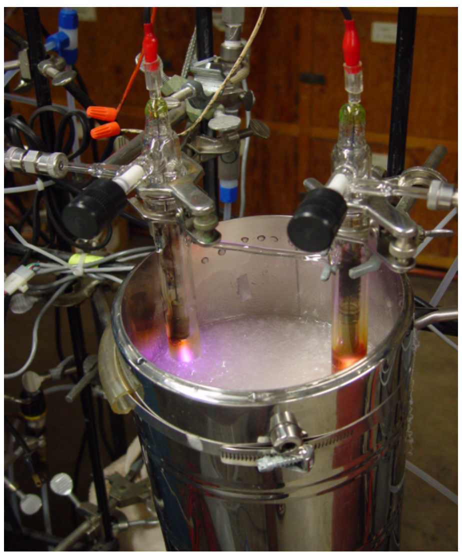
Chemical Analysis in the Titan Environment using High Performance Mass Spectrometry

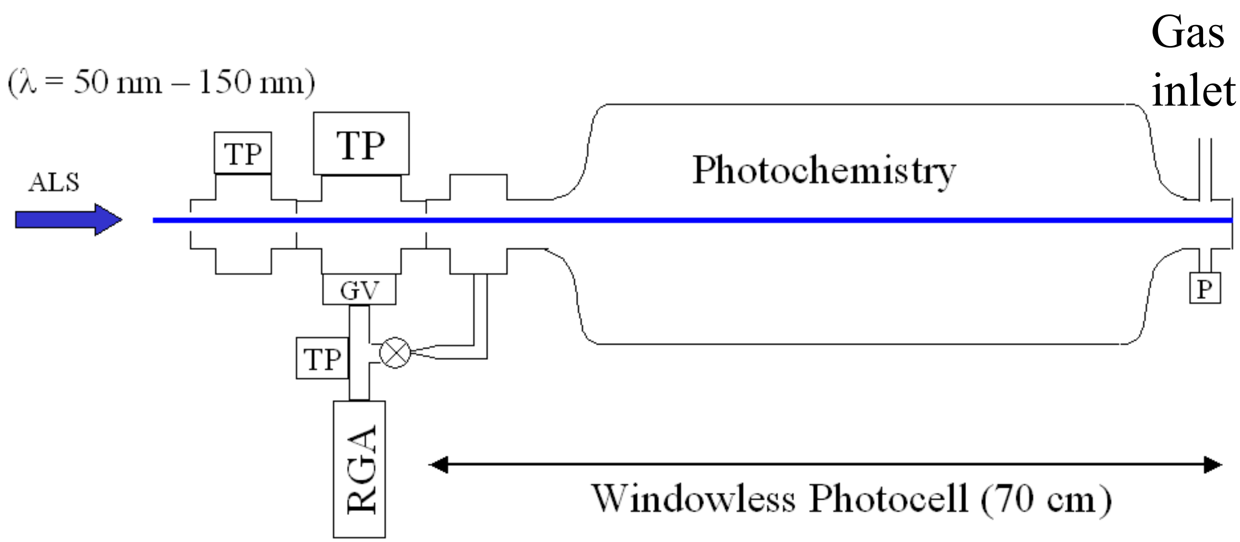
- Magnetic Sector Mass Spectrometer
- Quadrupole mass spectrometer
- Quadrupole Ion Traps
- Orthogonal Sampling Time of Flight Mass Spectrometer
- Fourier Transform MS: Orbitrap Mass Spectrometer

Laboratory Studies of The Organic Chemistry of Titan: The Titan Tholin Project

- Simulated Titan Chemistry (discharge and VUV)
- Spectroscopic characterization
- Separation and analysis
- Structural chemistry
- Reactivity (introduction of oxygen)

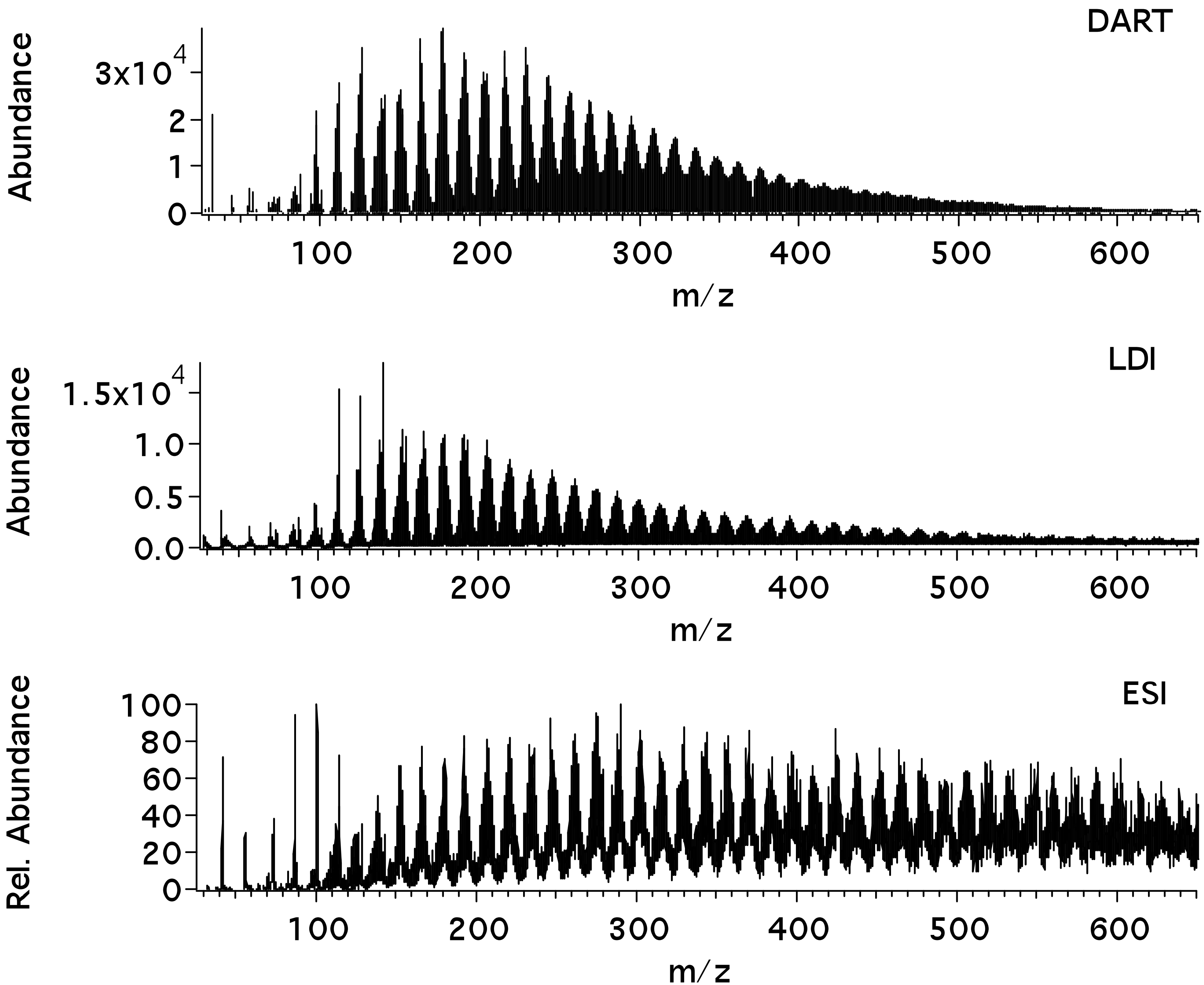


Discharge Source

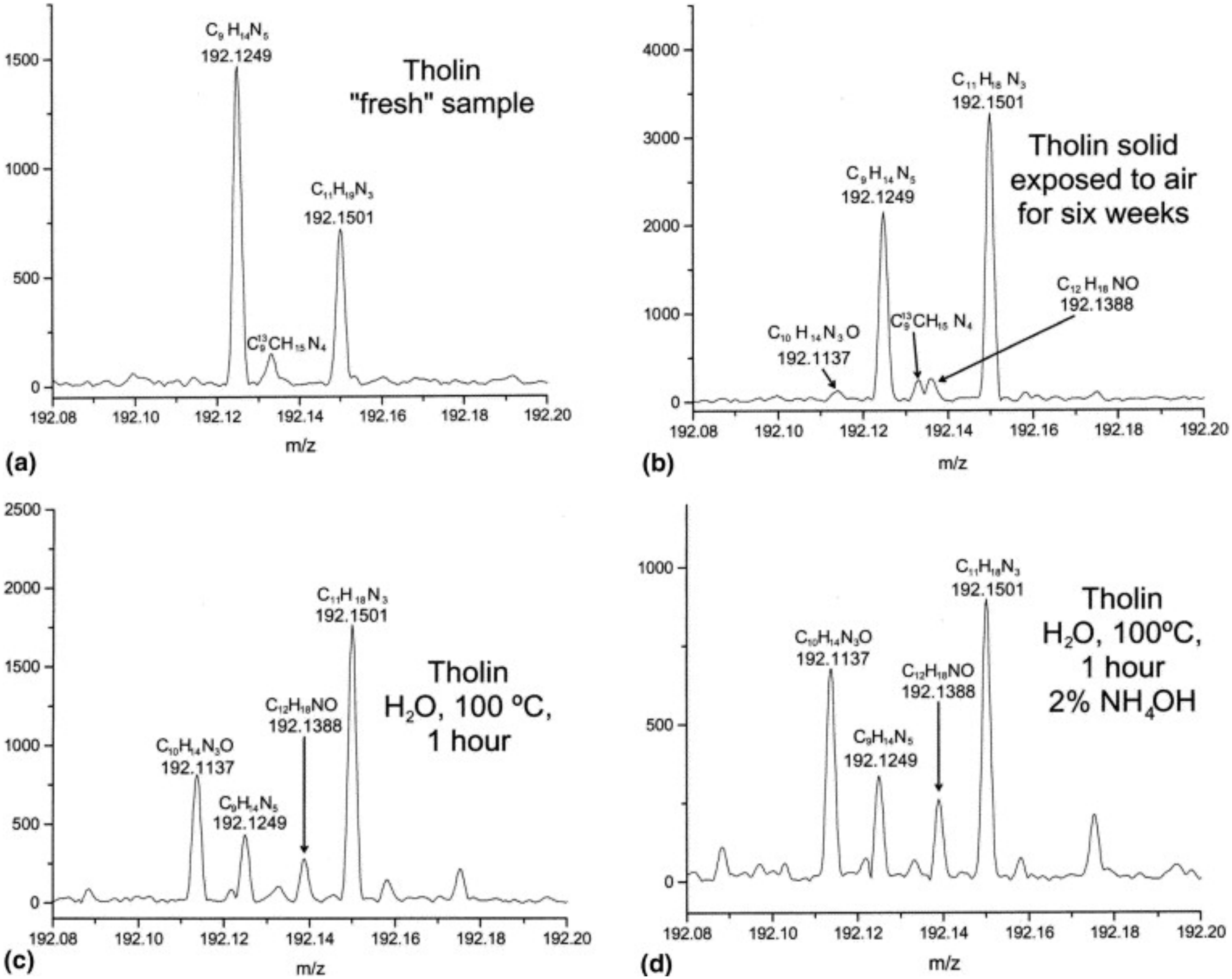


UV Photolysis (ALS)

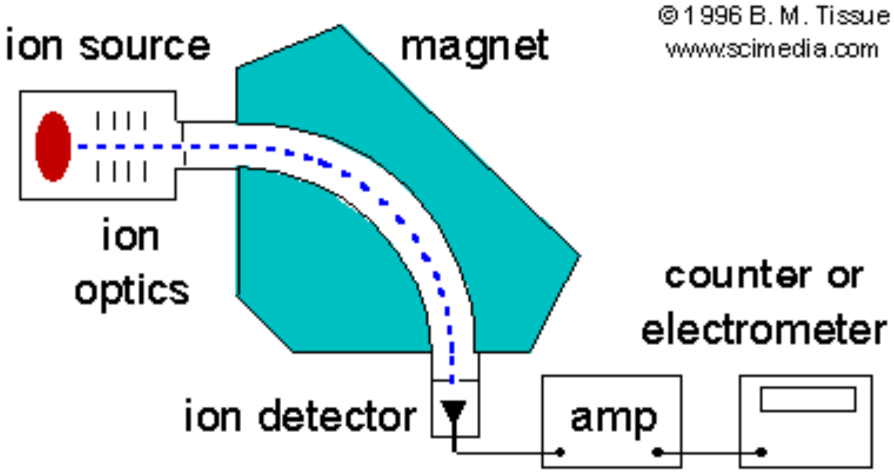
Tholin (Discharge) Analysis– Different Ionization Methods

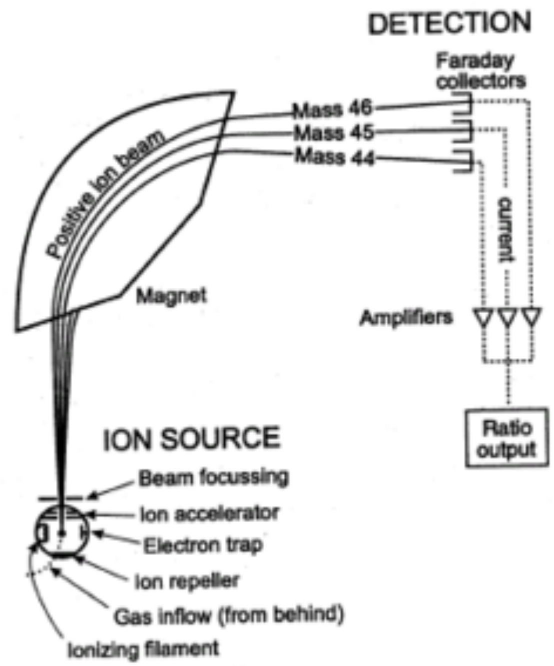


Tholin Analysis: ESI/FT-ICR Showing Oxygen Incorporation



Magnetic Sector Mass Spectrometer





Magnetic Sector Mass Spectrometer

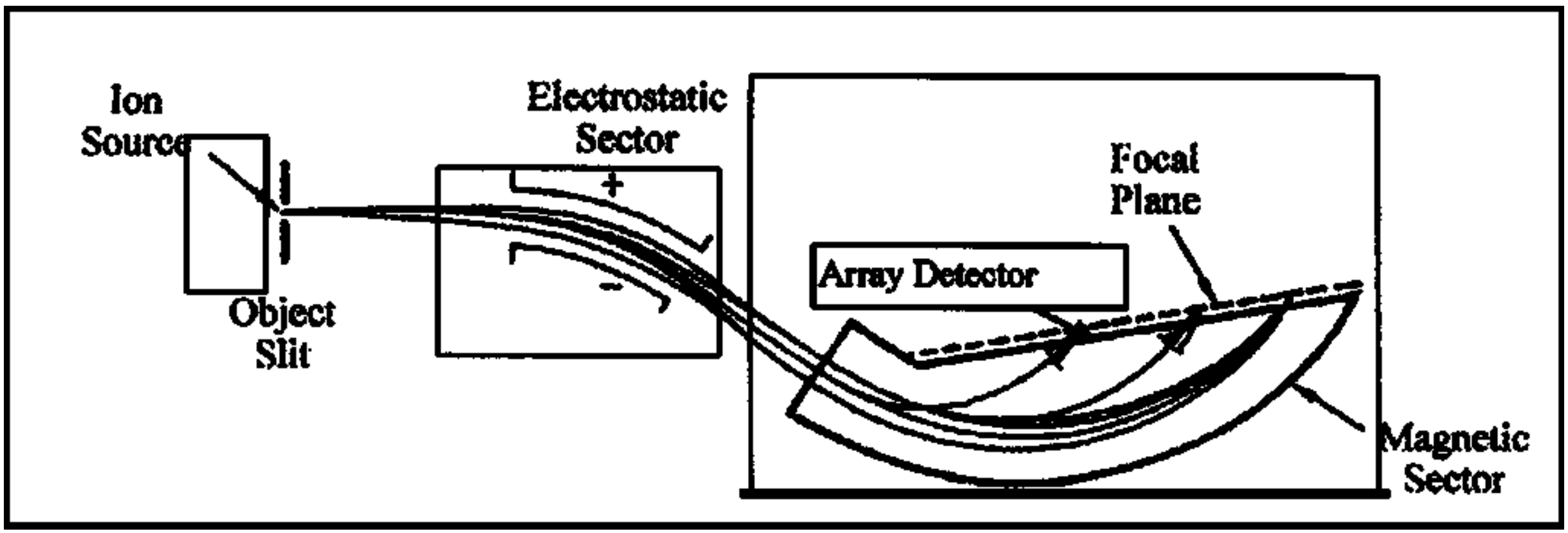
Nier’s ‘mass spectrometer in a briefcase’, constructed in the mid-1960s, was used to convince NASA officials that it was possible to include such instrumentation on spacecraft.

Magnetic Sector Mass Spectrometer

Miniature focal plane mass spectrometer with 1000-pixel modified-CCD detector array for direct ion measurement

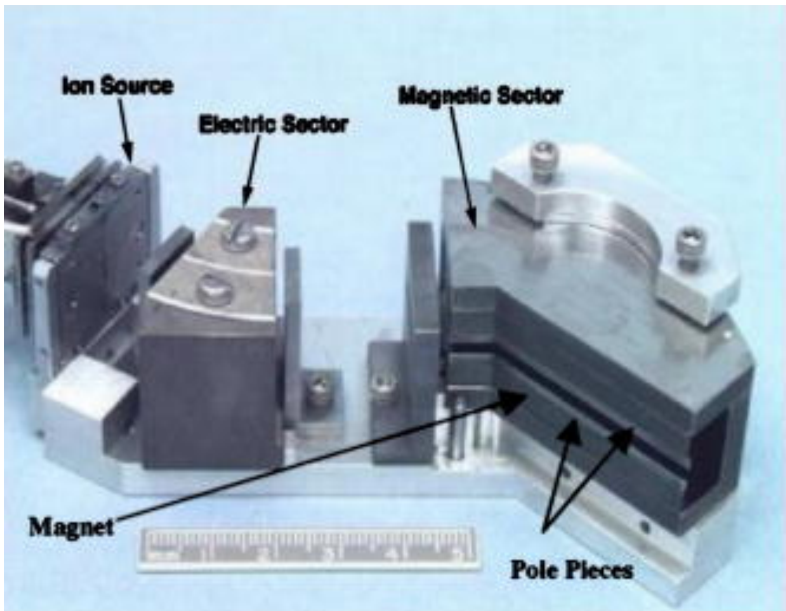
Mahadeva P. Sinha and Mark Wadsworth

Rev. Sci. Instrum. **76**, (2005); doi:10.1063/1.1840291



Schematic of the focal plane mass spectrometer of Mattauch–Herzog geometry

Magnetic Sector Mass Spectrometer

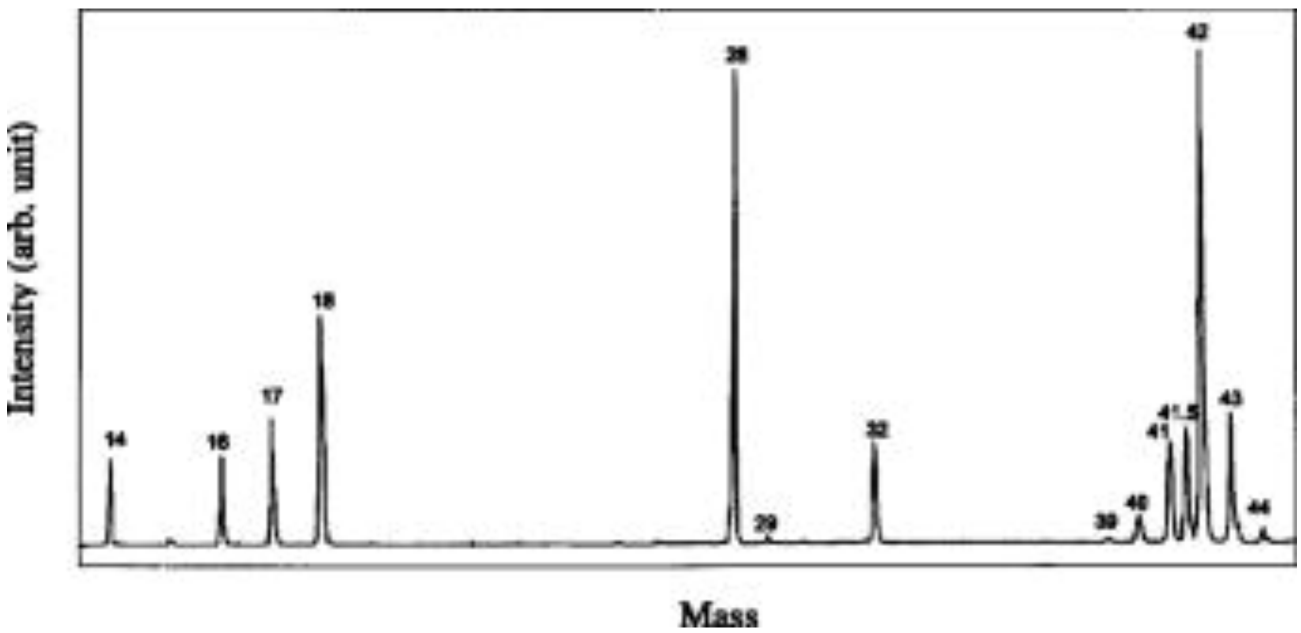


Photograph of the miniature mass spectrometer

Table I. MMS features and performance

MMS Mass	395 g (as shown in the photograph)
Dimensions	10 cm × 5 cm × 5 cm
Ion source	Thermionic
Mass range	2–250
Resolution	330 (50% valley definition)
Sensitivity	2 μA/Torr

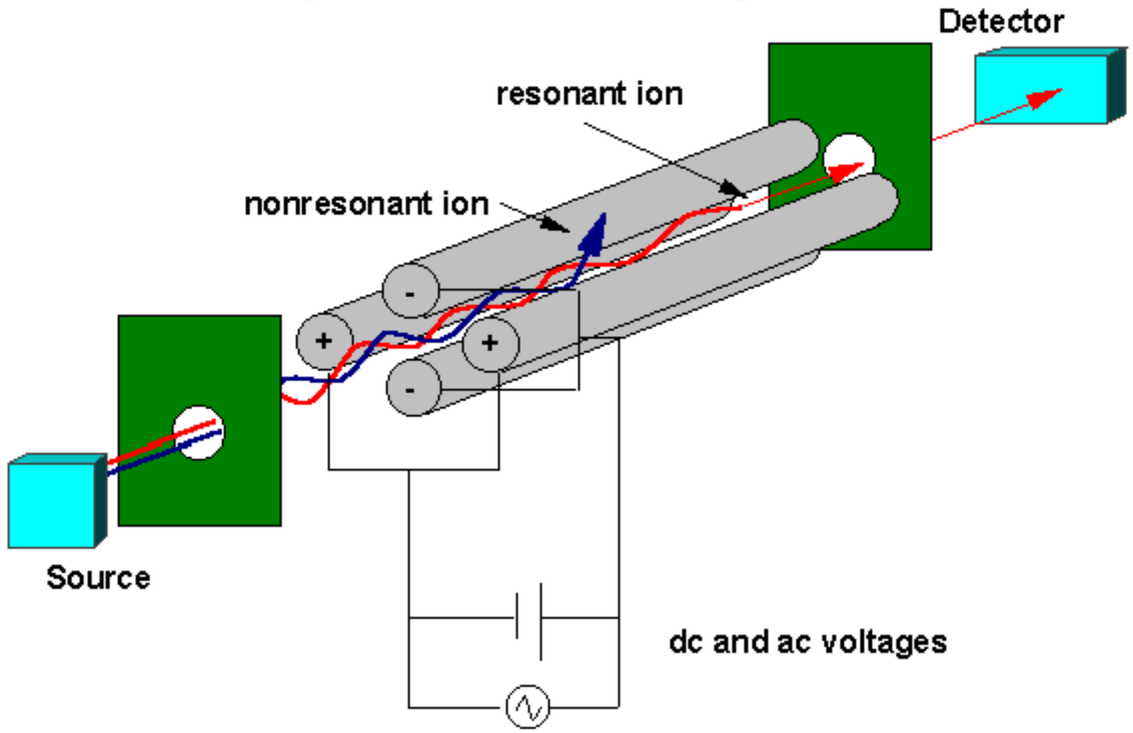
Magnetic Sector Mass Spectrometer



The spectrum measured by the translation of a single detector element along the focal plane. The peaks correspond to the residual gases in the vacuum chamber and the doubly charged ions arising from krypton gas introduced into the chamber.

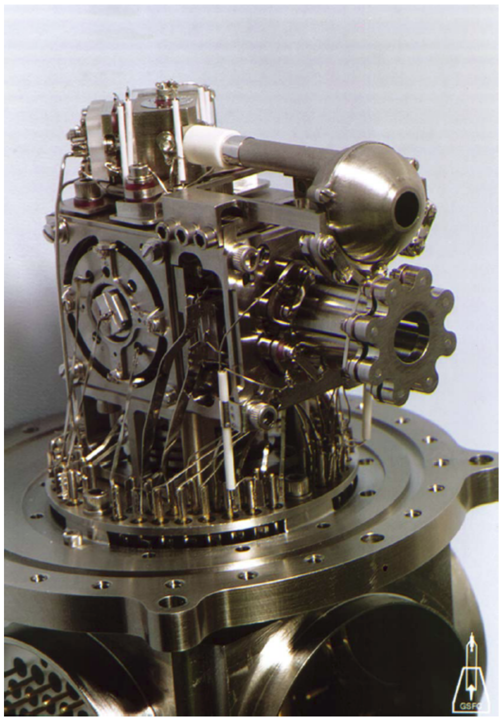
Rev. Sci. Instrum. 76, 025103 (2005)

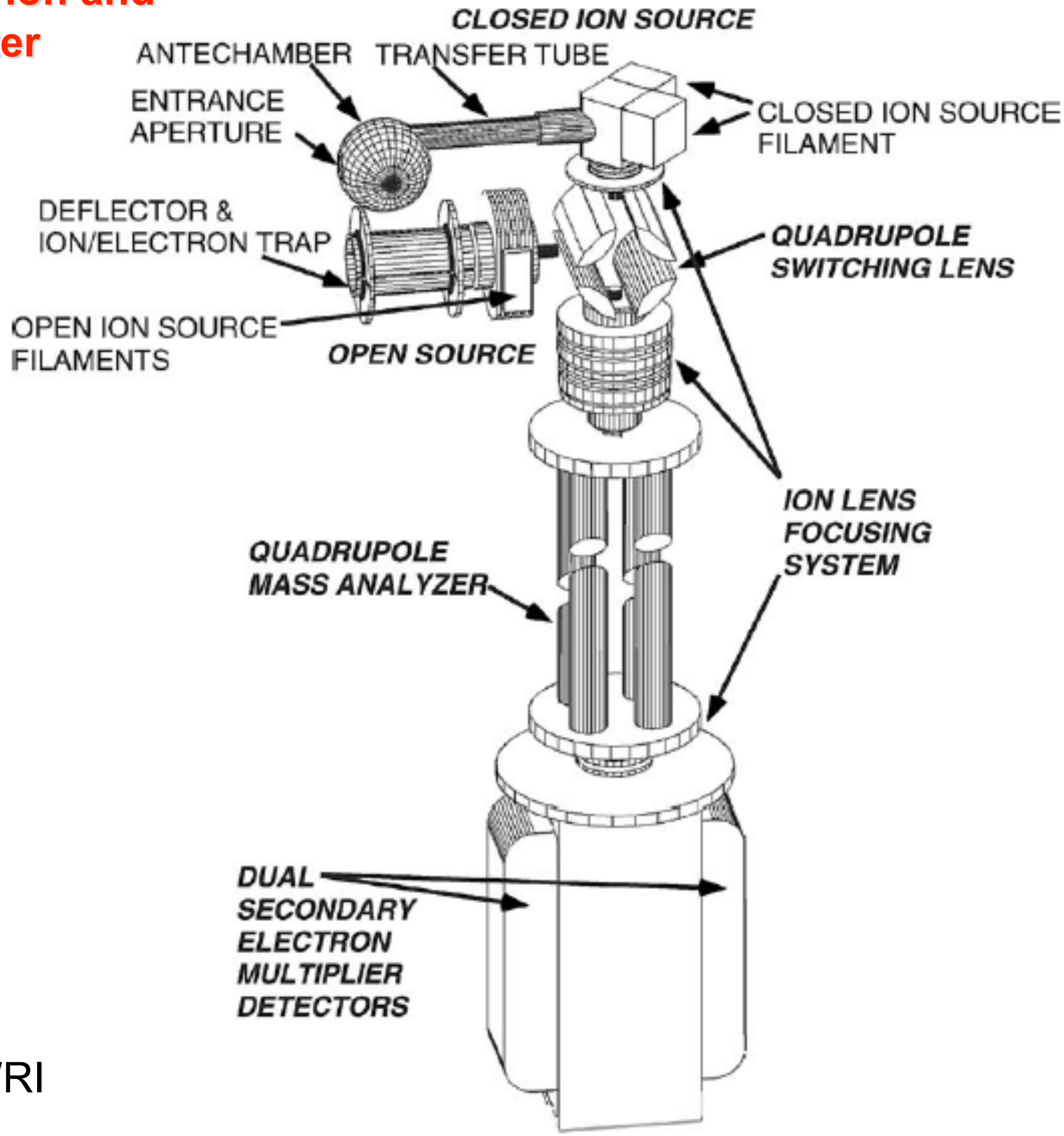
Quadrupole Mass Spectrometer



A quadrupole mass filter consists of four parallel metal rods. Two opposite rods have an applied potential of (U+Vcos(wt)) and the other two rods have a potential of -(U+Vcos (wt)), where U is a dc voltage and Vcos(wt) is an ac voltage. The applied voltages affect the trajectory of ions traveling down the flight path centered between the four rods. For given dc and ac voltages, only ions of a certain mass-to-charge ratio pass through the quadrupole filter and all other ions are thrown out of their original path. A mass spectrum is obtained by monitoring the ions passing through the quadrupole filter as the voltages on the rods are varied

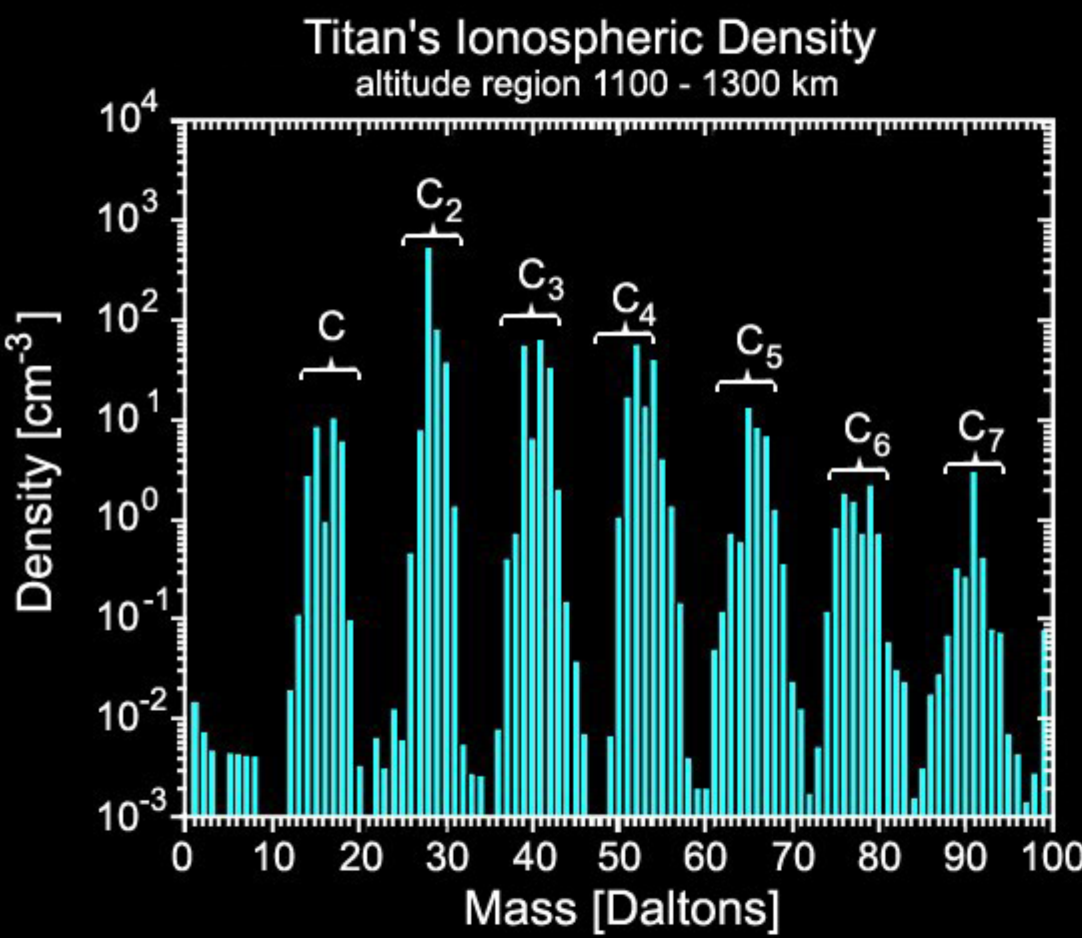
Schematic of the Cassini Ion and Neutral Mass Spectrometer (INMS).





PI: H. Waite, U. of MI/SWRI

Mass Spectrum Recorded in Close Approach (½ radius) of Cassini to Titan (INMS)



CH_3^+

CH_5^+

NH_4^+

$HCNH^+$

CH_3CNH^+

$C_6H_7^+$

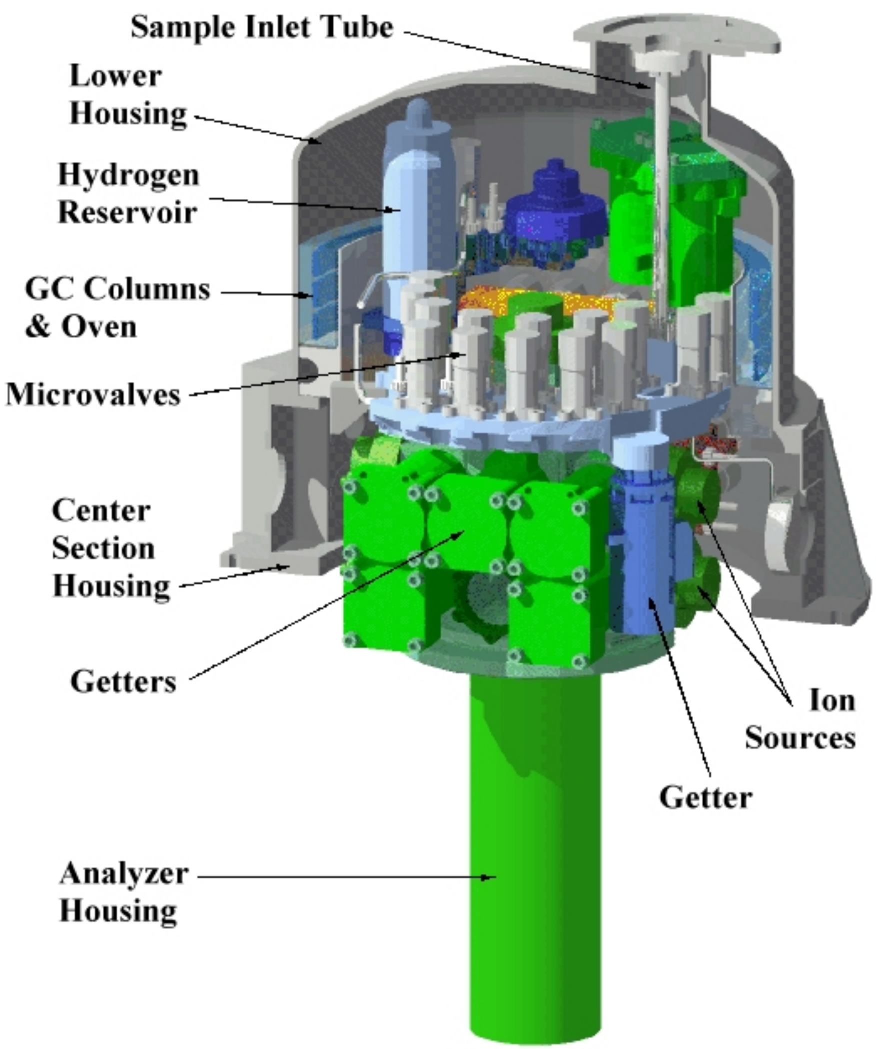
$C_6H_5CH_2^+$

http://www.esa.int

PROBE RELEASE December 24, 2004
PROBE DESCENT January 14, 2005

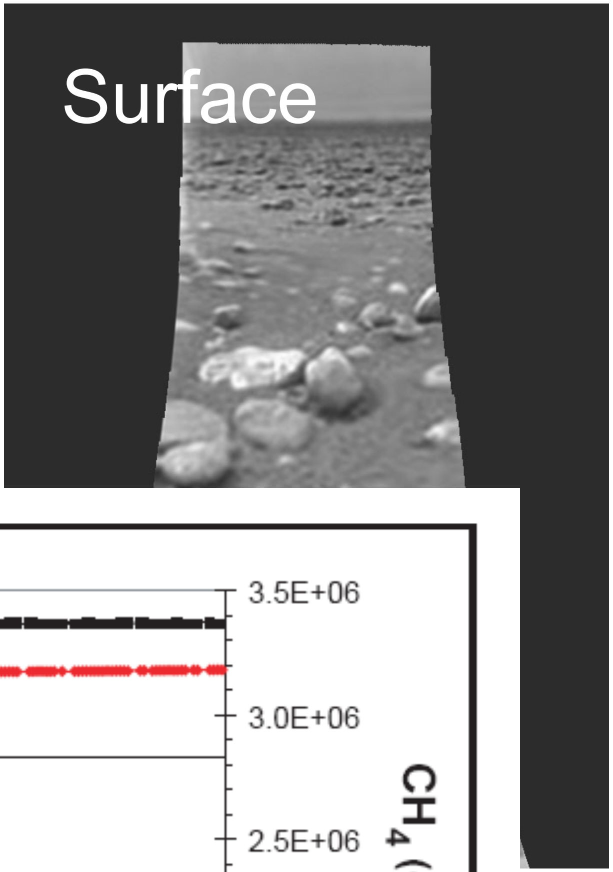
The probe was designed only for the atmospheric descent, with the possibility of another 3-30 minutes of transmission on the surface. The probe returned over 80 minutes of data on the surface.

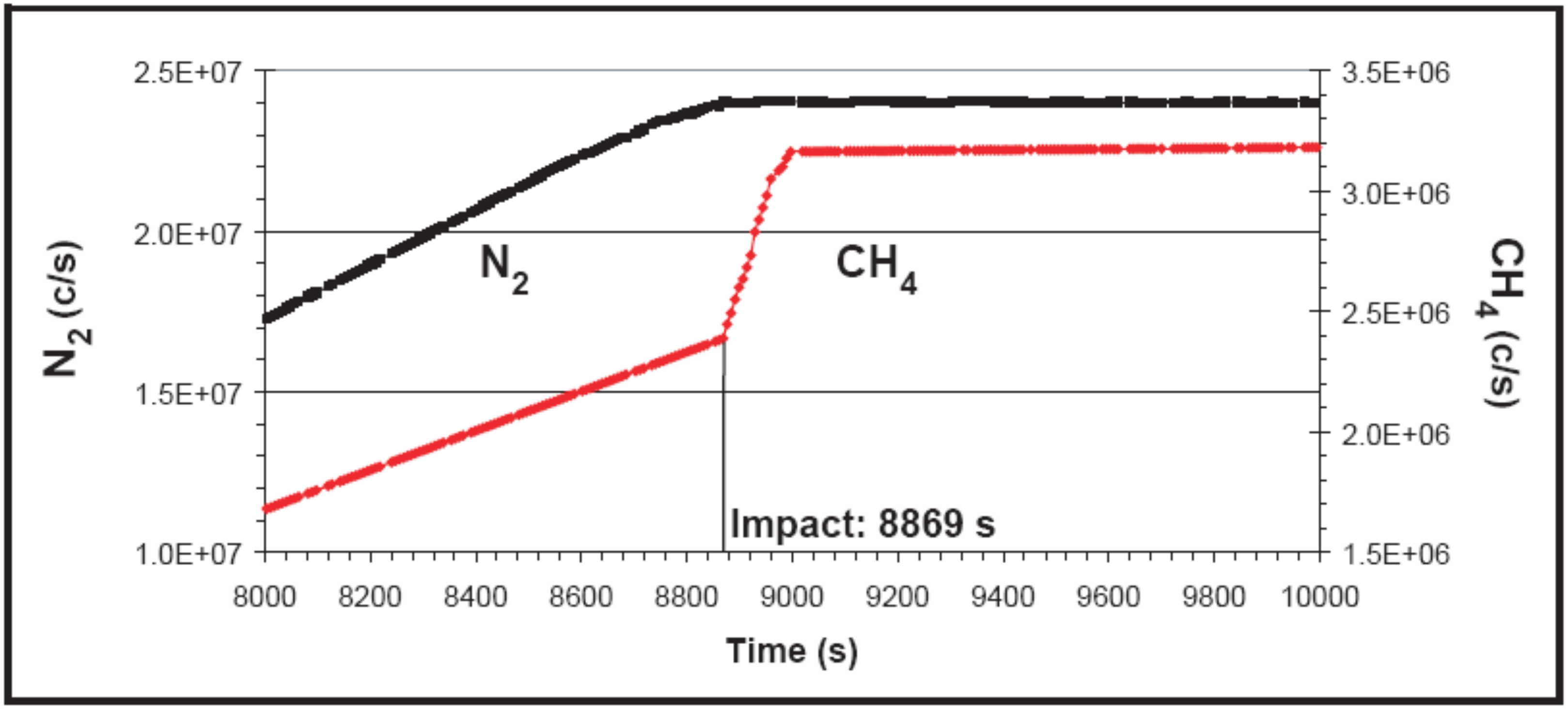
Huygens Probe Investigations



- Aerosol Collector Pyrolyser (ACP)
- Descent Imager and Spectral Radiometer (DISR)
- Doppler Wind Experiment (DWE)
- Gas Chromatograph and Mass Spectrometer (GCMS)
- Huygens Atmospheric Structure Instrument (HASI)
- Surface Science Package (SSP)

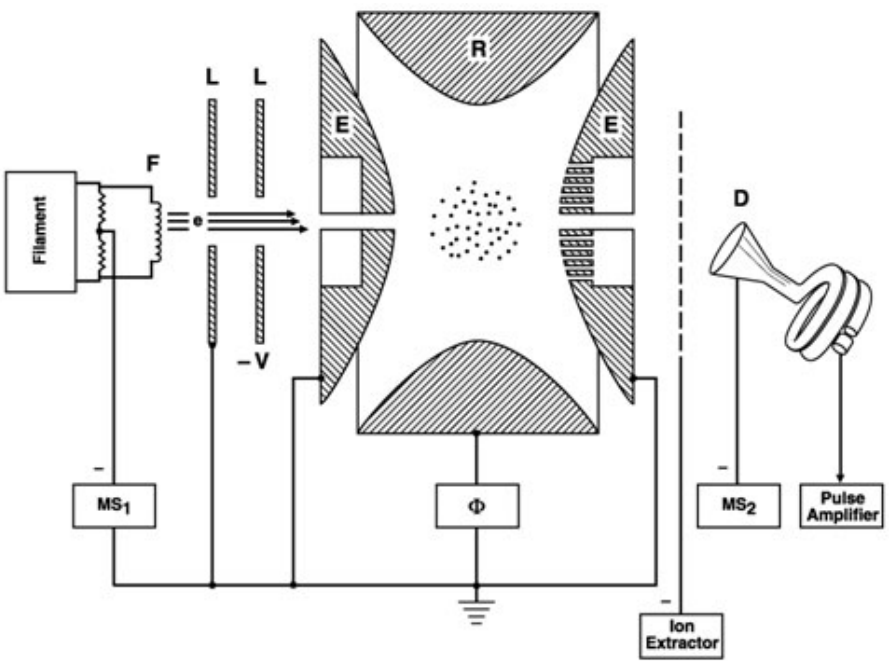

Photo taken
during descent


Surface


2.5E+07
2.0E+07
1.5E+07
1.0E+07
N2 (c/s)
3.5E+06
3.0E+06
2.5E+06
2.0E+06
1.5E+06
CH4 (c/s)
N2
CH4
Impact: 8869 s
8000
8200
8400
8600
8800
9000
9200
9400
9600
9800
10000
Time (s)

Quadrupole Ion Trap Mass Spectrometer

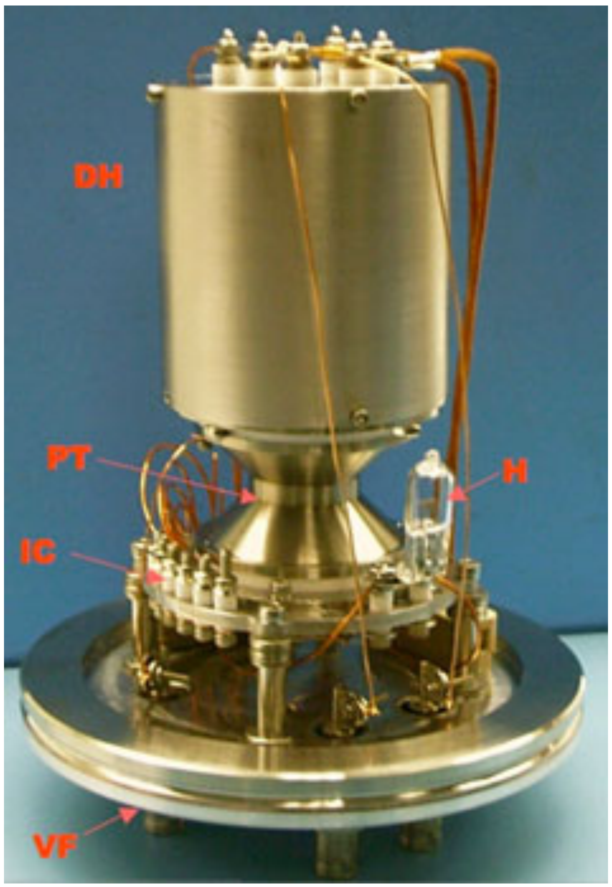
The Vehicle Cabin Atmosphere Monitor (VCAM) is a miniature gas chromatograph-mass spectrometer (GCMS) that is scheduled for a one-year test run in the International Space Station (ISS) beginning in 2010. Later versions are expected to be used to monitor the air in the Orion crew exploration vehicle and in habitats on the Moon and Mars. With each successive environment in which the instrument will be used, it will be designed to detect a wider assortment of chemicals.



Schematic diagram of the Paul ion trap mass spectrometer and electronics. The electron filament for the ionizing electrons (e) is denoted by *F*; the pulser which switches the filament bias voltage is MS1; that for switching the high voltage to the ion detector is MS2; the electron lens elements are *L*; the trap end caps are *E*; the trap ring is *R*; and the detector is *D*. The radiofrequency trapping potential is indicated as M.

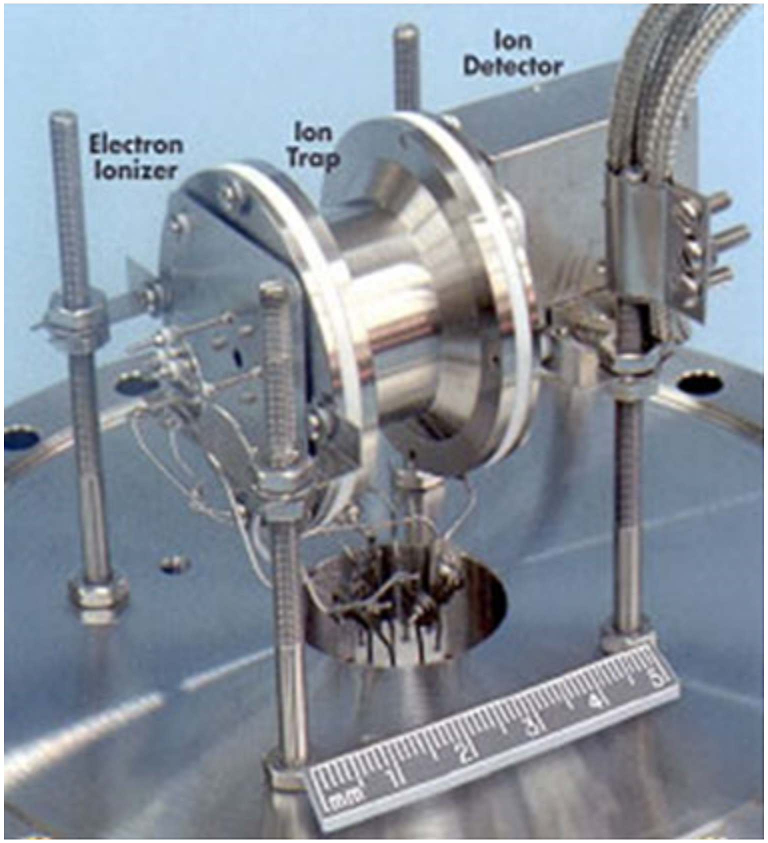
Quadrupole Ion Trap Mass Spectrometer

Above: The development unit for VCAM's preconcentrator/gas-chromatograph assembly. The base is 30.5 cm by 10.2 cm (about 12 inches by 4 inches).



Left: The development unit for VCAM's Paul ion trap. **DH** = detector housing, **H** = heater bulb, **IC** = ionizer connections, **PT** = Paul trap, **VF** = vacuum flange. The vacuum flange is less than 15 cm (about 6 inches) in diameter.

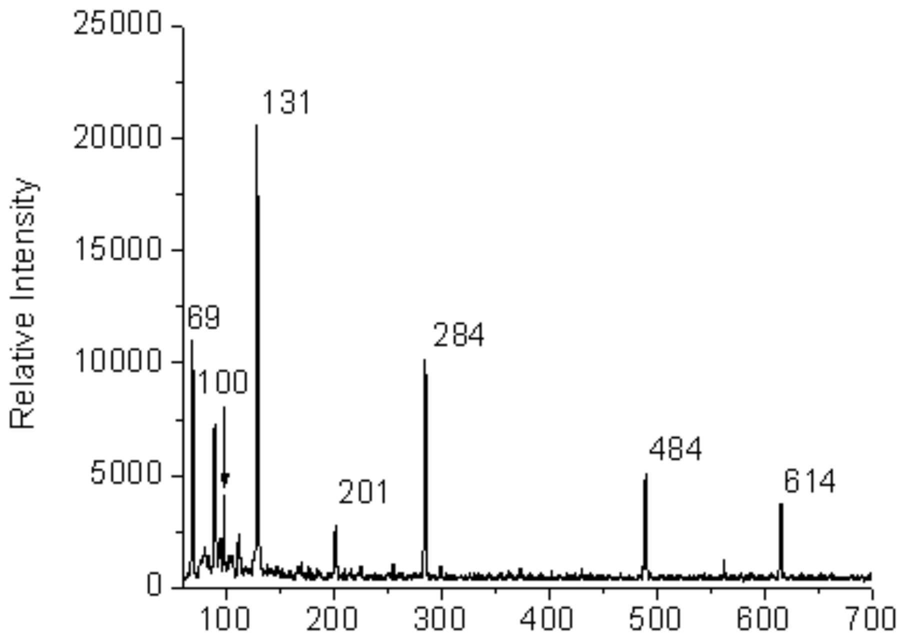
Quadrupole Ion Trap Mass Spectrometer



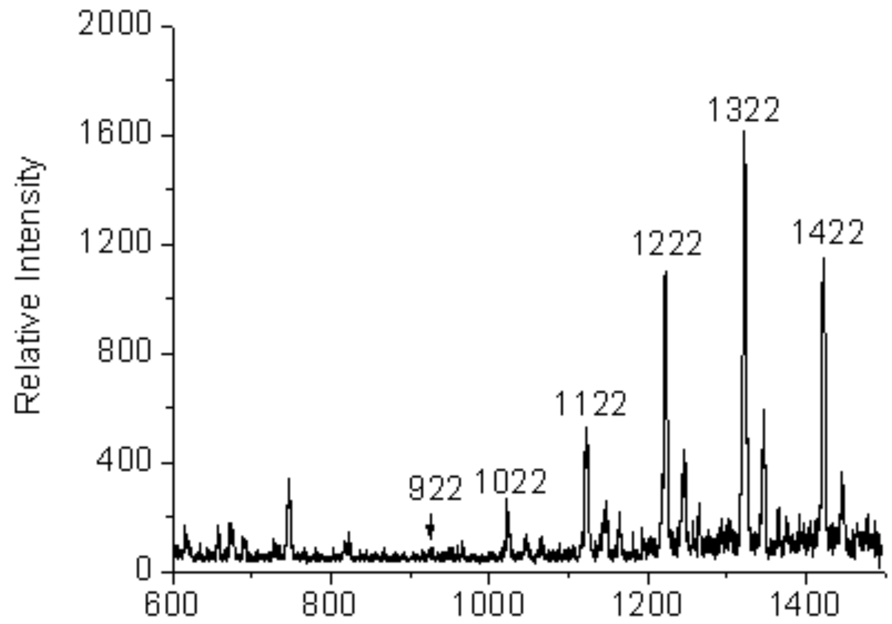
The ion trap mass spectrometer designed and tested at JPL is about the size of a tennis ball. The ions are formed directly inside the trap, so the trap does not suffer as great a loss in sensitivity as the quadrupole when miniaturized. However, as the trap size gets smaller, the number of ions it can hold decreases because the positively charged ions repel each other and resist being confined together in too high a density. This results in decreased sensitivity and dynamic range.

"Results from the Vehicle Cabin Atmosphere Monitor: A Miniature Gas Chromatograph/ Mass Spectrometer for Trace Contamination Monitoring on the ISS and Orion," Ara Chutjian, Murray Darrach, B.J.Bornsttein, A. Croonquist and E. Edgu-Fry, ICES 2008 (2008-01-2045) 2008.

Quadrupole Ion Trap Mass Spectrometer



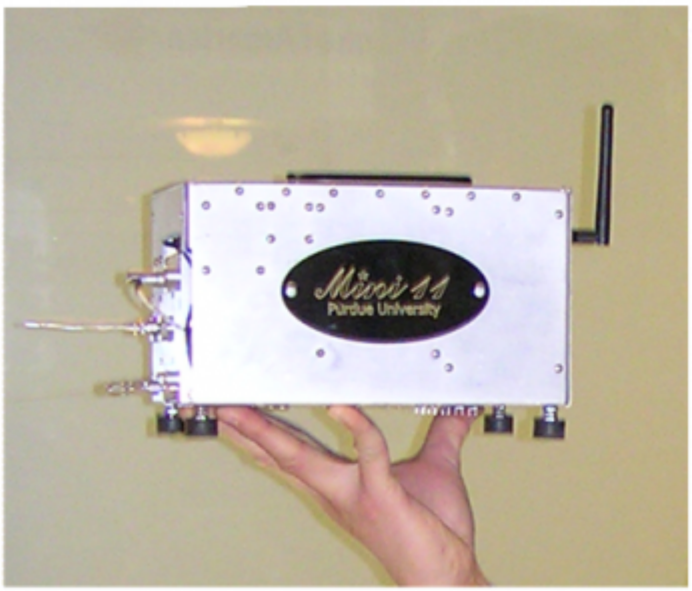
Mass spectrum of PFTBA obtained using GDEI internal ionization with an RF frequency of 1041 kHz

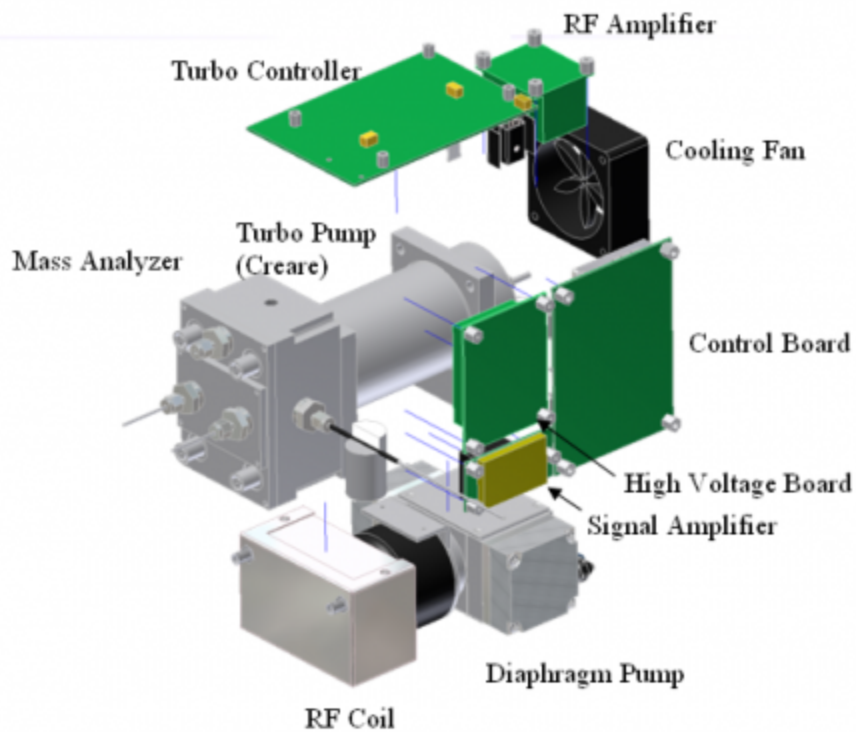


Mass spectrum of 100 ppm Ultramark obtained using a nano-ESI source in the external ionization mode with RF frequency at 695 kHz

Quadrupole Mass Spectrometer

("Mini 11" R. Graham Cooks, Purdue University)





Power: 35 Watts
Weight: 4 kg
Size: 0.2 ft^3

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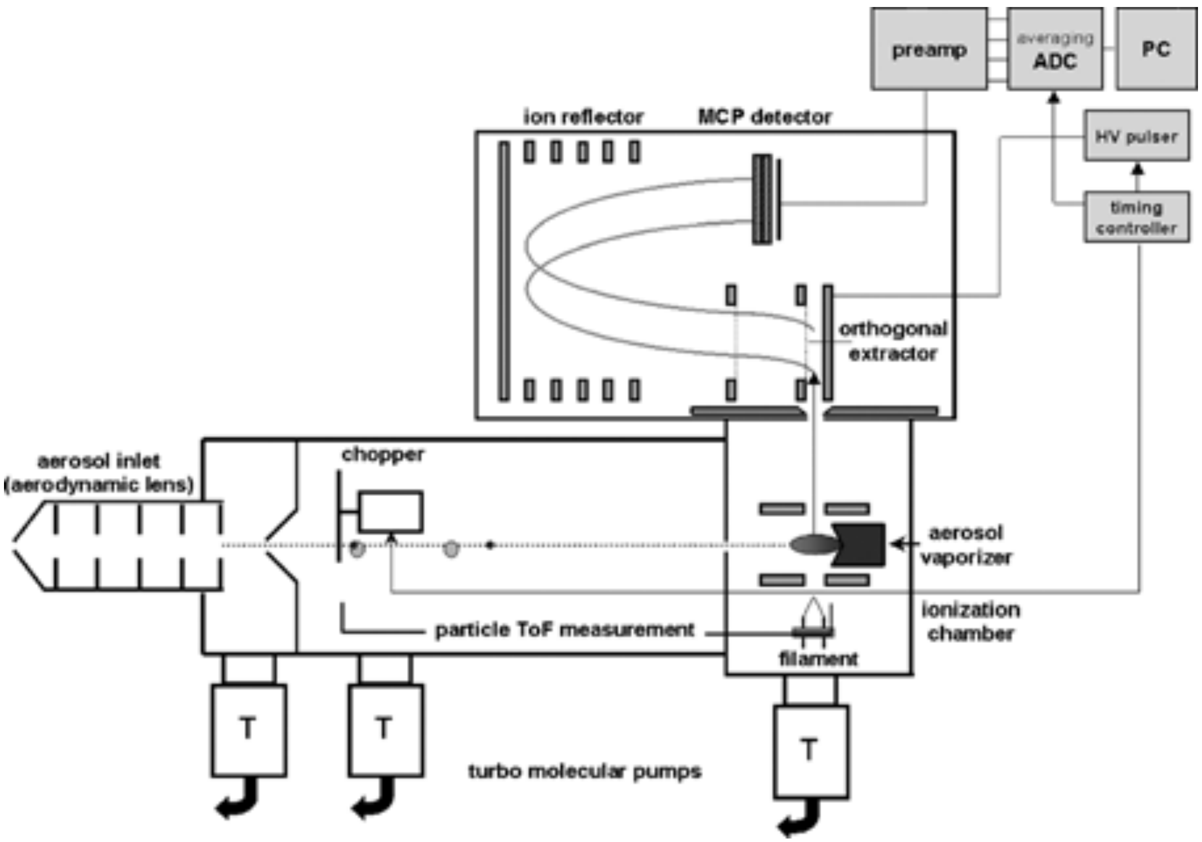
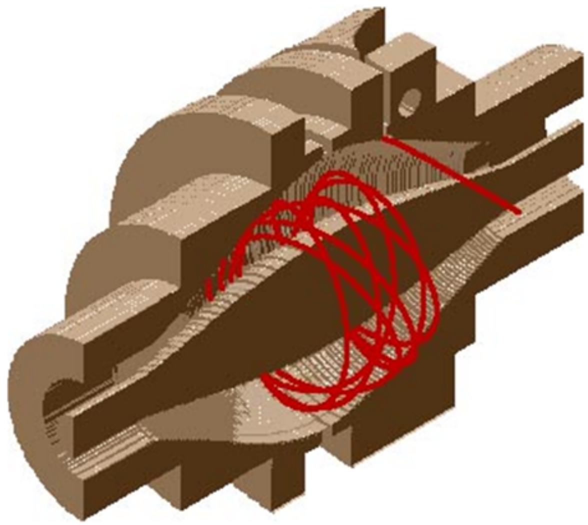
Orthogonal Sampling Time of Flight Mass Spectrometer



A New Time-of-Flight Aerosol Mass Spectrometer (TOF-AMS)—Instrument Description and First Field Deployment, Frank Drewnick; Silke S. Hings; Peter DeCarlo; John T. Jayne; Marc Gonin; Katrin Fuhrer; Silke Weimer; Jose L. Jimenez; Kenneth L. Demerjian; Stephan Borrmann;Douglas R. Worsnop, *Aerosol Science and Technology*, **39**, 2005, 637 – 658.

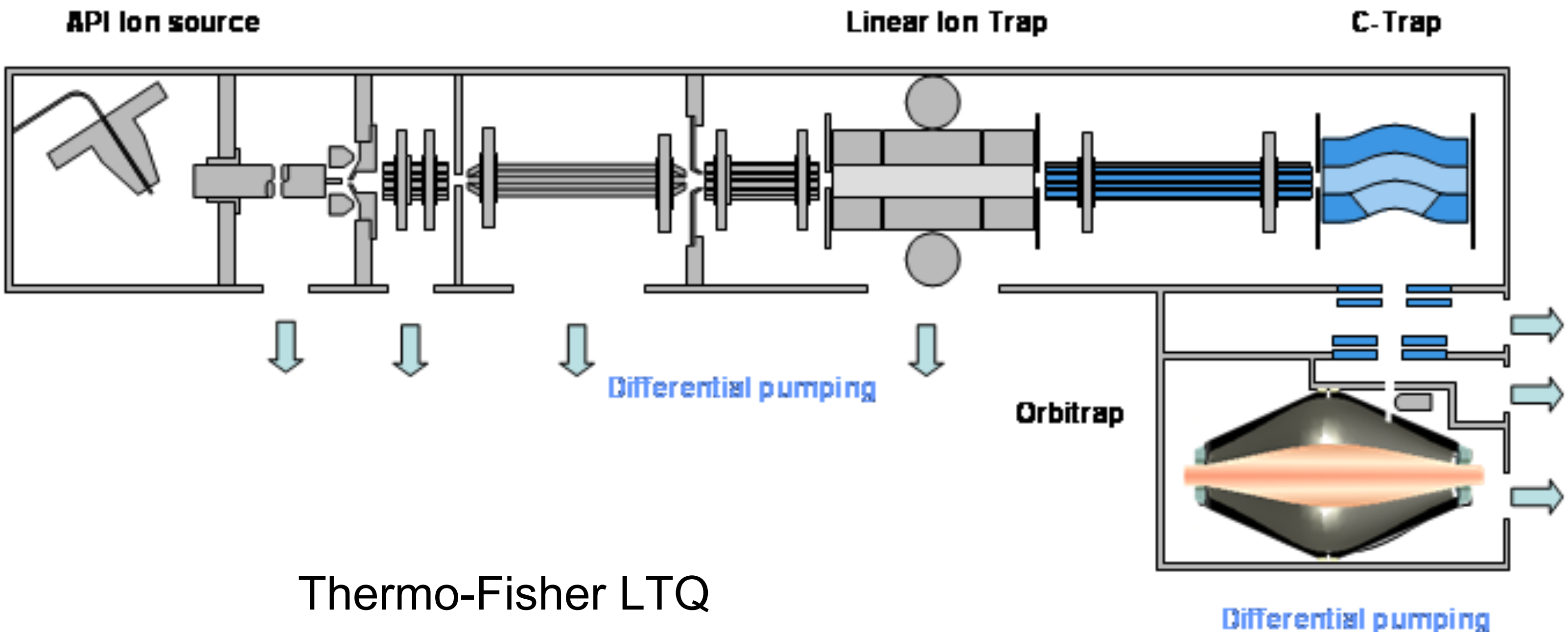
Fourier Transform MS: Orbitrap Mass Spectrometer



Capabilities
High performance instrument competitive with FT-ICR
mass resolution up to 200,000
mass range 50,000
high mass accuracy (1-2 ppm)

Thermo-Fisher LTQ Orbitrap Mass Spectrometer

Fourier Transform MS: Orbitrap Mass Spectrometer



Thermo-Fisher LTQ
Orbitrap Mass
Spectrometer