^{13}C NMR SPECTROSCOPY BASICS

A BIT ABOUT ^{13}C NMR….

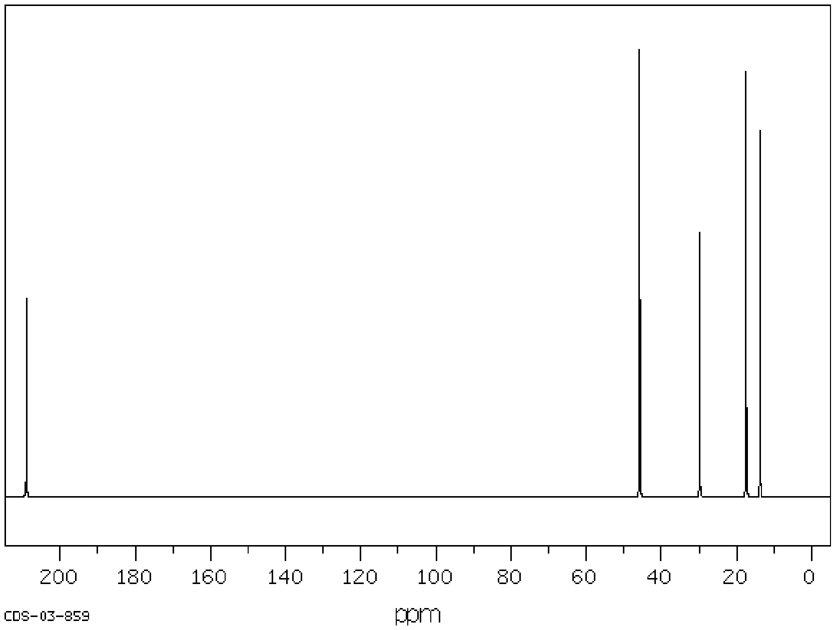
Carbon-13 nuclear magnetic resonance provides information about the different "types" of carbon atoms which are present in a sample and gives us clues about what type of functional groups might be present.

HOW IT WORKS (NOT ASSESSABLE)

When an organic compound is placed in a strong magnetic field the nuclei of any carbon-13 (^{13}C) atoms in the compound will align themselves either with the magnetic field or against the magnetic field.
Those nuclei which are aligned with the magnetic field can be made to flip so they are aligned against the field by absorbing a specific radio frequency. However, this radio frequency varies depending on the **chemical environment** of the carbon atom. This allows us to identify the different "types" of carbon atoms which are present in a sample, and also helps us determine what functional groups may or may not be present in the compound.

An example of a typical ^{13}C NMR is shown below. The x axis is the **chemical shift** (measured in ppm) which is related to the differences in radio frequency causing the nuclei of the different carbon nuclei to flip.

This ^{13}C NMR spectrum shows that there are **5 different types of carbon atom** in the compound being analysed as there are **5 PEAKS**



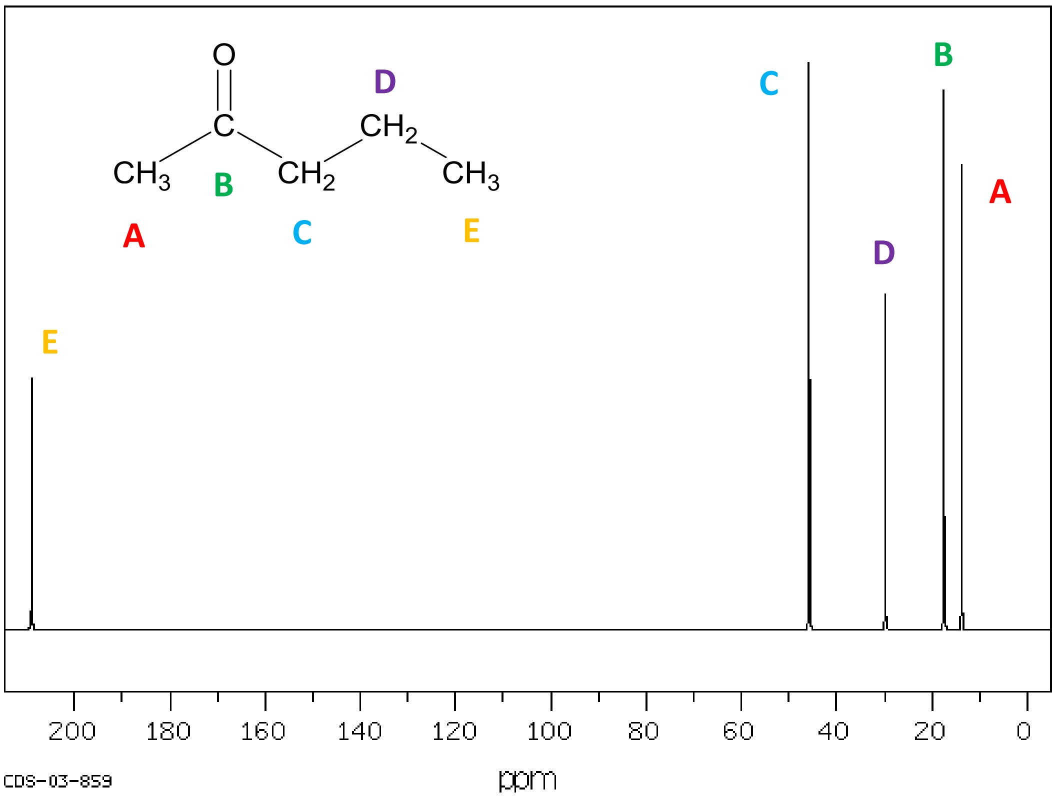
Why are we using ^{13}C and not ^{12}C atoms for NMR analyses?
In nature only ~1% of carbon atoms are ^{13}C, while most of the remaining ~99% are ^{12}C. So why doesn't NMR use ^{12}C atoms?

The simple answer is that ^{12}C atoms don't work. Only atoms with an odd number of protons and/or an odd number of neutrons in their nuclei work with NMR. As a ^{12}C nuclei has 6 protons and 6 neutrons it will not work with NMR, whereas ^{13}C has 6 protons and **7 neutrons** which allow it to generate the nuclear spin required for it to interact with the magnetic field of an NMR device.

EXAMPLES OF SPECTRA

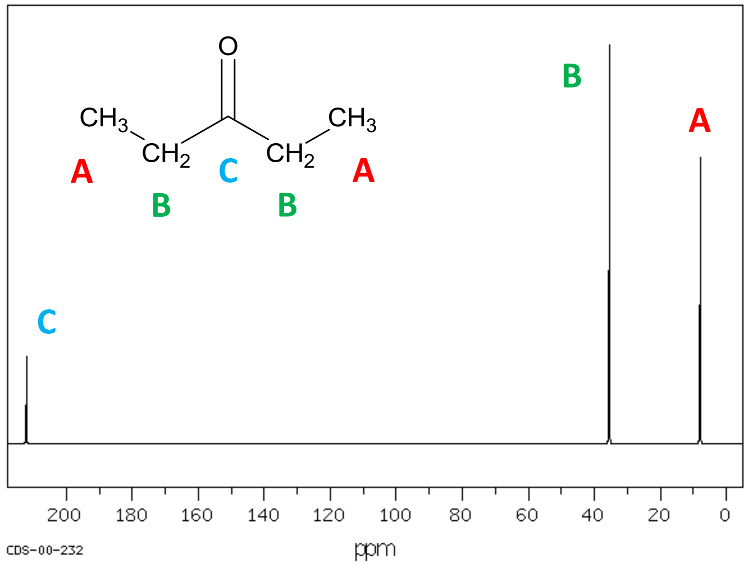
So let's take a closer look at this ^{13}C NMR spectrum which comes from 2-pentanone. Each peak (or line) on the spectrum represents a different carbon atom in the structure. These have been identified using the letters in the diagram below.

2-pentanone



Each C atom is different – surrounded by different groups. As there are 5 different C atoms, there are 5 peaks.

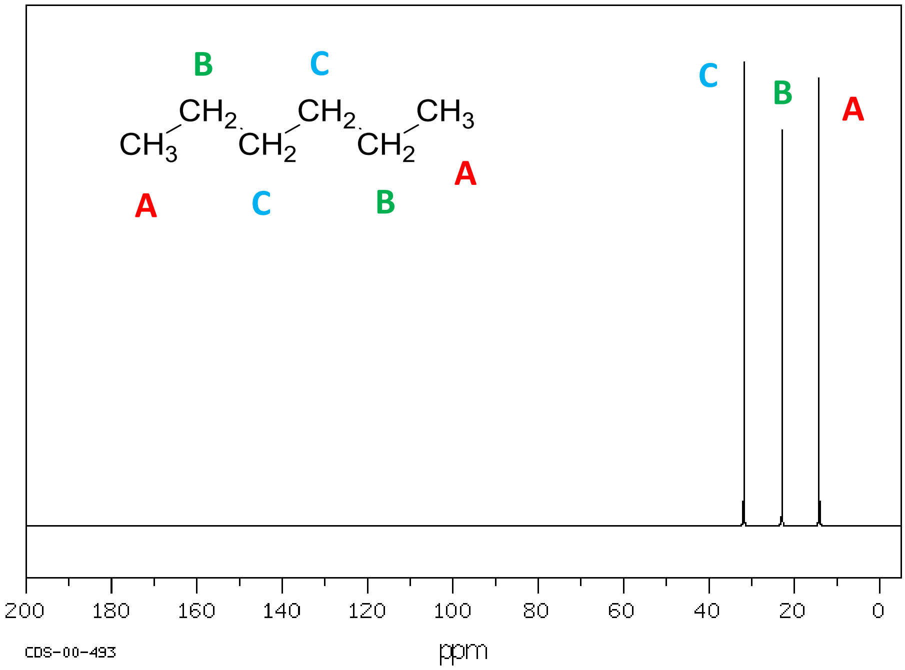
3-pentanone



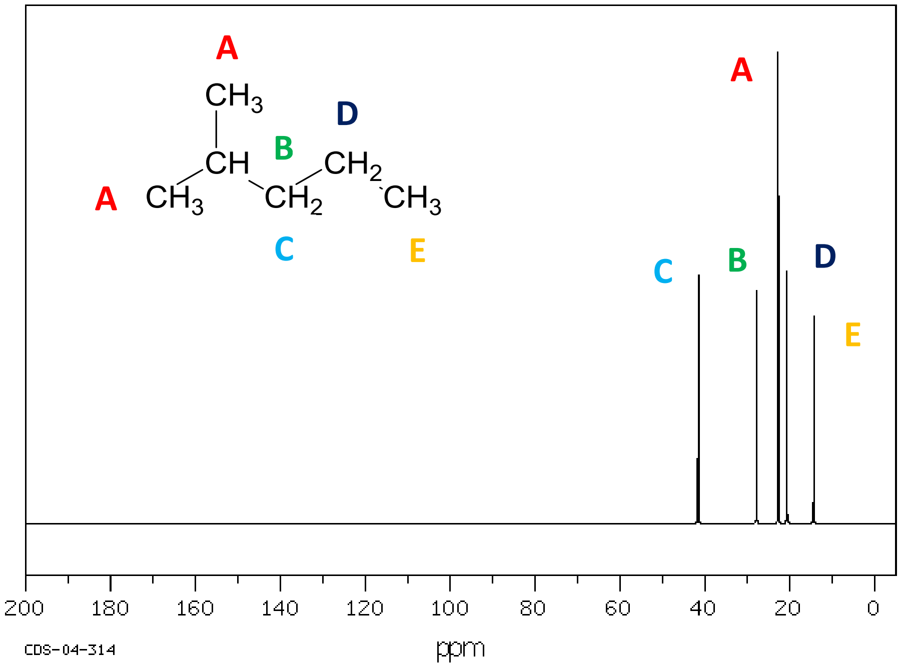
There are 3 peaks as there are 3 different types of C atom.

Isomers of C_6H_{12}

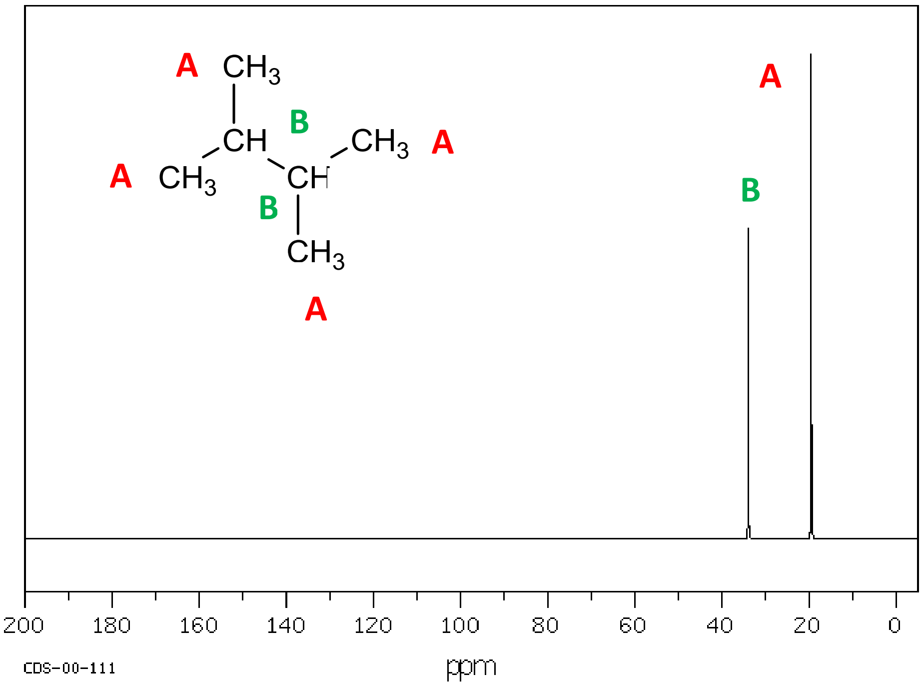
Hexane



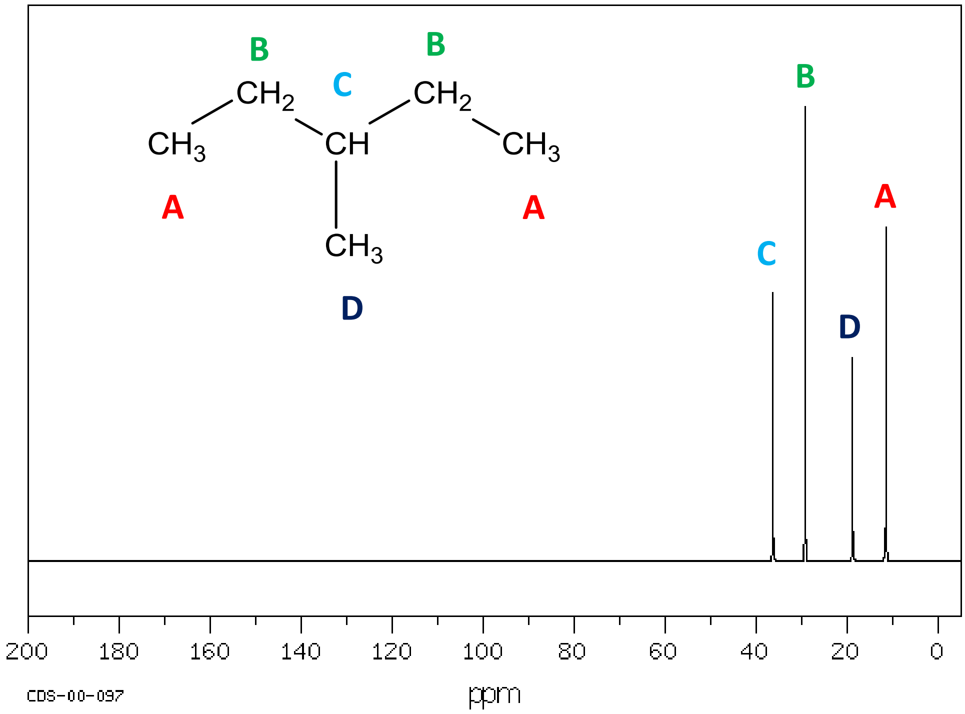
2-methylpentane



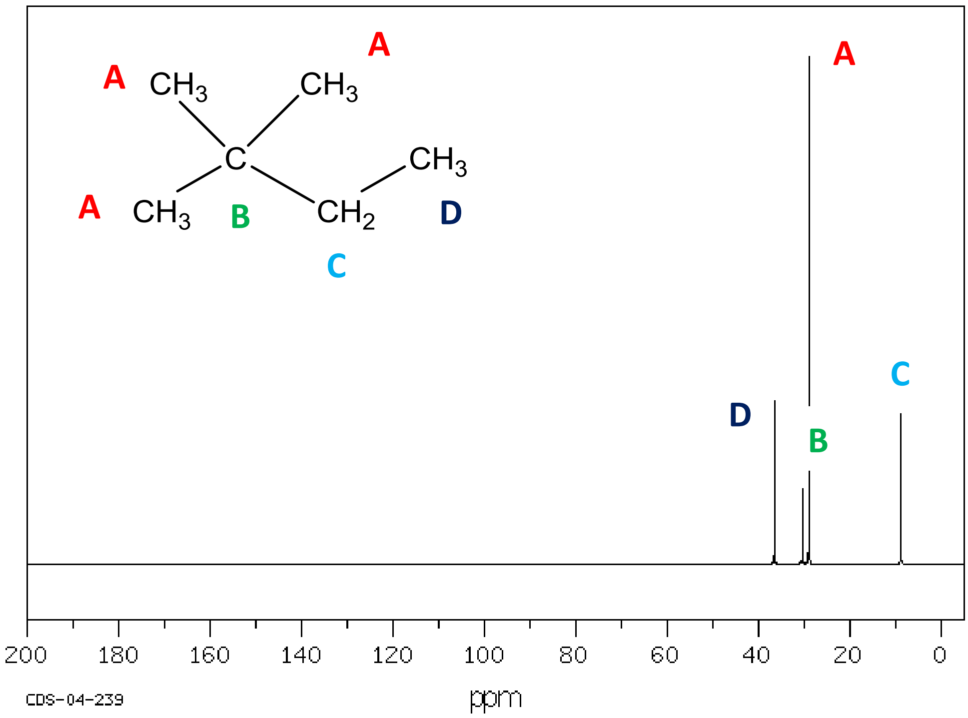
2,3-dimethylbutane



3-methylpentane



2,2-dimethylbutane



FUNCTIONAL GROUP INFORMATION

By examining the chemical shifts present in a ^{13}C NMR spectrum it will give us some idea of what functional groups may be present. Below is a diagram outlining the typical ranges of chemical shifts for different carbon atoms (e.g. from the table we can see that the carbon atom in an aldehyde would have a chemical shift between 190 and 220 ppm whereas the carbon attached to a Cl group would be between 30 to 50 ppm).

Typical ^{13}C Chemical Shifts