Development of an Ion Trap Mass Spectrometer with an Alternate Trapping Geometry

***Steve Lammert*, Marc Wise**

and Cyril Thompson

Chemical and Analytical Sciences Division
Oak Ridge National Laboratory
Oak Ridge, TN 37831-6120

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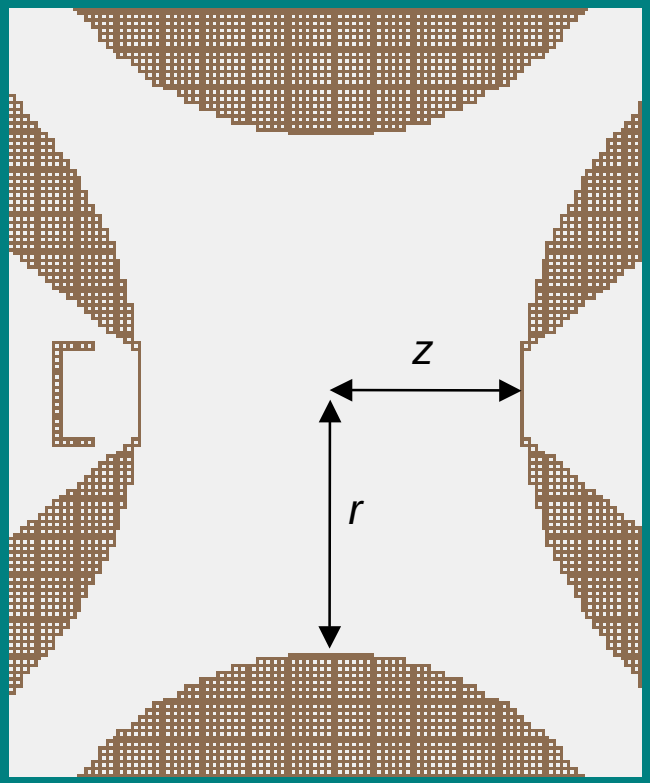
Ion Trap Parameters

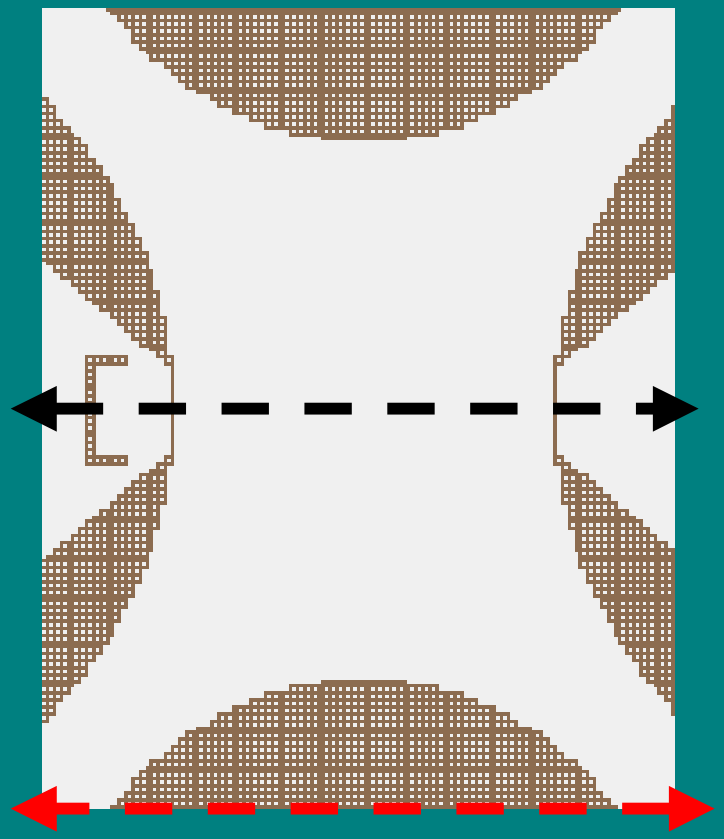
- 3-D Ion trap is an "Ion Bottle" with its <u>relative</u> dimensions (r_0 vs. z_0) fixed (at least somewhat).
- Optimized at

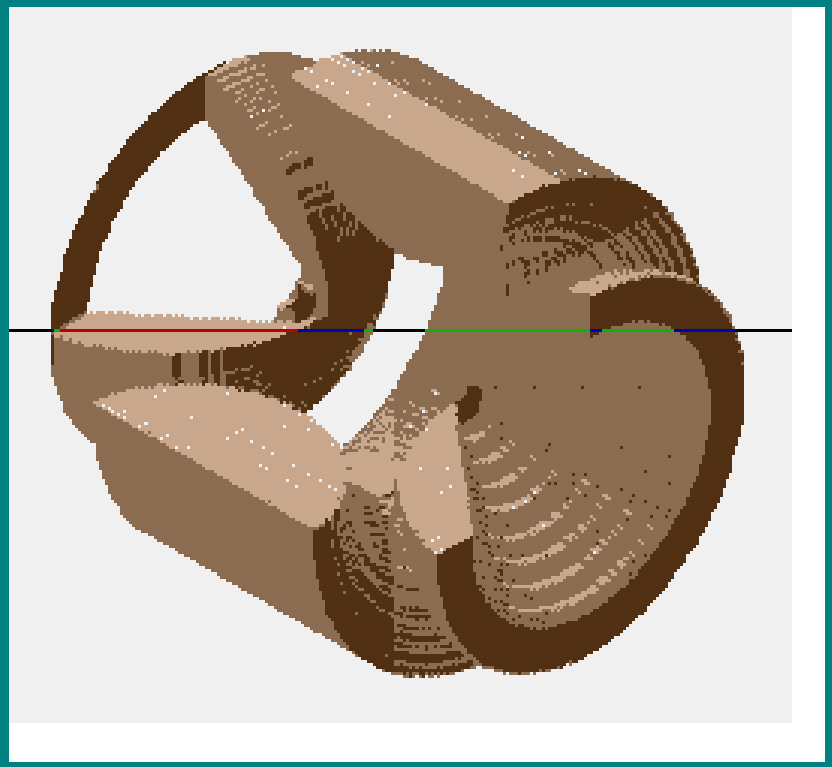
  r_0 =1cm, ~8.1kV$_{0\text{-}p}$
  - large increase in r_0 not practical due to high voltage arcing
  - reduced r_0 prone to space charge

$$q = \frac{-8 * e * V}{m * (r_0^2 + 2z_0^2) * \Omega^2}$$

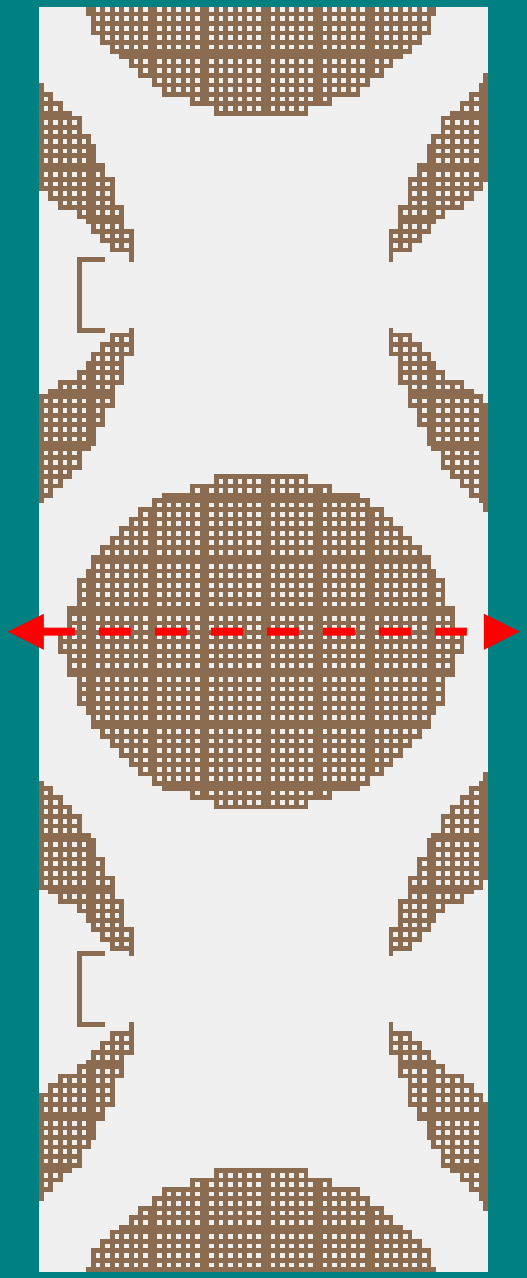


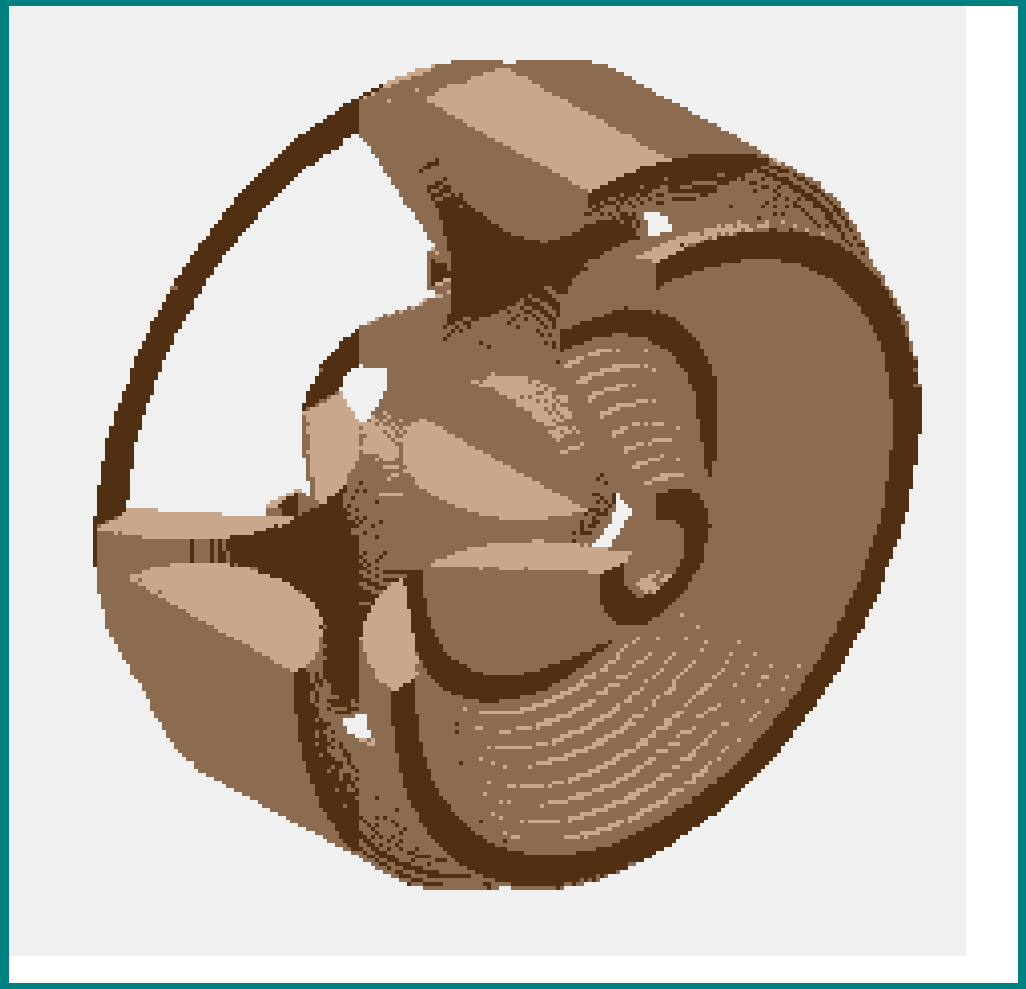
3-D Ion Trap Cross-section "Cylindrical Geometry"





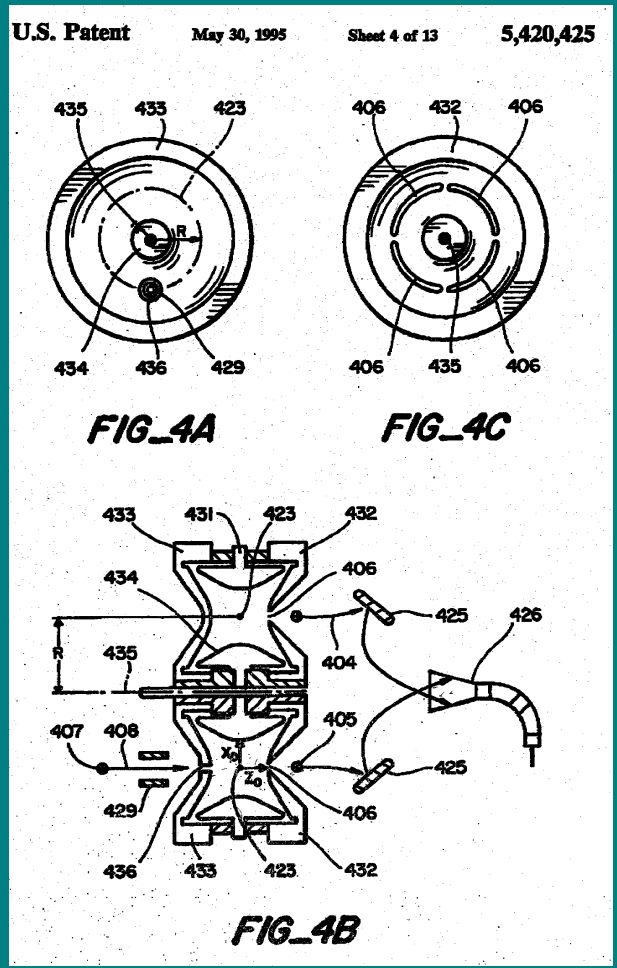
Ion Trap with "Toroid Geometry"





Related Work

- Mark E. Bier and John E.P. Syka - US Patent No. 5,420,525 on ion trapping systems using linear quadrupoles
  - started with <u>linear quad</u>
  - <u>possible</u> advantage in ion storage (rf only linear quadrupoles highly efficient in transmission)
  - unknown mass analysis capabilities
  - requires two rf signals (+/-) as in linear quadrupoles



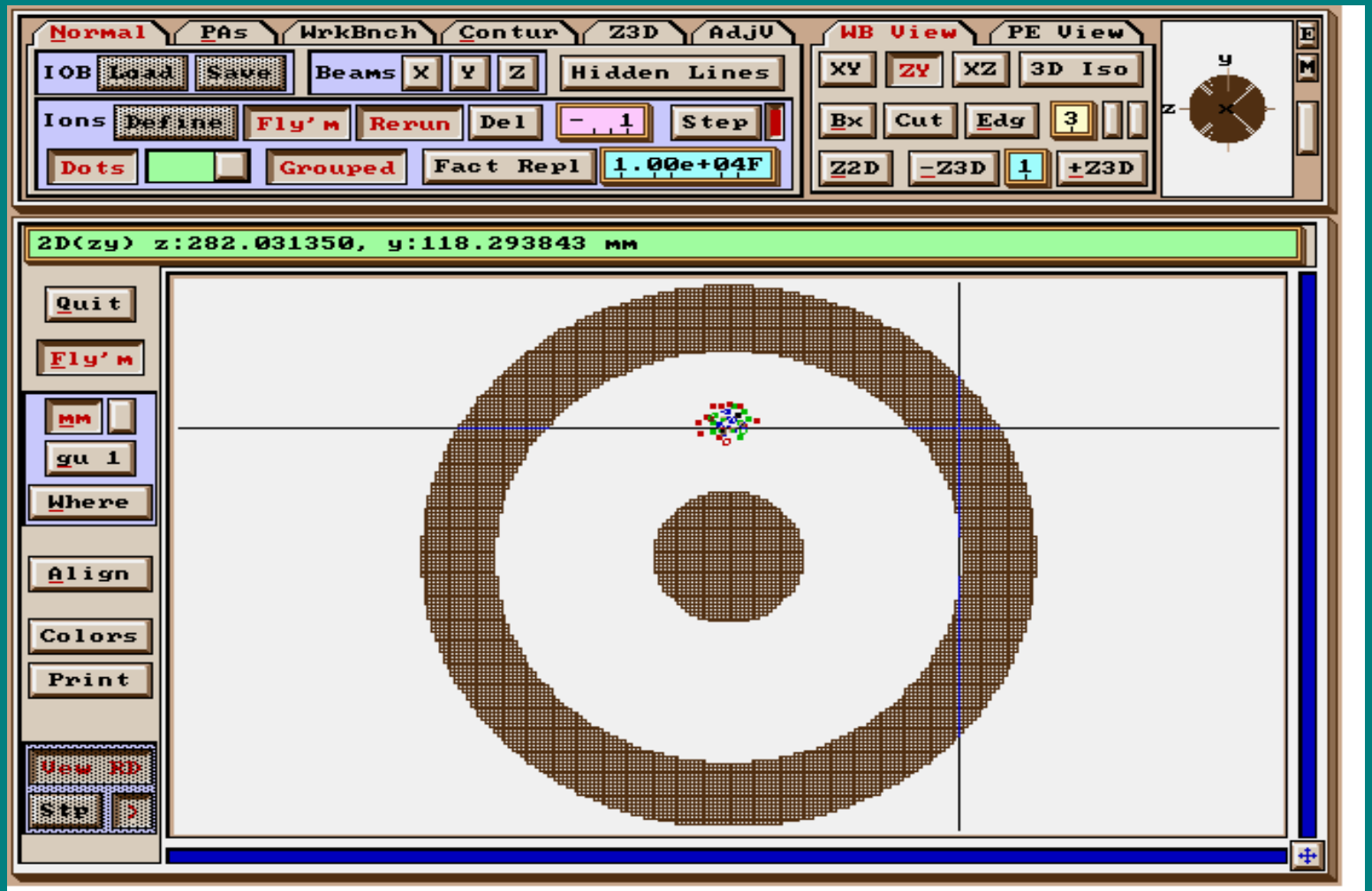
Characteristics of Toroid Analyzer

- Uses standard ITMS Electronics with few modifications
  - r_0 = 1 cm allows standard operating parameters
  - filament and resonance ejection circuitry directly compatible
- Capacitance of cell = 34 pf (compared to ca. 25 pf for std. Ion trap cell) which requires:
  - retapping coil (down 10 turns from previous setting)
  - modification of rf drive frequency to 986 kHz (from 1100 kHz)
- Requires annular detector (currently using custom multi-channel plate detector)

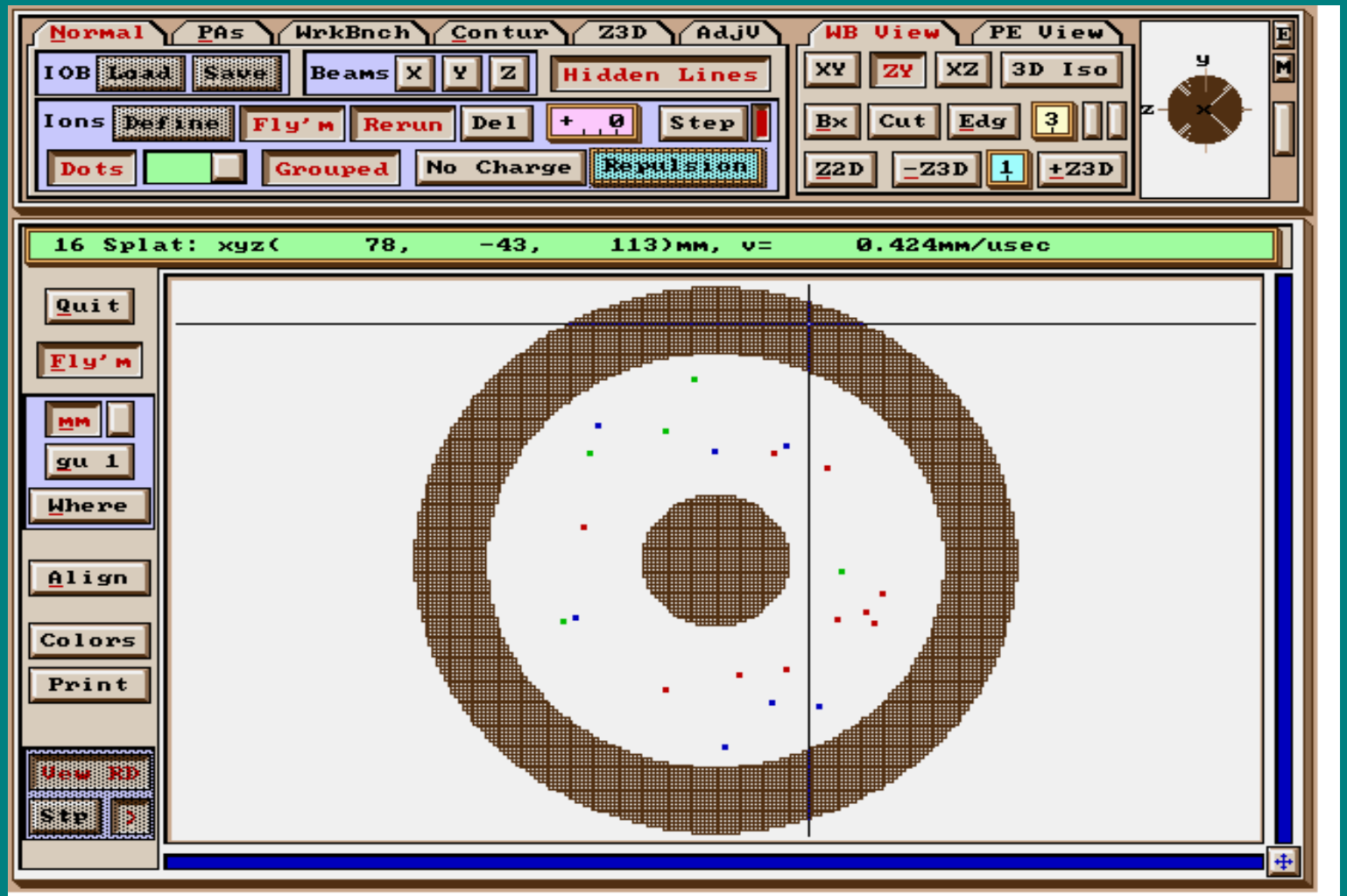
Toroid Enabling Features

- Significant increase in ion storage capacity for given device radius (ref: P. Hemberger's ion tomography experiments at LANL)
  - For standard size cells, 400-1000 fold increase assuming 1 mm dia. ion cloud
  - For reduced size cells - similar ion storage capacities but significantly reduced operating voltages. (8kV to 80 V with 10 x reduction in radius)
- New degree of freedom for ion motion
  - potential increased internal energy deposition for MS/MS experiments
- New mode for ion injection (tangential "orbital capture")

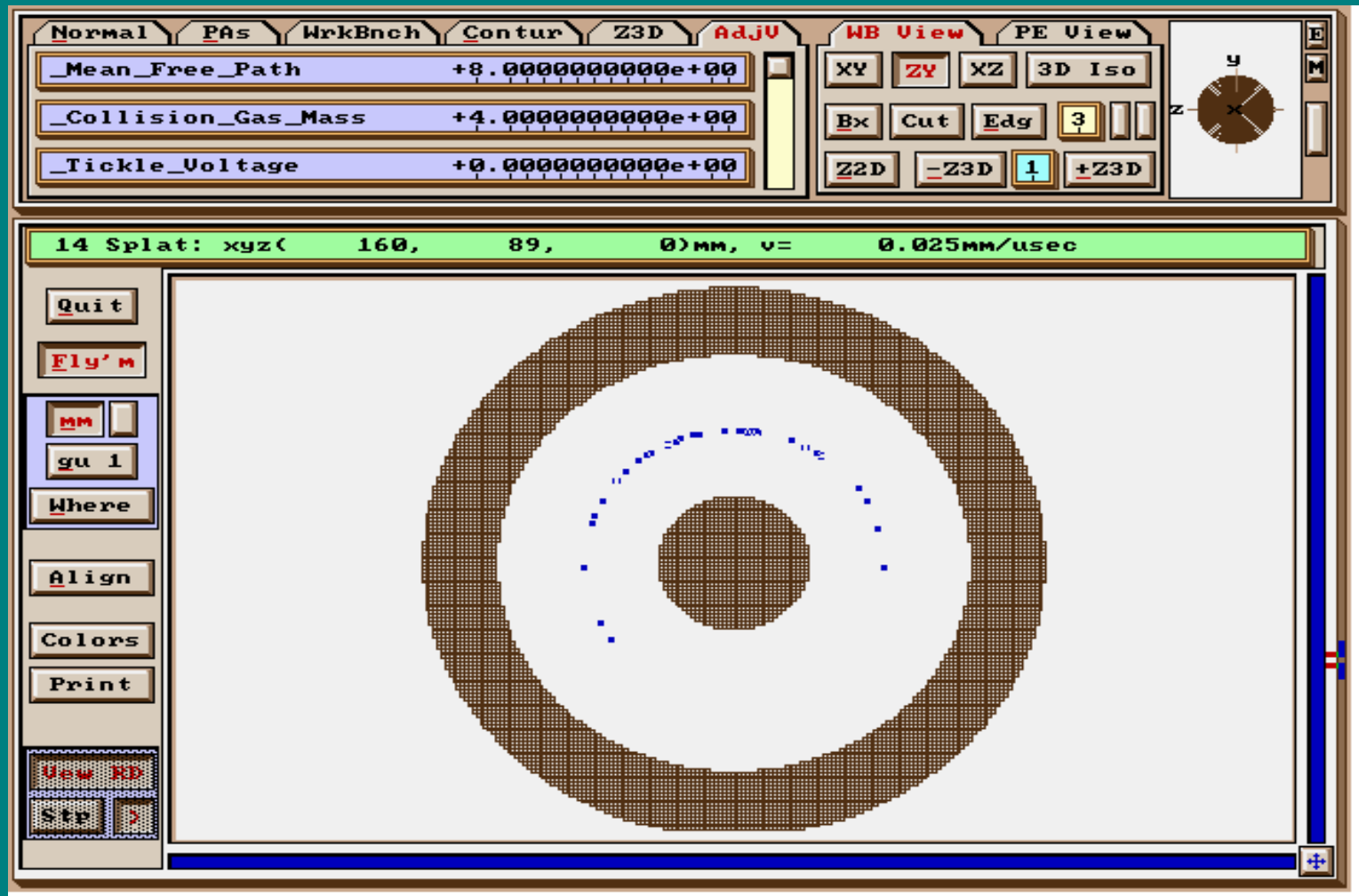
SIMION-3D6 Simulations-Ionization



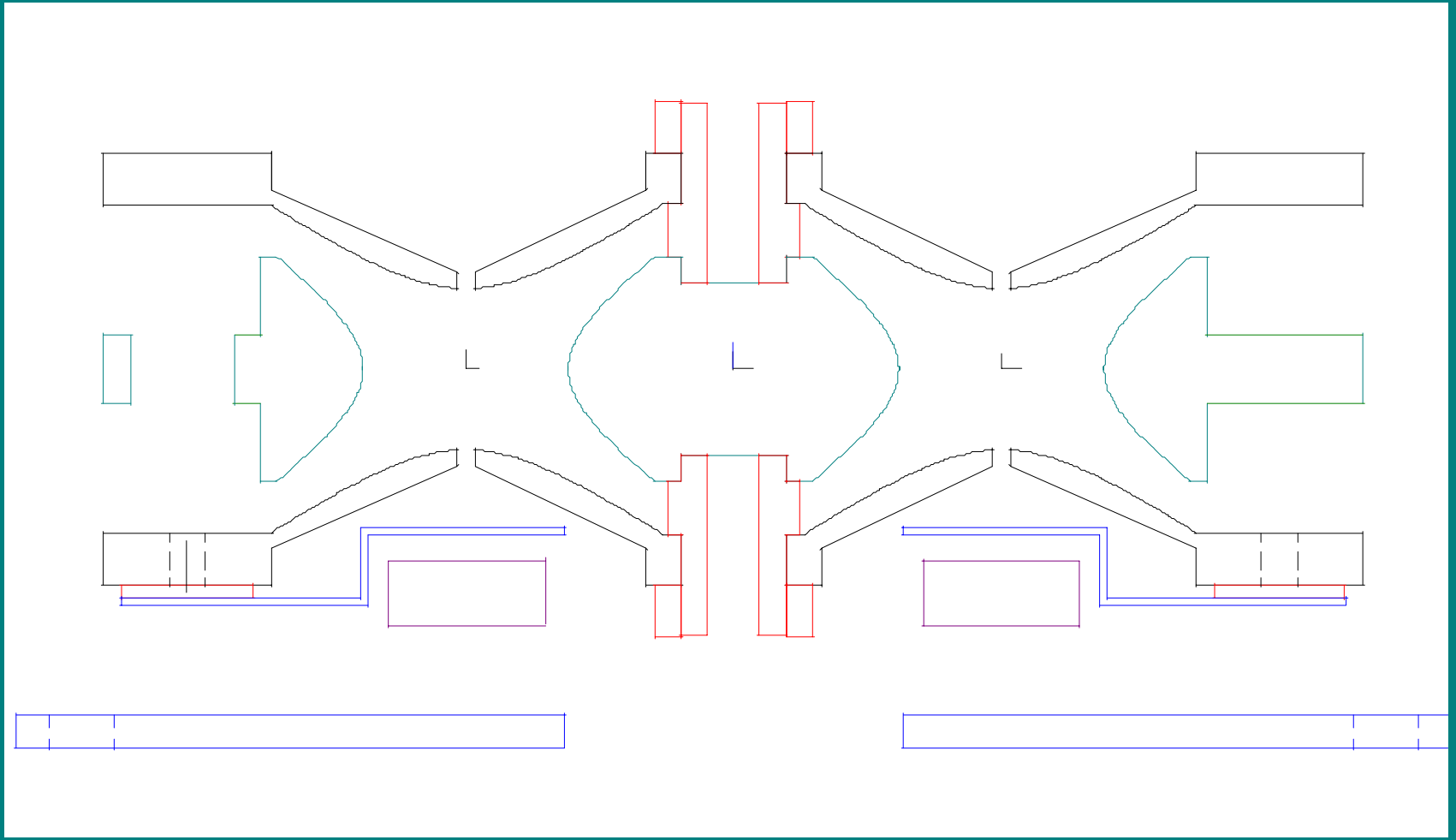
SIMION-3D6 Simulations-Diffusion



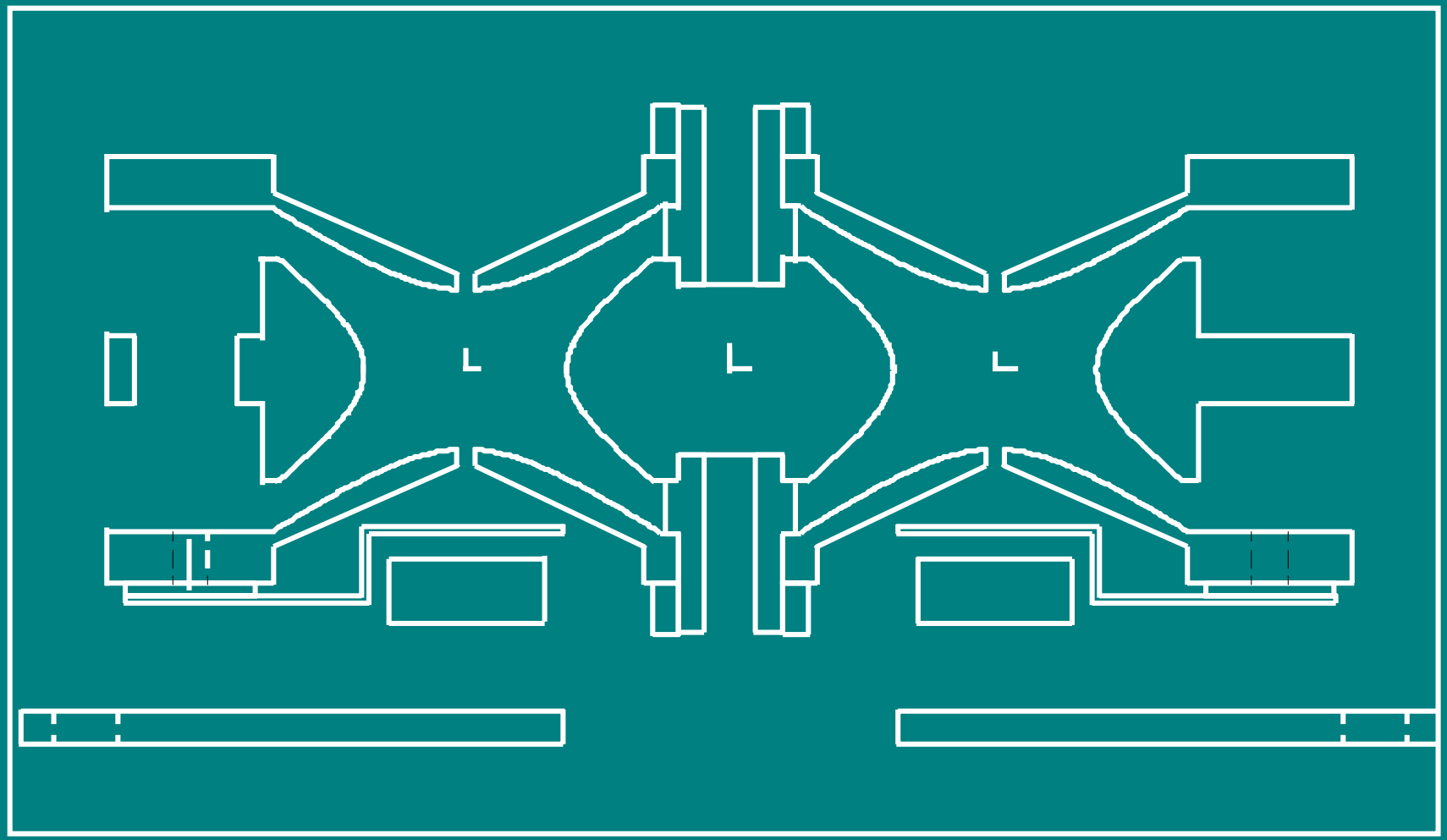
SIMION-3D6 Simulations-Collisional Cooling



Toroid Ion Trap Schematic



Toroid Ion Trap Schematic

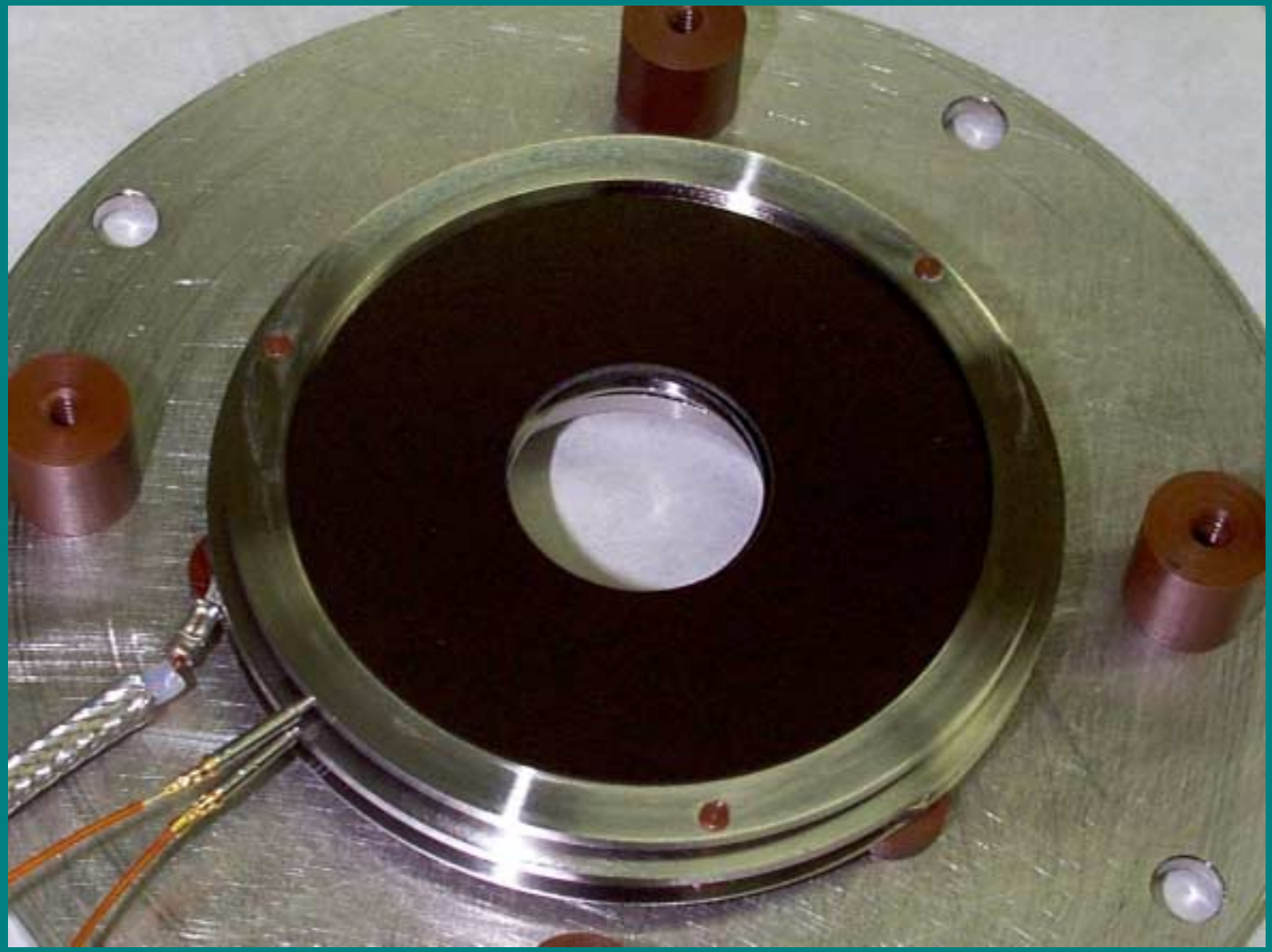


Comparison to Std. 3D Ion Trap

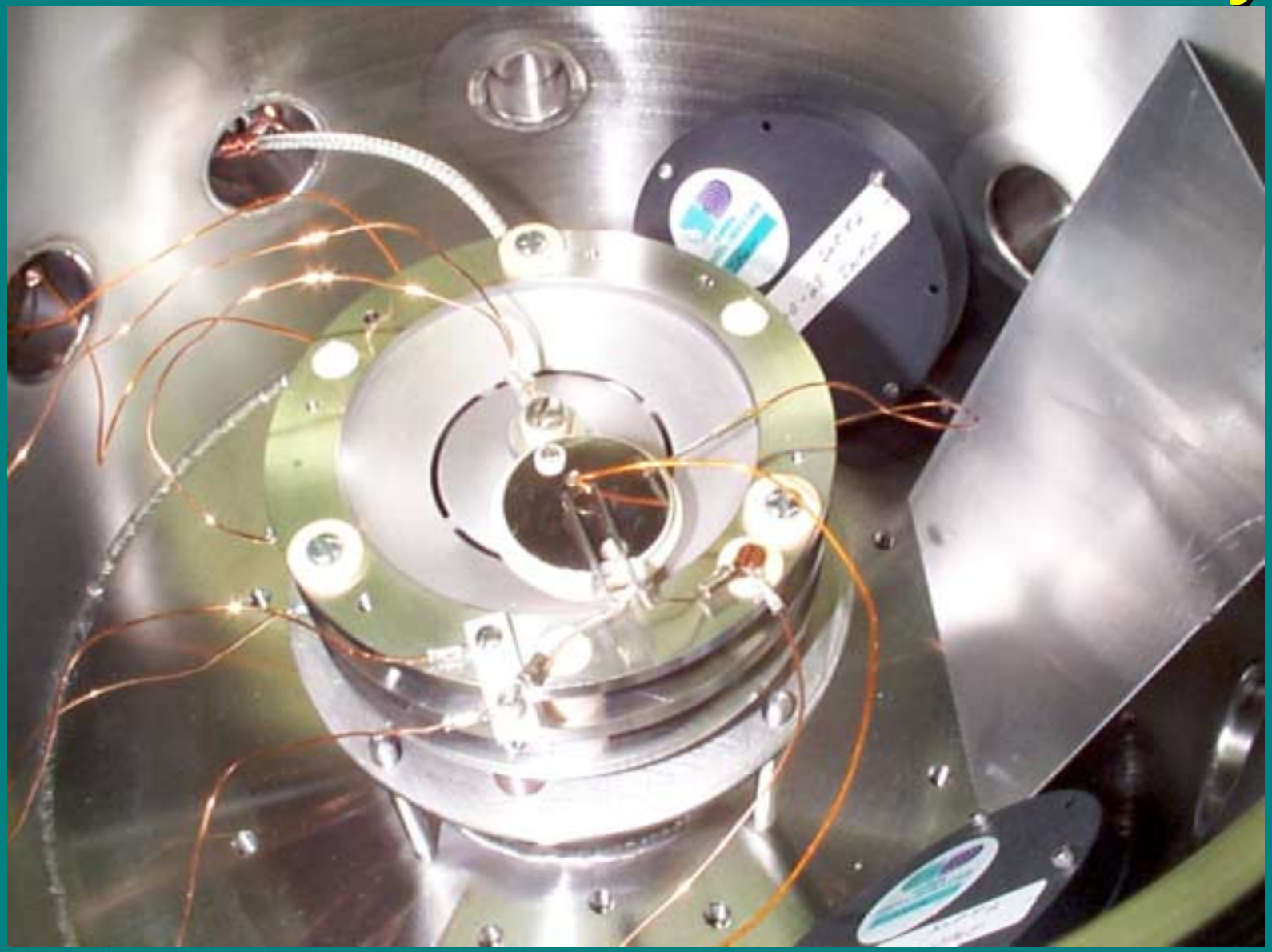
Toroid Ion Trap Analyzer

Trapping Region and Exit Slits

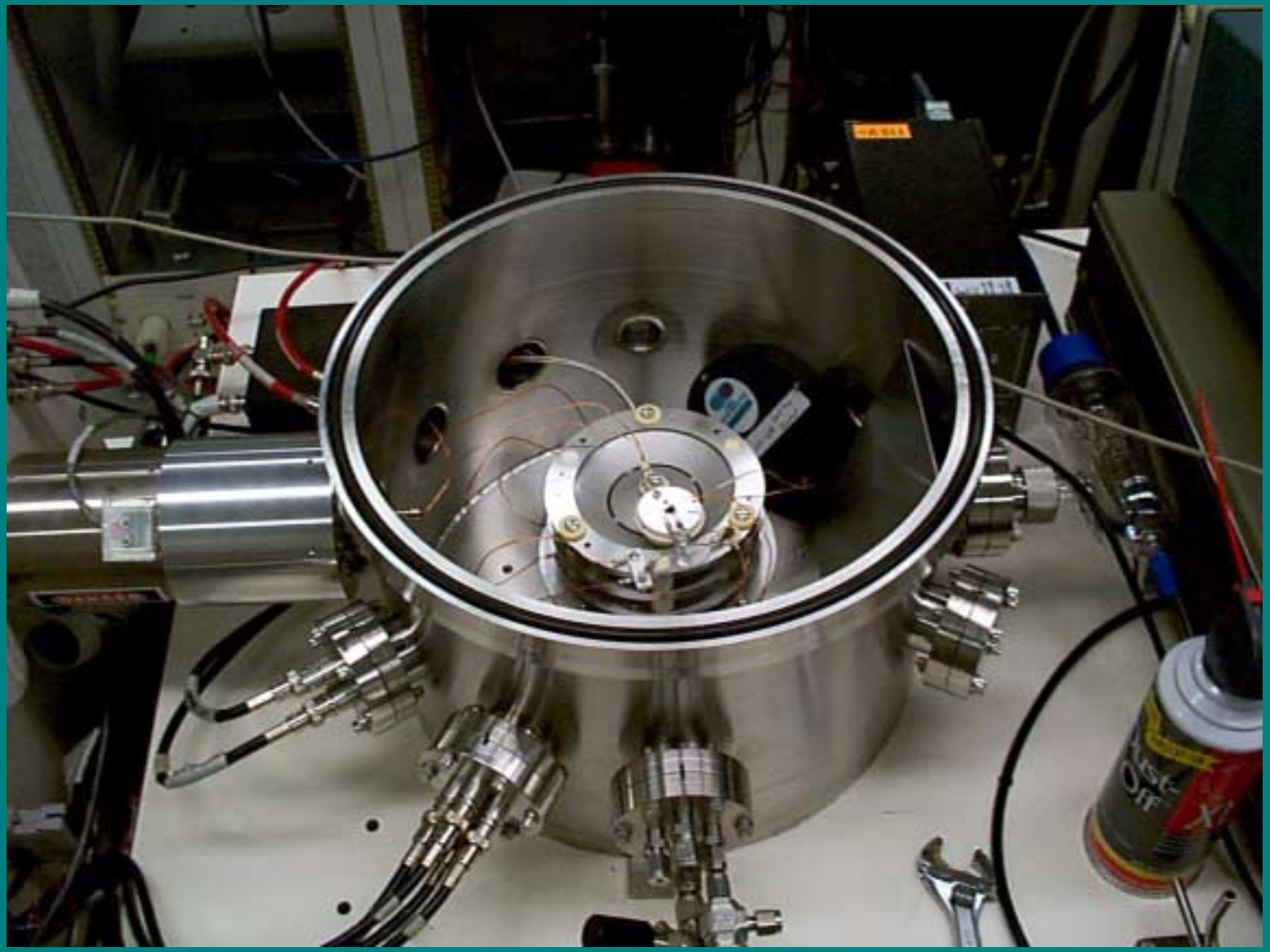
Annular MCP Detector



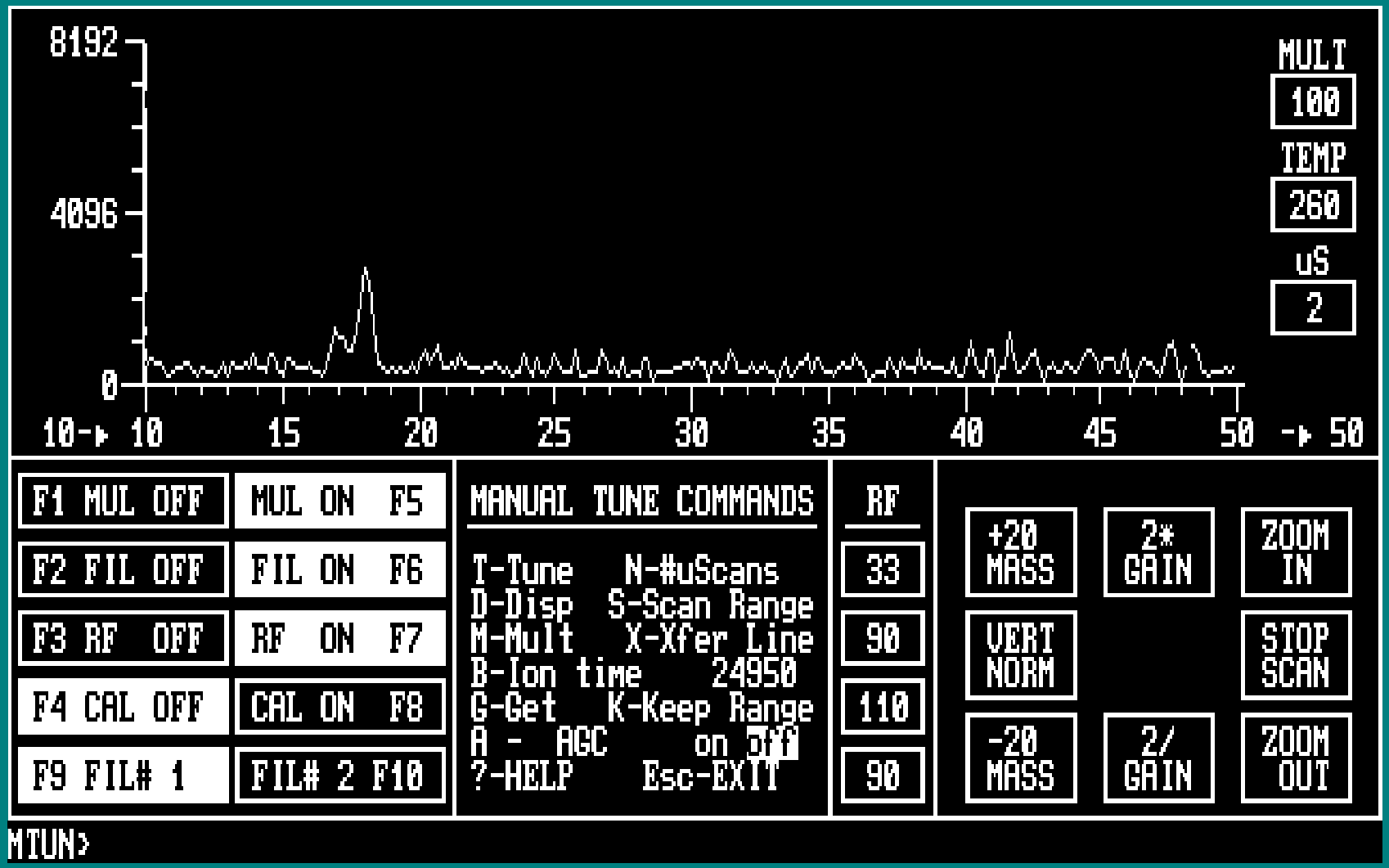
Modified ITMS Filament Ass'y



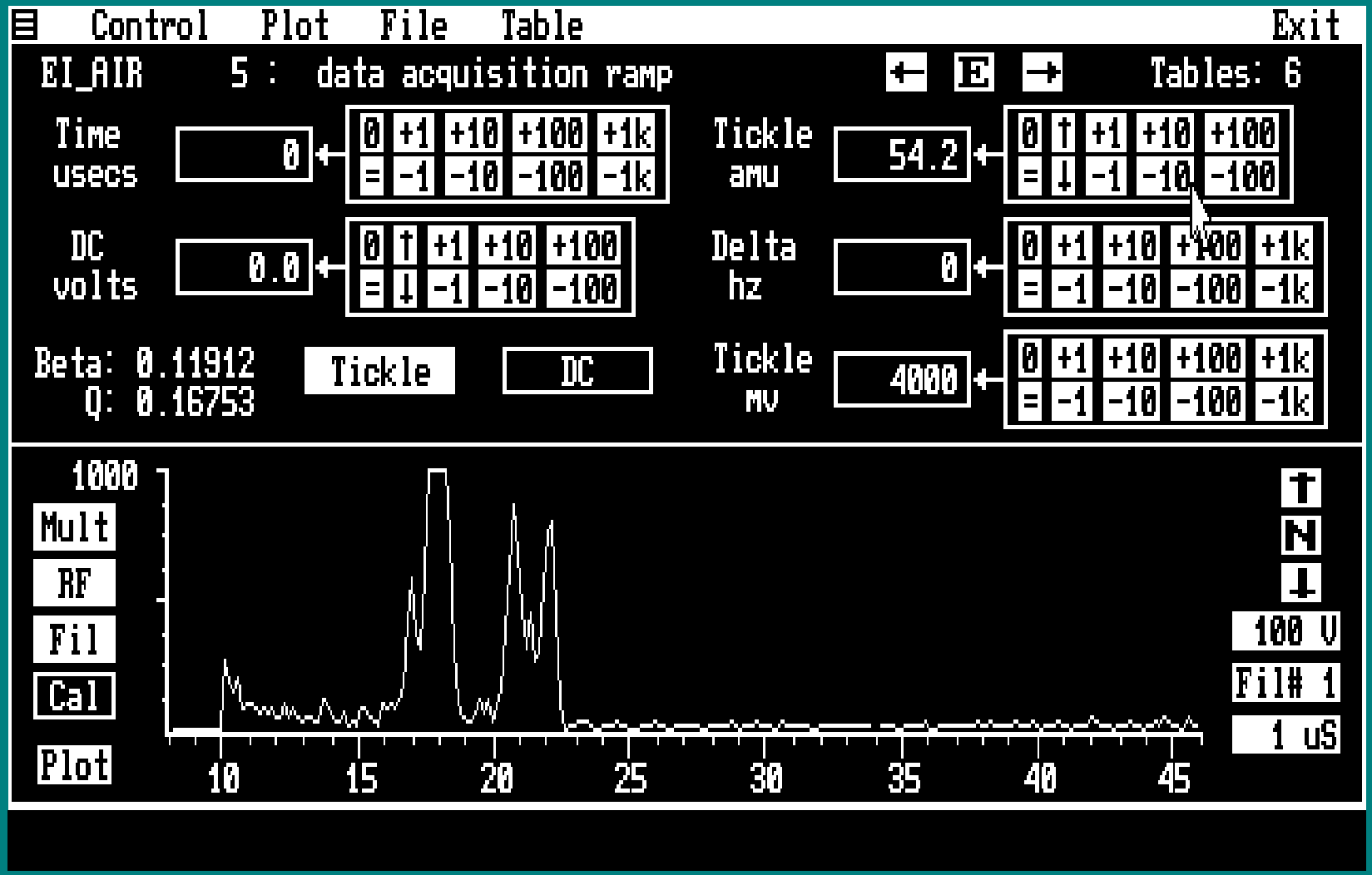
Toroid Vacuum Chamber



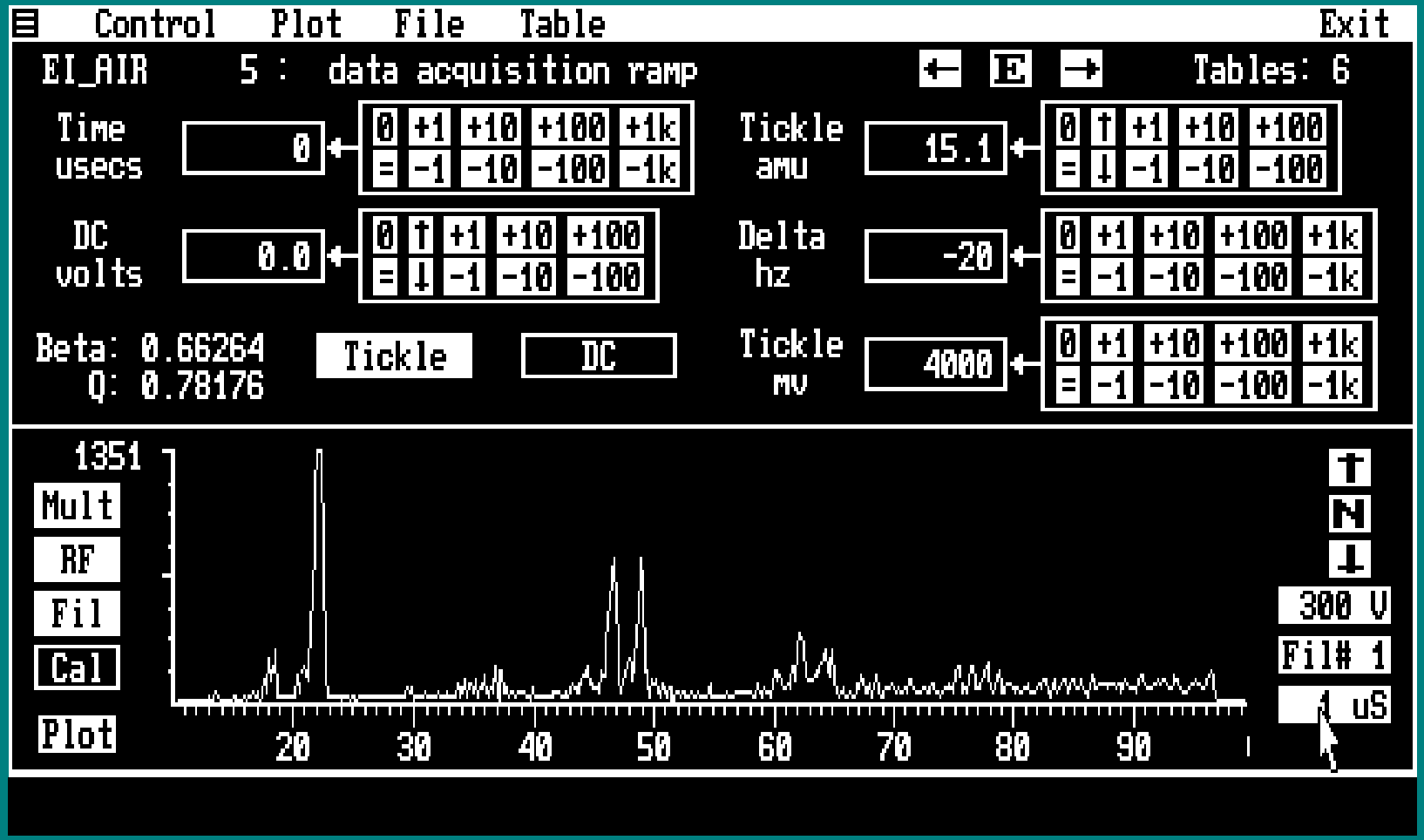
First Spectrum



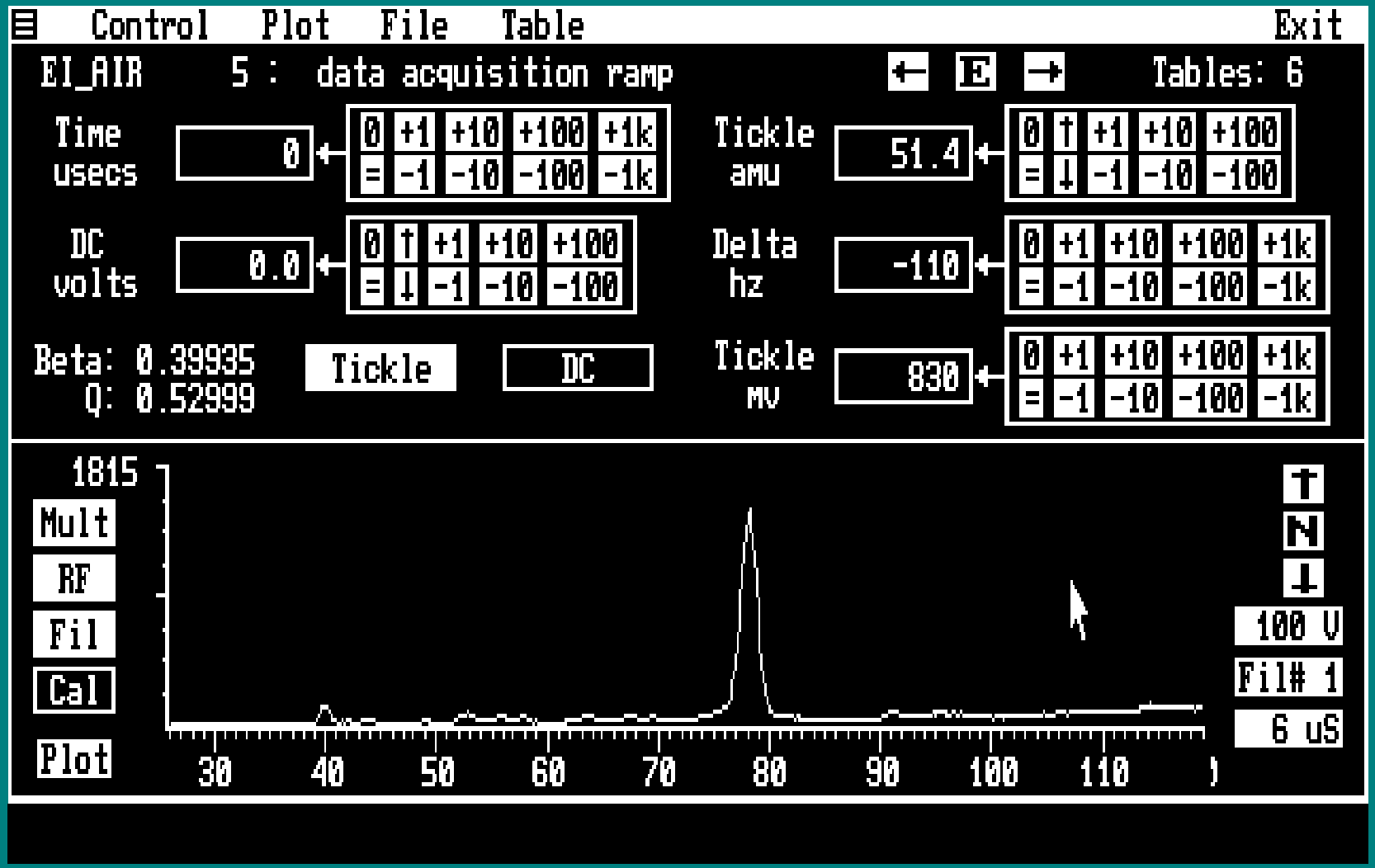
Air/Water Background Spectrum



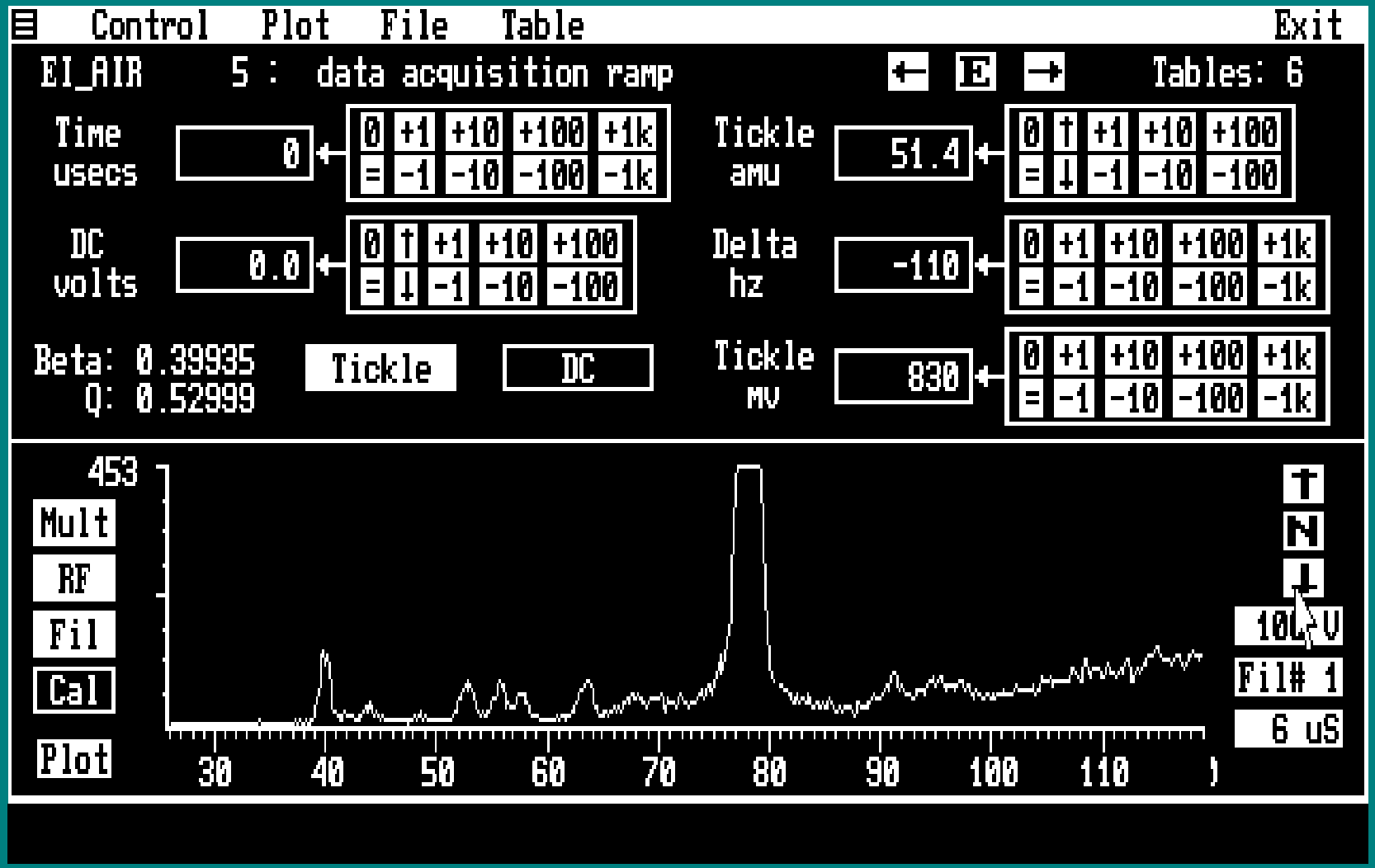
Background Spectrum



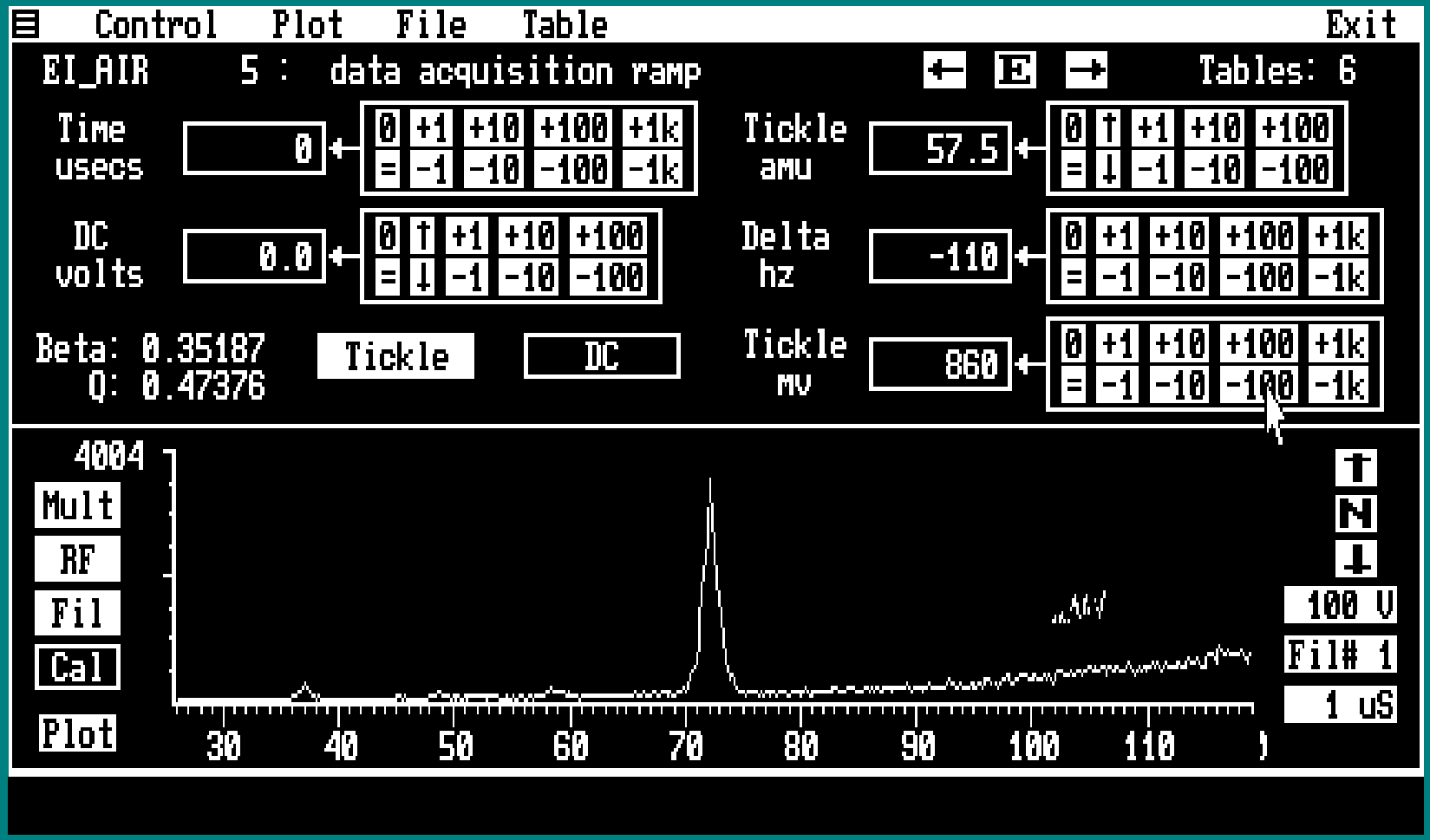
Benzene Spectrum



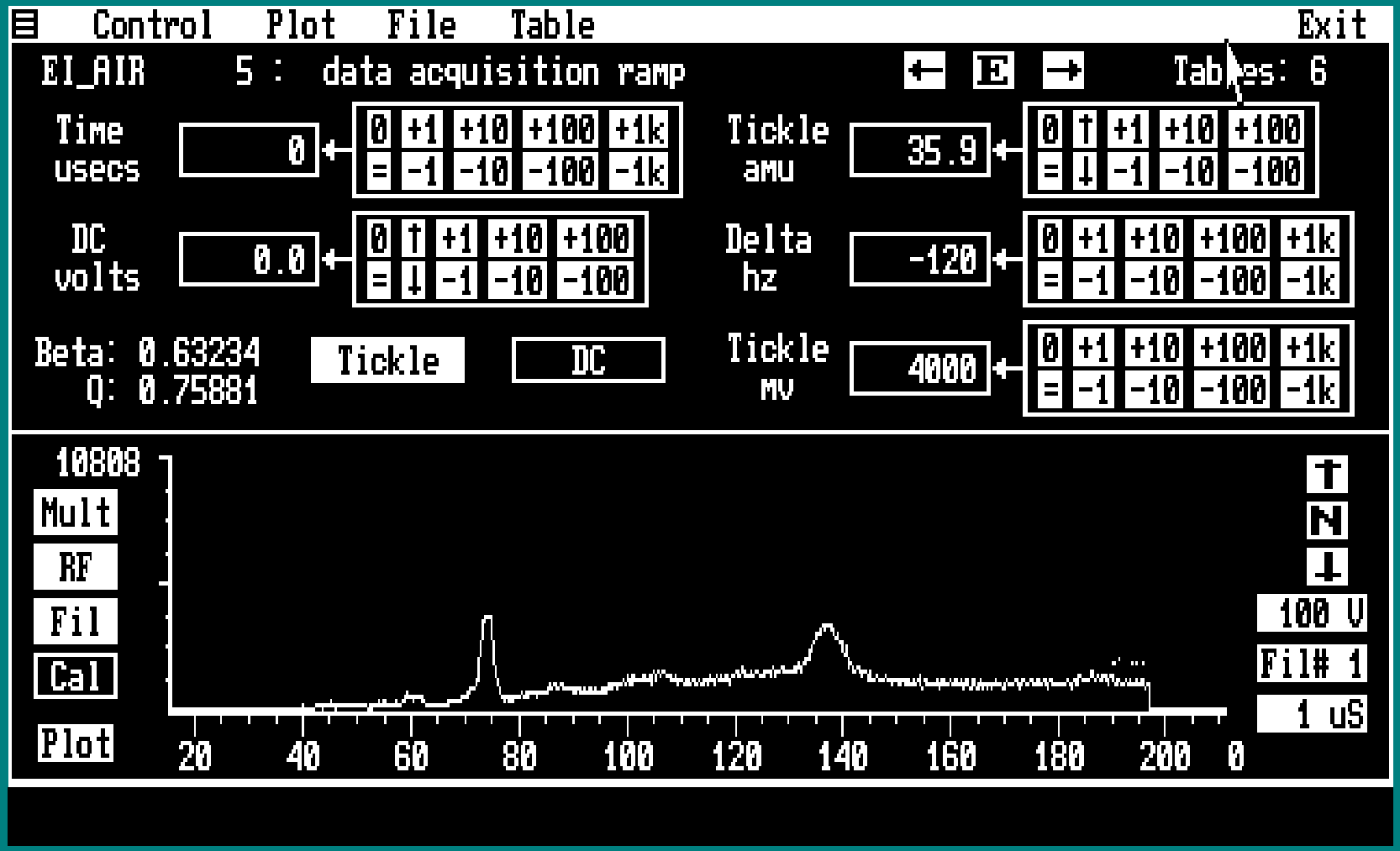
Benzene/Background Spectrum



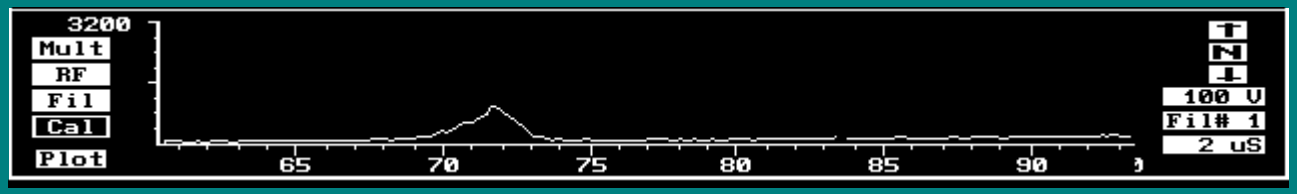
Improved Mass Resolution at $\beta_{eject} = 0.388$



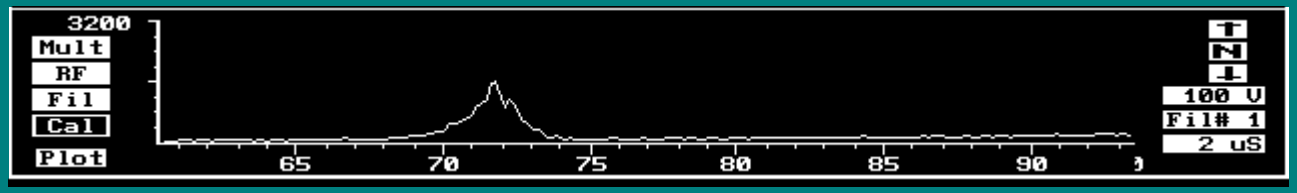
Naphthalene



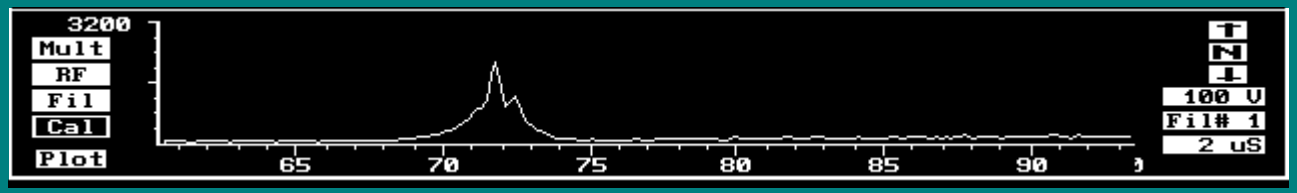
Effects of Ion Cooling Time



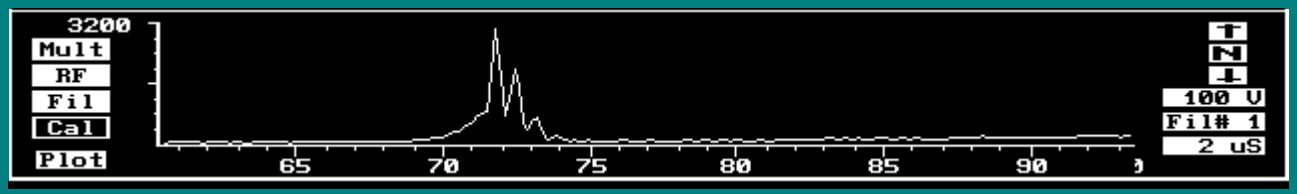
t=10 ms



t=50 ms

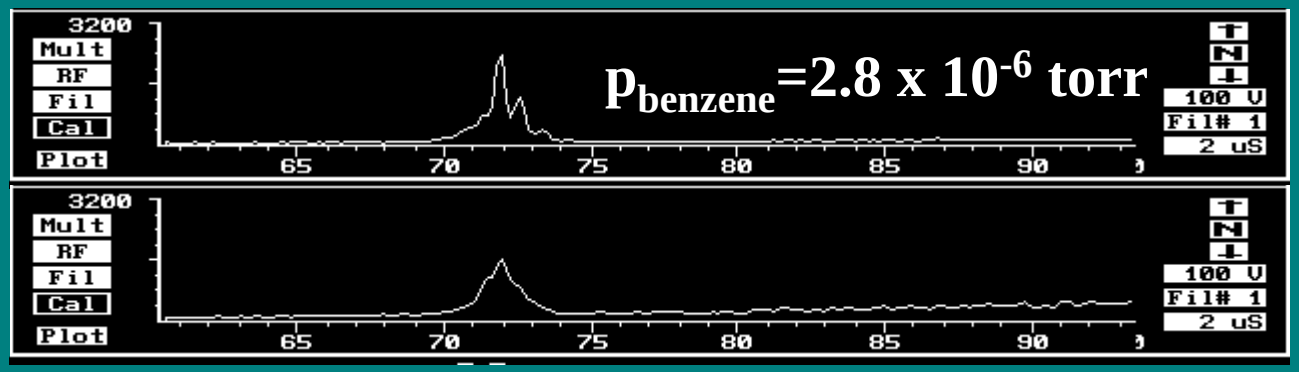


t=100 ms



t=250 ms

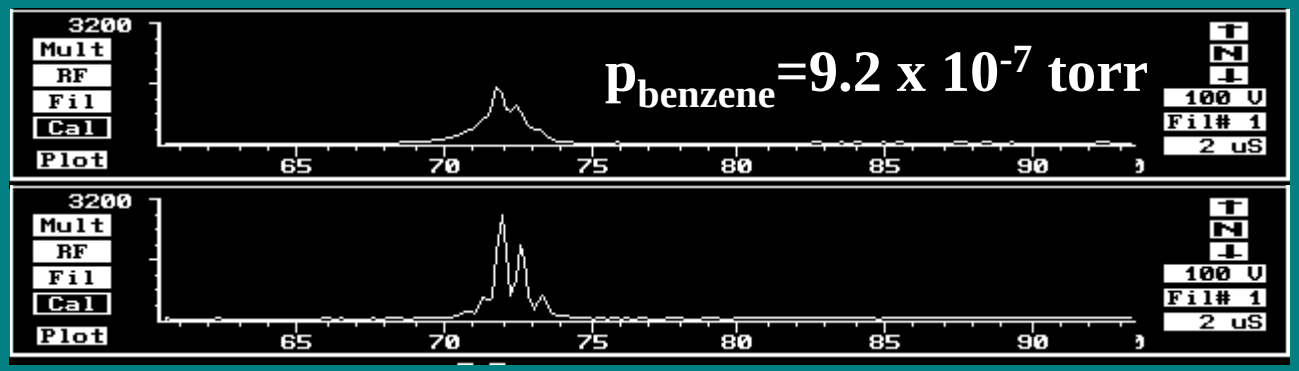
Effects of Pressure and Helium



$p_{benzene}$=2.8 x 10^{-6} torr

No helium

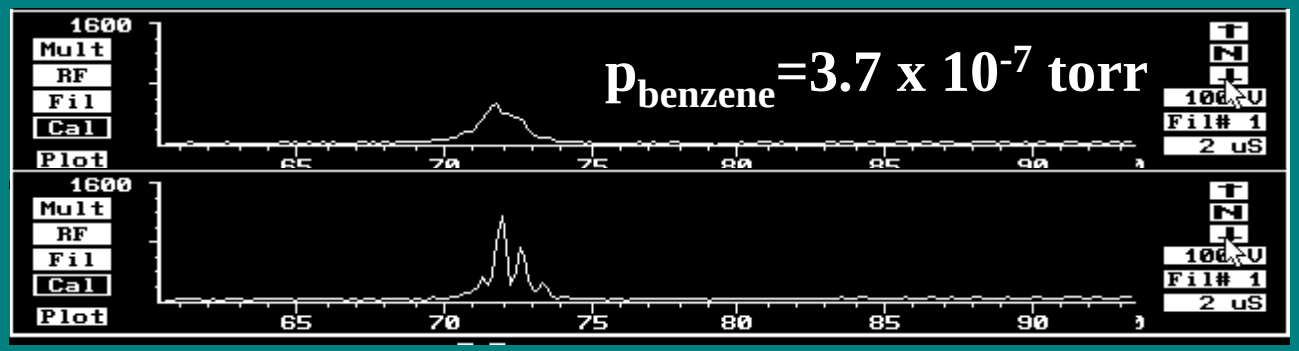
p_{helium}=2 x 10^{-5} torr



$p_{benzene}$=9.2 x 10^{-7} torr

No helium

p_{helium}=3 x 10^{-6} torr



$p_{benzene}$=3.7 x 10^{-7} torr

No helium

p_{helium}=3 x 10^{-6} torr

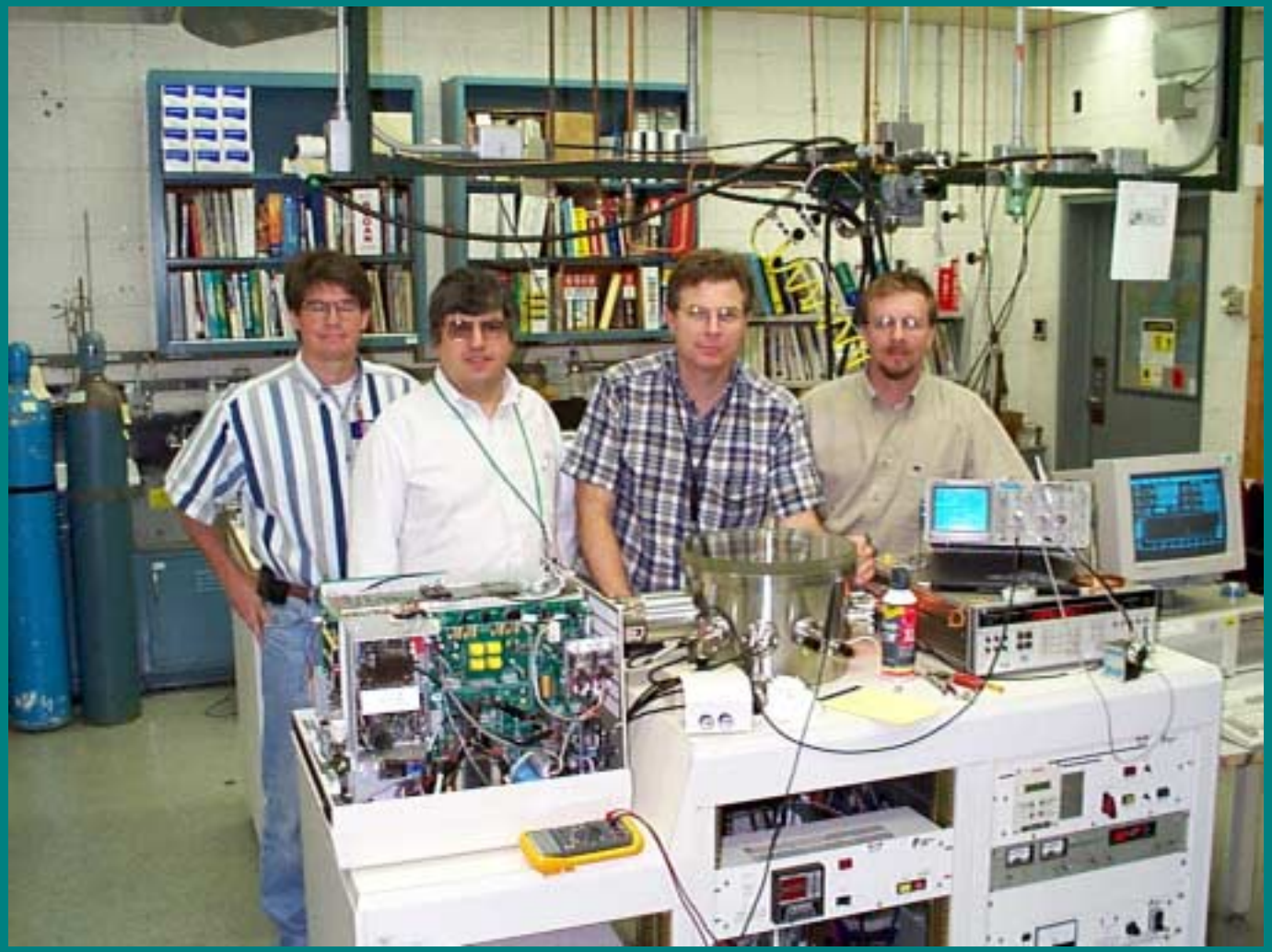
Current Status

- **Resolution: peak widths ca. 1-2 da. FWHM**
  - **<u>very</u> dependent on β_{eject}**
  - **split peaks at discrete values of β_{eject}**
- **Pressure > 3-5 x 10^{-6} torr causes large background current on MCP**
  - **currently operating with high dark current (detector surface area too large?)**
- **RF circuitry not yet optimized for masses > 350 da.**
- **Helium effects not yet understood**
  - **currently requires long ion cooling times**

New Areas of Research

- High intensity ion sources (ESI, ASGDI, IMS) coupled to new cell geometry
  - take advantage of potential increase in ion storage capacity
- New mode of higher internal energy deposition
  - activation <u>along</u> toroid path
- Tangential ion injection
  - counteract inertial tendency to “ride” out of cell
- High duty cycle version (stacked toroidal cells)
- Non-destructive ion detection
- Smaller r_0, low power sensor versions

Acknowledgements



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