# M.Sc Inorganic Chemistry (Special-III) Elective Paper-1
## Semester-IV

## Course Title: Spectral Techniques in Inorganic Chemistry
## Paper Code: 4101-A
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**Inorganic Group I and II**

# Mass Spectrometry

Syllabus

Mass spectrometry: Experimental arrangements and presentation of spectra, molecular ions, appearance and ionization potential, fragmentation, ion reactions and their interpretation, effect of isotopes on the appearance of a mass spectrum, molecular weight determination, thermodynamic data. Application of mass spectrometry to inorganic compounds.

# Introduction

A mass spectrometer is an instrument in which gaseous ions are produced from a sample, separated according to their mass-to-charge ratios (m/z) using electric and/or magnetic fields, and then detected in terms of their abundance.

Thus, a spectrometer is in principle very simple, consisting of an ion source, a mass analyzer and a detector.

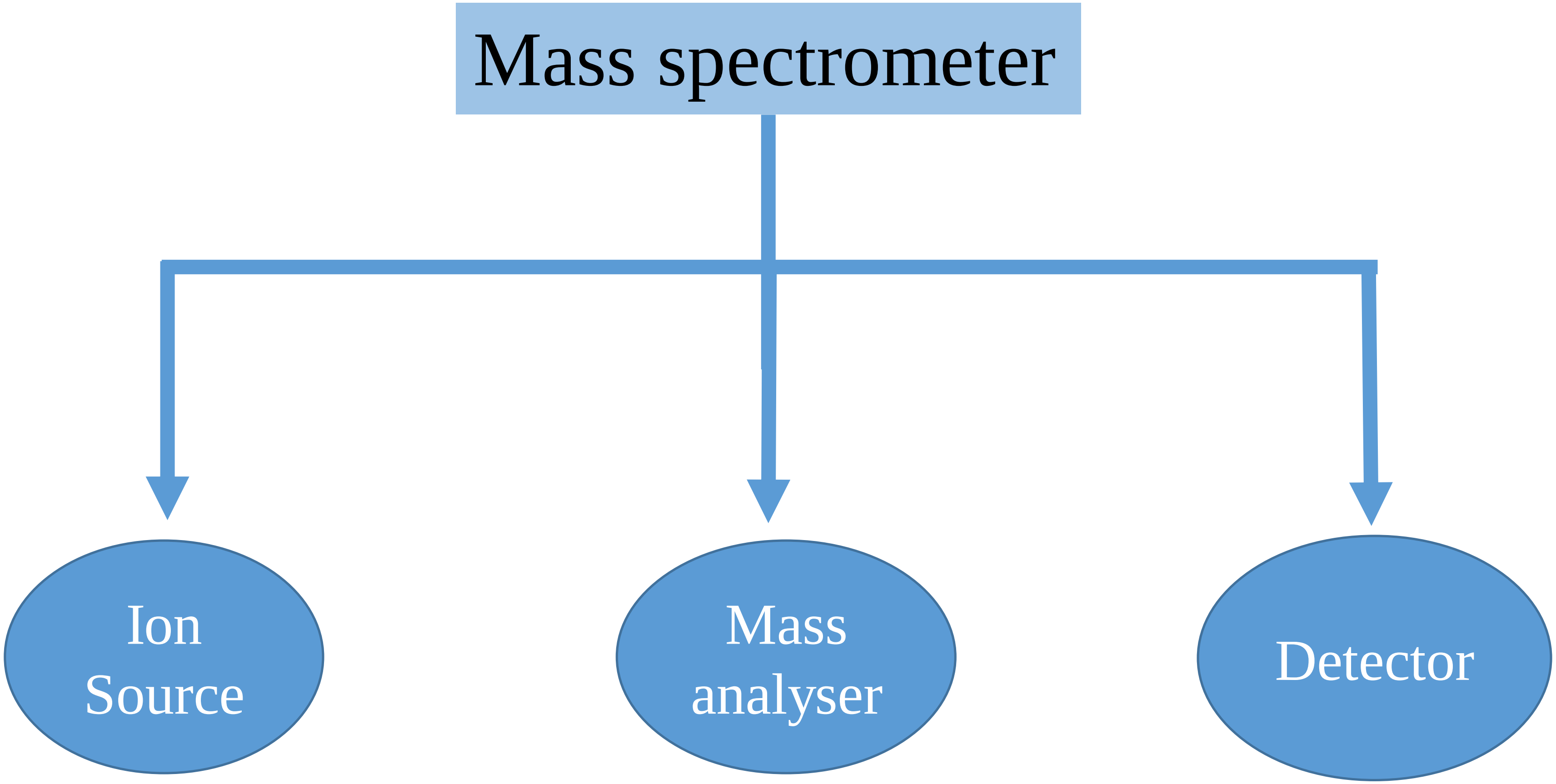
In practice there are many variations on this basic theme, and a high-resolution mass spectrometer is a sophisticated and expensive device.

One of the most useful pieces of information that can be provided by a standard mass spectrometer is the molecular mass of a compound with an accuracy of 1 dalton (Da) (1 Da = 1 unified atomic mass unit (u) = $1.660538921(73) \times 10^{-27}$ kg).

Even better, high-resolution mass spectrometry can provide us with accurate molecular masses, which are accurate to about $10^{-4}$ Da, depending on the total resolution of the spectrometer.

# Experimental arrangements

The mass spectrometer consists of three components an ion source, a mass analyzer and a detector.



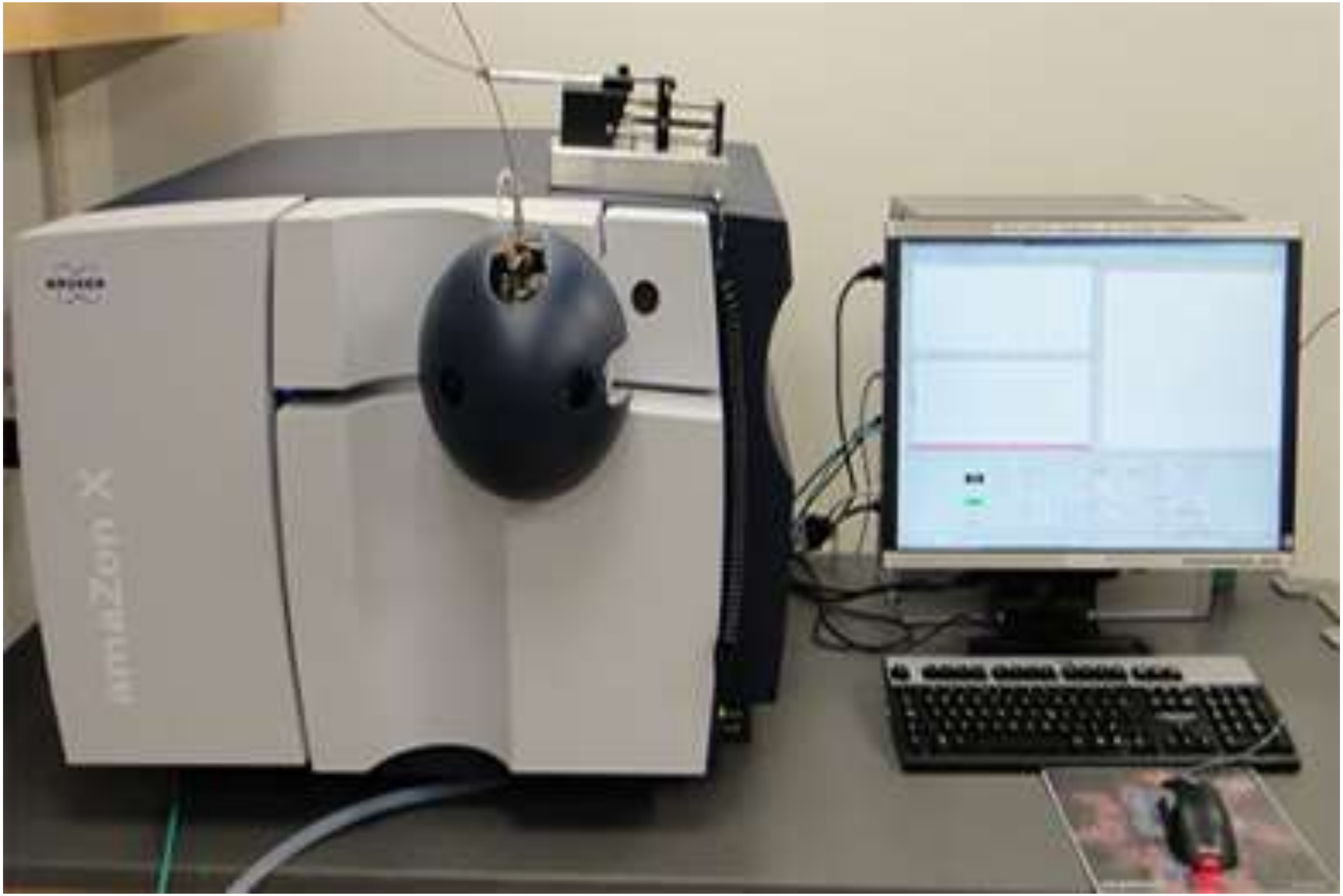
Mass spectrometer

Ion Source

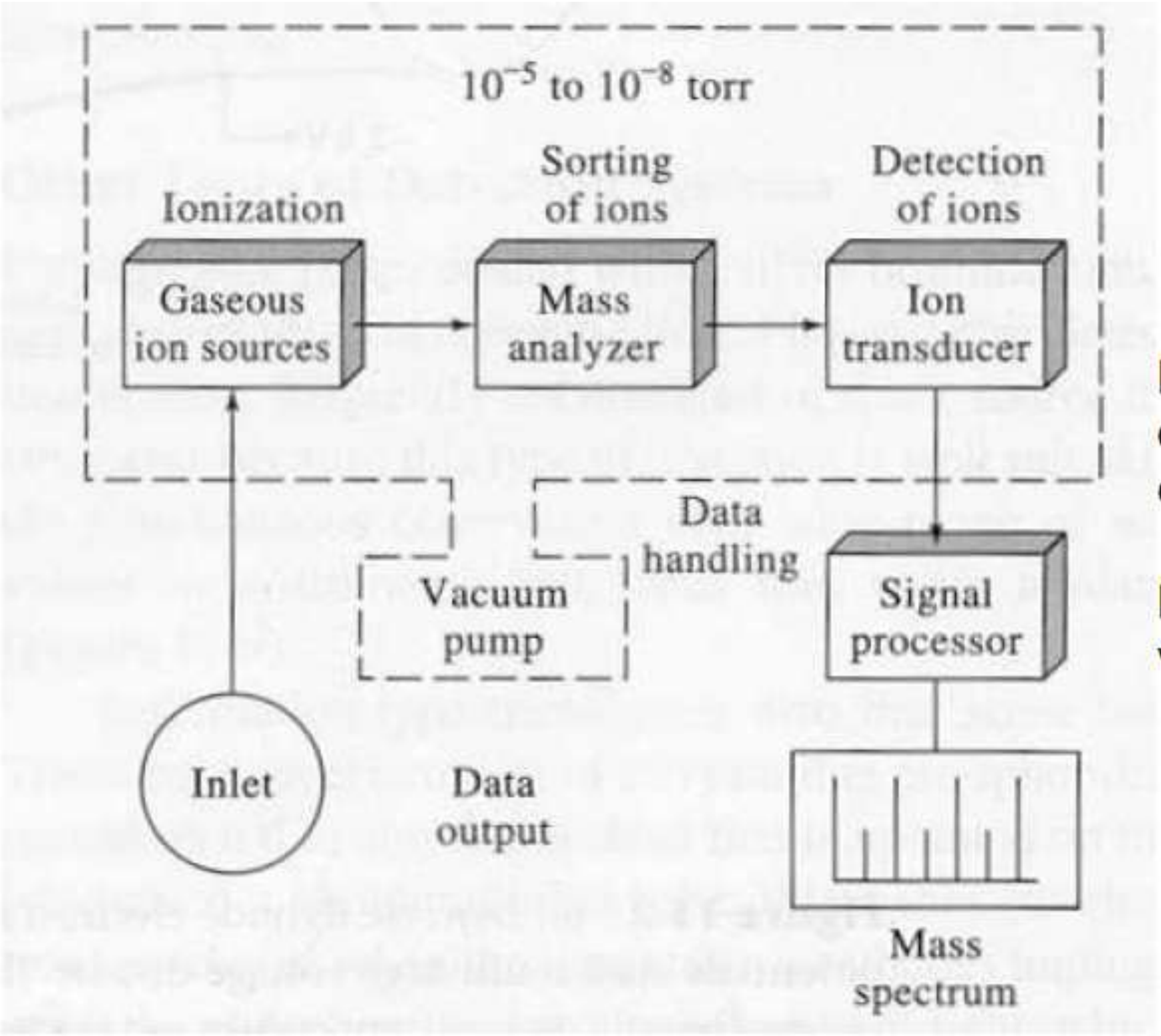
Mass analyser

Detector

# Bruker AmaZon X Ion Trap Mass Spectrometer



# Schematic diagram of a Mass Spectromerter



Basic MS design components

Note high vacuum

# Ion sources

The sample can be introduced as a solid, liquid or vapor into the ion source, where it is ionized and fragmented. There are many different types of ion source available, and which method to use depends on the nature of the sample to be analyzed and the type of information that is sought. With most methods, there is the possibility of creating positively or negatively charged ions, by the gain or loss of electrons or protons.

This results in a very flexible technique, with many specialized applications.

The majority of work undertaken in inorganic chemistry tends to use the positive-ion methods, but negative-ion methods can also give useful information, particularly relating to complex stabilization energies.

# Ion sources

Ion sources can be broadly grouped into two classes:

- Hard source
- Soft source

Hard source, in which the ionization method leaves the ion in an excited state, which invariably fragments upon relaxation.

Soft source, in which fragmentation is suppressed. The latter methods are therefore particularly well suited for recording the accurate masses of samples, and for the handling of large, fragile, complex samples such as macromolecules and biomolecules.

Moreover, as the ions formed by soft ionization methods tend to be multiply charged, this reduces the m/z ratio of the resultant ion stream so that heavier samples can be detected within the range of standard spectrometers.