

DESIGNING OF A REACTION MICROSCOPE TO STUDY DYNAMICS OF ATOMS AND MOLECULES

*Dissertation Submitted in Partial Fulfillment of the Requirements for the
Award of the degree of*

Master of Science

Submitted by

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DECLARATION

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APPROVAL SHEET

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Dedicated to

****Badminton Friends at IIT Hyderabad****

ABSTRACT

In this thesis the designing of high resolution Reaction Microscope (also known as COLTRIMS) to study dynamics of atoms and molecules is presented. COLTRIMS is a powerful technique that allows one to measure three dimensional momentum vectors of ions and electrons resulting from a single event of atomic or molecular fragmentation. The designing includes the trajectory simulation of charged particles to optimize the value of electric field. The designing of COLTRIMS and the trajectory simulation of ions and electrons is done by using commercial software SIMION 8.0. Further, a data analysis on Carbon monoxide molecule is done and the experimental results are compared with the simulated results. The experimental value matches quite well with simulation.

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Chapter 1

Designing the Reaction Microscope

1.1 Introduction (Recoil-ion and electron momentum spectroscopy: Reaction-microscopes)

Recoil-ion and electron momentum spectroscopy is a rapidly developing technique that allows one to measure the vector momenta of several ions and electrons resulting from atomic or molecular fragmentation. In a unique combination, large solid angles close to 4π and superior momentum resolutions around a few per cent of an atomic unit (a.u.) are typically reached in state-of-the art machines, so-called reaction-microscopes.

1.2 Principle of Momentum Spectrometry

Momentum and mass/charge ratio of the ions are determined by simultaneous spatial and temporal dispersion in a uniform electric field. The momentum spectrometer in our laboratory can be thought of as a single field time-of-flight mass spectrometer combined with a large area position-sensitive detector. The detector and the associated electronics is capable of recording the arrival of several ions in rapid succession.

The ionizing source crossed an effusive molecular gas beam at a right angle. Single collision condition is ensured. Ions and electrons formed in the collision region were extracted by a homogeneous electric field (along the z axis). Ions are detected by a large area position-sensitive detector (psd) whereas electrons are detected by a same kind of detector which was kept on the opposite side of the collision region.

Electron signal is generally used as a start pulse for the time-to-digital convertor and ion signal as a stop pulse. The stop/start time difference is the time-of-flight of the ion. During the flight the momentum components transverse to the electric field lead to a spatial dispersion (x, y) of the ions. The position of arrival of the ion on the psd (x, y) and the time-of-flight (t) were recorded as entries in a list mode data file.

The working principle of MCP and PSD is explained in the last section of this chapter.

1.3 Principle of Time-of-Flight Mass Spectrometer (TOF)

The time-of-flight spectrometer in its simplest form consists of an ion source and an ion collector fixed at two opposite ends of an evacuated tube.

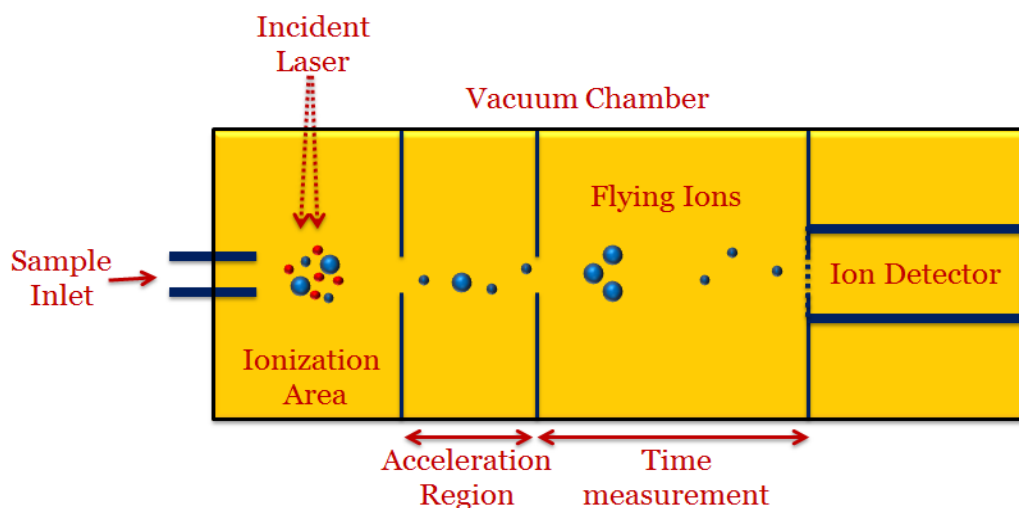


Figure 1.1: Schematic diagram of TOF mass spectrometer

The ions formed in the ion source, for example, in electron-atom/molecule collisions are extracted out and are made to move towards the collector under a constant or a pulsed electric field. In either case, the time-of-flight of the ions is proportional to $\sqrt{m/q}$, where q is the charge state and m is the mass of ions.

A time-of-flight spectrometer possesses the following salient features:

- (i) Speed of collection of ions at the collector is relatively fast ($< 1\mu\text{s}$),
- (ii) If a pulsed accelerating field is used, then for each accelerating pulse, the entire spectrum is recorded in one pulse event. Thus, it is possible to measure the relative intensities accurately, even though source conditions may vary rapidly.

1.4 Building the ion momentum vector

The TOF of an ion depends on the initial momentum component along the extraction axis, the length of the extraction region S , the length of drift region D , and the extraction field E_s . Let us first see how the TOF of an ion is obtained.

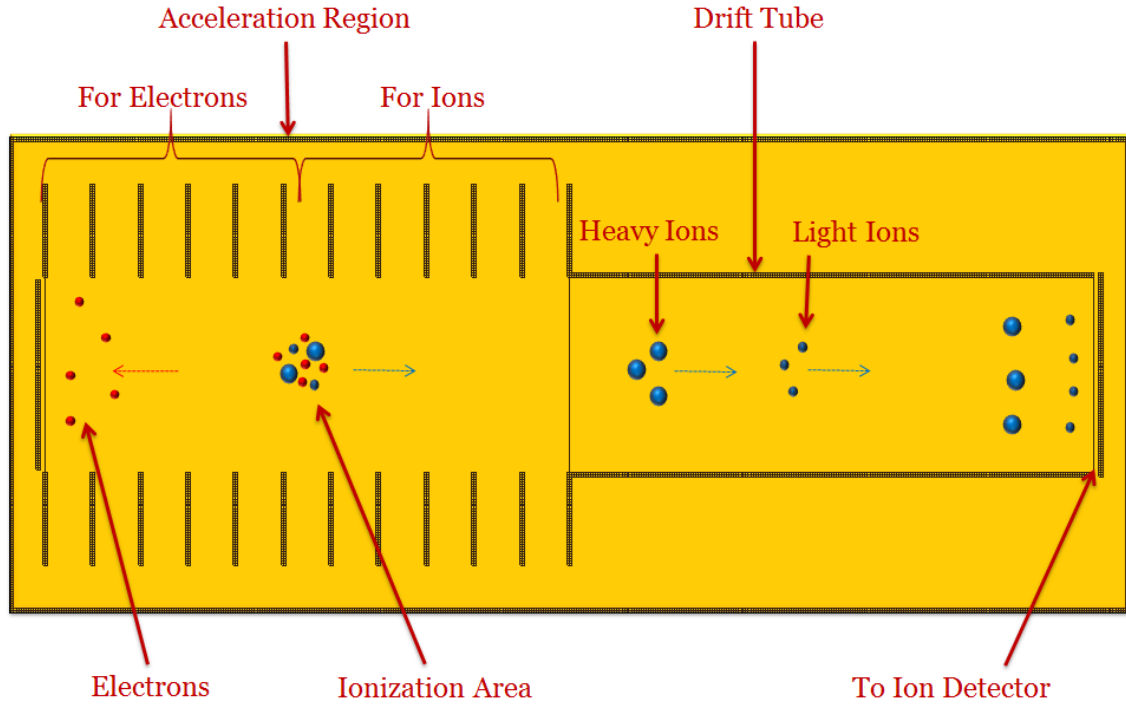


Figure 1.2: Movement of ions and electrons in a TOF mass spectrometer

Consider an ion that is created in the ionisation region, having charge q , mass m and initial momentum along the extraction axis p_z . The time t_s taken by the ion to cross the extraction region is given by Newton's 3rd equation of motion:

$$(s = ut + \frac{1}{2} at^2) \quad (1.1)$$

$$s = \frac{p_z}{m} t_s + \frac{1}{2} \frac{qE_s}{m} t_s^2 \quad (1.2)$$

Solving Eq. (1.2) gives the TOF in extraction region:

$$t_s = \frac{-p_z/m + \sqrt{[p_z/m]^2 + [qE_s/m]s}}{[qE_s/m]} \quad (1.3)$$

Now to calculate the final velocity when an ion leaves the extraction region and enters into the field free Drift region, again we use Newton's 1st equation of motion:

$$(v = u + at) \quad (1.4)$$

$$v = \frac{p_z}{m} + \left[\frac{qE_s}{m} \right] t_s \quad (1.5)$$

Now if D be the length of drift region, the time spent by the ion in the drift region is

$$t_D = D/v \quad (1.6)$$

Using equation (1.5) into (1.6) we get

$$t_D = \frac{D}{\sqrt{[p_z/m]^2 + [qE_s/m]s}} \quad (1.7)$$

So, the total time ion takes to reach the detector is given by

$$t = t_s + t_D = \frac{-p_z/m + \sqrt{[p_z/m]^2 + [qE_s/m]s}}{[qE_s/m]} + \frac{D}{\sqrt{[p_z/m]^2 + [qE_s/m]s}} \quad (1.8)$$

Setting the Wiley-McLaren condition ($2s = D$) gives

$$t = \frac{-p_z/m + \sqrt{[p_z/m]^2 + [qE_s/m]s}}{[qE_s/m]} + \frac{2s}{\sqrt{[p_z/m]^2 + [qE_s/m]s}} \quad (1.9)$$

The TOF (t_0), for ions which have zero initial energy ($p_z = 0$) is given by

$$t_0 = \frac{\sqrt{[qE_s/m]s}}{[qE_s/m]} + \frac{2s}{\sqrt{[qE_s/m]s}} \quad (1.10)$$

$$t_0 = 3 \times \sqrt{\left[\frac{m}{q} \right] \frac{s}{E_s}} \quad (1.11)$$

Cases in which $(p_z^2/2m) \ll qE_s$, the difference between the flight times of zero energy and non-zero initial velocity ions can be written in a simplified form. The condition is well satisfied in our spectrometer. Combining Equations (1.9) and (1.10), we get

$$p_z = qE_s(t - t_0) \quad (1.12)$$

Once the TOF (t) and the position (x, y) is obtained, the momentum vector of each registered ion can be derived. The momentum components parallel to the detector plane and perpendicular to the TOF axis are given by following expressions:

$$p_x = m \times (x - x_0) / t \quad (1.13)$$

$$p_y = m \times (y - y_0) / t \quad (1.14)$$

where (x_0, y_0) is the centroid of the interaction volume projected on the detector plane.

1.5 MCP and Delay Line detectors

1.5.1 General description

The Microchannel plate detector with delay line anode is a device for single particle counting, giving information on the position of each particle and its impact time with high precision. We can use it at the right end of the drift tube to detect ions. It uses an electron read-out scheme employing fast timing amplifiers, timing discriminators and digitizers.

The detector system is modular and comes in different sizes and versions. It operates under ultra-high vacuum and requires high voltage supplies.

1.5.2 Construction and operation

The detector consists of a pair of selected MCPs in chevron configuration and a helical wire delay line anode for 2D position readout [figure 1.3]. The MCP's are either supported by a pair of partially metallized ceramic rings or the MCP stack is mounted between a metal front ring and a rear side holder plate.

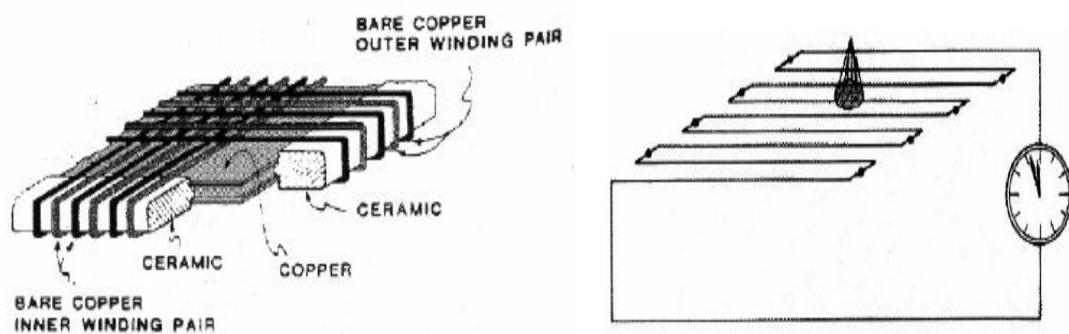


Figure 1.3: Operation principle of Delay line Anode

The operation requires two DC voltages for a MCP stack on front and back contacts and three voltages for the anode support plate (holder) and the wire array [10].

1.5.3 Position encoding

The position of the detected particle is encoded by the signal arrival time difference at both ends of each parallel pair delay line, for each layer independently. While the signal speed along the delay line is close to speed of light, one can define a perpendicular signal speed given by the pitch of one wire loop, and the time which a signal needs to propagate through this loop.

The difference between signal arrival times at the adjacent ends of each delay line is proportional to the position on the MCP in the respective direction.

1.6 Setting the dimensions

We are starting designing RIMS (Recoil Ion Momentum Spectrometer) with these parameters: accelerating region with voltage difference of 10 V/cm for a length of 130 mm and also the field free drift tube of the same length of 260 mm .

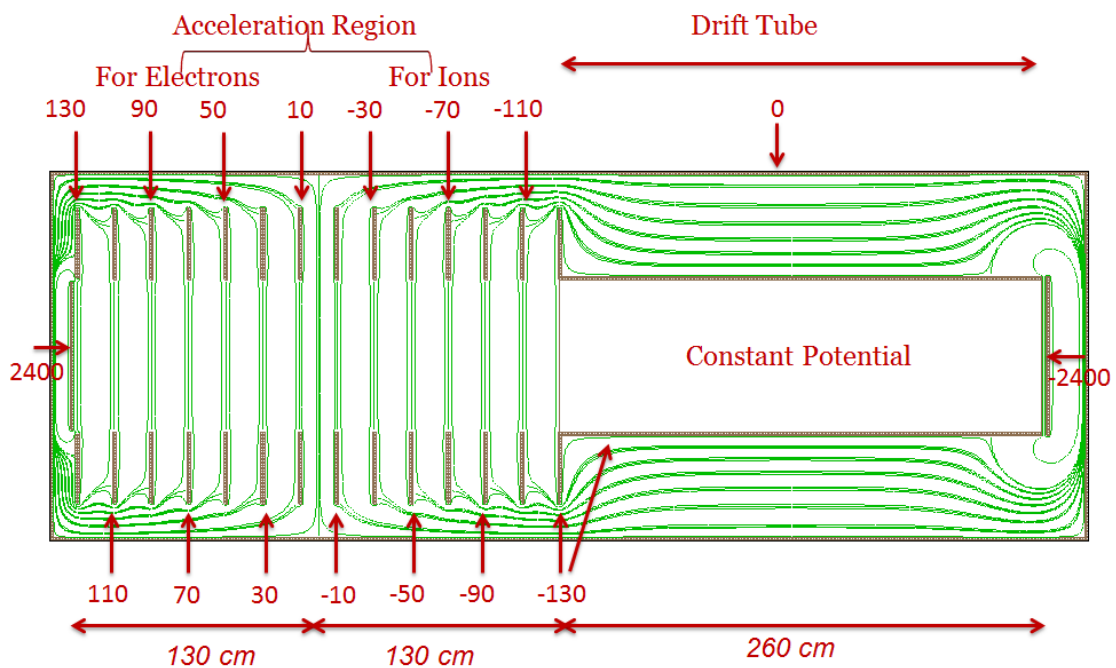


Figure 1.4: Two Dimensional view of RIMS

Referring to [figure.1.4], we assume that the ionization of molecules takes place at the centre of spectrometer, which is at ground potential by means of charged particles or photons impact. The acceleration region on electron side consists of various electrodes with positive potentials, which accelerates electrons to the left side of the

spectrometer, and after travelling through the acceleration region electrons are detected by an electron detector. Similarly, ions also travel through the acceleration region on the other side of the spectrometer which has the electrodes with negative potential and length of the acceleration region for electron and ions are same, i.e. 130mm. Ions travel an extra distance which is a field free region and we call it as drift region which is double the length of the extraction region and length is 260mm. At the end of the drift tube an ion detector is placed to detect ions.

The momentum spectrometer design satisfies the Wiley-McLaren condition ($2s = D$). *This condition nullifies the effect of time difference due to the place of birth of ions in reaction volume.*

Chapter 2

Simulations

2.1 Working with SIMION 8.0

Light optics can be modeled using physical optics benches and interior beam shapes can be seen with smoke, screens, or sensors. Ion optics hardware is generally internally inaccessible and must normally be evaluated via end to end measurements. Numerical simulation programs like SIMION allow the user to create a virtual ion optics bench and look inside much like physical light optics benches.

Hence, to design a microscope of our purpose, we chose to work on SIMION 8.0 because of the fact that it is intended to provide direct and highly interactive methods for simulating a wide variety of general ion optics problems.

2.1.1 Introduction

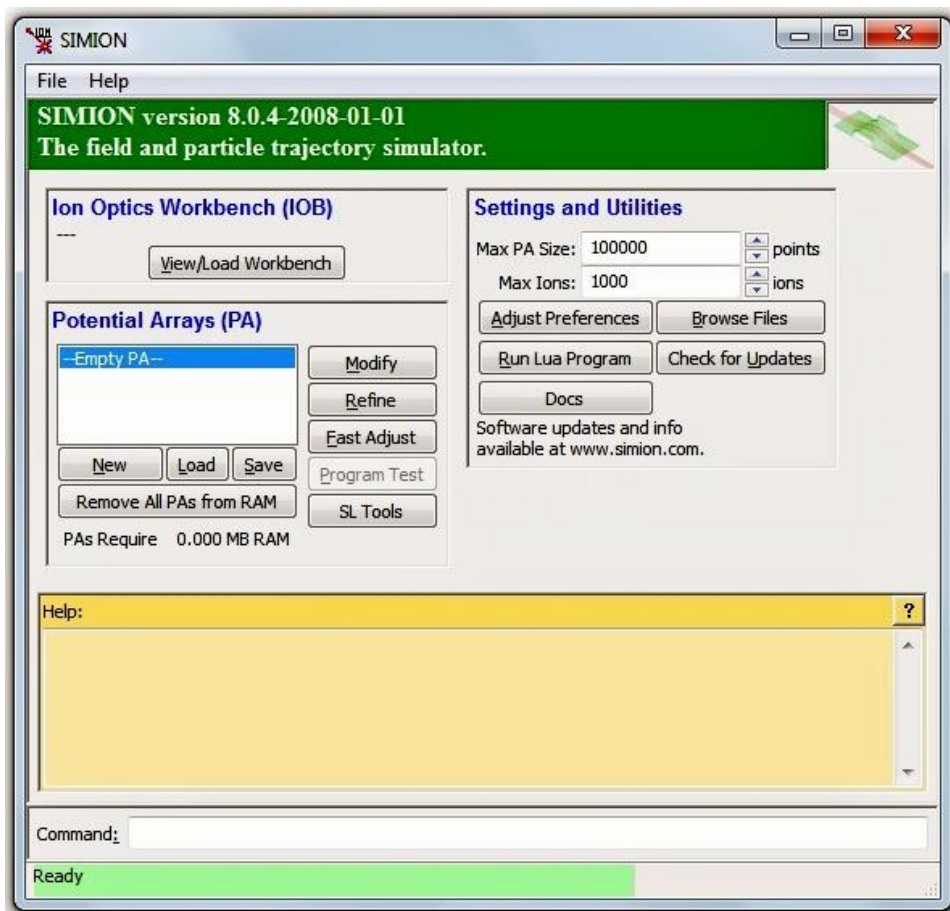


Figure 2.1: A starting view of SIMION 8.0

SIMION 8.0 [figure 2.1] is a software package used primarily to calculate electric fields, when given a configuration of electrodes with voltages, and calculate trajectories of charged particles in those fields, when given particle initial conditions, including optional RF, magnetic field, and collisional effects. In this, SIMION provides extensive supporting functionality in defining our system geometry and conditions, recording and visualizing results, and extending the simulation capabilities with user programming. It is a versatile platform, to simulate lens, mass spectrometer, and other types of particle optics systems [7].

2.1.2 How does it work?

SIMION makes use of *potential arrays* that define the geometry of electrodes (or magnetic poles) as well as the potentials both on the electrodes and in the empty space between the electrodes. Typically, the potentials on the electrodes are defined by us, and SIMION solves for the potentials in the space between the electrodes (as well as the fields defined by the gradient of those potentials). The potentials between the electrodes are determined by solving the Laplace equation by finite difference. In SIMION, this process is called *refining* the potential array.

Refined potential arrays can then be positioned as *potential array instances (3D virtual images)* into an *ion optics workbench* volume. Ions can be flown within the workbench volume, with their trajectories calculated from the fields inside the potential array instances they fly through. This basic approach is the foundation for simulating a wide variety of charged particle optics systems.

2.1.3 Determining Field Potentials

The electrostatic or magnetic field potential (*Volts or Mags - SIMION's magnetic potentials*) at any point within an electrostatic or static magnetic lens can be found by solving the Laplace equation with the electrodes or poles acting as boundary conditions. The Laplace equation assumes that there are no space charge effects and boundary conditions are sufficiently constrained.

2.1.4 The Potential Array

SIMION utilizes potential arrays to define electrostatic and magnetic fields. A potential array is an array of points organized so the points form equally-spaced square (2D) or cubic (3D) grids. Equally-spaced means that all points are equal distances from their nearest neighbour points. Figure shows a part of Modify function view of a 471 by 101 2D

potential array. Below is 3D view of partially clipped Potential array designed exclusively for this work [Figure2.2]:

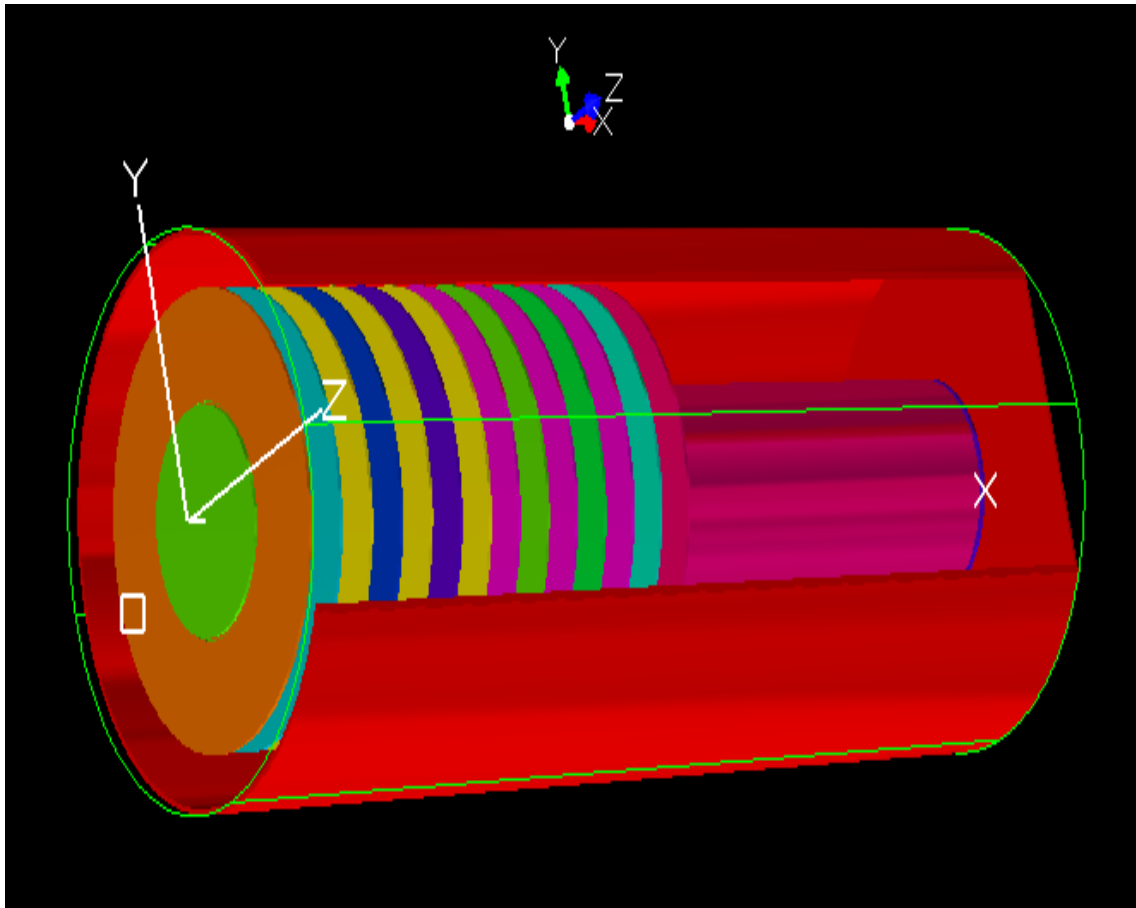


Figure 2.2: A '3D' view of designed potential array

2.1.5 PE View

We can use SIMION's potential energy view (*PE View*) of the einzellens to help us understand the electrostatic focusing process. Figure shows a potential energy view of the einzellens designed in this project below [Figure2.3]. Note that the potential energy surface is much like the surface of a golf course. Since ions react in much the same way to potential energy surfaces as golf balls react to hills and valleys it is quite easy to see why ions have the trajectories they do in this einzellens.

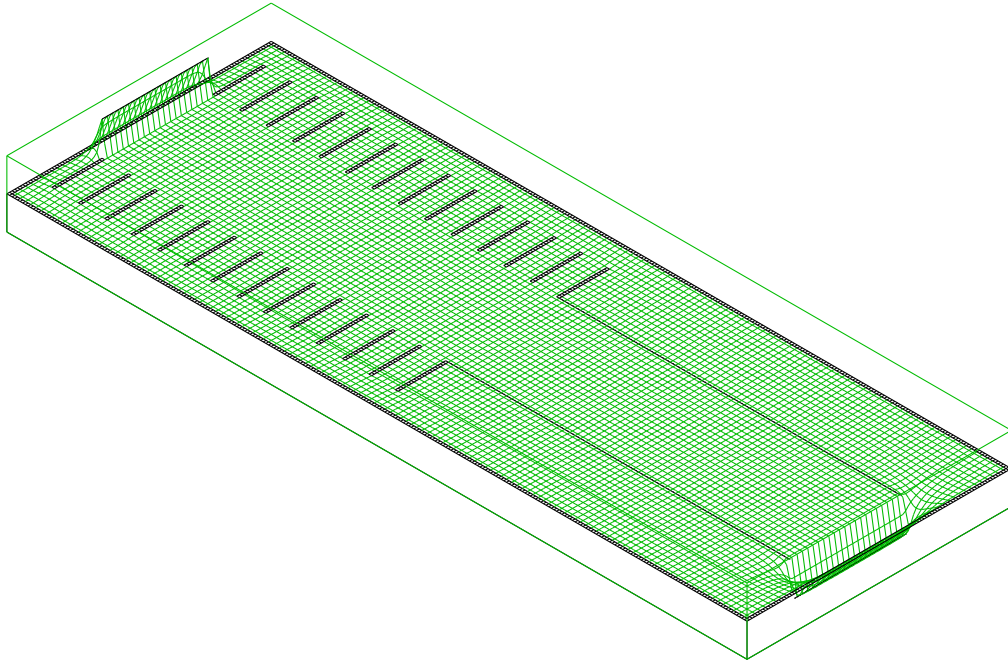


Figure 2.3: A potential energy view in XY dimensions

2.2 Basic Ion Optics Concepts

Ion optics utilizes the electrostatic and/or the magnetic forces on charged particles to modify ion trajectories.

2.2.1 Equations from Basic Physics

The movement of a particle i.e. its acceleration is defined by the force on it, as given by *Newton's Second Law*:

$$\begin{aligned} \text{force} &= \text{mass} \times \text{acceleration} \\ F &= m \times a \end{aligned} \tag{2.1}$$

This force applied over a distance of movement is *work* (consuming energy):

$$\begin{aligned} \text{work} &= \text{force} \times \text{distance} \\ \text{force}_{\text{avg}} &= \text{work} / \text{distance} \\ F &= dW / dr \end{aligned} \tag{2.2}$$

2.2.2 Coulomb's law/Motion from Electrostatic force

If Q_i be the particle's charge, forces between charged particles are given by *Coulomb's Law*:

$$F_e = k \frac{Q_i Q}{r^2} \quad (2.3)$$

(For a point charge)

$$F_e = k Q_i \sum_n \frac{Q_n}{r_n^2} \quad (2.4)$$

(For whole system of point charges)

The electric field intensity is the force per charge or in terms of work the change in work per charge (i.e. voltage) over distance:

$$E = F_e / Q_i = d(W / Q_i) / dr \quad (2.5)$$

$$E = \text{Volts} / \text{Meter}$$

$$\text{Volts} = \text{Joules} / \text{Coulomb}$$

Conversely, we may think of the electric field as the cause of the force on a charged particle:

$$F_E = -eE \quad (2.6)$$

(e : unit of positive charge)

Putting this together, the acceleration on a particle or its trajectory is determined by the electric field as such:

$$a = F / m \quad (2.7)$$

$$a = dV / dt = -eE / m = -E / (m / e) \quad (2.8)$$

2.2.3 The Laplace Equation

$$\nabla^2 V = \nabla \cdot \nabla V = 0 \quad (2.9)$$

$$\nabla V = (\partial V / \partial x)i + (\partial V / \partial y)j + (\partial V / \partial z)k = -E \quad (2.10)$$

$$\nabla^2 V = -\nabla \cdot E = \partial E_x / \partial x + \partial E_y / \partial y + \partial E_z / \partial z = 0 \quad (2.11)$$

The Laplace equation constrains all electrostatic and static magnetic potential fields to conform to a zero charge volume density assumption (no space charge). This is the equation that SIMION uses for computing electrostatic and static magnetic potential fields.

2.2.4 The Nature of Solutions to the Laplace Equation

The Laplace equation really defines the electrostatic or static magnetic potential of any point in space in terms of the potentials of surrounding points. For example, in a 2-dimensional electrostatic field represented by a very fine mesh of points the Laplace equation is satisfied to a good approximation when the electrostatic potential of any point is estimated as the average of its four nearest neighbour points:

$$V = (V_1 + V_2 + V_3 + V_4)/4 \quad (2.12)$$

2.3 Simulating the present work

2.3.1 Flying the ions

We develop two groups of charged particles- C+ Ions and Electrons. We put their respective charges and masses. We generate them just at the centre of the accelerating area. Due the positive potential on the left, electrons easily got accelerated towards left, whereas ions start accelerating towards right and after entering into field free region they start flying freely. Now we wish to collect all the ions which we generated, at the end of the drift tube and for this we keep setting different values of kinetic energy. We see the results of applying all possible values of kinetic energy. We also decide to fix various other parameters related to particles such as their 'Direction' of generation. To get generalized results we set it as 'uniform' and we choose Azimuthal angle ($0^\circ - 180^\circ$), Elevation angle ($0^\circ - 360^\circ$). Now we record ions' Time of Flight (TOF) at the end of the drift tube.

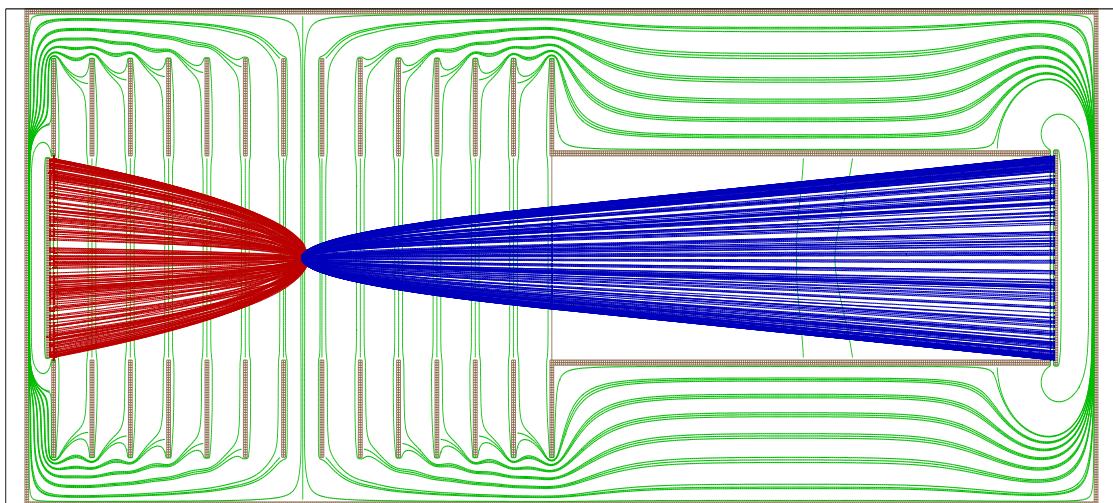


Figure 2.4: A particle flying view of workbench

2.3.2 Results

After designing the microscope and flying the charged particles we observe that the RIMS design with the present dimensions works for ions with maximum kinetic energy 0.8 eV and electron with the maximum kinetic energy 2.9 eV successfully.

Whereas the outcome for other applied potentials [Table 2.1] is listed below:

Table 2.1: Simulated Results

Electric field (V/cm)	C^+ Ion K.Energy (eV)	Electron K.Energy (eV)
10	0.80	2.90
20	1.60	5.90
30	2.40	8.85

Chapter 3

Data Analysis

3.1 Input data

The data which is plotted in following figure is taken from Physical Research Laboratory, Ahmedabad. This data is collected for Carbon monoxide molecule interaction with 1300 eV electron impact. The following graph shows the time of flight spectrum of ions which are formed due to the interaction.

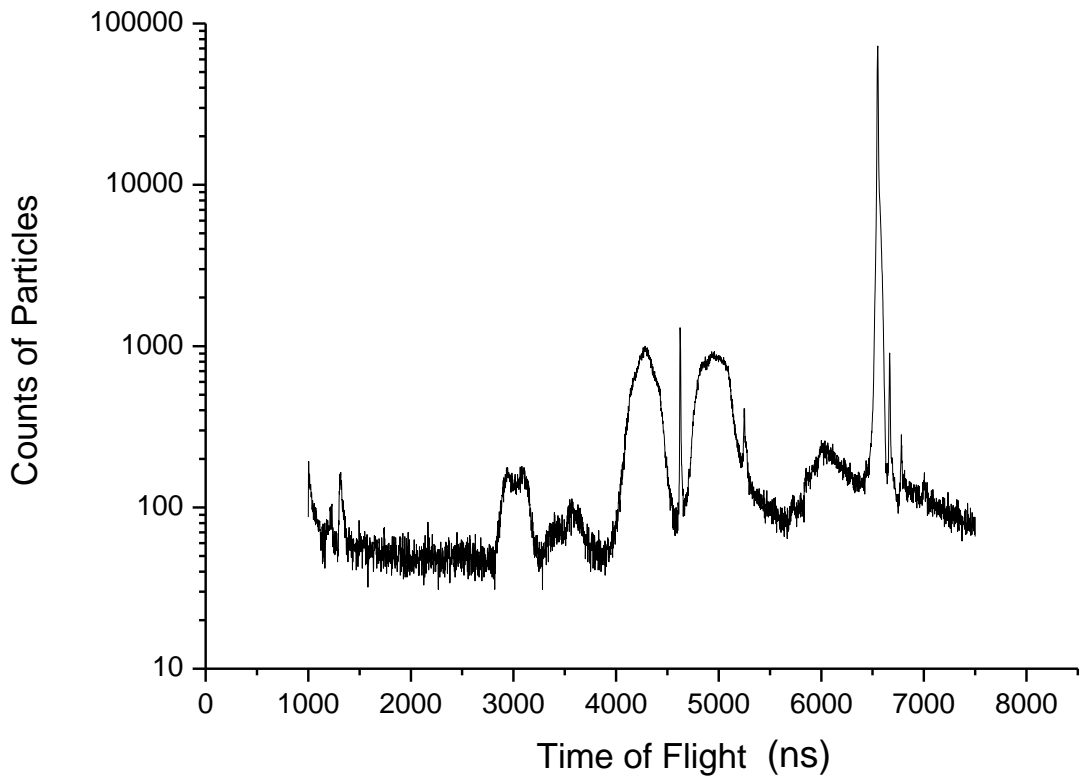


Figure 3.1: Graph showing the Data to be analysed

3.2 Analysing the data

We see there are two sharp peaks which we get at 4628 ns and 6550 ns , [Figure 3.1] with the information that these belong to $\sqrt{14}$ and $\sqrt{28}$ values of $\sqrt{m/q}$ respectively.

Now have a look on eq. (1.11)

$$t_0 = 3 \times \sqrt{\left[\frac{m}{q} \right] \frac{s}{E_s}} \text{ sec}$$

For our convenience we would like to convert mass units into 'amu' and charge units into 'e units'.

Thus we get,

$$t_0 = \frac{10165.1}{\sqrt{E_s}} \times \sqrt{\left[\frac{m}{q} \right]} \text{ nsec} \quad (3.1)$$

$$\therefore 1 \text{ amu} = 1.67 \times 10^{-27} \text{ kg}$$

$$\text{electronic charge } e = 1.6 \times 10^{-19} \text{ C}$$

$$s = 11 \times 10^{-2} \text{ m}$$

So, Now

Time of Flight is to be taken in *nsec*,

Electric Field is to be taken in *V/cm*,

Mass is to be taken in *amu*,

Charge is to be taken in *e*.

If we compare equation (3.1) with the Equation of Line

$$(y = mx + c) \quad (3.2)$$

(*m*: slope of the line $m = y/x$)

$$\therefore \frac{10165.1}{\sqrt{E_s}} = t_0 / \sqrt{\left[\frac{m}{q} \right]} \quad (3.3)$$

(Slope of equation 3.1)

3.3 Finding the unknown ions

Now, choosing the two peak values and plotting them with their respective $\sqrt{m/q}$ values, a linear fitted curve [Figure 3.2] gives the slope of the equation (3.1) as:

$$\frac{10165.1}{\sqrt{E_s}} = 1237.51789 \text{ nsec} \times \sqrt{(C/amu)} \quad (3.4)$$

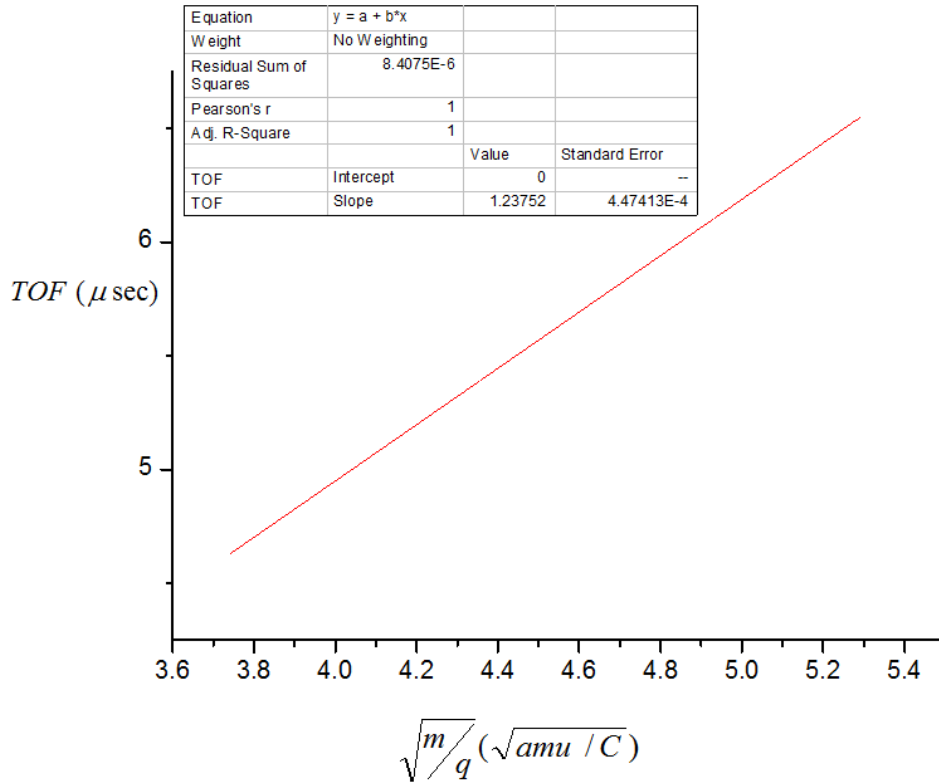


Figure 3.2: Graph showing linear fitted curve

Hence,

$$E_s = \left[\frac{10165.1}{1237.517} \right]^2 = 67.472 \text{ V/cm} \quad (3.5)$$

Now we use this data to design a microscope similar to the one which we designed earlier.

Now proceeding further to identify all the ions, we use *equation (3.1)*, which gives $\sqrt{m/q}$ values associated with t_0 values as [Table 3.1]:

Table 3.1: Calculated results

t_0 (nsec)	$\sqrt{m/q} \left(\sqrt{\frac{amu}{C}} \right)$
4284	3.46178
4948	3.99800
6028	4.87103
3066	2.47754

Analysing these values we get a clear picture of all ions having different peaks as shown [Figure 3.3]:

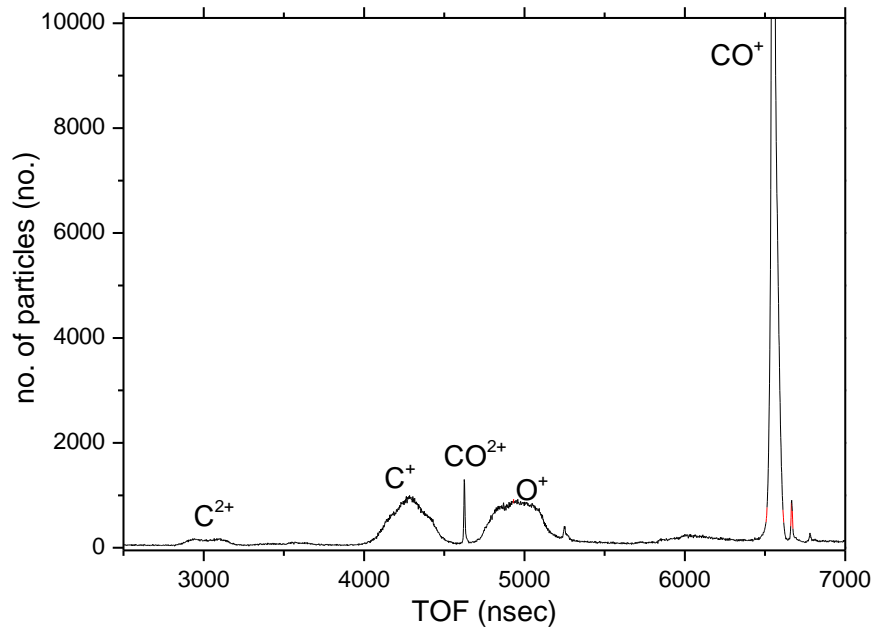


Figure 3.3: Graph showing identified peaks

This is how we identify all the ions which are formed in the reaction volume after interaction of molecules with charged particle.

3.4 Calculating the vector momenta and energy

Now we have to calculate the momentum vectors for C^+ ion, so first we observe the spread of the peak for the same ion. Then using *equation (1.12)*,

$$p_z = 0.958 \times 10^{-3} qE_s (t - t_0) \quad [3.6]$$

Also kinetic energy with respect to the counts of particles can be calculated as

$$K.E = p_z^2 / 2m \quad [3.7]$$

Hence, Kinetic energy distribution comes out to be [Figure 3.4]:

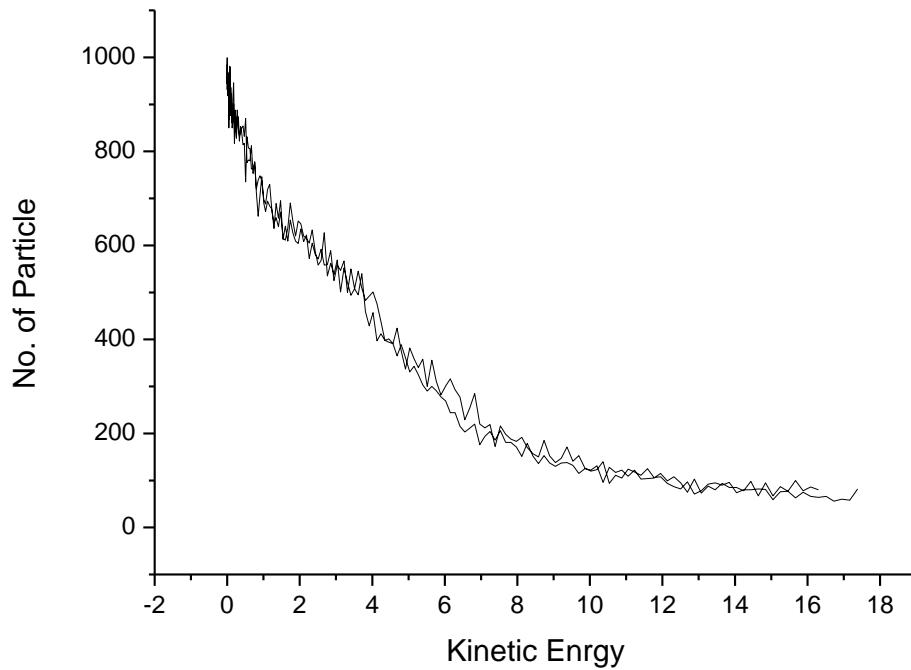


Figure 3.4: Graph showing Kinetic energy distribution

3.5 Results

Observing the kinetic energy distribution, the mean kinetic energy is coming out to be 5.65308 eV with *446 numbers of particles*.

Whereas when we simulated this data with SIMION 8.0, we found it to be 5.5 eV with Gaussian distribution (*Standard Deviation: 0.42, FWHM: 1 eV*) where maximum energy detected is 6.5 eV .

So we found that the experimental results are perfectly matching with the simulated results.

Chapter 4

A view into the future

The reaction dynamics of multiply charged ions- both in the gas phase and at the gas-surface interface, i.e. when the reactions are no longer unimolecular, are expected to be far more complicated because of the competition between different collision pathways. Such pathways include charge transfer, dissociative charge transfer, collision-induced dissociation and chemical reactions.

Measurements on propensities for each of the possible pathways, as a function of collision energy can be carried out, accompanied by accurate calculations of PES for the various electronic states involved in the collision process. These will lead us to understanding reactive chemistry and provide new insights into the interaction of multiply charged ions with other species.

References

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