Mass Spectrometry

Mass spectrometers are devices that are used for separating charged atoms and molecules based on their mass to charge ratio. The core component of a particular kind of these devices called Quadrupole Mass Spectrometer is a quadrupole mass filter that uses a combination of AC and DC voltages to create an electric field that only allows ions with a narrow range of mass-to-charge ratio pass through to reach the detector. As the name suggests, quadrupoles has four parallel rods with circular cross sections and with the same length that are positioned in a square geometry (see Figure below).

Opposite rods are electrically connected to each other and one pair has a potential of $V_{DC}+V_{AC}\text{Cos}(\omega t)$ while the other pair has a potential of $-V_{DC}-V_{AC}\text{Cos}(\omega t)$, where V_{DC} and V_{AC} are the amplitude of the DC and AC voltage and ω is the frequency of the AC voltage and t is time. Ion beam is directed towards the centre of the quadrupole in parallel to the rods and as they pass through the quadrupole they experience the effect of the electric field that is generated by the rods resulting in an equation of motion that is in the form of Mathieu's differential equation: $\frac{d^2u}{d\zeta^2} + [a_{DC} + 2q_{AC}\cos 2\zeta]u = 0$, where u is either x or y referenced from the centre of quadrupole, $a_{DC} = \frac{4eV_{DC}}{\omega^2 r_0^2 m}$, $q_{AC} = \frac{2eV_{AC}}{\omega^2 r_0^2 m}$, and ζ=t/2.

Mathieu's equation has a relatively large stability region for a given mass of m, and voltages of V_{DC} and V_{AC} can be further tuned to operate at a very narrow stability region and allow for only mass m±dm to pass through with dm<0.1amu which leads to a mass resolution that is needed for separating most ions.

This mass filter however works in a sequential fashion and only one mass can be resolved at a time and a time gap is needed for the ions to travel through the rods before the next mass can be measured. Also, achieving a high mass resolution for separating the isotopes that are less than one amu apart is not possible, as quadrupole has a very narrow spatial stability region and increasing the resolution leads to a significant loss in the number of ions that can reach the end of the quadrupole before they are destabilized. Any configuration of electrodes and electrical fields that can help address these issues can have a significant impact on this field of mass spectroscopy. A possible solution for addressing the sequential nature of this filter could be to create an electric field arrangement that leads to areal dispersion of ions based on their masses so that an area detector can resolve multiple masses at a time or to resolve the closely lying masses in space.

Detailed work on such topics needs numerical modelling to solve the differential equations but the general idea of the arrangement of fields that can be used to separate or disperse the ions has to be established before such detailed studies, and this is what we hope to accomplish in this workshop.