

## Using the Tandem Ionizer/Energy Filter to Separate Internal & External Ions

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### I. INTRODUCTION

The Tandem Ionizer/Energy Filter may be used to filter ions with different kinetic energies. The following experiment was set up to demonstrate the capabilities of this energy filter in two different experimental conditions. First, the energy filter was used with its integral ionizer to separate gas phase ions from Electron Induced Desorbed (EID) ions. Secondly, the energy filter was used to separate internal gas phase ions from external gas-phase ions. In this second part of the experiment, the “external” ions are those ions born in an ionizer mounted in front of the integral ionizer of the Tandem Ionizer/Energy Filter assembly. These external, gas-phase ions are analyzed to simulate how the Tandem assembly can separate ions of different energies regardless of the process in which they were born.

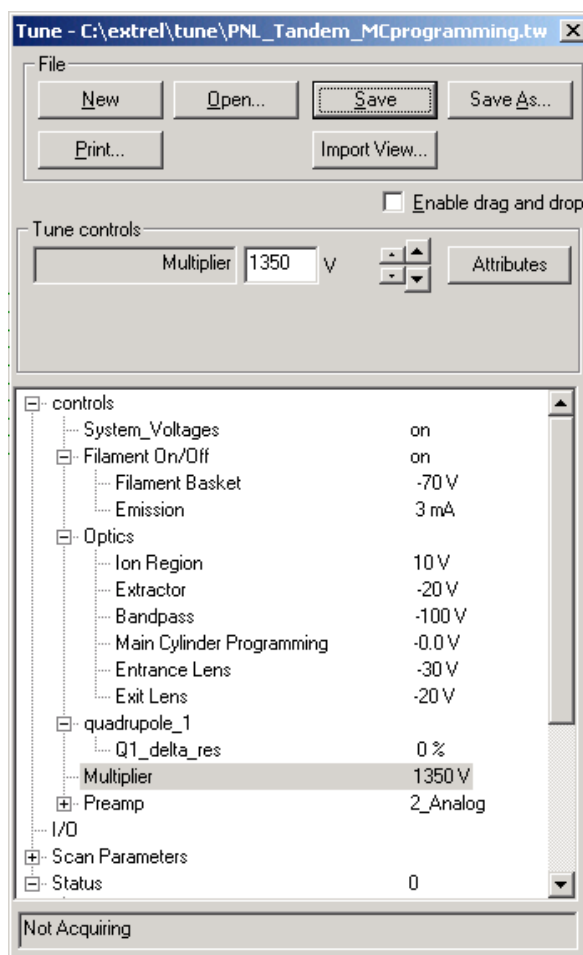
### II. EXPERIMENTAL

An external, Axial Molecular Beam Ionizer was set up on a chamber flange so that its focusing lenses would be facing the Tandem ionizer top plate as shown in Figure 3. In the first part of the experiment, gas phase ions were separated from EID ions to show that although the ions have the same  $m/z$  ratio, they may be separated because of differing kinetic energies.

The second part of the experiment was much more difficult, because of the distance between the external ionizer lens 3 and the entrance aperture of the Tandem ionizer. Compounding the problem was the fact that the ion region of the internal ionizer had to be used as an ion region potential and as a focusing lens for external ions. However, to show the filtering of ions born from different ionizers, gas phase ions from the external ionizer were separated from gas phase ions born in the Tandem ionizer itself.

In the first part of the experiment, the ionizer and optics were tuned to optimize the ion peak intensities of the gas phase ions. This was taken as the upper limit of peak intensities being analyzed. A macro was written so that the Main Cylinder voltage, Bandpass voltage and Quadrupole Pole Bias voltages would be ramped incrementally in software while

acquiring data. More information on this type of lens programming is explained under the “Virtual Elements” section of this paper.



**Figure 1: tuning parameters for separating internal gas phase ions from internal EID ions.**

Data was collected while ramping the Main Cylinder from  $-20\text{V}$  to  $20\text{V}$  while programming the Bandpass, and Pole Bias voltages to have this  $40\text{V}$  ramp ride on top of their respective settings. In other words, the above tune file was loaded and as the acquisition ran, the Main Cylinder Programming element ramped from  $-20\text{V}$  to  $20\text{V}$ . This programmed the Bandpass

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to ramp from -120V to -100V and the Pole Bias to ramp from -20V to 20V, since its starting setting was 0V.

### A. Virtual Elements

Programming one lens with respect to another lens is done easily in the Merlin Automation Data System. A “Virtual Element” was created that calls a macro every time it is adjusted. The macro then determines how much the element was changed and changes other elements by the same delta. This makes it easy to program the Bandpass and Pole Bias, according to the Main Cylinder, when doing SIMS experiments. However, the user is still able to program the Extractor, Lens 1/3, Lens 2, Quad Entrance and Exit lenses according to the Ion Region when doing Molecular Beam or Residual Gas Analysis (RGA) work.

### B. Results of Experiment 1

The following is the actual plot of the data collected during the first experiment.

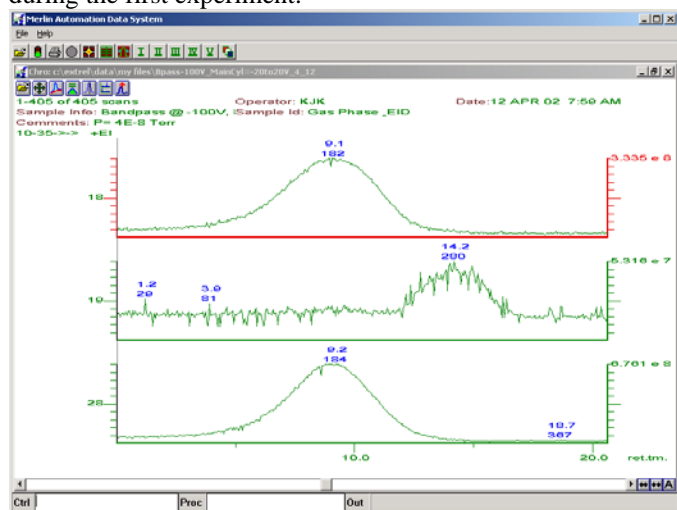


Figure 2: results of first experiment, separating internal gas phase ions from internal EID ions.

It is easy to see from the above plots that m/z 19 has a completely different kinetic energy than m/z 18 & 28. The EID compound, m/z 19 is actually fluorine from the tuning compound Perfluorotributylamine (PTA). The amine group of PTA sticks to the steel of the ionizer. Stray electrons hit the metal and knock off molecules containing fluorine. Since this fluorine is a result of an impact with the surface, its kinetic energy is higher than that of the gas phase molecules. An ion region voltage of zero (0) volts is used so that the ions born in the ionizer have only their ionization energy. There is no other potential placed on the ions born in this process. Therefore, the plots are representative of the different energies since the time plot is linearly related to the ramping main cylinder voltage. The higher energy species passes through the energy filter at a higher voltage

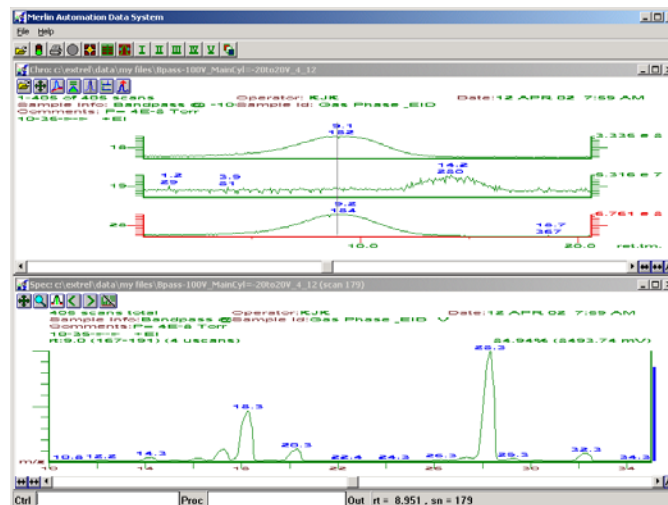


Figure 3: Spec view of mass spectrum at the point of the cursor. Knowing that the experiment was done with a Main Cylinder programming ramp of -20 to 20V, it is easy to determine the voltage at scan 179 = -2.1V.

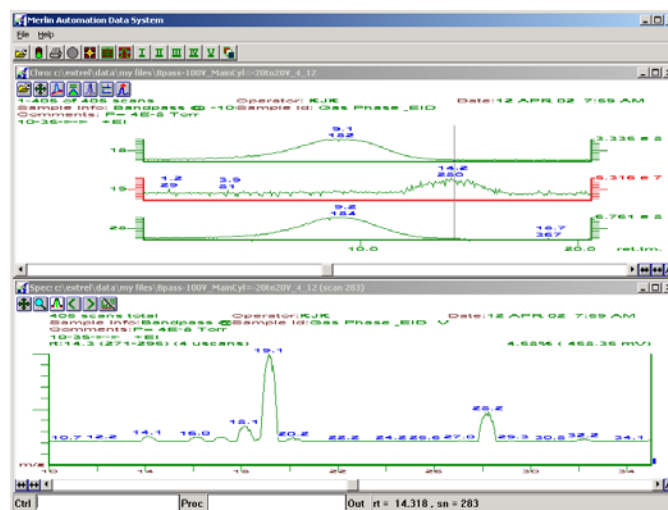


Figure 4: mass spectrum at scan #283, which is a main cylinder voltage of +8.3V.

### C. Experiment #2

The second part of this experimental involves the use of an external ionizer. The physical setup of the ionizers is shown in Figure 3 below.

A tune table was set up so that both ionizers could be on. The tune table shown in Figure 4 was used. The tuning parameters for this part of the experiment are different in that the ion region of the tandem ionizer has to be at a negative potential



in order to focus the external ions. Because of this, the ion region, and pole bias were initially set to  $-10V$ . This allows for a zero potential on the ions born in the tandem ionizer, because the difference between the tandem ionizer ion region and pole bias is zero. It also allows for a negative voltage on the ion region with respect to the external ionizer.

During acquisition, the main cylinder was ramped from  $-15V$  to  $10V$ . This in turn ramped the Bandpass from  $-115V$  to  $90V$ , and pole bias from  $-15$  to  $10V$ . This puts a  $+5V$  potential on the internal ion region (with respect to pole bias) at the beginning of the experiment. As the acquisition progressed, internal ion energy drops to zero because the ion region was held at  $-10V$  while the pole bias was being ramped with the Main Cylinder. The external gas phase ions had a higher energy because of the  $+10$  volts on the external ion region.

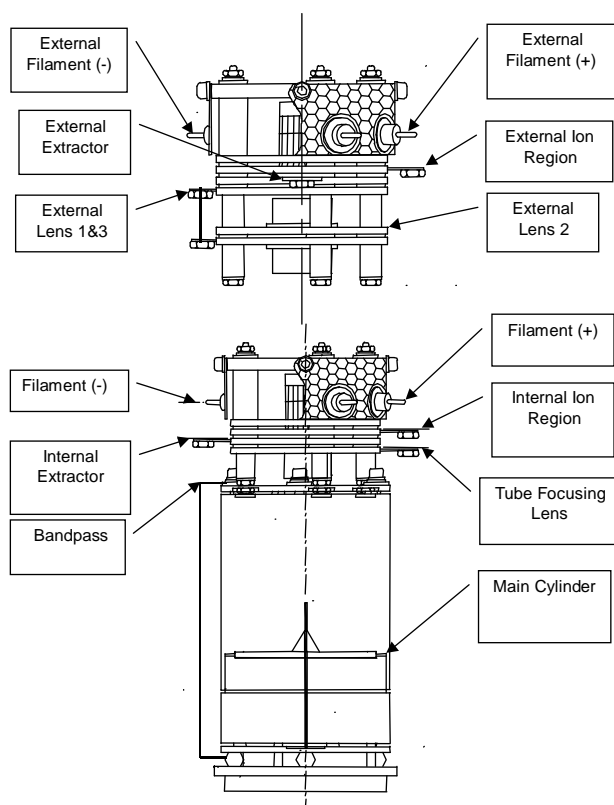


Figure 5: Ionizer setup used for external ions experiment.

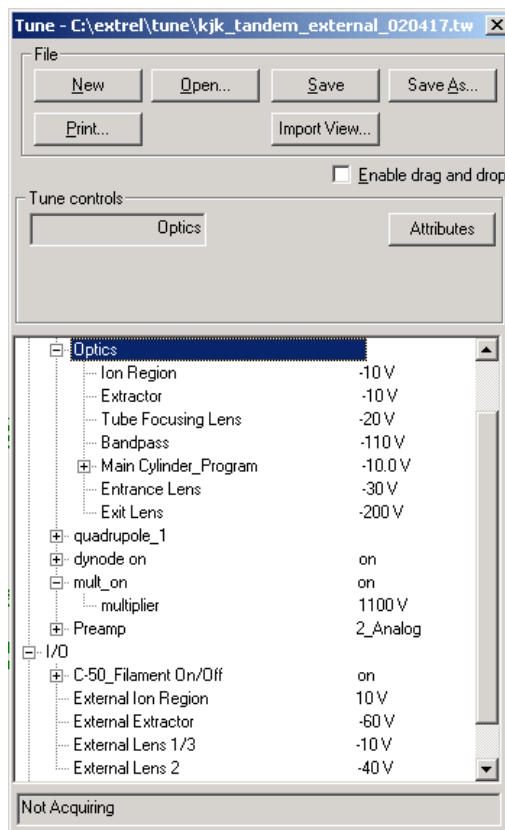


Figure 6: tuning parameters for second part of experiment.

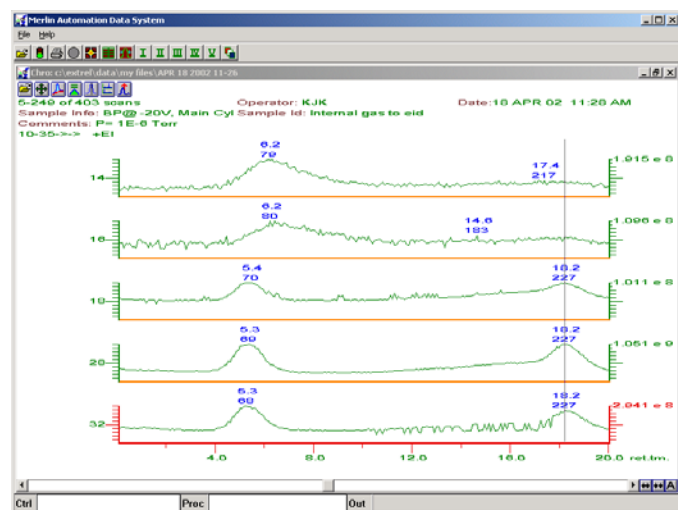


Figure 7: results of second experiment, separating external gas phase ions from internal gas-phase ions.

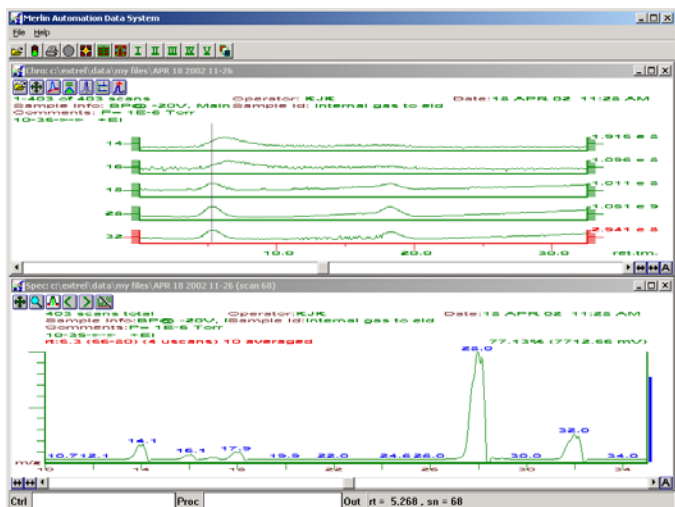


Figure 8: The Spec View shows the spectrum collected at the time of the cursor shown in the Chro View. Notice the large gas phase peaks, m/z 28 and 32.

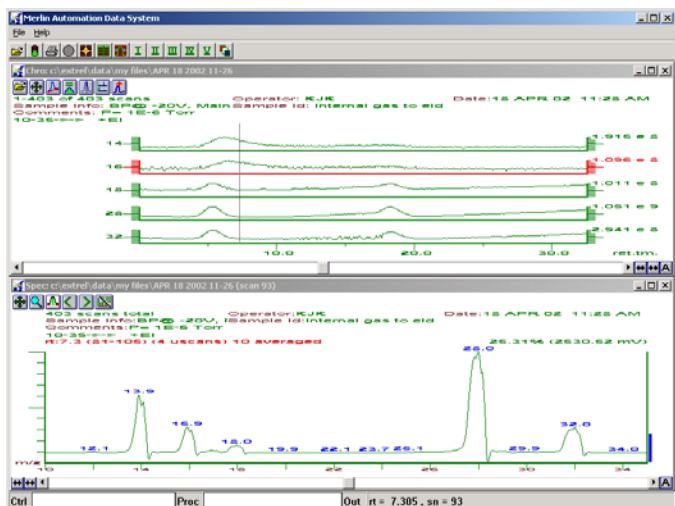


Figure 9: Spec view of scan #93. With an energy ramp of -20 to 20V, it is easy to calculate the Main Cylinder programming voltage of -10.7V.

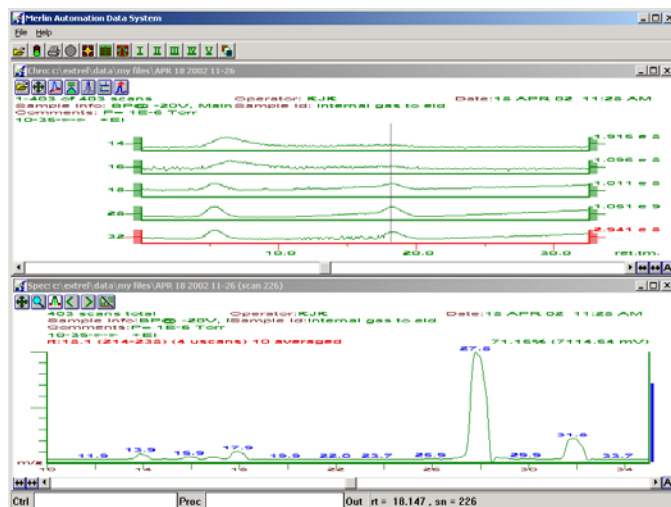


Figure 10: Spec view of scan #226. This translates to a Main Cylinder programming voltage of +2.6V.

#### D. Results of Experiment 2

The plots shown in Figures 7-10 show a clear distinction between the internal and external gas phase ions. The internal gas phase ions pass through the energy filter at a lower energy. The peaks in the chromatograph for m/z 16 & 18 may be the dissociated, monatomic ions. These monatomic dissociated ions will have a slightly higher energy and a wider energy range than the respective parent ions. This can be seen in the plots of m/z 14 & 16.

It is unlikely that any EID ions at m/z 14 would be present. Although m/z 16 is a common EID ion, it is very unlikely that EID 16 and gas phase dissociated m/z 14 would have similar energies. Therefore, it is likely that m/z 14 and 16 are both dissociated gas phase products of the parent ions m/z 28 and 32, respectively.

The external gas phase ions come through the energy filter at a higher energy because of the +10V placed on the ion region of the external ionizer.

### III. CONCLUSIONS

Our results demonstrated that the Tandem Ionizer Energy Filter is an efficient means of separating ions of different kinetic energy. The Merlin Automation Data System, which was used to collect the experimental data and control the mass spectrometer, made it extremely easy to design the experiment. Use of software macros enabled easy customizable control over both ionizers and the quadrupole itself.

#### IV. Appendix

The following macro was used to acquire data and ramp all lens voltages.

```
# lens_ramp.pml
# Created 020327 by KJK
# This macro is designed to scan the Main Cylinder of a
# Tandem Ionizer
# It is set up to be run either from the Ctrl line or from
# within an acquisition.
# The command should look like lens_ramp 0,25,25,10,501
# where the first variable is the
# starting voltage, the second parameter is the end voltage,
# the third parameter
# is the number of steps, the fourth parameter is number of
# averages, and the fifth
# parameter is the element ID number of the element you
# want to control.
# The macro is designed to ramp the Main Cylinder in a
# given step size.
# If this macro is run from within an acquisition, the
# acquisition will end when the macro ends.
```

# First make sure that the Pict and List views are visible.

```
VIEW_ADD:"list":cr
```

# Then clear the list view.

```
list_clear
```

```
old_volt = mlens %5
```

# Next, set the Main Cylinder to the starting voltage.

```
volt_to_lens = %1
volt_step = (%2-%1)/%3 #and determine the step size
```

```
"scanning"; ?%5; "with increment of";?volt_step; "volt";cr
```

# doze 3 #doze so the user can read the output line.

# Now, begin the loop and incremental voltage changes.

```
while volt_to_lens<=%2
```

```
mlens %5 = volt_to_lens
```

```
avmode = 2
```

```
average = %4
```

```
repeat 9: fish: end
```

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```
collect_resume
```

```
fish
```

```
collect_pause
```

```
list_append(volt_to_lens,1)
```

```
" Element"; ?%5; ?volt_to_lens; "Volts"; cr #This is an
# output to let you know what the voltages
#while the macro is running.
```

```
volt_to_lens += volt_step
```

```
mlens %1 = volt_to_lens
```

```
doze 0.5
```

```
end
```

```
COLLECT_STOP
```

```
#Stop the acquisition when the macro ends.
```

```
avmode=0
```

```
mlens %5 = old_volt
```

```
"Element"; ?%5; "reset to original voltage"; ?old_volt;
"volts"; cr
```

```
end
```

```
# The following copies any traces into List to make it easier to
# plot peak Intensity
# against energy.
```

```
chro_to_list(1,2)
```

```
chro_to_list(2,3)
```

```
chro_to_list(3,4)
```

```
chro_to_list(4,5)
```

```
chro_to_list(5,6)
```

```
chro_to_list(6,7)
```

```
chro_to_list(7,8)
```

```
end
```

