Mass Spectrometry

The mass spectrometer is used to determine

- the of a molecule.
- the of isotopes.
- the of a compound.

Infrared Spectroscopy

Infrared spectroscopy provides information on the different types of bond in a molecule and from this the functional groups present.

NMR Spectroscopy

An NMR spectrometer provides information on the and types of environments in a molecule or the number and types of environments and from this the detailed molecular structure can be deduced.

In chemical analysis these techniques are used in combination with each other to fully identify a compound. However, the NMR spectrum gives more detailed information than any of the others.

NMR Spectroscopy

Nuclear magnetic resonance or NMR spectroscopy is a powerful analytical technique for examining molecular structures in detail, but it also has other applications such as in , where it is more commonly called .

The two most common types of NMR spectroscopy are Proton NMR spectroscopy and Carbon-13 NMR spectroscopy, both of which rely on the use of isotopes with an uneven number of nucleons (and) in their nucleus - ^{1}H and ^{13}C.

These nuclei are used because they are able to generate a . Other isotopes used include Fluorine-19 and Phosphorus-31.

Isotopes:

Formula	Neutrons	Protons	Electrons
^{1}H			
^{13}C			
^{19}F			
^{31}P			

The nuclei in these atoms are able to absorb and emit low energy radio waves which are then picked up by the spectrometer and used in the analysis to produce an NMR spectrum. When these nuclei absorb energy they are said to or are from a low energy state to a high energy state. When the nuclei return to the low energy state the process is known as . This continual excitation and relaxation is called . This is what is measured.

The electrons in an atom will shield the nucleus from the applied magnetic field in the spectrometer and the extent of shielding will vary according to the in neighbouring atoms or groups. The environment of a nucleus will have an effect on how much radiation it absorbs in "flipping".

Key Terms

Chemical shift

this is the frequency of radiation at which a nucleus absorbs energy. This frequency is measured in and is compared to a ( ).

TMS

this stands for tetramethylsilane and it is the chemical used as a standard in NMR spectroscopy.

It is given a value of .

TMS has (the same) . This gives rise a peak that can be easily .

TMS is chemically and so it can be easily removed from a sample.

Deuterated solvent

A solvent containing rather than Hydrogen (H) so that the solvent's molecular structure does not interfere with the analysis as D atoms do not produce an NMR signal. E.g. $CDCl_3$. It has an number of . Therefore does not produce a .

Peak

the line at a particular in an NMR spectrum

Spin-spin splitting

this is the pattern of of a peak in a spectrum, resulting from its atoms.

Integration trace

this indicates the of the number of protons of a particular type in a Proton-NMR spectrum