RICE UNIVERSITY

NOVEL PERMANENT-MAGNET PENNING TRAP
FOR STUDIES OF DIPOLE-BOUND NEGATIVE IONS

by
Leonard Suess

MASTER OF SCIENCE

HOUSTON, TEXAS
DECEMBER, 2001
RICE UNIVERSITY

Novel Permanent-Magnet Penning Trap
for Studies of Dipole-Bound Negative Ions

by

Leonard Suess

A THESIS SUBMITTED
IN PARTIAL FULFILLMENT OF THE
REQUIREMENTS FOR THE DEGREE

Master of Science

APPROVED, THESIS COMMITTEE:

F.B. Dunning, Chair
Professor of Physics

G.K. Walters, Sam and Helen Worden
Professor of Physics, Emeritus

P. Padley
Assistant Professor of Physics

HOUSTON, TEXAS
DECEMBER, 2001
ABSTRACT

Novel Permanent-Magnet Penning Trap for Studies of Dipole-Bound Negative Ions
by Leonard Suess

Low-energy electron transfer between a Rydberg atom and a target molecule can result in formation of long-lived metastable negative ions. Here we describe a novel permanent-magnet Penning trap designed to examine the lifetime of such long lived metastable negative ions. With the help of ion trajectory calculations, the characteristics of the trap have been investigated and the most effective methods for ion injection have been established. Collisions with SF$_6$, which has a high electron attachment rate, result in the formation of SF$_6^{-*}$ ions which are known to have a long intermediate lifetime. Comparisons between experimental SF$_6^{-*}$ trapping data and ion trajectory calculations are discussed that demonstrate the capabilities of the trap. Future experimental studies are also proposed.
Acknowledgments

A big thank you to Dr. Barry Dunning for his guidance and insight. Priya, thanks for sharing your knowledge with me and for being such a wonderful friend. I am grateful to Shannon Hill whose tireless efforts allowed a detailed investigation of the trap used in this work. I have also benefited greatly from the interactions of all the other graduate students and post docs in the laboratory. Their advice and contributions are greatly appreciated.

I would like to thank my family for their love and support. I am grateful to my parents, who have constantly pushed me to better myself.

Most importantly, my deepest thanks go to my wife, Jessica. Her constant support and love continues to push me forward.
# Table of Contents

Abstract iii

Acknowledgments iv

List of Figures vii

1 Introduction 1
   1.1 Electron Attachment Processes .......................... 1
   1.2 Rydberg Atom Properties ............................... 2

2 Ion Kinematics in an Ideal Penning Trap 4
   2.1 Introduction .................................... 4
   2.2 Equations of Motion for an Ion in an Ideal Penning Trap .......... 5
      2.2.1 Radial Motion .................................. 6
      2.2.2 Axial Motion .................................. 7
   2.3 Trapping Requirements ................................ 8
   2.4 Cylindrical vs. Ideal Penning Trap ....................... 8

3 Experimental Apparatus 11
   3.1 Vacuum System .................................. 13
   3.2 Potassium Source ................................ 13
   3.3 Laser System ................................... 14
   3.4 Permanent-Magnet Cylindrical Penning Trap ................. 16
      3.4.1 Cladding Design ............................. 18
      3.4.2 Trap Electrode and Electronics ................. 24

4 Simulating Ion Trajectories – SIMION 28
   4.1 Experimental Model in SIMION ........................ 28
   4.2 Loop Cycle .................................... 29
   4.3 Electric Potential Distributions for Trap Electrodes .......... 30
   4.4 Simulations .................................... 30

5 Experimental and Analytical Techniques 33
   5.1 Experimental Procedure ............................... 33
   5.2 SF₆⁺ Results .................................... 35

6 Conclusion and Future Work 40
   6.1 Conclusion .................................... 41
List of Figures

2.1 Ideal Penning trap with hyperbolic electrodes. .......................... 4
2.2 Magnetron motion superimposed on the cyclotron motion. ............... 5
2.3 Graph of expansion coefficients $D_2$ and $D_4$ as functions $\frac{\omega}{z_0}$. .... 10

3.1 Experimental setup. ..................................................................... 12
3.2 Comparison of different magnetic materials. ................................. 17
3.3 Magnetic Ohm’s analog. ................................................................. 19
3.4 Cladding magnet. ................................................................. 20
3.5 Cross-sectional view of clad magnet. ............................................. 21
3.6 Comparison of unclad and clad magnetic structures. ...................... 22
3.7 Magnetization of the magnet assembly. ........................................... 23
3.8 Axial magnetic field within the magnet. ........................................... 25
3.9 Cross-section of trap electrode. ...................................................... 26
3.10 Schematic of switching circuit. .................................................... 27

4.1 SIMION model of experimental setup. ............................................. 28
4.2 Potentials on trap electrodes for various modes ............................... 31
4.3 Extraction of axial frequency for SF$_{6}^{-*}$. ................................. 32

5.1 Pulse sequence for the bottom grid of the interaction region............. 34
5.2 TOF for 300$\mu$s trapped SF$_{6}^{-*}$ ions. ........................................ 36
5.3 Arrival time spectrum for trapping times 185,300, and 416$\mu$s. .......... 37
5.4 Arrival time spectrum for a trapping time of 358$\mu$s. ................. 38
5.5 Stability of SF$_{6}^{-*}$ in Penning trap. .............................................. 39

A.1 Electrode numbers for SIMION ................................................. 47
Chapter 1

Introduction

1.1 Electron Attachment Processes

The study of electron-molecule interactions has grown significantly over the past several years due to their importance in biological, chemical, and physical systems [1, 2]. For example, electron attachment is important in atmospheric studies involving pollutants such as polycyclic aromatic hydrocarbons and multiply halogenated methane and ethane compounds. Studies of their interaction with free electrons provide rate constant data used for modeling their behavior in the atmosphere [3, 4].

Electron attachment to molecules can lead to reactions of the form,

\[ e^- + ABC \rightarrow ABC^{-*} \rightarrow ABC + e^-, \]  
\[ e^- + ABC \rightarrow ABC^{-*} \rightarrow AB + C^-, \]  
\[ e^- + ABC \rightarrow ABC^{-*} \rightarrow ABC^-. \]  

In reaction 1.1.1, the transient negative ion formed reverts back into a neutral molecule and an electron (autodetachment). In reaction 1.1.2, the intermediate dissociates producing a neutral and a charged fragment. In reaction 1.1.3, the intermediate is stabilized by intramolecular vibrational relaxation leading to formation of long-lived metastable negative ions. For the present study, particular attention is paid to the formation of long-lived anions.

Here we study the properties of negative ions that are created through electron transfer in collision with potassium atoms in high-lying Rydberg states. Rydberg atoms, atoms in states of high principal quantum number \( n \), exhibit exaggerated properties. Typically, the
separation between the core ion and the excited electron is such that the target molecule views the highly-excited atom as two independent scatters.

One of the major benefits in utilizing Rydberg atom techniques for studying electron attachment processes is the extremely low energy of the attaching electron. Its mean kinetic energy, which is equal to its binding energy, can be varied from a few meV down to \( \mu \text{eV} \) by changing the principal number, \( n \), of the atom. The velocity of the electron in its orbit is high compared to the relative velocity of the atom and the target molecule at thermal temperatures; thus, the energy (velocity) of the electron dominates the interaction.

### 1.2 Rydberg Atom Properties

The physical characteristics of Rydberg atoms are quite different from those of atoms in ground or low-lying excited states. This is illustrated by Table 1.1 which lists a number of atomic properties, their dependence on \( n \), and representative values for each at several \( n \).

<table>
<thead>
<tr>
<th>Property</th>
<th>scaling (a.u.)</th>
<th>( n=1 )</th>
<th>( n=15 )</th>
<th>( n=30 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean radius</td>
<td>( n^2 )</td>
<td>( 5.3 \times 10^{-9} \text{ cm} )</td>
<td>18nm</td>
<td>48nm</td>
</tr>
<tr>
<td>Orbital period</td>
<td>( 2\pi n^3 )</td>
<td>( 1.5 \times 10^{-16} \text{ s} )</td>
<td>0.5ps</td>
<td>4.5ps</td>
</tr>
<tr>
<td>Binding Energy</td>
<td>( \frac{1}{2n^2} )</td>
<td>13.6eV</td>
<td>60meV</td>
<td>15.1meV</td>
</tr>
<tr>
<td>Radiative Lifetime</td>
<td>( \tau_0 n^3 )</td>
<td>6.78ns</td>
<td>22.9( \mu \text{s} )</td>
<td>183( \mu \text{s} )</td>
</tr>
</tbody>
</table>

Table 1.1: Properties of Rydberg atoms.

The large size of the Rydberg atom indicates a large separation between the excited electron and the core ion. For \( n \gtrsim 10 \), the separation between the core ion and the excited
electron is greater than the range typical of either electron/molecule or ion/molecule interactions; therefore, during collision with a neutral target, the Rydberg core and excited electron act as independent scatters leading to the so-called essentially-free electron model.
Chapter 2

Ion Kinematics in an Ideal Penning Trap

2.1 Introduction

![Diagram of an ideal Penning trap with hyperbolic electrodes.](image)

Figure 2.1: Ideal Penning trap with hyperbolic electrodes.

The confining of ions in a trap has been extensively studied since 1936 when Francis Michel Penning applied an axial magnetic field to an electric discharge to increase the path length of electrons [5]. The basic structure of a Penning trap consists of three electrodes: two end-cap electrodes and a ring electrode, as shown in Figure 2.1 immersed in a homogenous axial magnetic field. This axial field causes ions to move in circular cyclotron orbits confining them in the radial direction [6]. Axial confinement is achieved by applying constant electric potentials to the electrodes. The superposed $\mathbf{E}, \mathbf{B}$ fields trap the ion, but introduce another particle motion due to $\mathbf{E} \times \mathbf{B}$-terms called the magnetron motion. The magnetron motion is superimposed on the cyclotron motion as seen in Figure 2.2 and ultimately determines trap lifetime [5].
2.2 Equations of Motion for an Ion in an Ideal Penning Trap

In an ideal hyperbolic Penning trap as shown in Figure 2.1 with endcaps separated by a distance $2z_0$ and a ring of radius $r_0$, these parameters are related by, $r_0 = \sqrt{2}z_0$.

For a charged particle in a constant electric field and a magnetic field orientated along the $\hat{z}$ axis, the scalar potential $\phi$, and the magnetic field $\mathbf{B}$ are given by,

$$\mathbf{B} = B_0\hat{z}, \quad (2.2.1)$$

$$\phi = \frac{V}{2z_0^2 + r_0^2}(2z_0^2 - x^2 - y^2) = \phi_1, \quad (2.2.2)$$

where $V$ is the potential applied to the endcap electrodes with respect to the ring electrode, $B_0$ is the magnetic field strength inside the trap and $\phi_1$ is the electric potential inside the trap generated by the endcaps.

The Lorentz force felt by a charged particle of mass $m$ and charge $q$ is,

$$\mathbf{F} = q(\mathbf{E} + \mathbf{v} \times \mathbf{B}), \quad (2.2.3)$$
taking the dot product with x, y and z respectively yields,

\[ F_x = m \ddot{x} = q \left( -\nabla \phi_1 \cdot \hat{x} + (v \times B) \cdot \hat{x} \right), \quad (2.2.4) \]

\[ F_y = m \ddot{y} = q \left( -\nabla \phi_1 \cdot \hat{y} + (v \times B) \cdot \hat{y} \right), \quad (2.2.5) \]

\[ F_z = m \ddot{z} = q \left( -\nabla \phi_1 \cdot \hat{z} + (v \times B) \cdot \hat{z} \right). \quad (2.2.6) \]

Using \( v = (\dot{x}, \dot{y}, \dot{z}) \) and \( B = (0, 0, B_0) \) yields,

\[ \ddot{x} = \omega_c \dot{y} + \frac{1}{2} \omega_{0z}^2 x, \quad (2.2.7) \]

\[ \ddot{y} = -\omega_c \dot{x} + \frac{1}{2} \omega_{0z}^2 y, \quad (2.2.8) \]

\[ \ddot{z} = -\omega_{0z}^2 z, \quad (2.2.9) \]

where \( \omega_{0z} \) is the axial frequency,

\[ \omega_{0z} = \sqrt{\frac{4qV}{m (r_0^2 + 2z_0^2)}}, \quad (2.2.10) \]

and \( \omega_c \) is the cyclotron frequency,

\[ \omega_c = \frac{qB_0}{m}. \quad (2.2.11) \]

### 2.2.1 Radial Motion

To determine the radial motion of the ion in the Penning trap, solving the coupled differential equations 2.2.7 and 2.2.8 would be necessary as \( r = x\hat{i} + y\hat{j} \). Introducing the variable \( u \) defined by,

\[ u \equiv x + iy, \quad (2.2.12) \]

allows for the “decoupling” of equations 2.2.7 and 2.2.8. Differentiating this equation twice yields,

\[ \ddot{u} = -i\omega_c \dot{u} + \frac{1}{2} \omega_{0z}^2 u. \quad (2.2.13) \]
Using \( u = e^{-i\omega t} \), the following characteristic equation is obtained,

\[
2\omega^2 - 2\omega_c\omega + \omega_{0z}^2 = 0,
\]

(2.2.14)

the roots of which are,

\[
\omega_{\pm} = \frac{1}{2} \left( \omega_c \pm \sqrt{\omega_c^2 - 2\omega_{0z}^2} \right).
\]

(2.2.15)

If \( \omega_c^2 - 2\omega_{0z}^2 < 0 \), then \( u \) will be characterized by an exponential decay and the ion will no longer be trapped (i.e., loses its harmonic characteristic). Defining,

\[
\omega_{01} = \sqrt{\omega_c^2 - 2\omega_{0z}^2},
\]

(2.2.16)

we obtain two frequencies,

\[
\omega_+ = \frac{1}{2} (\omega_c + \omega_{01}),
\]

(2.2.17)

\[
\omega_- = \frac{1}{2} (\omega_c - \omega_{01}),
\]

(2.2.18)

where \( \omega_+ \) is the modified cyclotron frequency and \( \omega_- \) is the magnetron frequency. The general solution of Eq. 2.2.13 is [5],

\[
u = Ae^{-i\omega_+ t} + Be^{-i\omega_- t},
\]

(2.2.19)

squaring and adding the \( x \) and \( y \) components of Eq. 2.2.19 gives,

\[
x^2 + y^2 = |A|^2 + |B|^2 + 2|A||B| \cos \theta.
\]

(2.2.20)

Since \( 1 \leq \cos \theta \leq -1 \), this equation implies that the radial motion of the ion will oscillate between an outer radius of \( |A + B| \) and an inner radius of \( |A - B| \).

**2.2.2 Axial Motion**

The axial motion of the ion can be extracted from Eq. 2.2.9 which represents the equation of a harmonic oscillator with natural frequency \( \omega_{0z} \). The particle will therefore oscillate in the axial direction with frequency given by Eq. 2.2.10.
2.3 Trapping Requirements

From the above analysis, three independent and uncoupled degrees of motion are apparent: cyclotron, magnetron and axial motions. Conditions for trapping an ion in an ideal Penning trap are [5],

\[ \omega_+ \approx \omega_c \gg \omega_{0z} \gg \omega_- \quad (2.3.1) \]

Under realistic conditions, it is sufficient that Eq. 2.2.15 be satisfied,

\[ \omega_c > \sqrt{2} \omega_{0z} \quad (2.3.2) \]

What does Eq. 2.3.2 represent in terms of experimental parameters? Using the definitions of \( \omega_c \) and \( \omega_{0z} \) the answer is,

\[ V < \frac{B_0^2 e d_0^2}{2m} \quad (2.3.3) \]

where \( d_0^2 = \frac{1}{2} \left( z_0^2 + \frac{1}{2} r_0^2 \right) \). Table 2.1 shows various voltages for differing masses in a 0.3T B-field,

<table>
<thead>
<tr>
<th>( B_0 ) (T)</th>
<th>mass (amu)</th>
<th>Voltage (V)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.3</td>
<td>1</td>
<td>5,350</td>
</tr>
<tr>
<td>0.3</td>
<td>35</td>
<td>153</td>
</tr>
<tr>
<td>0.3</td>
<td>146</td>
<td>36.6</td>
</tr>
</tbody>
</table>

Table 2.1: Maximum trapping voltage for an ion of mass \( m \) in a 0.3T B-field.

2.4 Cylindrical vs. Ideal Penning Trap

Ideal Penning traps are difficult to engineer, so the hyperbolic electrodes are frequently replaced using planar end caps and a cylindrical center electrode. How does a real cylindrical Penning trap differ from its ideal counterpart? Consider a Penning trap with a cylindrical ring electrode of radius \( r_0 \) and two endcaps separated by a distance \( 2z_0 \). Near the center
of the trap, the electric potential, $V$, may be expanded as \[7, 8\],

$$V = \frac{1}{2} V_0 \sum_{k=0}^{\infty} D_k \left( \frac{r}{d_0} \right)^k P_k (\cos \theta),$$

(2.4.1)

where $V_0$ is the potential applied between the endcaps and the ring electrode, $d_0$ is the characteristic trap dimension defined as $d_0^2 = \frac{1}{2} \left( z_0^2 + \frac{1}{2} r_0^2 \right)$, and $P_k (\cos \theta)$ are the Legendre polynomials. All expansion coefficients $D_k$ except for $D_2$ vanish for an ideal quadrupole configuration due to cylindrical symmetry. The first few even terms in the expansion Eq. 2.4.1 are thus the important terms. $D_0$ is small and thus negligible, while the second term ($D_2$) determines the axial oscillation frequency $\omega_z$. For a particle of charge $q$ and mass $m$, this frequency is given by \[7\],

$$\omega_z = \sqrt{\frac{q V_0 D_2}{m d_0^2}}.$$  

(2.4.2)

Trap anharmonicities are quantified through $D_k$ terms higher than 2nd order, and the most important of these is $D_4$ which gives rise to a shift in $\omega_z$,

$$\frac{\Delta \omega_z}{\omega_z} = \frac{3 D_4}{2 D_2} \frac{E_z}{m \omega_z^2 d_0^2},$$

(2.4.3)

where $E_z$ is the axial energy. Minimizing Eq. 2.4.3 is essential since it depends on the ion-oscillation amplitude, i.e. $E_z$. The ratio of the axial energy and the axial well depth $m \omega_z d_0^2$ is typically very small, but just how small Eq. 2.4.3 will be is determined by the ratio of $D_4$ to $D_2$. The $D_k$ can be obtained as a series expansion of Bessel functions,

$$D_k = \frac{(-1)^{k/2} \pi^{k-1}}{k! 2^{k-3}} \left( \frac{d_0}{z_0} \right)^{k} \sum_{n=0}^{\infty} \frac{(-1)^{n+1} (2n + 1)^{k-1}}{J_0(i \pi (n + \frac{1}{2}) z_0))},$$

(2.4.4)

which is discussed in detail in \[9\]. The values of $D_2$ and $D_4$ are plotted in Figure 2.3 as a function of $\frac{r_0}{z_0}$ \[7\].

An important feature of Figure 2.3 is that when $r_0 \sim 1.20 z_0$, $D_4 = 0$ and $\frac{\Delta \omega_z}{\omega_z}$ is close to zero, greatly reducing the trap anharmonicities.
Figure 2.3: Graph of expansion coefficients $D_2$ and $D_4$ as functions of $\frac{r_0}{z_0}$.
Chapter 3

Experimental Apparatus

The apparatus used in this work is shown in Figure 3.1. A collimated beam of potassium atoms from an effusive source is photoexcited to selected Rydberg states using a frequency-doubled tunable ring dye laser. Excitation of the potassium atoms usually occurs in the presence of target gas near the center of an interaction region defined by two parallel plates containing fine-mesh copper grids. The laser output is chopped into a train of pulses (~2µs width) and measurements are conducted in pulsed mode to incorporate time of flight techniques. Following each laser pulse, the Rydberg atoms are allowed to interact with target gas for ~2µs before an extraction voltage is applied to the bottom plate of the interaction region to extract any negative ions that may result from this interaction. The negative ions travel through a drift region, located below the interaction region, held at a constant DC voltage (typically ~100V). Upon exit from the drift region, the negative ions traverse a second drift region at the entrance of the Penning trap. Initially the entrance grid of the trap is held positive to allow negative ions to enter. The exit grid is held negative to prevent the ions from escaping the trap. Once the ions have entered the trap, a negative voltage is applied to the entrance grid to trap them. Typical voltages are +5V and -5V. After a predetermined time in the Penning trap, a positive extraction voltage is applied to the bottom mesh. Ions are accelerated through an exit drift region, and are detected by a position sensitive detector (PSD) [10] which records their arrival positions and times. Positive ions produced in collisions travel through a time of flight mass spectrometer (TOFMS), located above the interaction region and are again detected using a PSD.
Figure 3.1: Experimental setup.
Data acquisition is accomplished using a Macintosh Quadra 800 system interfacing with a CAMAC (Computer Automated Measurement And Control) bus via a KSC (Kinetic Systems Corporation) 2932 CAMAC/Macintosh card. The KSC 2932 supports the KSC 3922 CAMAC Crate controller. Particle arrival times are recorded with a Bi-Ra model 2205 Quad Event Timer (QET) that measures the time difference between up to 4 stop signals and a common start signal using a digital counter. The QET has a 10ns resolution and a 41µs range. Particle arrival positions are digitized by a 12-bit Jorway model 32 analog-to-digital converter (ADC). The spatial resolution of the PSD is 50-100µm. Ion confinement and motion in the trap was modeled using SIMION software on an i586 AMD PC platform.

3.1 Vacuum System

Creating an effusive Potassium beam, photo-exciting it to selected Rydberg states and ultimately detecting collision products requires the use of a high vacuum environment. The vacuum system consists of two differentially-pumped stainless steel chambers, the source chamber and the main chamber. The background pressure in the main chamber is typically $\sim 2 \times 10^{-7}$ Torr. A gas manifold allows the introduction of the target gas, its pressure being controlled using a needle valve. The target gas pressure in the main chamber is limited to $\lesssim 5 \times 10^{-5}$ Torr by the characteristics of the diffusion pumps that evacuate the main chamber.

3.2 Potassium Source

Potassium, like all alkali metals, is a hydrogen-like atom with a single $n$s electron in its outer-most shell. Due to this configuration, the outer-most electron can be easily photoexcited to a high-lying $n$ state. The necessary frequencies for photoexcitation of potassium
are well matched with the tuning ranges that can be obtained using commercial dye laser systems.

To produce the ground state atomic beam, potassium metal packaged in 1 gram ampoules is heated in a stainless steel oven. The oven consists of an enclosed reservoir with a $\sim 0.5$mm diameter beam exit hole. Simple resistive heating cartridges are used to heat the oven to $\sim 300^\circ$C while the exit hole is maintained $\sim 20^\circ$C hotter to prevent potassium condensation from occurring and blocking the beam exit.

The effusing beam is further collimated by a $\sim 1$mm diameter aperture before it enters the interaction region resulting in a beam divergence of $\lesssim 1^\circ$. A hot wire detector is placed beyond the interaction region to monitor the potassium beam flux and beam density, which is estimated to be $\sim 10^{10}$ cm$^{-3}$ at the center of the interaction region.

3.3 Laser System

The wavelengths needed to excite ground-state potassium atoms to high Rydberg states in a single photon transition are in the range $\sim 285$-295nm, which can be obtained using a Coherent model CR699-21 Rhodamine 6G dye laser with a model 7500-06 doubling package.

The output of an Argon-ion pump laser is focused on a flat stream of dye which fluoresces over a broad frequency range. For this work, Rhodamine 6G (Rh6G) dye dissolved in ethylene glycol is pumped by 10W of 514.5nm radiation from a Coherent Innova 400 Argon Ion laser. The tuning range for Rh6G is 560-640nm. The circulating visible radiation is partially converted into UV radiation through second harmonic generation in a nonlinear potassium dihydrogen phosphate (KDP) crystal. Power output at the frequency range relevant to this work (285-295)nm is typically $\sim 2$-4 mW. Single frequency operation is accomplished through the use of 3 tuning elements: a 3 plate birefringent filter with a
passive bandwidth of 380GHz, a thin etalon with 200GHz free-spectral-range (FSR) and a thick etalon with 10GHz FSR. This combination allows for tuning through the lasing range of the dye in a series of 20GHz-wide steps and provides an effective line width of < 500kHz [11]. An optical diode made up of an optically active element and a Faraday rotator is used to ensure unidirectional operation.

The CR699-21 is actively stabilized by locking it to a temperature controlled Fabry-Perot etalon. Fast deviations are corrected by a piezoelectric translator (PZT) mounted mirror and long term drifts are corrected by a vertex mounted brewster plate. Servomechanisms correct the laser short-term jitter by altering the effective cavity length using these two components. Long term stability is limited to \(~40\text{MHz/hr}\) [11] by drift in the 699-21 reference cavity.

For the present work, this long term stability is not sufficient. An external locking device termed “Superlock” [12] is used to reduce the drift to \(\leq 1\text{MHz/day}\) in the fundamental. This is achieved by locking the dye laser output frequency to a frequency stabilized Helium-Neon laser via a temperature controlled Fabry-Perot etalon, which scans at 50Hz using a PZT. The etalon outputs two series of sharp transmission peaks, one associated with each input wavelength. Any change in the frequency of the dye laser results in a change in the relative spacing of the peaks and is used to generate an error signal that restores the dye laser frequency to its original value.

The continuous output of the laser is chopped into pulses typically \(~2\mu\text{s}\) long by an acousto-optic modulator (AOM). The AOM consists of a PZT transducer mounted on a fused quartz block and is operated as a Bragg device. The transducer generates a high frequency RF acoustic traveling wave inside the glass. The resulting periodic variation of the refractive index produces a diffraction grating which can deflect up to 90% of the light
out of the zero order. To produce a pulse of light, the sound wave is pulsed to deflect the light into the first order.

### 3.4 Permanent-Magnet Cylindrical Penning Trap

Some negative ions such as SF$_6^{-}$ are known to have long-lifetimes. To study such lifetimes an ion trap is required and a cylindrical Penning trap was chosen. As will be demonstrated, this trap provides storage times $\gtrsim 100$ms allowing a broad range of ion lifetime studies.

Designing a magnet to produce a strong, uniform magnetic field over some localized volume with little or no magnetic field outside this region would have been next to impossible without utilizing some of the newer magnet technologies. The magnetic field for the current experiment is produced by exploiting the properties of rare-earth-permanent-magnets (REPMs). The remarkable characteristics of REPMs stem from two fundamental attributes: (1) large intrinsic magnetic moments per unit volume, and (2) extremely high resistance to demagnetization by external or internal fields [13]. As a result, REPMs can be manipulated into shapes that would cause other materials to demagnetize. The two possible choices of REPMs for the present magnet are: SmCo and NdFeB. Both of these choices surpass older magnetic materials in areas such as residual flux density, maximum energy product, and intrinsic coercivity, to name a few. Campbell [14] and McCraig [15] describe the crystalline structures and explain the different properties of the most common magnet types. Figure 3.2 shows the comparison of REPMs and older magnet materials. From this figure, it is apparent that REPMs offer superior performance. The presence of a reverse field has little effect on REPMs and thus magnet assemblies can incorporate several magnets with fields orientated in many directions; which is crucial for magnet designs that
Figure 3.2: Comparison of different magnetic materials.
incorporate cladding as will be described in the following sections.

Properties of REPMs allow for construction based on a magnetic analog of Ohm’s law. This approach was used in the past in elementary general physics courses. One of the major differences between REPMs and older materials such as Alnico is that REPMs are not affected by strong external or internal fields, thus allowing REPMs to be viewed as a source of constant magnetomotive force (mmf) i.e., a magnetic battery. Materials such as soft iron with a high permeability can be viewed as near-perfect flux conductors, and materials with low permeability and air gaps can be viewed as magnetic resistors. Some of the more important quantities are given in Table 3.1. A detailed derivation of the magnetic Ohm’s law starting from Ampere’s law is described in Leupold and Potenziani II [16].

3.4.1 Cladding Design

In most magnetic circuits, magnetic flux generated by REPMs is wasted along unwanted flux paths. Using the electric circuit analog, current (i.e., magnetic flux) along unwanted paths can be eliminated either by insulation or by utilizing a compensating potential. These compensating potentials in a magnetic circuit are referred to as cladding. Figure 3.3 shows a basic magnetic circuit and its corresponding analog.

Following Leupold and Potenziani [16], the two magnets are represented by batteries and the flux paths through air by resistors in the circuit. Of particular interest is the

<table>
<thead>
<tr>
<th>Electric Quantity</th>
<th>Magnetic Analogue</th>
</tr>
</thead>
<tbody>
<tr>
<td>I(Electric Current)</td>
<td>Φ(Magnetic Flux)</td>
</tr>
<tr>
<td>V(Electric Potential)</td>
<td>F(m.m.f)</td>
</tr>
<tr>
<td>G(Conductance)</td>
<td>P(Permeance)</td>
</tr>
<tr>
<td>R(Resistance)</td>
<td>R(Reluctance)</td>
</tr>
</tbody>
</table>

Table 3.1: Electrical and magnetic analogous quantities.
air gap between the magnetic poles. Obviously much of the flux is lost to the external surroundings. To restrict flux to the air gap, the outer surfaces of the pole faces must be kept at the same magnetic potential using so-called “cladding” magnets. In order to determine the configuration for the cladding magnets, assume flux suppression has been accomplished and work backwards.

If the flux produced by the magnets is confined to flow within the cross-section of the structure, the flux can be written using the magnetic analog of Ohm’s law as,

$$\Phi = \frac{F}{R_t} = \frac{-2L_m H_{BC}}{(R_m + R_g)} = \frac{2L_m B_r}{(R_m + R_g)},$$

(3.4.1)

where $L_m$ is the length of one magnet, $B_r$ is the remanence, $R_m$ and $R_g$ the reluctance of the magnet and the air gap respectively and $H_{BC}$ is the coercivity which approximately equals $-B_r$ for REPMs. Total flux confinement requires that every point external to or on
the surface of the magnet structure must be at the same potential. Cladding is required only around the magnets and the air gap, and is such that the potential difference between any point on the surface of the cladding and any point on the iron yoke must be zero. Consider path ABC as shown in Figure 3.4. If the potential difference between A and C equals zero, then the mmf along the path must also equal zero,

$$F_{ABC} = F_{AB} + F_{BC} = 0.$$  \hspace{1cm} (3.4.2)

Given that,

$$F_{AB} = \frac{F_m \cdot x}{2L_m}, \hspace{1cm} (3.4.3)$$

$$F_{BC} = H_d \cdot y, \hspace{1cm} (3.4.4)$$

where $F_m$ is twice the mmf across one of the magnets, $H_d$ is the radial magnetic flux inside the cladding, and $y$ is the cladding thickness at point $B$, Eq. 3.4.2 can be written as,

$$\frac{F_m \cdot x}{2L_m} + H_d \cdot y = 0. \hspace{1cm} (3.4.5)$$

Using the magnetic Ohm’s law,

$$F_m = \Phi \cdot R_m, \hspace{1cm} (3.4.6)$$
in Eq. 3.4.5 yields,
\[ \frac{F_{BC}}{H_d} = \frac{-F_{AB}}{H_d} = -\frac{\Phi}{2L_m} \cdot \frac{x}{H_d}. \] (3.4.7)

The radial flux density in the cladding must equal zero by assumption that no flux flows to the exterior. At zero flux density, \( H_{BC} = -B_r \) for an REPM. Substituting for \( \Phi \) from Eq. 3.4.1 into Eq. 3.4.7 yields,
\[ y = -\frac{2L_m B_r R_m x}{2L_m H_d (R_m + R_g)} = \frac{R_m \cdot x}{(R_m + R_g)}. \] (3.4.8)

This relationship between \( y \) and \( x \) indicates that the surface of the cladding is a truncated cone with a half angle of \( \tan^{-1} \left( \frac{R_m}{R_m + R_g} \right) \). Figure 3.5 shows the cross-sectional shape of the cladding magnets. The thickness \( y \) reaches a maximum at the magnets edge and declines beyond the edge since the field in the gap, \( H_g \), is opposite that in the magnet \( H_m \). The potential decreases linearly with distance, \( z \), from the gap edge as,
\[ \Delta F = -z H_g = z B_m = \frac{z \Phi}{A_m}, \] (3.4.9)
where \( A_m \) is the cross-sectional area of the gap. Using Eq. 3.4.1 for \( \Phi \) gives the result,
\[ \Delta F = \frac{-z L_m B_r}{A_m (R_m + R_g)}. \] (3.4.10)
Midway through the gap, the mmf is zero, implying that the cladding thickness is minimal. The potential changes polarity which means cladding of opposite polarity must be used to compensate for the potential change. The shape of the cladding is symmetric about the center of the air gap.

To illustrate the effectiveness of cladding, consider Figure 3.6. The unclad magnet has a $0.8T$ B-field, while the clad magnet structure has a B-field of $\sim 2T$. Approximately 55kg of material would be needed in the unclad configuration to obtain field densities of $\sim 1.6T$. The same field would be generated by 7kg of material in a proper clad configuration.

The magnetic structure used to generate the magnetic field in the current Penning trap is shown in Figure 3.7. Seven different REPMs and two iron discs make up the magnet design.
Figure 3.7: Magnetization of the magnet assembly.

Arrows on Figure 3.7 indicate the direction of magnetization of each piece. The iron discs provide magnetic equipotentials at either end of the field region. The central tube magnet establishes the axial field while cladding is achieved using six REPMs. Confinement of the axial field is accomplished by ensuring that the outer surface of the magnet is a magnetic equipotential by the opposing magnetization of the cladding discs outside the iron discs and by the two tapered, conical shaped cladding magnets. Cladding rings surrounding the central tube further confine the field by opposing diagonal fields leaking from the central tube. The resultant field due to this arrangement is a 0.3T uniform, axial magnetic field from end-disc electrode to end-disc electrode. Figure 3.8 illustrates the actual field within the trap. Measurement of the axial magnetic field was performed with a gaussmeter and
hall-probe mounted on a translational stage.

To ensure all cladding magnets are in contact with the central disc, the use of several screws on each end of the aluminum support structure was used. The amount of force, as calculated by Finch [17], required to hold all the magnetic pieces together is $\gtrsim 90\text{lbs}$. Measurements made by the manufacture of the magnetic trap (Magnet Sales and Manufacturing) suggest that the repulsive force may be twice as large.

3.4.2 Trap Electrode and Electronics

Figure 3.9 shows a cross-sectional view of the electrodes which are made of oxygen-free-high-conductivity (OFHC) copper. The two end disc electrodes consist of copper plates supporting 70 lines per inch (lpi) fine mesh Cu grid material. The ring electrode is a Cu tube with an inner radius ($r_0$) of 4.2cm and a length ($2z_0$) of 8.0cm. The end disc electrodes and ring electrode, which are separated by specially designed Teflon spacers, can be individually biased.

An electronics module has been designed and built to allow for injection(ejection) of ions into(out of) the trap. The end disc electrodes are used as gates which are opened and closed via a fast voltage switch. Depending on the charge of the trapped ion, an attractive voltage potential(of opposite polarity to that of the ion) admits the ion into the trap while a repulsive voltage potential is applied to the opposite end disc electrode to prevent the ion from escaping through the bottom. To extract ions from the trap, an attractive voltage is applied on the bottom electrode. The circuit responsible for this switching is shown in Figure 3.10.

The switching circuit operates off a $\pm 24\text{V}$ power supply, which is regulated by two 3-terminal adjustable regulators, one for the positive and one for the negative rail. This
Figure 3.8: Axial magnetic field within the magnet.
Figure 3.9: Cross-section of trap electrode.
regulated voltage is used to power two ADG436 Analog switch chips. The ADG436 is able to switch from one input voltage to the other with a turn on time of $\lesssim 200\text{ns}$. The output voltage of each switch chip is directly sent to the end plates of the trap. Three input reference voltages, shown in Figure 3.10, are supplied by external DC regulated power supplies. The unit is triggered by a Stanford Research Systems(SRS)DG535 pulser.

![Figure 3.10: Schematic of switching circuit.](image-url)
Chapter 4

Simulating Ion Trajectories – SIMION

In order to reduce the time spent optimizing the trap parameters experimentally, simulations using the program SIMION 3D version 6 were undertaken. SIMION 3D is a 3 dimensional electrostatic lens analysis program developed at the Idaho National Engineering Laboratory. Figure 4.1 illustrates the current apparatus as modeled into SIMION 3D. Various adjustable parameters are input before every flight of an ion. Switching between various trap modes (i.e., injection, trap, and ejection) is accomplished by updating the potentials applied to the various electrodes at the appropriate time. Simulations stepping in time increments of $\frac{1}{100} \mu s$ with an ion mass of 146 amu ($SF_6^-$) and 35 amu ($Cl^-$) are discussed below.

Figure 4.1: SIMION model of experimental setup.

4.1 Experimental Model in SIMION

An accurate 1:1 scale representation of the experimental apparatus was entered into SIMION. For example, the separation between the bottom grid of the interaction region
and the top grid of the bottom drift region is \( \sim 0.5 \text{cm} \), and this is the value separating these two components in the SIMION model. To simulate the axial magnetic field, two magnetic “grids” with a potential difference of \(-2950 \text{ mags} \) (SIMION unit for magnetic potential) is used. The magnetic grids are placed near the endcaps of the cylinder yielding a uniform magnetic field of \( \sim -3000 \text{ Gauss} \) within the trap.

### 4.2 Loop Cycle

The ion in question is created at the center of the interaction region and allowed to sit unperturbed for a small amount of time called interact time. Following this, an extraction subroutine is called and the ion begins to accelerate towards the trap. To ensure the negative ion enters the trap in a reasonable amount of time \( (\Delta t \lesssim 35 \text{ µs}) \), the drift region immediately following the interaction region and the drift region prior to the trap are set to +100V and +140V respectively. A +5V DC electric potential is applied to the entrance grid of the trap to reduce the ion’s velocity. The exit grid of the trap has -5V DC electric potential applied to further ensure that the negative ion remains within the trap. It is desirable to have the negative ion within a small localized volume near the center with only a few meV kinetic energy. An electric potential of +1.5V DC is applied to the ring electrode of the trap to offset the zero in the electric potential distribution. This process of admitting negative ions into the trap is termed “injection mode”. After a time called switch time, the entrance grid electric potential is changed from +5V to -5V to enable “trap mode”. The voltage difference during the switch between injection and trap mode must also be small \( (\Delta V \sim 10V) \) in order to ensure the ion’s energetics are not perturbed greatly. The negative ion will remain trapped \( (\text{trap time}) \) until the exit grid of the trap is switched from -5V to +18V (“extraction mode”). To accelerate the negative ions to the PSD, a +140V
DC electric potential is applied to a drift region immediately following the trap. These simulations allow us to probe ion motions within the trap and determine the turning points and axial frequency. These simulations also provide a method for investigating stable or unstable trajectories within the trap.

4.3 Electric Potential Distributions for Trap Electrodes

The electric equipotentials for the various modes of the trap are shown in Figure 4.2. One major feature of Figure 4.2 is the difference in equipotential spacings in the trap and extraction modes. In the extraction mode, the equipotential spacing near the top of the trap is much greater than that near the bottom of the trap, corresponding to a much smaller $E$ field. Thus the force felt by the ion near the top of the trap would be small compared to the force felt if the ion is near the bottom of the trap. The temporal distribution of the extracted ions; therefore, will be broader if they are extracted when originally near the top as opposed to near the bottom. This can provide insight into the spatial distribution of ions in the trap at the time the extraction potential is applied.

4.4 Simulations

Simulations for ions with a mass of 146 amu are discussed below. Experimentally, ions can originate within a finite volume near the center of the interaction region. To simulate this in the SIMION model, a “grid” of 15 ions are used and the behaviors of each modeled. Three ions are placed at the center of the interaction region with one ion located at the exact center, one located 1mm above the exact center, and the other ion located 1mm below the exact center. Six ions, in sets of three, are located 1mm to the right and left of these center ions. The next six ions, in sets of three, are located 2mm to the left and right of the
Figure 4.2: Potential configurations for the various modes of the trap: a). injection mode, b). trap mode, and c). ejection mode.
Measuring the axial frequency of the ion in the trap is accomplished by plotting the temporal spread of the extracted ions vs. the trap storage time as shown in Figure 4.3 for SF$_6^{-*}$. The minima observed periodically in Figure 4.3 correspond to the axial frequency which is $\sim 10^4$Hz.
Chapter 5

Experimental and Analytical Techniques

The experimental and analytical techniques will be discussed below. Rydberg atoms are allowed to undergo electron transfer with SF$_6$ leading to the formation of long-lived SF$_6^{-*}$ negative ions. SF$_6$ is used as the target gas because of its high electron attachment rate ($k \approx 4 \times 10^{-7}$ cm$^3$s$^{-1}$) [18]. The spatial and temporal distributions of ions extracted from the trap are measured using a Position Sensitive Detector (PSD). The negative ion time of flight distribution at the PSD is compared with the results of SIMION simulations.

5.1 Experimental Procedure

To extract product ions, the top interaction grid is held at 0V while the bottom interaction grid is pulsed from 0V to 4V back to -2V using a WaveTEK model 801 50MHz pulse generator. Since potassium Rydberg atoms have a long radiative lifetime $\sim 150\mu$s for $n=30$, negative ion production can continue over an extended time period. Thus, the $E$ field in the interaction region is reversed following initial ion extraction to obtain a well defined group of ions and to prevent further negative ion collection. The voltage pulse applied to the bottom interaction grid is shown in Figure 5.1.

For this experiment, the Rydberg atoms are allowed to interact with SF$_6$ background gas for $2\mu$s ($t_0$) before the extraction pulse is applied. Time $t_1$ was optimized with the aid of SIMION simulations and had a value such that $\Delta t = t_1 - t_0 = 10\mu$s. Experimentally, $\Delta t$ is determined by reducing the width of the extraction pulse until no SF$_6^{-*}$ ions are detected on the PSD (i.e., the ions do not escape the interaction region prior to field reversal). The
extraction pulse is then extended by \( \sim 2 \mu s \) to ensure that an SF\(_6\)\(^{−} \) ion can exit the bottom grid of the interaction region.

Switching the voltages on the trap electrodes for the various modes (injection, trap and ejection) is performed by the switching circuit shown in Fig 3.10 which is triggered by a Stanford Research System (SRS) pulser model DG535. The system start pulse from the computer (which triggers the laser pulse) is used to trigger \((T_0)\) the SRS pulser. The SRS pulser DG535 has four trigger outputs (labeled A, B, C, and D) and a reference trigger input \((T_0)\). Currently, the configuration of the SRS pulser trigger outputs are,

- A: triggers injection→ trap mode,
- B: triggers trap→ ejection mode.
Trigger outputs C and D are used to trigger the start and stop of the QET, respectively, used in this experiment since the maximum time that can be recorded by the QET is $41\mu s$.

Trigger output A is referenced to the system start pulse ($T_0$), B is referenced to A, C is referenced to B, and D is referenced to C. For trapping $\text{SF}_6^{-\ast}$ ions with the above voltages, the following settings are input into the SRS pulser,

- A: $T_0 + 35\mu s$,
- B: $A + \text{traptime}$,
- C: $B + \text{QET offset}$,
- D: $C + 60\mu s$,

where traptime is the amount of time between closing and opening the trap, and the QET offset compensates for the ion flight time out of the trap and to the PSD.

### 5.2 $\text{SF}_6^{-\ast}$ Results

Using the above settings and QET offsets, $\text{SF}_6^{-\ast}$ ions could be trapped in the Penning trap for extended periods with ease. If the negative ions are trapped for $300\mu s$, the time-of-flight (TOF) distribution of the extracted ions is narrow $\sim 2\mu s$ FWHM. This is illustrated in Figure 5.2 which represents a total of one million experimental cycles at a target gas pressure of $3.0 \times 10^{-5}$ Torr. A comparison between theory and experiment provides a simple test of our model of the Penning trap. Using Eq 2.4.2, the period for one axial oscillation of an ion is,

$$T_z = \frac{2\pi}{\omega_z} = 2\pi \sqrt{\frac{m d_0^2}{q V_0 D_2}}. \quad (5.2.1)$$

Using $D_2 \sim 1.1$, and $d_0^2 \sim 1.921\text{in}^2$, Eq 5.2.1 gives,

$$T_z = 21.5\mu s \sqrt{\frac{m(\text{amu})}{V_0(V)}}. \quad (5.2.2)$$
Using $m = 146$ amu and $V_0 = 5V$ in Eq 5.2.2, an axial oscillation period of $116\mu s$ is obtained. If the trapping time is set to $300\mu s \pm 116\mu s$, the SF$_6^{-*}$ ion should be at the same location in the trap when the ion is extracted, thus giving the same TOF spectrum. Figure 5.3 shows the TOF spectra for trap times of $185\mu s$, $300\mu s$, and $416\mu s$ respectively. Note that the data for the $185\mu s$ TOF spectrum is half the number of experimental cycles. An important feature to notice in Figure 5.3 is how well defined the TOF spectrum is for these particular trapping times. Since the TOF spectra are well defined, this implies that the ions are near the exit grid of the trap when they are extracted. To test whether this is the case, the ions have also been extracted at a time when they are near the entrance grid. Figure 5.4 shows the arrival time spectrum resulting from trapping SF$_6^{-*}$ for $358\mu s$, which is $300\mu s + \frac{1}{2} T_z$. In Figure 5.4, the data are offset by $35\mu s$. This offset is needed because it takes the ions a longer time to exit the trap when they are extracted from near the top. The broad feature of Figure 5.4 can be understood by considering the electric field created during extraction as shown in Figure 4.2c. Ions near the top of the trap will initially experience a relatively small extraction field as compared to those ions extracted near the bottom.
Figure 5.3: Arrival time spectrum for SF$_6^+$ ions after trapping times of 185\,µs (top), 300\,µs (middle), and 416\,µs (bottom). The extraction field is turned on at t=0.
Figure 5.4: Arrival time spectrum of extracted SF$_6^{−*}$ ions after a trapping time of 358µs. The extraction field is turned on at t=0.

To determine the axial frequency spread due to trap anharmonicities, Eq 2.4.3 may be used. With $D_4 \sim 0.1$, the spread in the axial frequency is given by,

$$\frac{\Delta \omega_z}{\omega_z} \approx 3.6 \frac{E_z (eV)}{m (amu)},$$

where $E_z$ is the axial energy of the ion in the trap. SIMION simulations give a maximum value of $\sim 1.3$eV for $E_z$. This results in a spread of $\Delta \omega_z \approx 0.0321 \omega_z$, which corresponds to $\approx 3.2\%$ spread in $\omega_z$ for every oscillation cycle.

SF$_6^{−*}$ intermediates are known to have a long lifetime so a natural question would be to ask: how long can SF$_6^{−*}$ be trapped? This was examined by varying the trapping time and measuring the extracted ion signal. Ions injected far off axis have more erratic trajectories and may ultimately strike a trap electrode. Also, scattering by background target gas can lead to trap loss. This can be reduced by differential pumping of the trap. The signal decays only slowly with time corresponding to a trap lifetime $\gtrsim 20$ms. Some loss is to be expected. A fraction of the SF$_6^{−*}$ ions may undergo autodetachment or be scattered to the electrodes. Figure 5.5 shows a plot of normalized signal vs trapping time.
Figure 5.5: Time dependence of the trapped SF$_6^{-*}$ ions signal.
Chapter 6

Conclusion and Future Work

To date, SF$_6^-$ has been used as the target gas due to its high electron attachment rate. One drawback for using a molecular ion is the possibility of charge exchange with SF$_6$ in the trap itself. To avoid this possibility, it would be advantageous to use a target which produces an atomic negative ion. One such target is C$_2$Cl$_4$ which undergoes the reaction,

$$e^- + C_2Cl_4 \rightarrow C_2Cl_4^- \rightarrow C_2Cl_3 + Cl^-.$$  \hspace{1cm} (6.0.1)

Charge exchange would not occur when trapping Cl$^-$ and the mass of Cl$^-$ is much lighter than SF$_6^-^*$ (35 amu for Cl$^-$). Another improvement is to incorporate differential pumping which would allow the examination of effects associated with collisions in the trap. To achieve this, the trap would have to be differentially pumped allowing a second gas, which may be different from the target gas to be introduced into the trap.

With the current experimental apparatus, the lifetime of intermediate negative ions in the range of tens of microseconds to tens of milliseconds can be determined. Initial target species of interest include C$_7$F$_{14}^-$ and C$_6$F$_6^-$. Studies involving the trapping of multipole bound negative ions could also be performed. There is evidence which suggests that multipole bound states act as “doorway” states to valence bound states [19]. Since dipole bound states ionize in strong E fields, it will be possible by including a region of high electric field near the trap exit, to test whether transitions to a valence bound state occur.
6.1 Conclusion

Rydberg atoms provide a unique source of low-energy electrons which can be used to create excited metastable negative ions whose properties can be examined using a permanent-magnet Penning trap. This work shows that such ions can be stored in a Penning trap for well over 10ms, and the properties of the trap are well understood. The understanding of ion injection into the trap has been achieved, thus allowing future lifetime studies to be more efficient. The changes in the TOF spectrum of the extracted SF$_6^{-*}$ ions with varying trap time are also well understood.
References


Appendix A

SIMION Code for Simulations

;;ion trapping program
;;modeled after current penning trap

;;-----the following are adjustable parameters called when fly'm is depressed-----

defa inject_voltage 6 ;;injection voltage(V) on the trap entrance
defa ejection_voltage 20 ;;ejection voltage(V) on the trap exit
defa trapping_voltage -13 ;;trap voltage(V) used on the trap entrance
defa switch_time 33 ;;time for injection->trap mode (microsec)
defa trapping_time 300 ;;amount of time for trapping ions (microsec)
defa tau_time .8 ;;characteristic time for switch ramp (micro)

;;-----the following are static parameters called when fly'm is depressed-----
defs update_flag 1

;;-----this routine will fast adjust voltages (injection->trap->ejection)-----

seg fast_adjust
    rcl inject_voltage ;;initializes electrodes:3,5,16,17
    sto adj_elect16
    rcl trapping_voltage
    sto adj_elect17
    rcl inject_voltage
    sto adj_elect05
    rcl trapping_voltage
    sto adj_elect03 ;;finishes the initialization
rcl switch_time
rcl ion_time_of_flight
x>y gosub inject ;;if tof<switchtime, then inject
rcl switch_time
rcl ion_time_of_flight
x>y gosub trap ;;if tof>switchtime, then trap
rcl switch_time
rcl trapping_time
add ;;total trap time is
rcl ion_time_of_flight ;;switch_time+trapping_time
x>y gosub eject ;;if tof> total trap time, then eject
exit ;;when cycle complete, exit

;;---thus ends the fast adjustment routine-------------------------------

;;---this is the inject subroutine that the program will call upon-------

lbl inject
rcl inject_voltage ;;this subroutine recalls voltages
sto adj_elect05 ;;defined by inject_voltage and
rcl inject_voltage ;;trapping_voltage for ion's injection
sto adj_elect16 ;;into trap.
rcl trapping_voltage
sto adj_elect03
rcl trapping_voltage
sto adj_elect17
rtn ;;when all is done return to program

;;---this is the trap subroutine that is called upon by the program------

lbl trap
rcl ion_time_of_flight ;;this subroutine performs the trap
rcl switch_time ;;ramp and stores it as volt_voltage
subtract ;;which is later used in electrode#5
chs
rcl tau_time
1/x ;;1/(tau_time)
multiply ;;-(tof-switchtime)/(tau_time)
e"x ;;e^-((tof-switchtime)/(tau_time))
chs ;;-e^-((tof-switchtime)/(tau_time))
1
add ;;1-e^-((tof-switchtime)/(tau_time))
rcl inject_voltage
rcl trapping_voltage
subtract ;;(inject_voltage-trapping_voltage)
multiply ;;(Vin-Vtr)(1-e^-((tof-switchtime)/(tau_time)))
chs ;;(Vin-Vtr)(1-e^-((tof-switchtime)/(tau_time)))
rcl inject_voltage
add ;;Vin-(Vin-Vtr)(1-e^-((tof-switchtime)/(tau_time)))
sto volt_voltage
rcl volt_voltage
sto adj_elect05  ;;above voltage is stored in electrodes#:
                rcl volt_voltage       ;;5,16 (which is the entrance to the trap).
sto adj_elect16
rcl trapping_voltage    ;;trapping_voltage is stored in electrodes#:
sto adj_elect03       ;;3, 17 (which is the exit to the trap).
rcl trapping_voltage
sto adj_elect17
rtn                ;;when all is done, return to program

;;---this is the eject subroutine that the program so gladly uses-----

lbl eject
rcl trapping_voltage  ;;this subroutine switches the exit electrode
sto adj_elect16       ;;of the trap from trap mode to ejection mode
rcl trapping_voltage  ;;electrodes#: 16, 5 stay in trap mode, but
sto adj_elect05       ;;electrodes#: 17, 3 switch from trap to
rcl ejection_voltage  ;;ejection mode (i.e., trapping_voltage
sto adj_elect17       ;;->ejection_voltage)
rcl ejection_voltage  ;;return to program when all is done
sto adj_elect03
rtn

seg tstep_adjust     ;;this routine adjusts the time step of the
rcl ion_time_step 0.01 ;;calculations.
x>y exit           ;;if 0.01>ion_time_step then exit
sto ion_time_step   ;;else store the ion_time_step

lbl pe_update
rcl update_flag
x=0 rtn
0 sto update_flag
1 sto Update_PE_Surface
rtn
Figure A.1: Electrode numbers for SIMION code reference.
Appendix B

Important Trap Dimensions and Characteristics

B.1 Trap Dimensions and Quantities

\[ z_0 = 4 \text{cm} \quad (B.1.1) \]
\[ r_0 = 4.2 \text{cm} \quad (B.1.2) \]
\[ B_0 = .3 \text{T} \quad (B.1.3) \]
\[ d_0^2 = 12.4 \text{cm}^2 \quad (B.1.4) \]
\[ D_2 = 1.1 \quad (B.1.5) \]
\[ D_4 = 0.1 \quad (B.1.6) \]

where \( z_0 \) is one half the trap length, \( d_0^2 = \frac{1}{2} \left( z_0^2 + \frac{1}{2} r_0^2 \right) \), and \( D_2 \) and \( D_4 \) are expansion coefficients in Eq. 2.4.1.

\[ V < \frac{5.35 \times 10^3 \text{V}}{m(\text{amu})} \quad (B.1.7) \]
\[ \omega_c = \frac{28.9 \text{MHz}}{m(\text{amu})} \quad (B.1.8) \]
\[ \omega_z = 292 \text{kHz} \sqrt{\frac{V_0(V)}{m(\text{amu})}} \quad (B.1.9) \]
\[ T_z = 21.5 \mu\text{s} \sqrt{\frac{m(\text{amu})}{V_0(V)}} \quad (B.1.10) \]
\[ \frac{\Delta \omega_z}{\omega_z} = 0.124 \frac{E_z(\text{eV})}{V_0(V)} \quad (B.1.11) \]