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IS37. THE MASS SPECTROMETER: HOW IT WORKS?

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The mass spectrometer is an analytical tool which can measure the masses and relative concentrations of atoms and molecules. It makes use of the basic magnetic force on a moving charged particle.

The sample has to be introduced into the ionization source of the instrument. Once inside the ionization source, the sample molecules are ionized, because ions are easier to manipulate than neutral molecules. These ions are extracted into the analyzer region of the mass spectrometer where they are separated according to their mass (m) -to-charge (z) ratios (m/z). The separated ions are detected and this signal sent to a data system where the m/z ratios are stored together with their relative abundance for presentation in the format of a m/z spectrum.

The four essential sections of a mass spectrometer, and the associated components, are:

1. Sample Introduction: Gas or liquid chromatography column, flow injection
2. Ionisation: Gas phase ions are made in the ion source
3. Mass Anayser: Ions are separated by their mass to charge ratio (m/z) in the mass analyzer
4. Detector: Only charged molecules (ions) are detected

Sample Introduction

The method of sample introduction to the ionization source often depends on the ionization method being used, as well as the type and complexity of the sample. The sample can be inserted directly into the ionization source, or can undergo some type of chromatography in route to the ionization source. This latter method of sample introduction usually involves the mass spectrometer being coupled directly to a high pressure liquid chromatography (HPLC), gas chromatography (GC) or capillary electrophoresis (CE) separation column, and hence the sample is separated into a series of components which then enter the mass spectrometer sequentially for individual analysis.

Ionisation

Many ionization methods are available and each has its own advantages and disadvantages the ionization method to be used should depend on the type of sample under investigation and the mass spectrometer available.

Ionization methods include the following:

Electrospray ionization (ESI), Atmospheric Pressure Chemical ionization (APCI), Electron Impact (EI),

Chemical Ionization (CI, Fast Atom Bombardment (FAB), Field Desorption / Field Ionization (FD/FI), Matrix Assisted Laser Desorption Ionization (MALDI)

The ionization methods used for the majority of biochemical analyses are ESI, APCI, EI (especially GC MS) and MALDI.

With most ionization methods there is the possibility of creating both positively and negatively charged sample ions, depending on the proton affinity of the sample. Before embarking on an analysis, the user must decide whether to detect the positively or negatively charged ions.

Mass Anayser

The main function of the mass analyzer is to separate, or resolve, the ions formed in the ionization source of the mass spectrometer according to their mass-to-charge (m/z) ratios. There are a number of mass analyzers currently available, the better known of which include quadrupoles, time-of-flight (TOF) analyzers, magnetic sectors, and both Fourier transform and quadrupole ion traps.

These mass analyzers have different features, including the m/z range that can be covered, the mass accuracy, and the achievable resolution. The compatibility of different analyzers with different ionization methods varies.

Tandem (MS-MS) mass spectrometers are instruments that have more than one analyzer and so can be used for structural and sequencing studies. Two analyzers have all been incorporated into commercially available tandem instruments, and the analyzers do not necessarily have to be of the same type, in which case the instrument is a hybrid one. More popular tandem mass spectrometers include those of the quadrupole-quadrupole, magnetic sector-quadrupole, and more recently, the quadrupole-time-of-flight geometries.

Detector

The detector monitors the ion current, amplifies it and the signal is then transmitted to the data system where it is recorded in the form of mass spectra. The m/z values of the ions are plotted against their intensities to show the number of components in the sample, the molecular mass of each component, and the relative abundance of the various components in the sample. The type of detector is supplied to suit the type of analyzer; the more common ones are the photomultiplier, the electron multiplier and the micro-channel plate detectors.

Mass spectrometers are used in industry and academia for both routine and research purposes. The following list is just a brief summary of the major mass spectrometric applications:

Biotechnology: the analysis of proteins, peptides, oligonucleotides

Pharmaceutical: drug discovery, combinatorial chemistry, pharmacokinetics, drug metabolism

Clinical: neonatal screening, hemoglobin analysis, drug testing, steroid hormones,

Environmental: Polycyclic aromatic hydrocarbons, polychlorinated biphenyls, water quality, food contamination.

Geological: oil composition

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