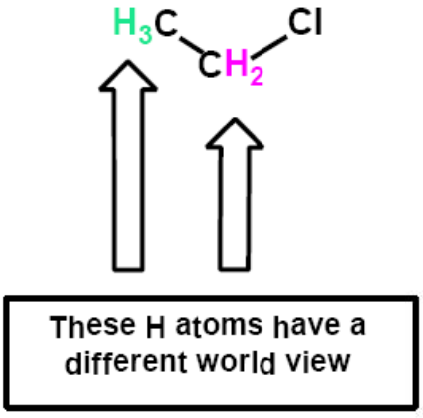
No significant UV absorption above 210 nm

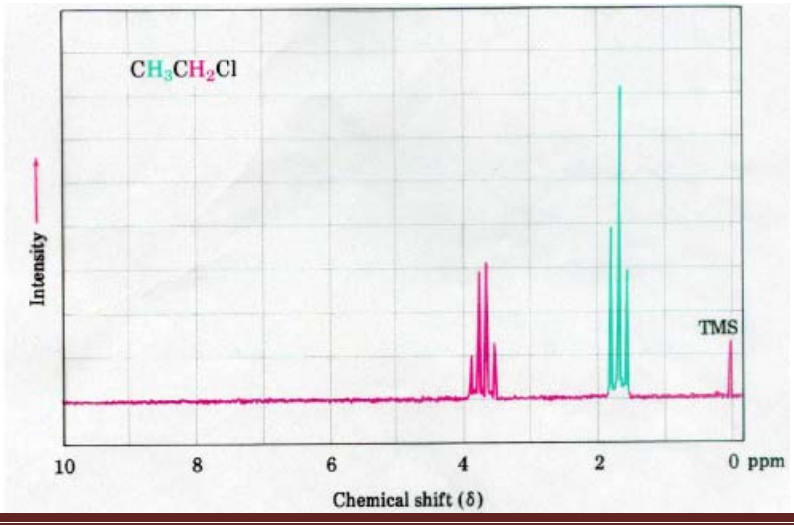
- The pop quiz above is quite difficult – it's a mixture between NMR, mass spectrometry and IR spectroscopy.
  - ➔ Drop at ~3000 and ~1700 suggest the presence of a C-H and C=O bonds (ketone or aldehyde).
  - ➔ Lack of a drop at ~3300 suggest that there's no –OH group.
  - ➔ The structure is methoxyacetaldehyde (below).



Lecture 6: ^{1}H NMR

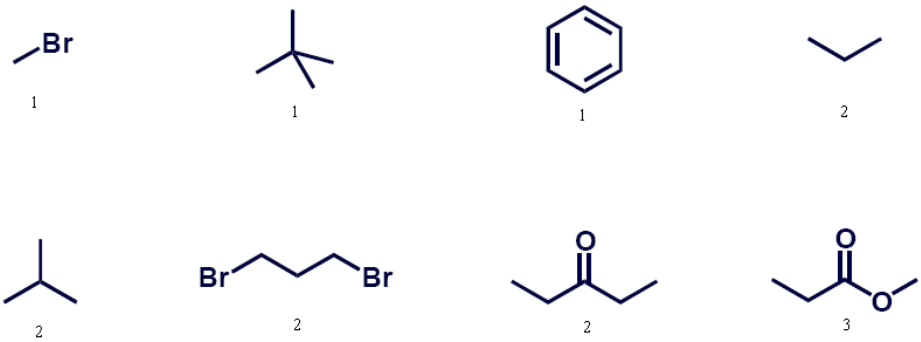
- The same principle in ^{13}C NMR can be used for ^{1}H NMR.
  - ➔ ^{1}H is NMR active.
  - ➔ Number of signals corresponds to the number of types of ^{1}H atoms.



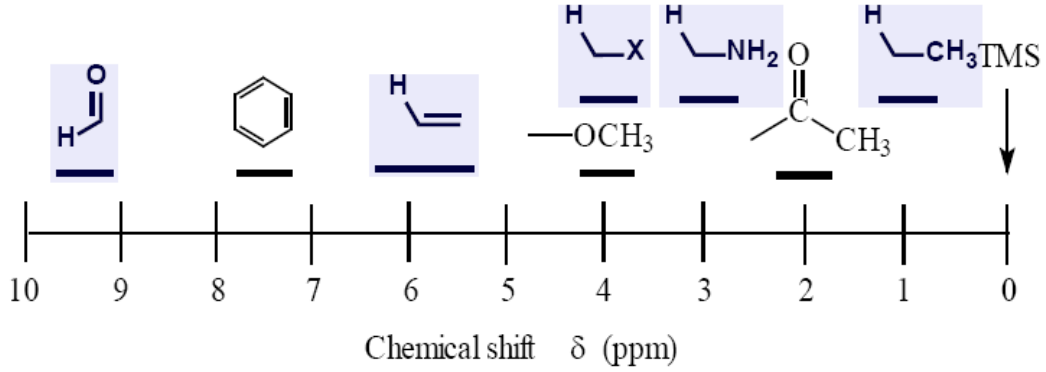


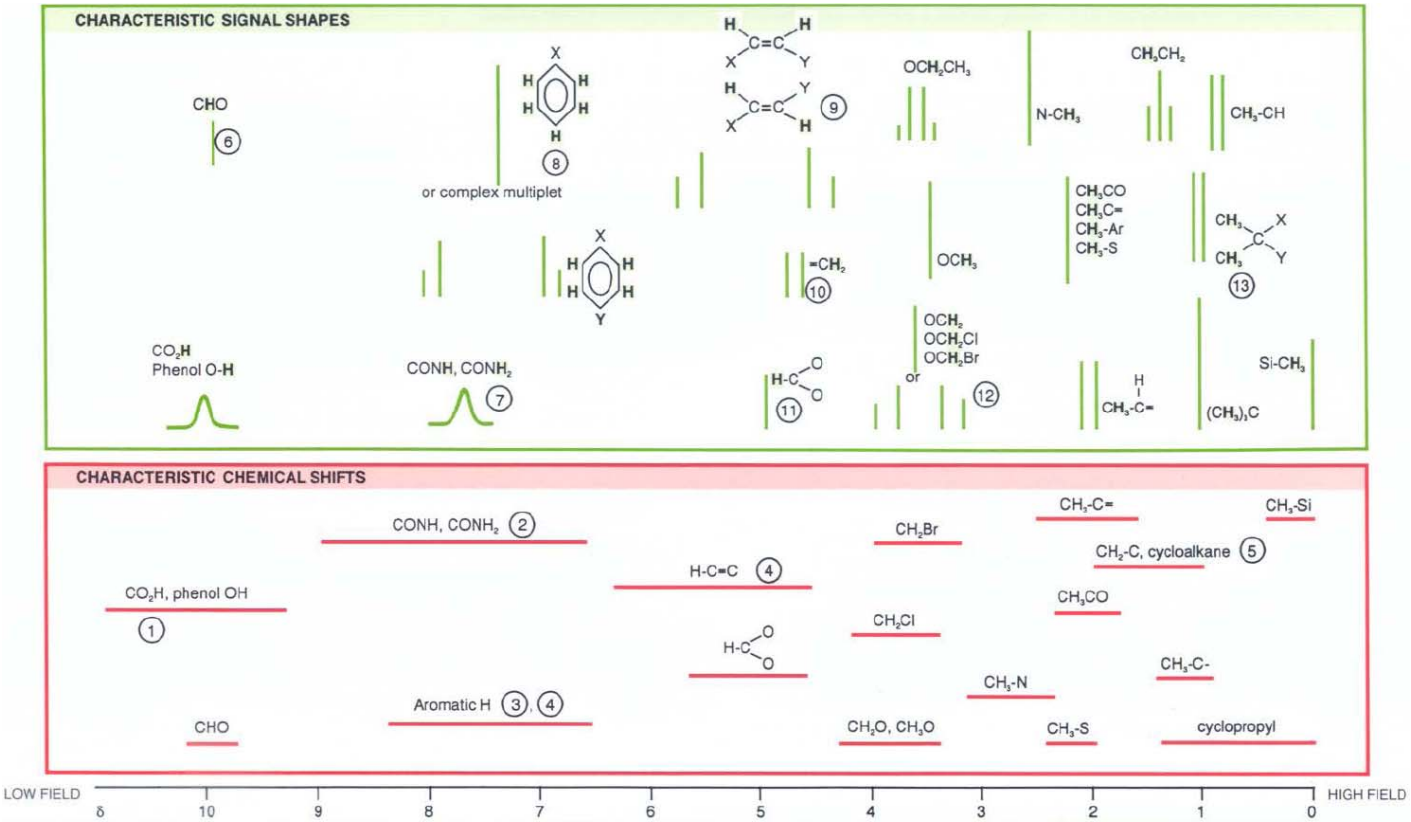
- The pop quiz below:

So how many ^{1}H NMR signals would you expect from these guys?



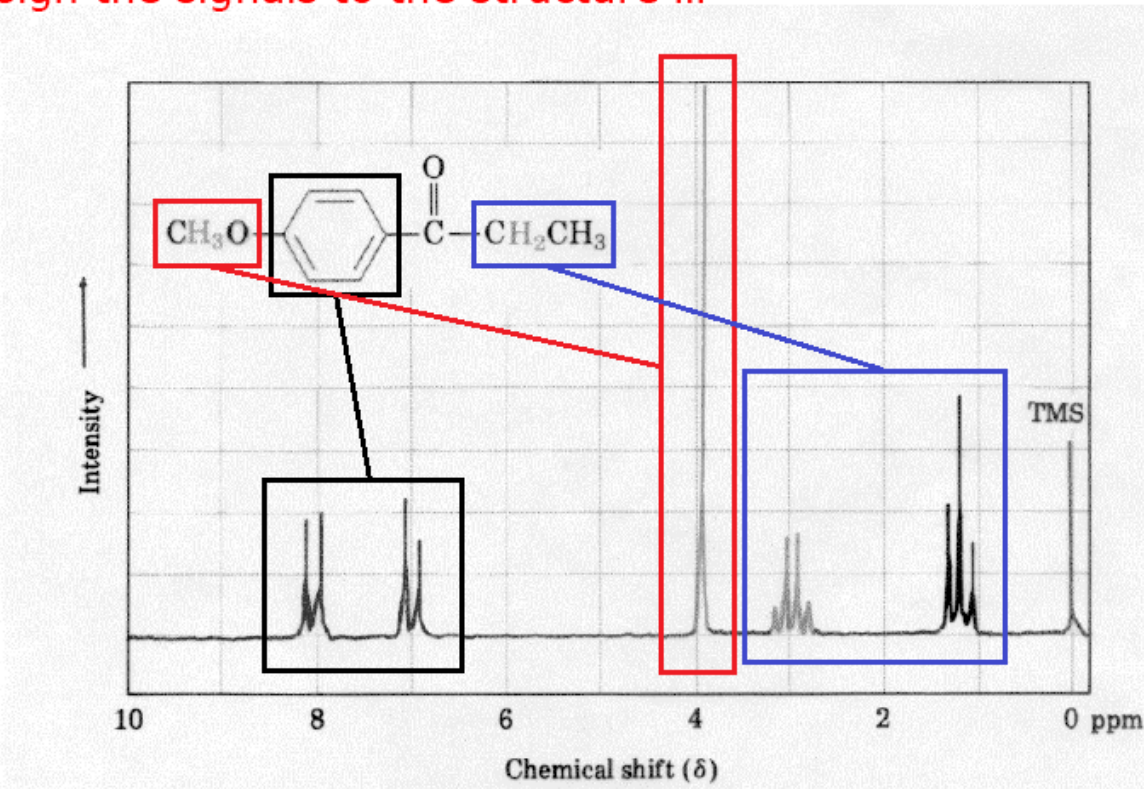
- The frequency axis (δ scale) calibrated in parts per million (ppm).
  - ➔ A reference compound, tetramethylsilane (TMS) or $(CH_3)_4Si$, and is set to 0.00ppm.
  - ➔ The difference between a signal arising from a sample and the TMS signal is called the *chemical shift*.





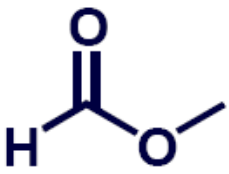
- In the above, the upper shows shapes of various signals and the lower part gives the region of NMR where they may be found – use the lower to find possible origins then use the top to determine possible features.

Assign the signals to the structure …

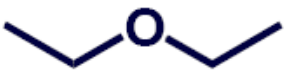


- You can solve this by looking at the number of neighbouring hydrogen atoms (equivalent protons are not spin splitting protons).
  - ➔ For the blue, the CH_2CH_3 group would produce two signals, a quartet and a triplet.
  - ➔ For the red (CH_3 group) is a singlet.
  - ➔ For the black, it is a benzene group and has a split signal (previous graph).
- There are two more sources of information in a ^1H spectrum.
  - ➔ The integral is the integrated peak area of ^1H signals – the intensity is directly proportional to the number of hydrogen.
  - ➔ The multiplicity is the splitting of peaks and tells you how many neighbouring protons there are.

What's the ratio of signal sizes in the ^1H NMR spectra of these?

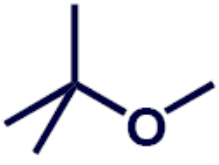


3 to 1



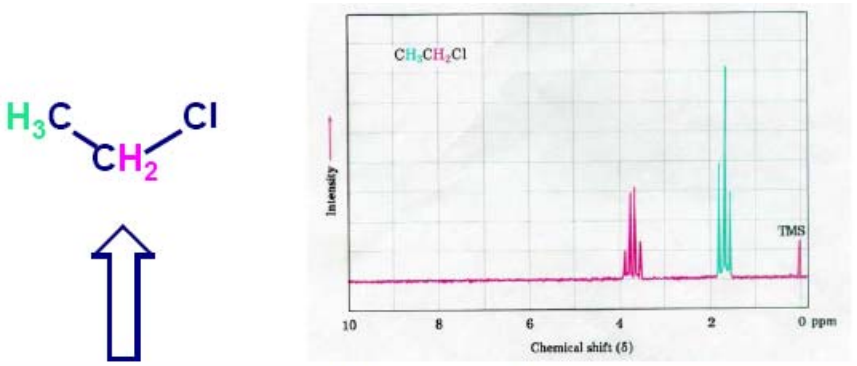
3 to 2

2 to 1



3 to 1

- It is important to understand equivalent hydrogen atoms and hydrogen atoms attached to neighbouring carbon atoms.
  - ➔ If X has n equivalent hydrogens on neighbouring carbons, X's signal will be split into n+1 peaks.



These H atoms have **three** neighbouring H's ⇒ Their signal shows up as a **quartet**