

Mass Spectrometry

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27 October 2015

1 What is mass spectrometer?

Mass spectrometry, also called mass spectroscopy, analytic technique by which chemical substances are identified by the sorting of gaseous ions in electric and magnetic fields according to their mass-to-charge ratios. The instruments used in such studies are called mass spectrometers and mass spectrographs, and they operate on the principle that moving ions may be deflected by electric and magnetic fields. The two instruments differ only in the way in which the sorted charged particles are detected. In the mass spectrometer they are detected electrically, in the mass spectrograph by photographic or other nonelectrical means; the term mass spectroscopy is used to include both kinds of devices. Since electrical detectors are now most commonly used, the field is typically referred to as mass spectrometry.

Mass spectroscopes consist of five basic parts: a high vacuum system; a sample handling system, through which the sample to be investigated can be introduced; an ion source, in which a beam of charged particles characteristic of the sample can be produced; an analyzer, in which the beam can be separated into its components; and a detector or receiver by means of which the separated ion beams can be observed or collected.

1.1 How does mass spectrometer work?

There are numerous different kinds of mass spectrometers, all working in slightly different ways, but the basic process involves broadly the same stages.

1. You place the substance you want to study in a vacuum chamber inside the machine.
2. The substance is bombarded with a beam of electrons so the atoms or molecules it contains are turned into ions. This process is called ionization.
3. The ions shoot out from the vacuum chamber into a powerful electric field (the region that develops between two metal plates charged to high voltages), which makes them accelerate. Ions of different atoms have different amounts of electric charge, and the more highly charged ones are accelerated most, so the ions separate out according to the amount of charge they have. (This stage is a bit like the way electrons are accelerated inside an old-style, cathode-ray television.)

4. The ion beam shoots into a magnetic field (the invisible, magnetically active region between the poles of a magnet). When moving particles with an electric charge enter a magnetic field, they bend into an arc, with lighter particles (and more positively charged ones) bending more than heavier ones (and more negatively charged ones). The ions split into a spectrum, with each different type of ion bent a different amount according to its mass and its electrical charge.

5. A computerized, electrical detector records a spectrum pattern showing how many ions arrive for each mass/charge. This can be used to identify the atoms or molecules in the original sample. In early spectrometers, photographic detectors were used instead, producing a chart of peaked lines called a mass spectrograph. In modern spectrometers, you slowly vary the magnetic field so each separate ion beam hits the detector in turn.

1.2 Equation

Mass analyzers separate the ions according to their mass-to-charge ratio. The following two laws govern the dynamics of charged particles in electric and magnetic fields in vacuum:

$$\mathbf{F} = Q (\mathbf{E} + \mathbf{v} \times \mathbf{B}) \text{ (Lorentz force law);}$$

$\mathbf{F} = m\mathbf{a}$ (Newton's second law of motion in non-relativistic case, i.e. valid only at ion velocity much lower than the speed of light).

Here \mathbf{F} is the force applied to the ion, m is the mass of the ion, \mathbf{a} is the acceleration, Q is the ion charge, \mathbf{E} is the electric field, and $\mathbf{v} \times \mathbf{B}$ is the vector cross product of the ion velocity and the magnetic field

Equating the above expressions for the force applied to the ion yields:

$$(m/Q)\mathbf{a} = \mathbf{E} + \mathbf{v} \times \mathbf{B}.$$