Mass Spectrometric Investigations of the Atmospheres of Giant Planets

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UNIVERSITÄT BERN

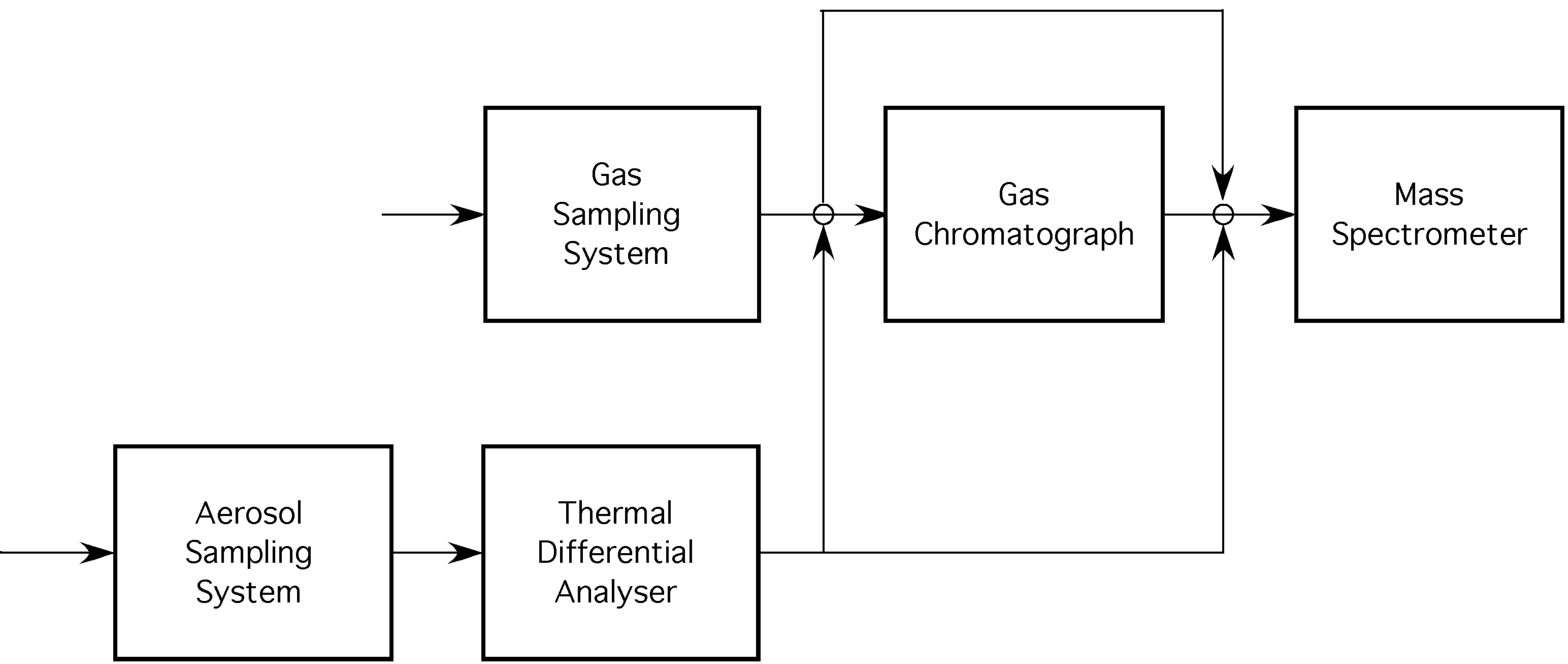
Science Objectives

Scientific Objective[1]	Measurement Objective[1]	Measurement Requirements[1]
Constrain our models and understanding of Saturn's formation and subsequent evolution in situ measurement of elemental constituents and isotopic abundances for comparison with elemental compositions observed in the Sun, meteorites, and other planetary atmospheres	Determine fractional abundance of helium relative to H_2	H_2/He ratio to an accuracy of 1%[2]
	Determine atmospheric abundance ratios of C, H, O, N, and noble gases	C/H, N/H, O/H to a precision of ±10% or better Ne/He, Ar/He, Kr/He, Xe/He to a precision of ±30% or better
	Determine isotopic ratios of C, H, O, N, and noble gases	$^{13}C/^{12}C$, $^{18}O/^{16}O$ to ±1% or better D/H, $^{15}N/^{14}N$ in major molecular species to ±1% to 5% Isotopic ratios of He, Ne, Ar, Kr, Xe to ±5% to ±10% or better[3]
Determine the strength of vertical mixing in Saturn's atmosphere	Determine the vertical abundance profiles of CH_4, NH_3, PH_3, and H_2S	Measure abundances with uncertainty of a factor of 2 or less[4]
Constrain models of cloud formation and structure	Determine abundances of condensable species below cloud base	e.g., H_2O, NH_3, and H_2S to a factor of 2 or better[4]

[1] from *A Strategy for the Exploration of the Outer Planets*, 1986-1996 (NRC, 1986)
[2] RFI requires H/He to 5%
[3] "... except for ^{21}Ne, ^{78}Kr, and $^{124,126}Xe$, where this accuracy may not be attainable" (*A Strategy*, p.23).
[4] from *A Strategy* but not included in the RFI list

Note: The RFI calls for measurement of sulfur to ±10% precision. This requirement does not appear in the COMPLEX report, but can, like the enhanced requirement for neon at 1% of solar, be satisfied by MASPEX. The reason for inclusion of $^{20}Ne/^{22}Ne$ in the "Baseline Enhancements" is not clear. The $^{20}Ne/^{22}Ne$ example is not used in the COMPLEX report (p. 23) to argue for "more precise or additional measurements," but to illustrate why a 10% error is better than a 30% error. An accuracy of 5-10% is already identified in the report (and the RFI) as the requirement for the noble gas isotopes (see above).

Instrument Overview



Galileo Probe Mass Spectrometer Experiment

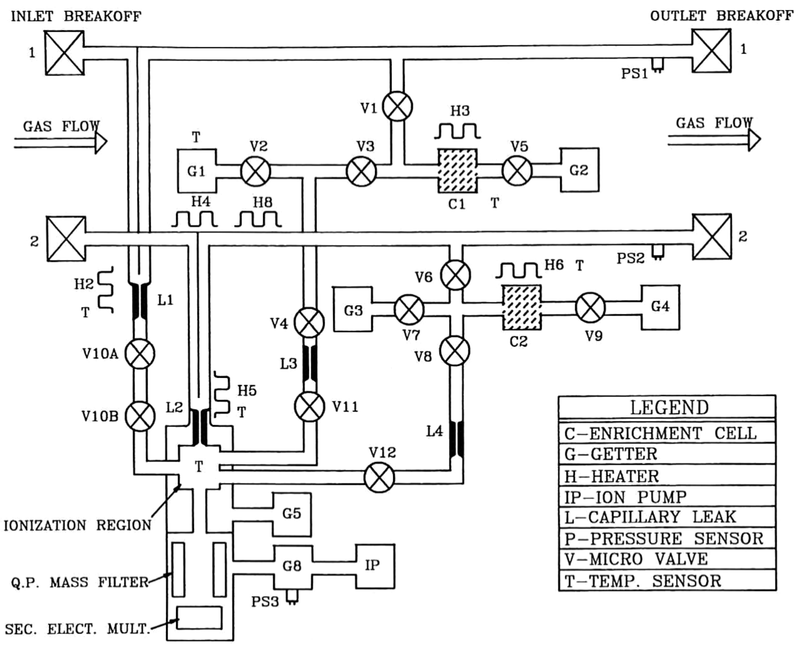


Fig. 1. Schematic of the gas inlet system and connection to the mass spectrometer sensor. Two parallel gas inlet/outlet systems are employed to provide gas samples to the direct leaks, L1 and L2, and to the two sample enrichment systems centered around C1 and C2.

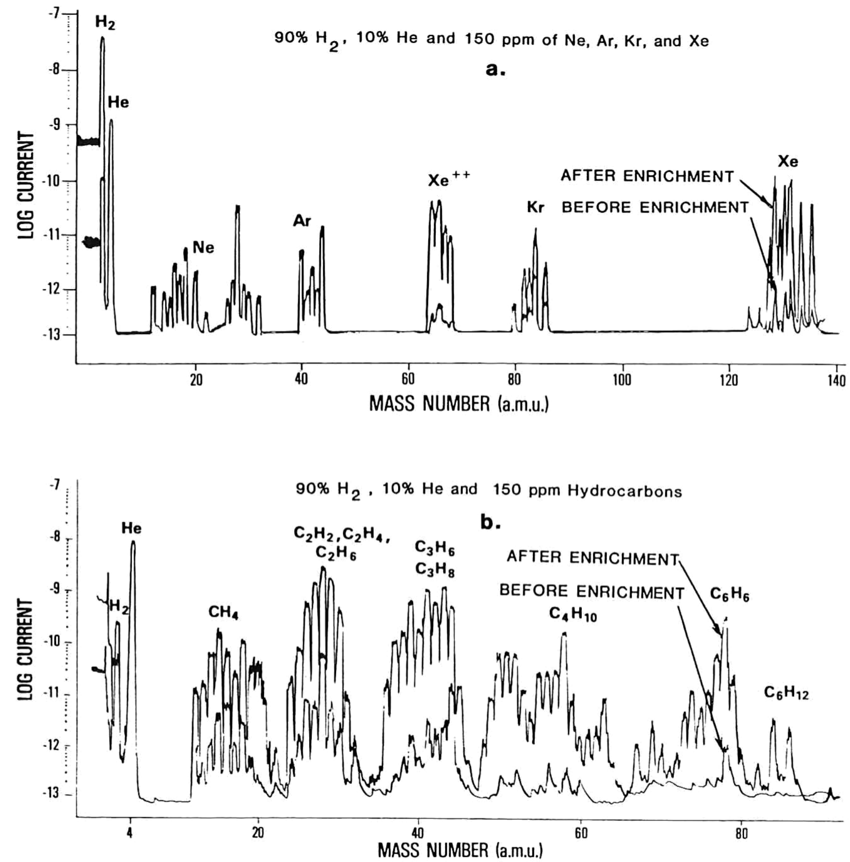


Fig. 2. Mass spectra showing enrichment obtained when gas processing is used to remove the major constituent H_2 from a 90% H_2 and 10% He mixture containing constituents each of 150 ppmv. (a) Rare gas enrichment. Note the substantial enrichment of Xe obtained. Expected Xe ratios are marginably measurable by direct analysis. (b) Hydrocarbon enrichment. There is a substantial enrichment of the C_3–C_4 hydrocarbons with a somewhat less enrichment for methane. For illustration the spectra were recorded analog with laboratory recording equipment.

H.B. Niemann, D.N. Harpold, S.K. Atreya, G.R. Cargnan, D.M. Hunten, T.C. Owen, Galileo Probe Mass spectrometer Experiment, Sp. Sci. Rev. 60 (1992) 111–142.

The Gas Chromatograph Mass Spectrometer for the Huygens Probe

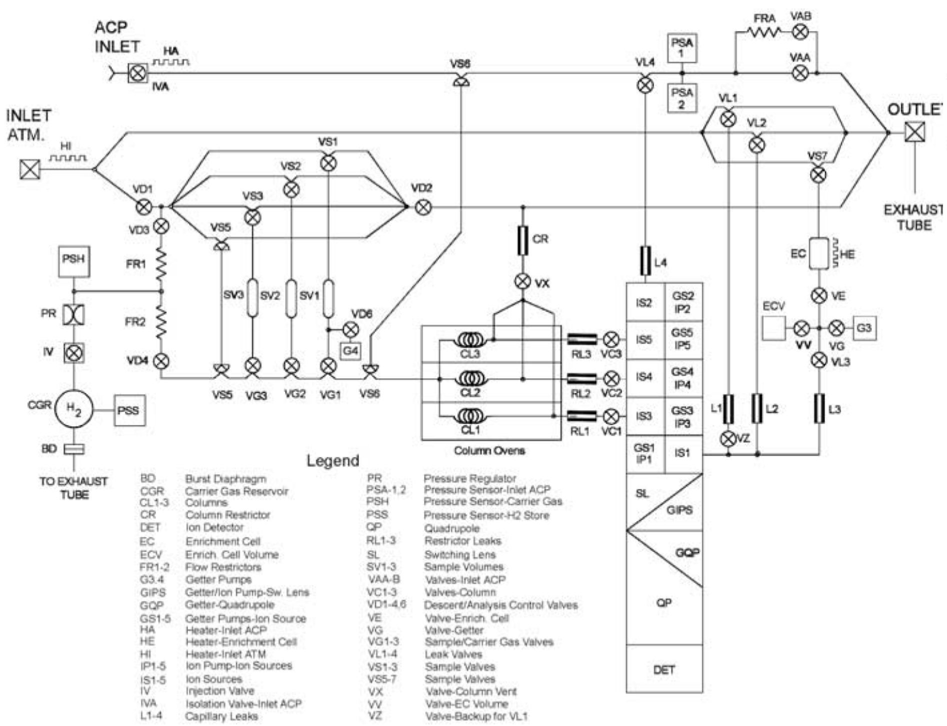


Figure 3. Schematic of the Gas Chromatograph Mass Spectrometer. Details of the Aerosol Collecto
Pyrolyser are shown in an accompanying paper in this volume.

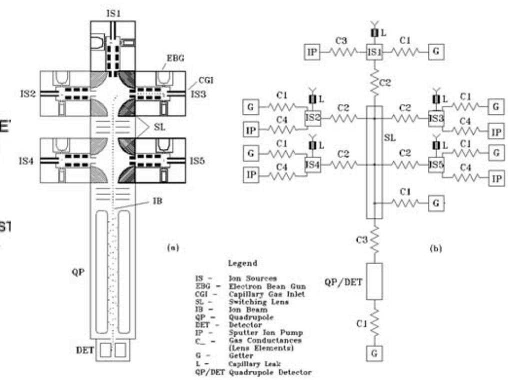


Figure 5. Illustrations of ion source configuration and sche
differential vacuum pumping system.

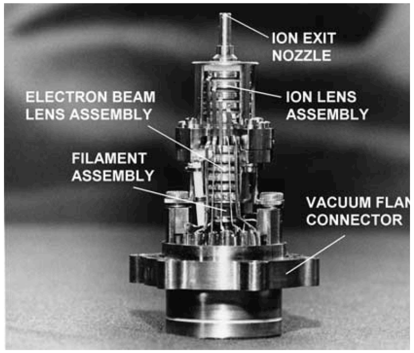


Figure 6. An ion source showing the electron and ion focusi
The overall height is 63 mm.

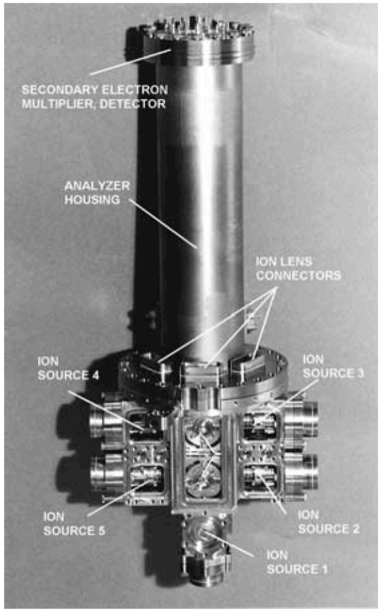


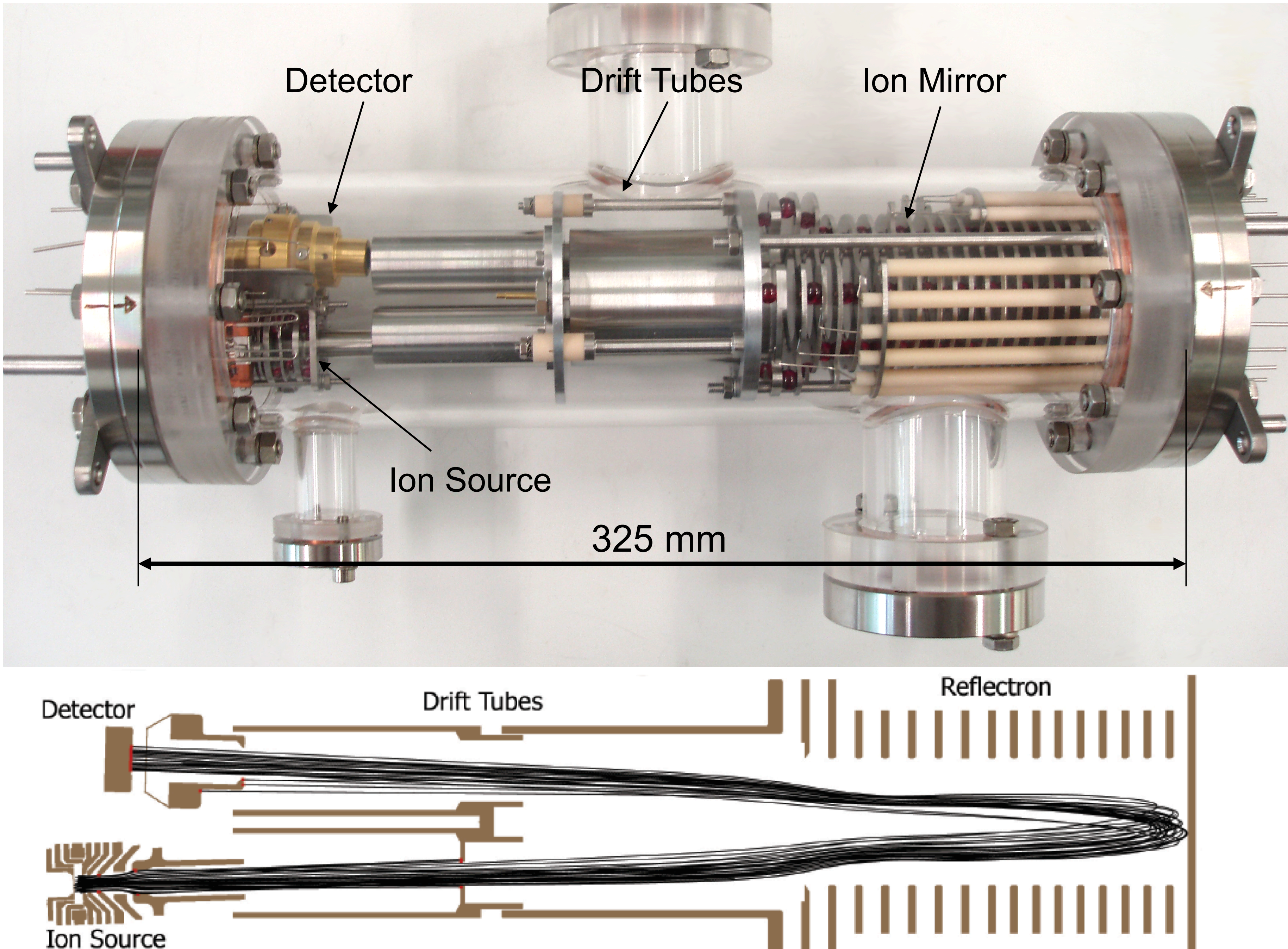
Figure 7. The ion source system, showing the individual ion sources and the switching lenses in the partially assembled ion source housing before installation of the getter housings and the gas inlet manifolds. The overall length is 357 mm.

H.B. Niemann, et al., The Gas Chromatograph Mass Spectrometer for the Huygens Probe, Sp. Sci. Rev. 104 (2002) 553–591.

Possible Future Developments

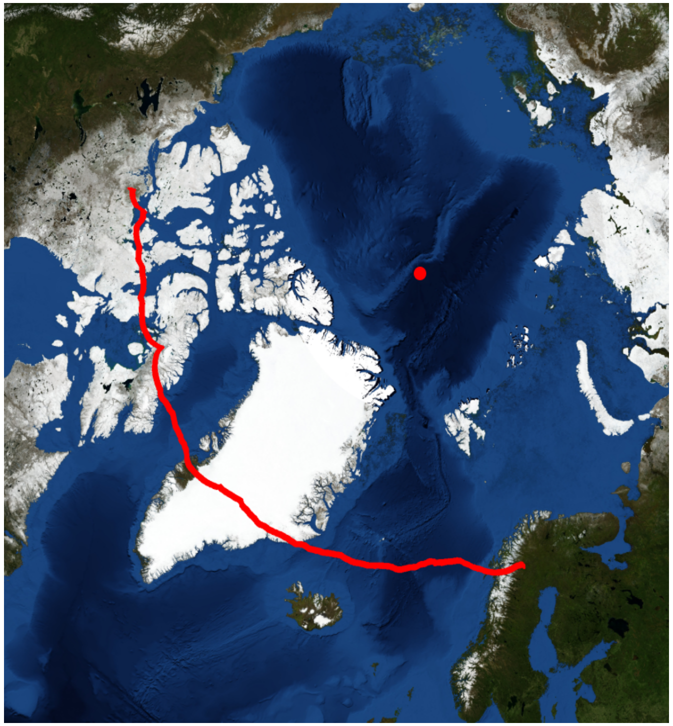
- Increase in sensitivity
- Increased mass range
- Increase in mass resolution
- Reduced complexity
- Reduced instrument resources

Increase in Sensitivity



D. Abplanalp, P. Wurz, et al., Adv. Space Res. 44 (2009) 870–878.

P-BACE on the MEAP platform



Background image: NASA, http://visibleearth.nasa.gov/

- Balloon provided by Esrange Space Center to test beyond line of sight flight
- Semicircular flight following the summer polar vortex
- Launched from Esrange, Sweden, on 28 June 2008
- Altitude 33 ... 38 km
- Landed in Canada, near Umingmaktok, on 3 July 2008.
- Recorded ~ 4500 mass spectra in stratosphere

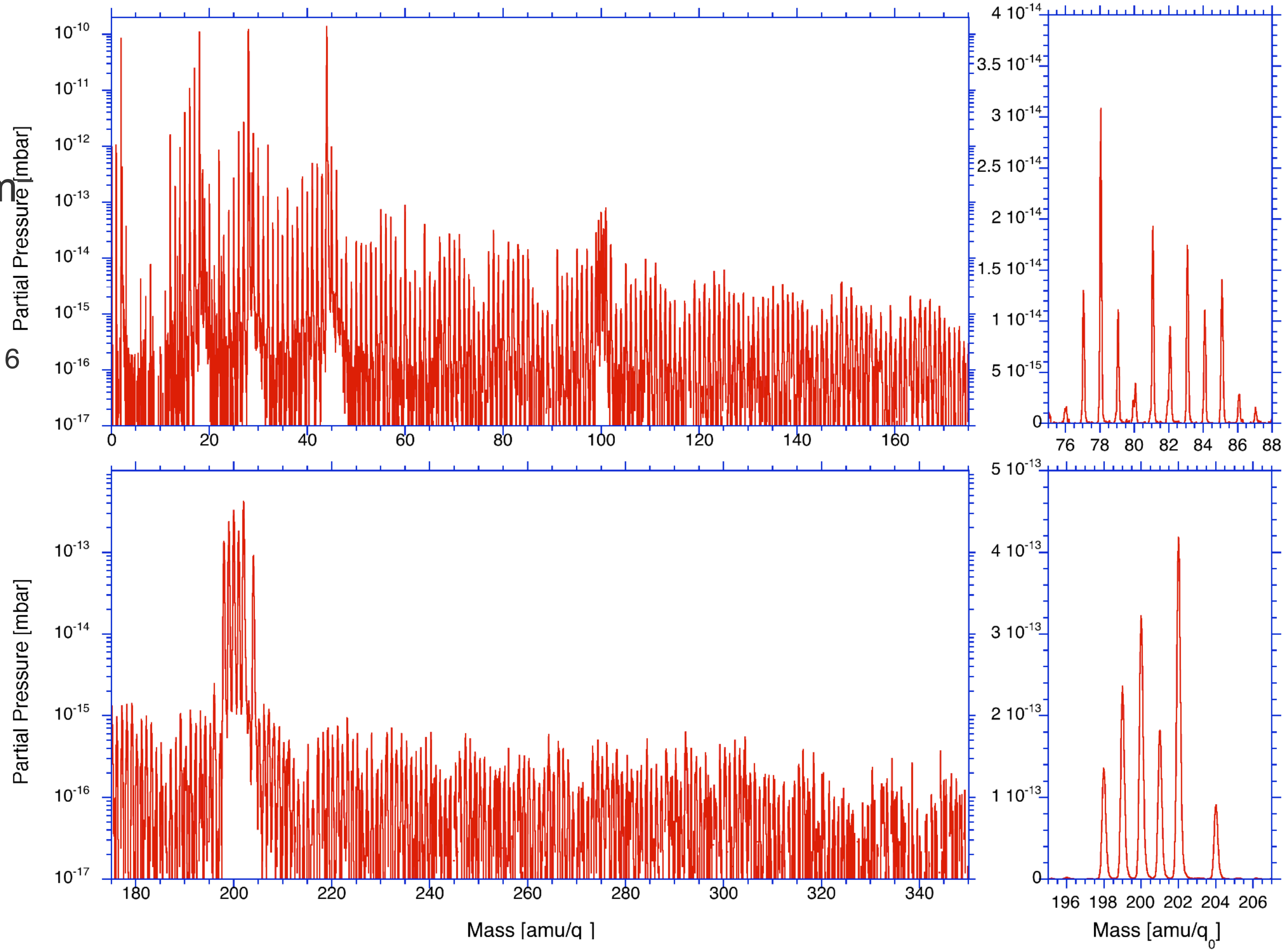
Species	Measurement 100 spectra (20080701/ 18:50 –20:40)	Meas. Error [%]	Literature value	Remarks
$^{36}Ar/^{38}Ar$	5.313	7	5.35	
$^{36}Ar/S_{tot}$	28 ppm	7	32 ppm	
$^{36}Ar/^{40}Ar$	$7.2\cdot10^{-4}$	7	$3.38\cdot10^{-3}$	Discrimination of small signals (ADC-card)
$^{21}Ne/S_{tot}$	0.053 ppm	21	0.049 ppm	Possible interference with H_2F^+
$^{20}Ne/^{22}Ne$	40	80	9.782	Interferences with $^{40}Ar^{++}$ and CO_2^{++}
$^{78}Kr/^{84}Kr$	0.010	50	0.006	
$^{80}Kr/^{84}Kr$	0.040	50	0.040	
$^{82}Kr/^{84}Kr$	0.200	11	0.203	
$^{83}Kr/^{84}Kr$	0.200	11	0.202	
$^{86}Kr/^{84}Kr$	0.300	7	0.304	
Kr_{tot}/S_{tot}	1.15 ppm	6	1.14 ppm	
$^{129}Xe/^{132}Xe$	0.9615	14	0.9833	
$^{131}Xe/^{132}Xe$	0.8846	14	0.7877	
$^{134}Xe/^{132}Xe$	0.3462	22	0.3882	
$^{136}Xe/^{132}Xe$	0.3077	22	0.3299	
Xe_{tot}/S_{tot}	0.3 ppm	8	0.087 ppm	Consideration of the large cross section for Xe gives a ratio of ~0.08 ppm
$^{196}Hg/^{202}Hg$	0.020	82	0.005	
$^{198}Hg/^{202}Hg$	0.367	14	0.334	
$^{199}Hg/^{202}Hg$	0.600	14	0.565	
$^{200}Hg/^{202}Hg$	0.800	14	0.774	
$^{201}Hg/^{202}Hg$	0.467	14	0.441	
$^{204}Hg/^{202}Hg$	0.233	14	0.230	
Hg_{tot}/S_{tot}	1.72 ppm	6	--	Source unknown (gondola)
O_3/S_{tot}	0.59 ppm	21	8 ppm	Pronounced fragmentation
H/D (H_2/HD)	8800	14	8694	
$^{23}Na^+/S_{tot}$	0.99 ppm	11	?	Probably oceanic NaCl
$^{40}Ca^{16}O_2^+/S_{tot}$	0.07 ppm	21	?	Contamination or meteorite material

P. Wurz, D. Abplanalp, M. Tulej, M. Iakovleva, V.A. Fernandes, A. Chumikov, and G. Managadze, "In Situ Mass Spectrometric Analysis in Planetary Science," Sol. Sys. Res. (2012) in press.

Neutral Gas Mass Spectrometer Luna-Resurs / Luna-Glob

Sensitivity

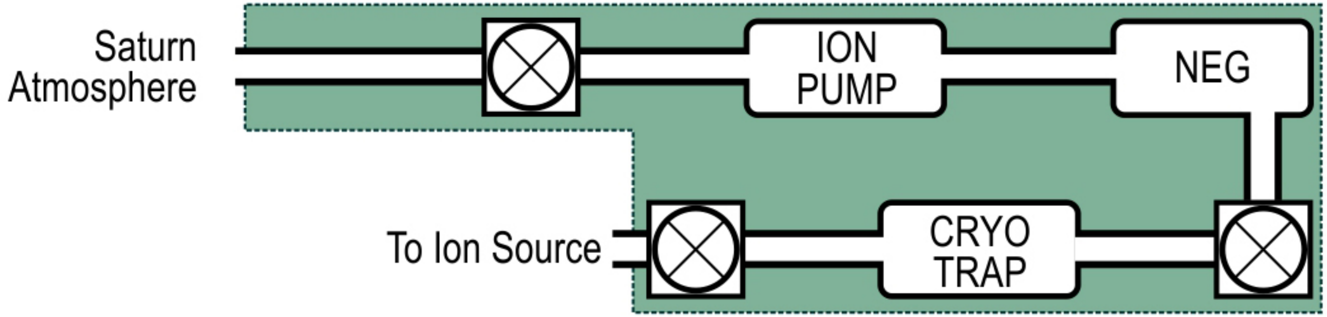
- Detection threshold: ≈ 1 cm^{-3} for 10 second integration
- Detection threshold: ≈ 10^{-16} mbar for 10 second integration



P. Wurz, D. Abplanalp, M. Tulej, and H. Lammer, "A Neutral Gas Mass Spectrometer for the Investigation of Lunar Volatiles," Planet. Sp. Science (2012) in print.

Noble Gas Sample Concentration: Cryotrap

- Sample concentration
  - Even though a TOF-MS is over 1000 times more sensitive than Cassini INMS (10x from ion source efficiency and 100 x from better duty cycle), calculations show that it would take longer than the probe descent time to provide the counting statistics required for the isotopes of Kr and Xe with sufficient accuracy
  - The noble gas enhancement can be achieved by using a combination of a cryotrap, ion pump, and non-evaporable getter (NEG: SAES 172).
  - The NEG removes all constituents except methane and the noble gases.
  - The cryotrap traps the products of the NEG process, except for helium and some neon.
  - The ion pump then operates to pump away the helium, which is the second highest source of gas, thus enhancing the remaining noble gases ~ 200 times.
  - Helium and neon are measured using a separate mode.

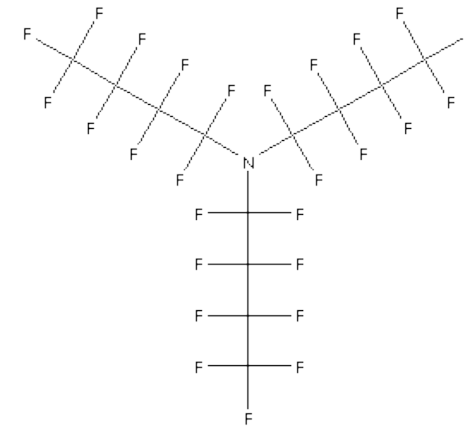


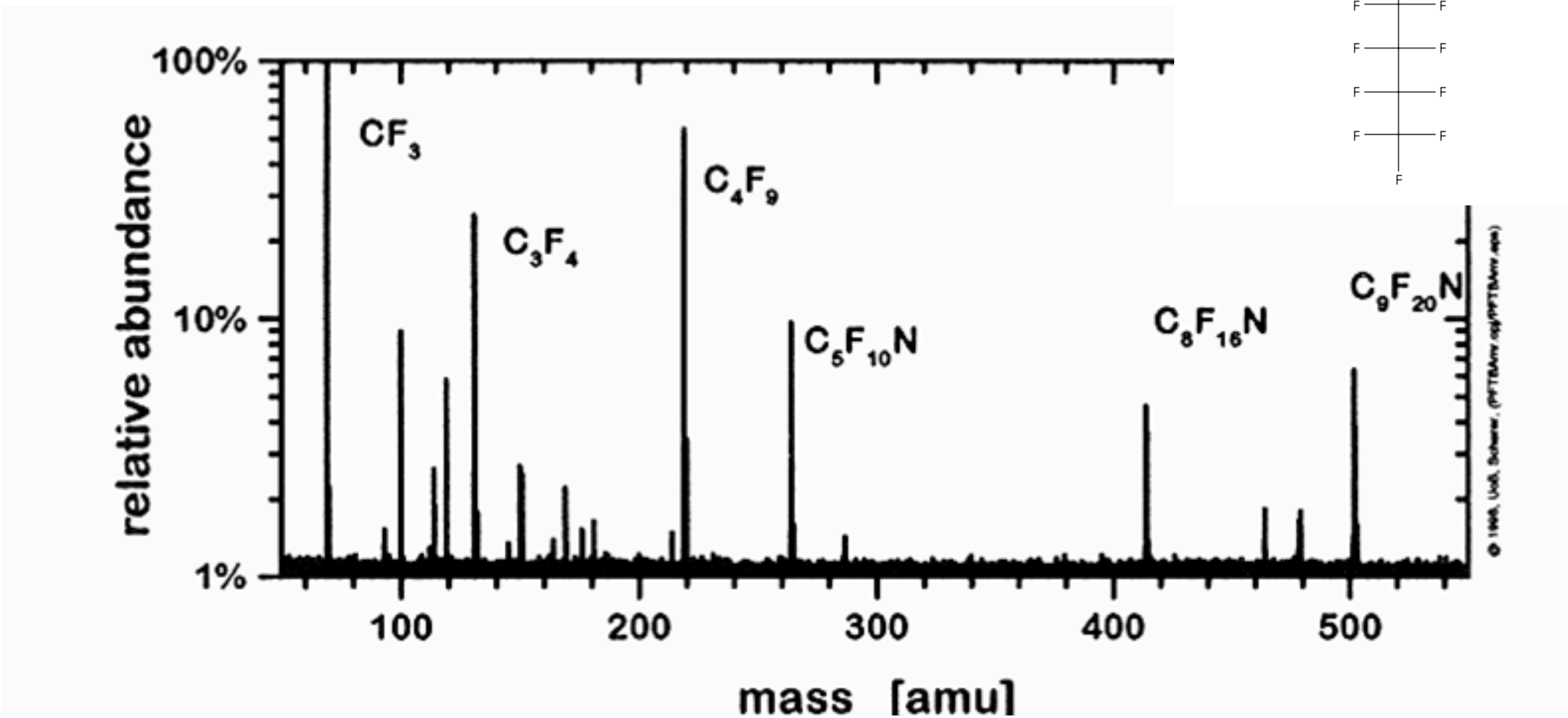
CEAMS / SwRI, H. Waite

Increased Mass Range

RTOF / ROSINA / Rosetta
Mass Range

$CF_3(CF_2)_3)_3N$



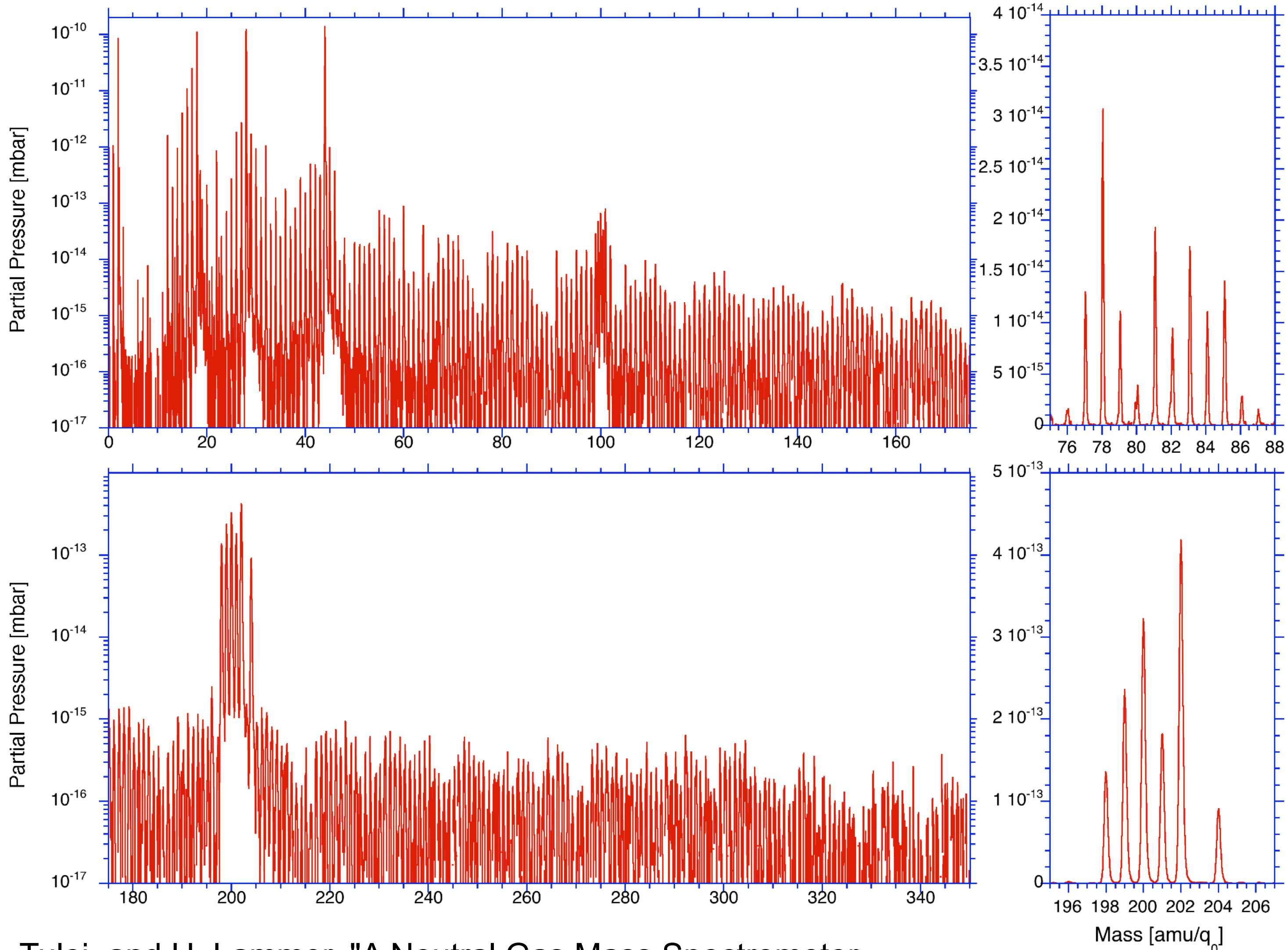


RTOF mass spectrum (prototype) of the calibration compound heptacosafluorotributylamine, a compound to demonstrate mass range. Mass range is unlimited by sensor itself, data acquisition memory however limits the mass range that can be covered. In case of RTOF, the mass range is up to 1000 amu.

S. Scherer, K. Altwegg, H. Balsiger, J. Fischer, A. Jäckel, A. Korth, M. Mildner, D. Piazza, H. Rème, and P. Wurz, "A novel principle for an ion mirror design in time-of-flight mass spectrometry," Int. Jou. Mass Spectr. 251 (2006) 73-81.

Neutral Gas Mass Spectrometer Luna-Resurs / Luna-Glob

Mass range
- 1 – 300 amu (low mass range mode)
- Can be increased in flight by command, if necessary, to 1000 amu (high mass range mode).
- Mass range is only limited by memory for accumulation

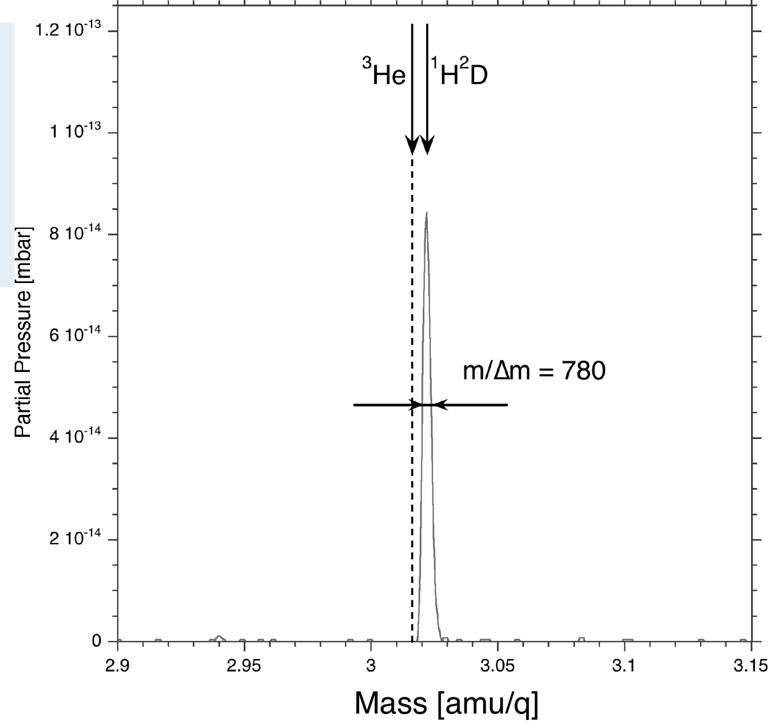


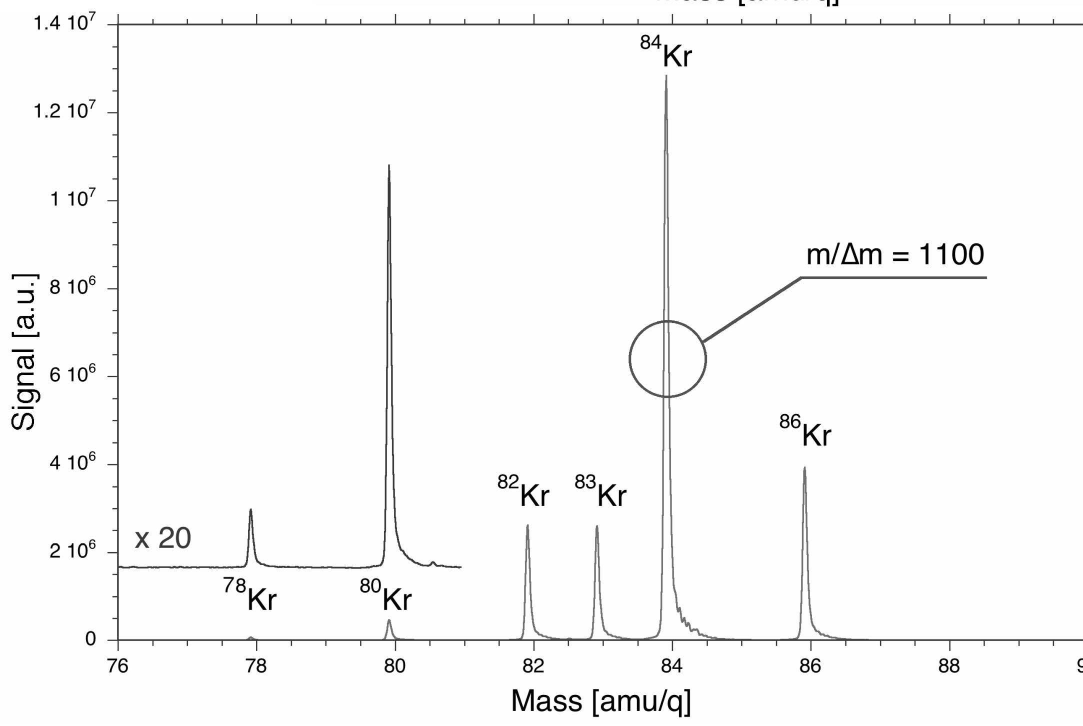
P. Wurz, D. Abplanalp, M. Tulej, and H. Lammer, "A Neutral Gas Mass Spectrometer for the Investigation of Lunar Volatiles," Planet. Sp. Science (2012) in print.

Increased Mass Resolution

Increased Mass Resolution

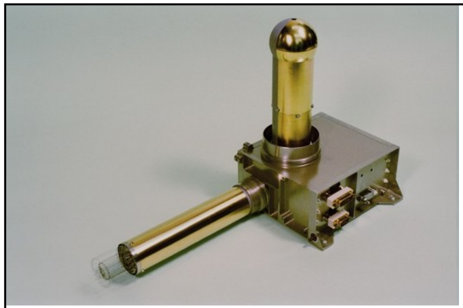
- **m/Δm ≈** 100 (50%)
  - there is separation of low-mass chemical species
- **m/Δm ≈** 1000 (50%)
  - there is a separation of peaks of different nominal mass (e.g., 325 amu versus 326 amu)
- **m/Δm ≈** 10000 (50%),
  - separation of peaks for nominally isobaric species (i.e., molecules of the same nominal mass differing in elemental composition), e.g., N_2 versus CO, both ~28 amu.
  - resolution of small (**<** 2500 amu) peptides of the same nominal mass differ by one amino acid (except for isomeric leucine and isoleucine)
- **m/Δm ≈** 100000 (50%),
  - there is a separation of peaks for nominally isobaric species, e.g. for complex carbon chemistry





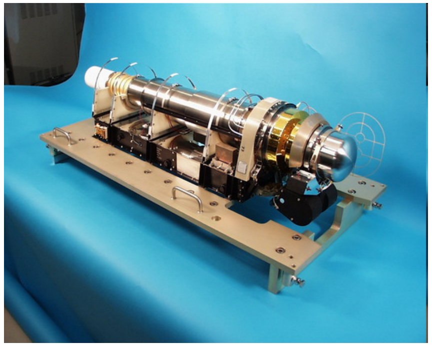
P. Wurz, D. Abplanalp, M. Tulej, and H. Lammer, "A Neutral Gas Mass Spectrometer for the Investigation of Lunar Volatiles," Planet. Sp. Science (2012) in print.

Rosetta / ROSINA Instruments



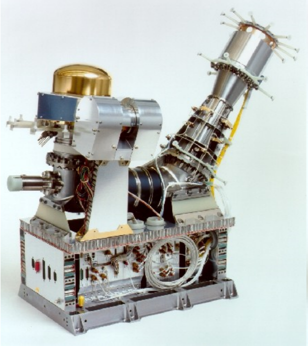
COPS:

- Measures the total neutral particle density and the ram pressure (the cometary gas flux)
- Measures the total pressure down to densities of 10^4 cm^{-3} in 10s



RTOF:

- Covers mass range from 1 to > 300 amu/e
- Mass resolution m/Δm > 3000 (at 50% peak height)
- Detects particle densities of 10^2 cm^{-3} within 10–1000s for a complete spectrum

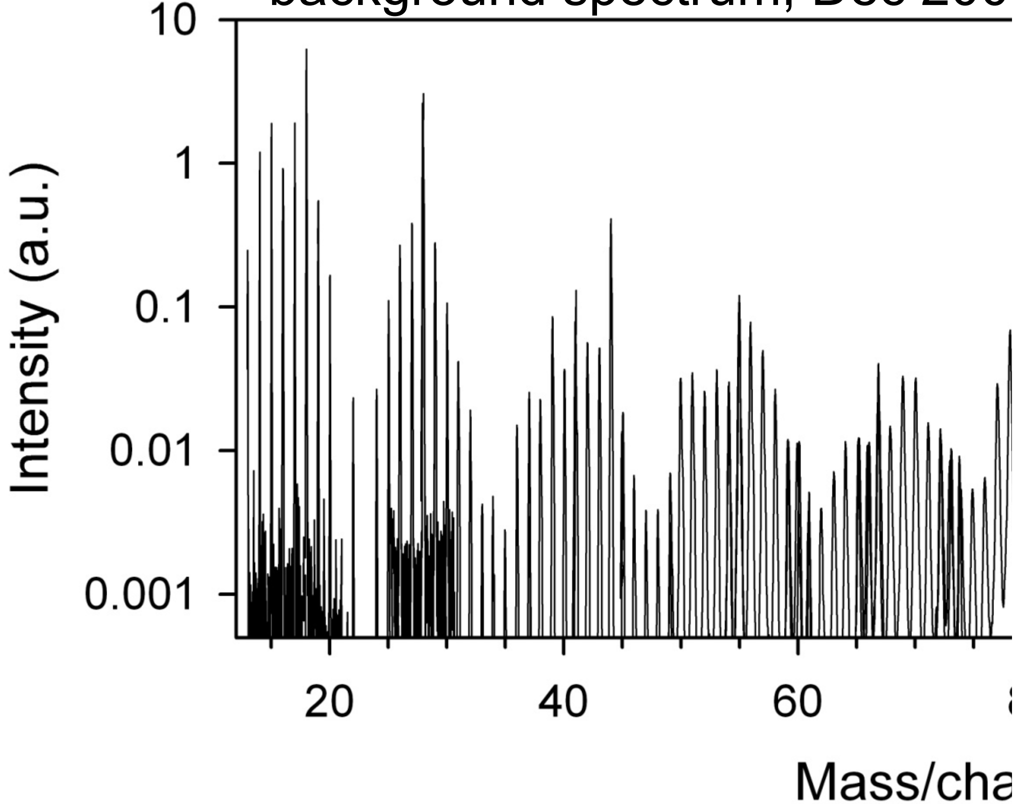


DFMS:

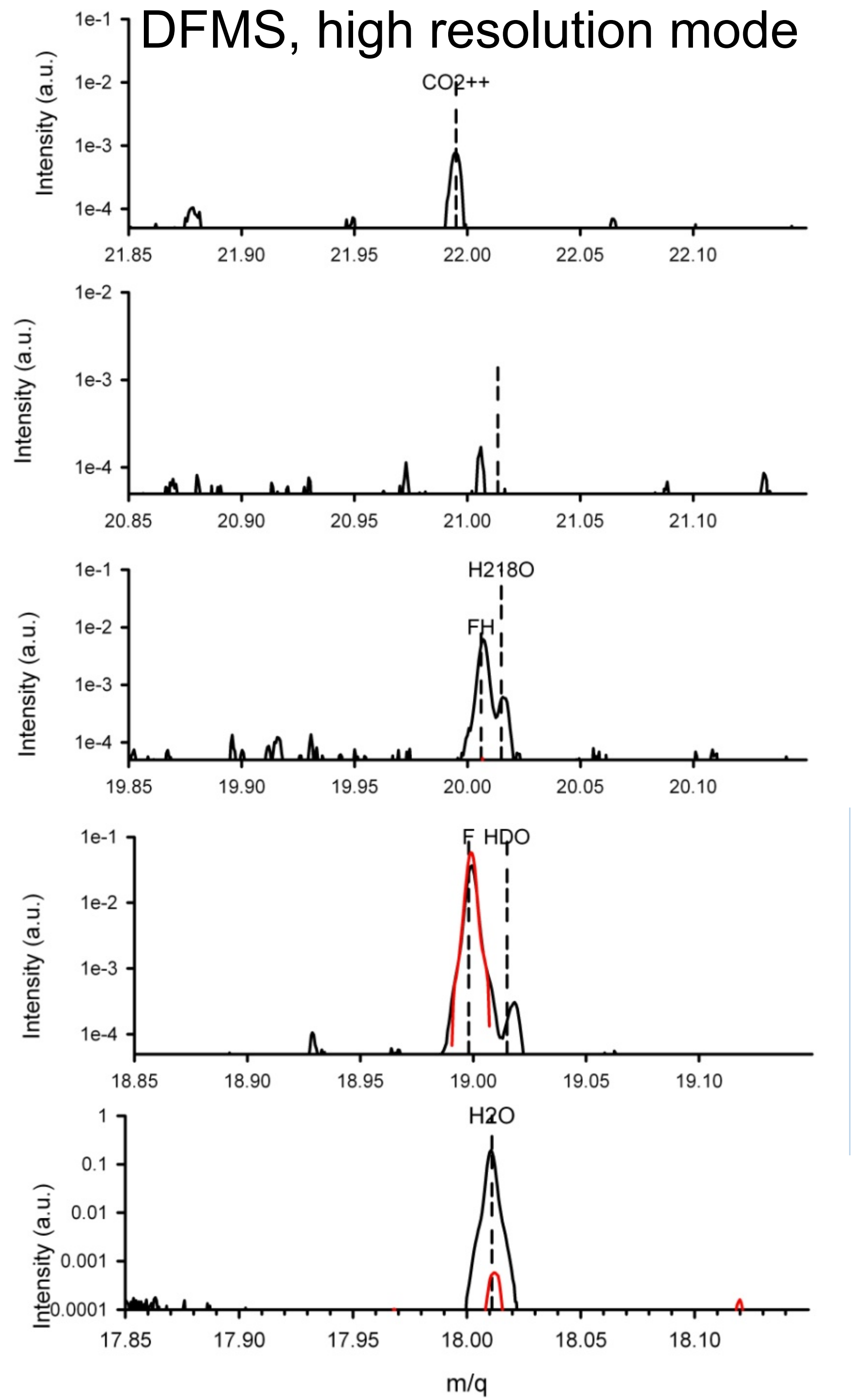
- Covers mass range from 12 to 150 amu/e
- Mass resolution m/Δm > 9000 (at 50% peak height)
- Detects particle densities of 1 cm^{-3} within 20 s for one mass line
- Complete mass spectrum ~ 20 min

H. Balsiger, et al., **"ROSINA - Rosetta Orbiter Spectrometer for Ion and Neutral Analysis,"** Space Science Review 128 (2007), 745-801.

Rosetta / ROSINA: Active chec
Double Focussing Mass Spect



B. Schläppi, K. Altwegg, H. Balsiger, M. Hässig, A. Jäckel, P.
Berthelier, J. DeKeyser, H. Rème, and U. Mall, "The influenc
tenuous atmospheres with in situ mass spectrometry," Jou. (



Rosetta / ROSINA: Active checkout PC4 Double Focussing Mass Spectrometer (DFMS)

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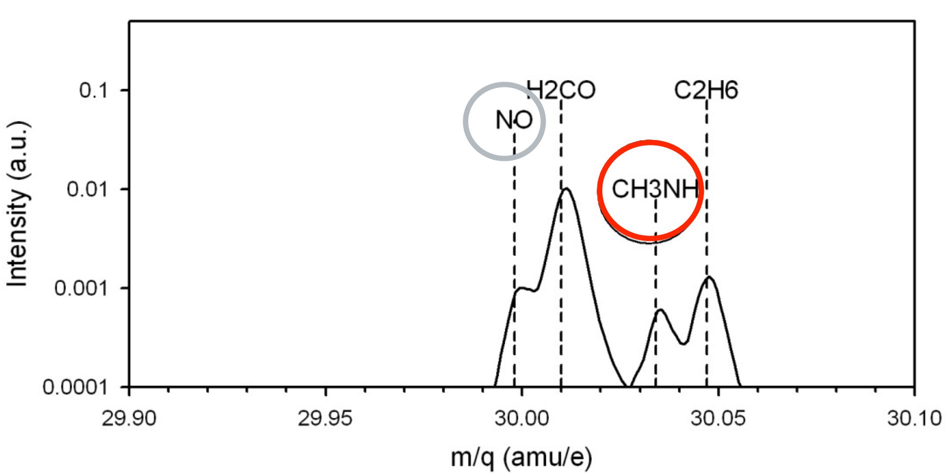
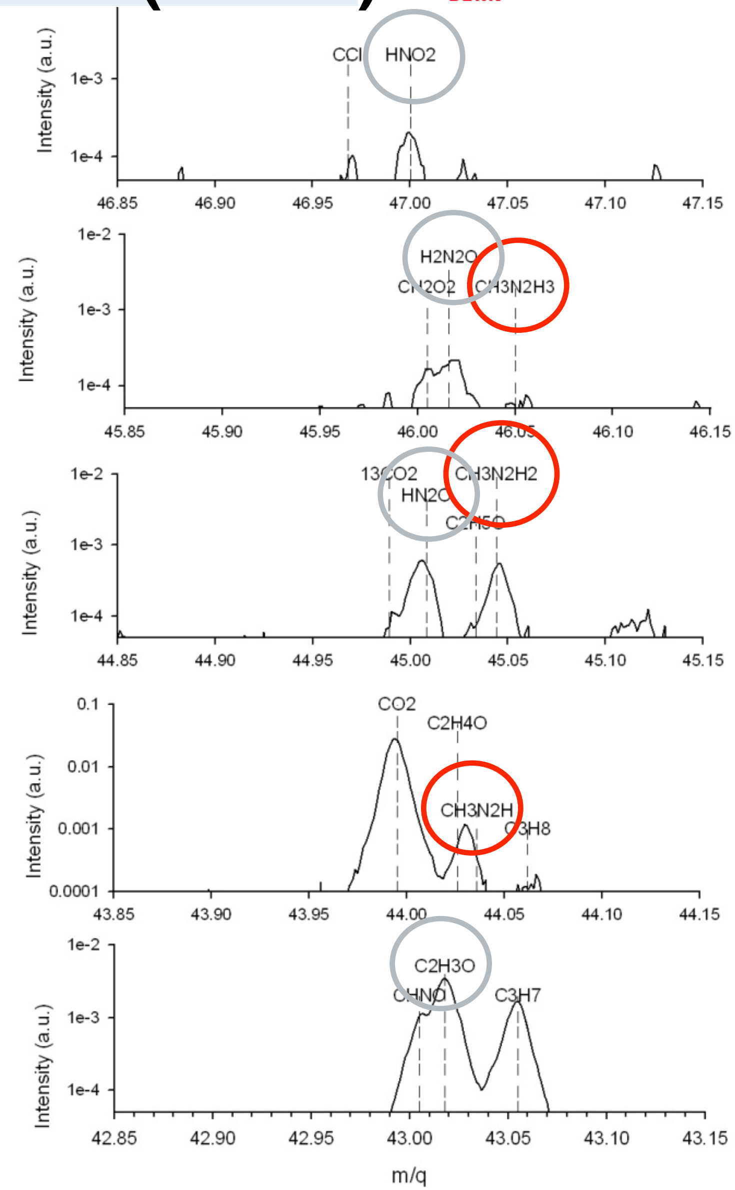
Traces of hydrazine $CH_3N_2H_3$, its oxidant N_2O_4, and products, 20 h after thruster firing

ROSINA-DFMS high resolution masss spectrum, Dec. 2006



$P_{total} \sim 4 \times 10^{-11}$ mbar, $p_{hydrazine} \sim 1 \times 10^{-12}$ mbar



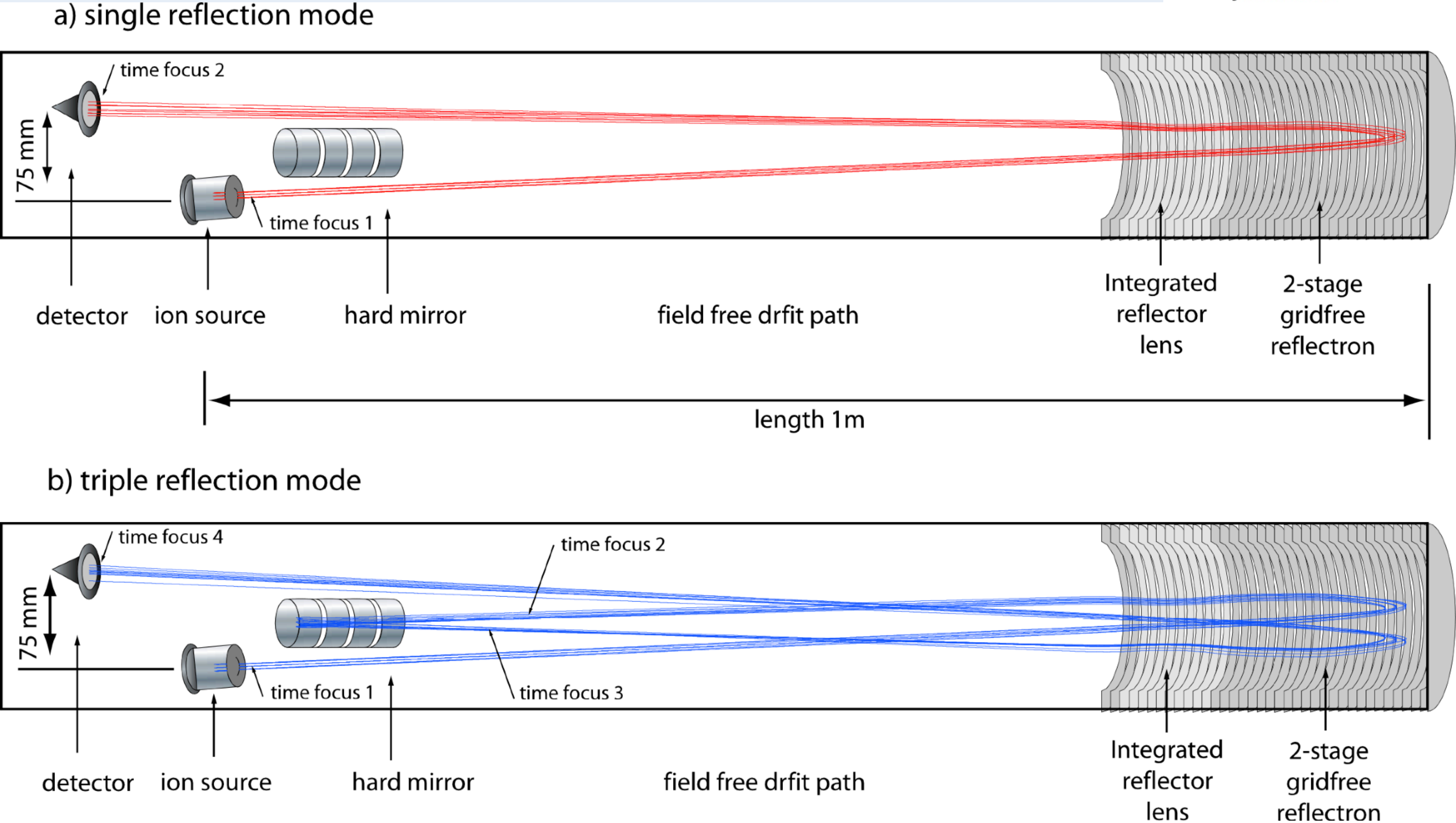
Some identified molecules and fragments in the vicinity of Rosetta S/C

Carbohydrates					PAH		N-H	Hydrazine	C-N	Oxygen	N-O
	C2	C3	C4	C5			N	CN		O	NO
CH	C_2H	C_3H	C_4H	C_5H	C_6H		NH	CHN	C_2H_2N	OH	CNO
CH_2	C_2H_2	C_3H_2	C_4H_2	C_5H_2	C_6H_2		NH_2	CH_2N	C_2H_3N	OH_2	HCNO
CH_3	C_2H	C_3H_3	C_4H_3	C_5H_3	C_6H_3	C_7H_3	NH_3	CH_3N	C_2H_4N	ODH	H_6CNO
CH_4	C_2H_4	C_3H_4	C_4H_4	C_5H_4	C_6H_4	C_7H_4	N_2	CH_3NH		$^{18}OH_2$	NO_2
	C_2H_5	C_3H_5	C_4H_5	C_5H_5	C_6H_5	C_7H_5		CH_3NH_2	C_5H_4N	O_2	HNO_2
	C_2H_6	C_3H6	C_4H_6	C_5H_6		C_7H_6		CH_3N_2H	C_5H_5N		H_4NO_2
		C_3H_7	C_4H_7	C_5H_7		C_7H_7		$CH_3N_2H_2$	C_5H_6N		$CHNO_2$
		C_3H_8	C_4H_8	C_5H_8		C_7H_8, Toluene		$CH_3N_2H_3$	C_5H_7N		CH_3NO_2
			C_4H_9	C_5H_9		C_8H_{10}			C_5H_8N		CH_4NO_2
			C_4H_{10}	C_5H_{10}		C_9H_{12}					C_2H_6NO
				C_5H_{11}					$C_4H_4N_2$		H_2N_2O
				C_5H_{12}							C_2N_2O
											C_2HN_2O
											$C_2H_2N_2O$
											$C_2H_3N_2O$
											$C_2H_5N_2O$
											$C_2H_6N_2O$
											$C_2H_7N_2O$
											$C_2H_8N_2O$

Yellow: Possible fragments from Monomethylhydrazine and N_2O_4

Green: Solvents

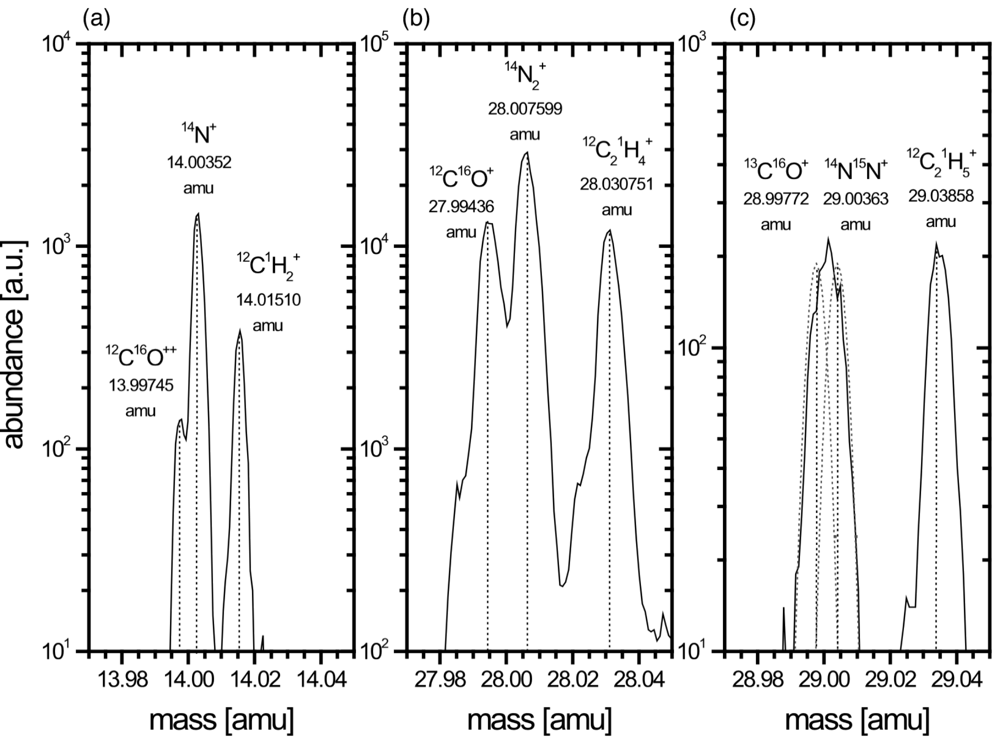
RTOF / ROSINA / Rosetta

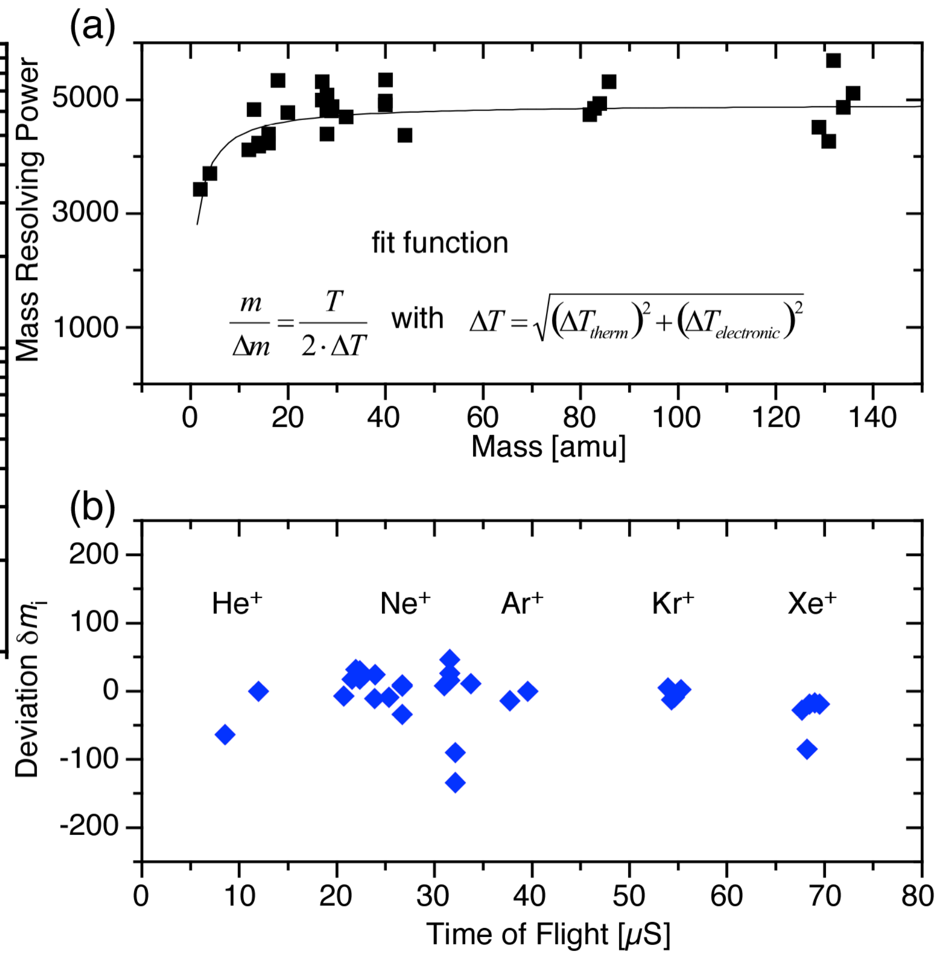


M. Hohl, P. Wurz, S. Scherer, K. Altwegg, and H. Balsiger, Int. J. Mass Spectr. 188 (1999), 189–197.

S. Scherer, K. Altwegg, H. Balsiger, J. Fischer, A. Jäckel, A. Korth, M. Mildner, D. Piazza, H. Rème, and P. Wurz, Int. Jou. Mass Spectr. 251 (2006) 73–81.

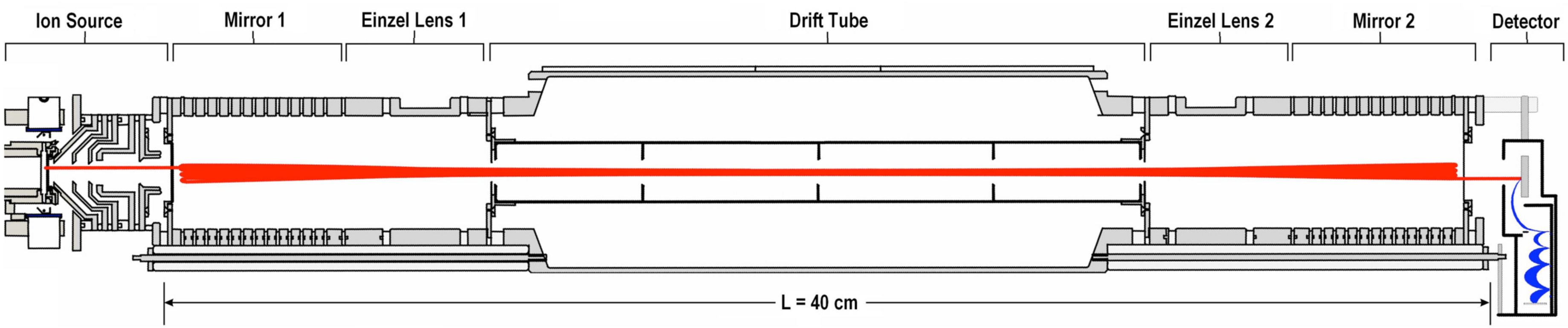
Rosetta / ROSINA / RTOF





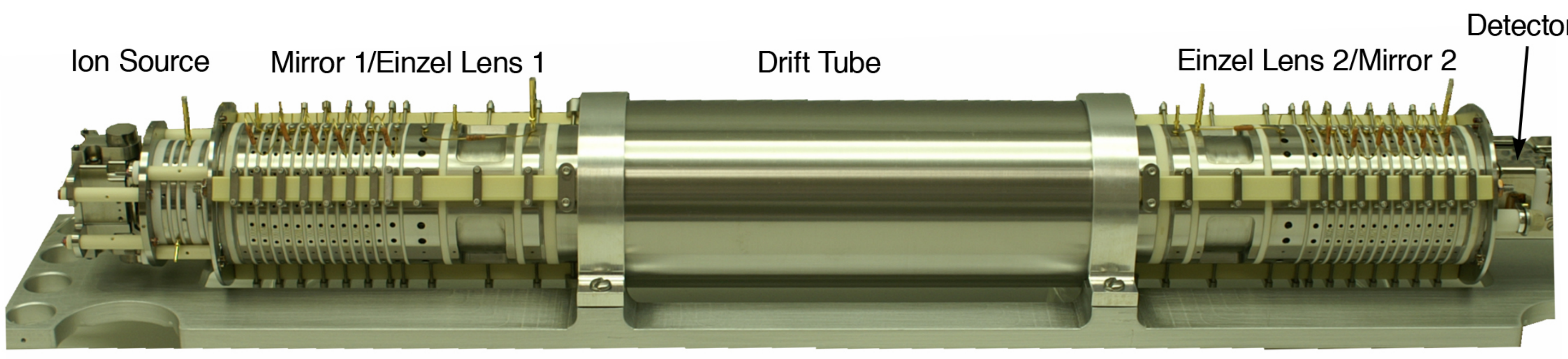
S. Scherer, K. Altwegg, H. Balsiger, J. Fischer, A. Jäckel, A. Korth, M. Mildner, D. Piazza, H. Rème, and P. Wurz, "A novel principle for an ion mirror design in time-of-flight mass spectrometry," Int. Jou. Mass Spectr. 251 (2006) 73-81.

Multi-Bounce time-of-flight mass spectrometer (MASPEX) Ion Optics Simulations and Prototype



Numerical simulations of ion trajectories showing focusing of multi-bounce ion packets.

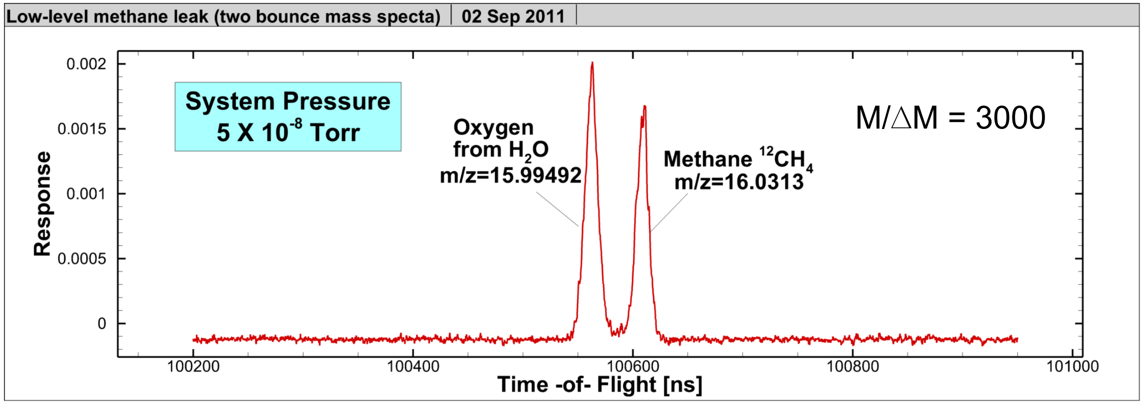
$$m/\Delta m(N) = NT_o/2(Dt+NdT)$$

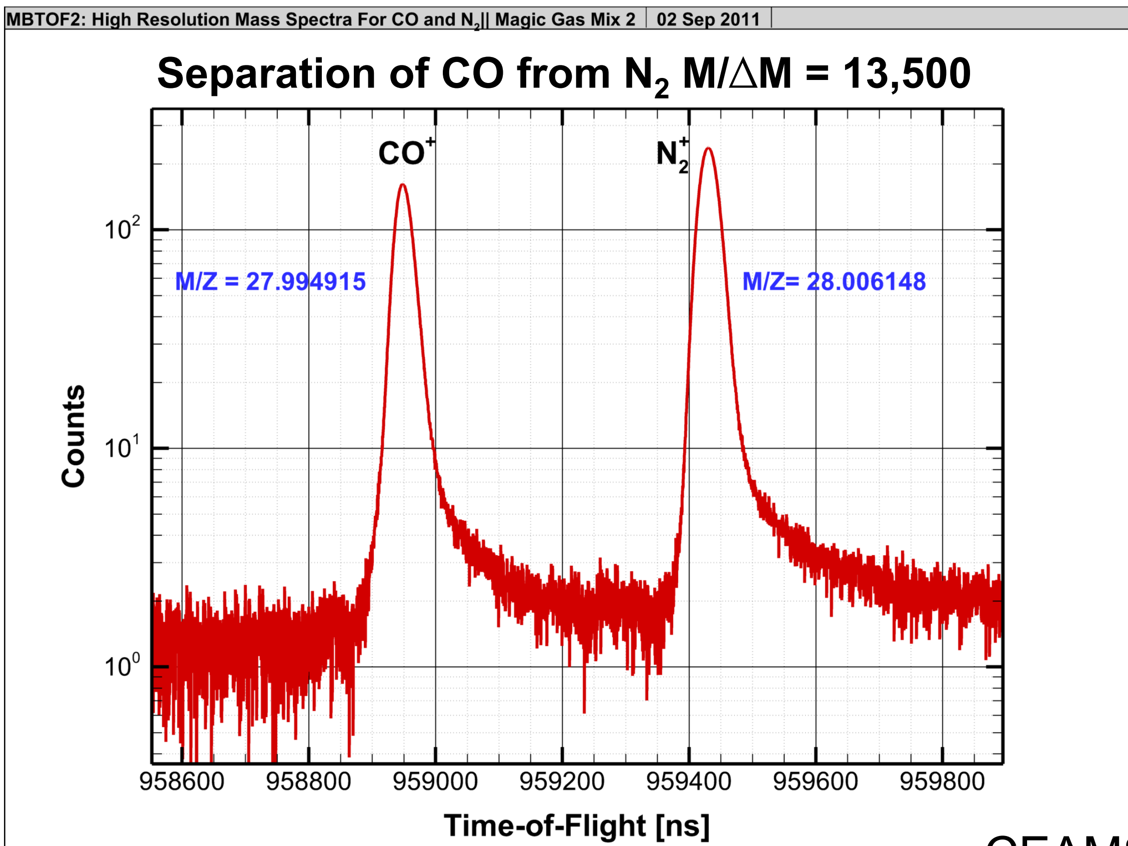


Third generation MBTOF has successfully undergone vacuum and vibration tests.

CEAMS / SwRI, H. Waite

MASPEX Performance (High-Resolution Mode)

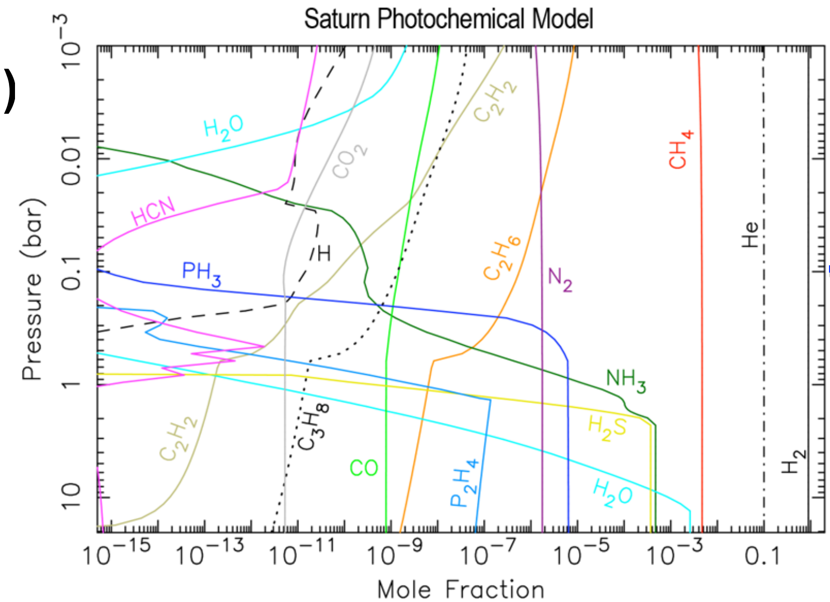




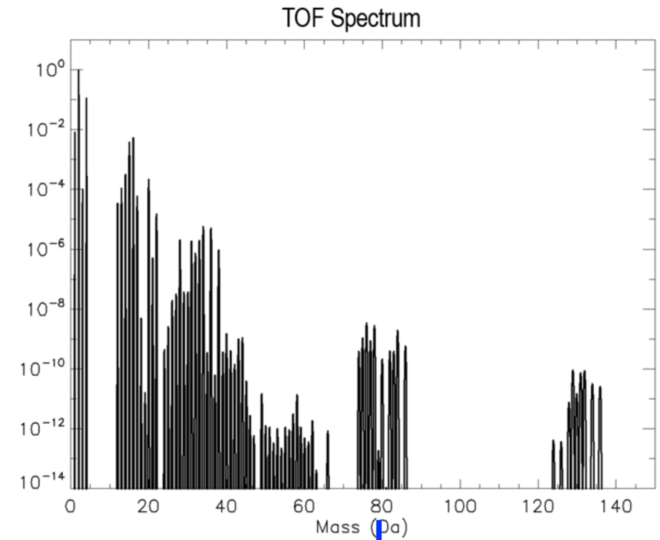
CEAMS / SwRI, H. Waite

Scientific Requirements

1)



2)



STEP 1: Saturn atmosphere model (J. Moses) produced as the basis for estimating the mass spectrometric measurement requirements (over 100 compounds from 0.5 to 20 bars).

STEP 2: Simulated mass spectrum generated using empirical laboratory data (line shapes) from mass spectrometer combined with NIST fragmentation and ionisation data and solar isotopic abundance information (H. Waite).

STEP 3: Spreadsheet programme developed to determine mass resolution and measurement time needed to satisfy the requirements and thus generate a realistic operational scenario (H. Waite).

3)

Results for the Measurement of Ambient Gas at 0.5 bar

Molecule	Specific isotope	Exact mass	Principal isotope	Molecular abun-dance	Mixing fraction	Min required acquisition time	Target precision	Minimum bounces required
		RMM						
		g/mol				sec		
H2	$^{1}H_2$	2.0	P	0.895	0.895	<0.1	5%	0
H2	$^{1}H^{2}H$	3.0	2H	0.895	3.58E-5	<0.1	5%	4
He	^{3}He	3.0	3He	0.1	4.64E-5	<0.1	10%	4
He	^{4}He	4.0	P	0.1	0.1	<0.1	5%	0
CH4	$^{12}C^{1}H_4$	16.0	P	0.005	0.005	<0.1	1%	0
CH4	$^{13}C^{1}H_4$	17.0	13C	0.005	5.25E-5	1.7	1%	0
CH4	$^{12}C^{1}H_3{}^{2}H$	17.0	2H	0.005	3.72E-7	9.7	5%	21
N2	$^{14}N_2$	28.0	P	1.75E-6	1.74E-6	0.3	10%	3
Ne	^{20}Ne	20.0	P	2.06E-4	1.92E-4	<0.1	10%	0
Ne	^{22}Ne	22.0	22Ne	2.06E-4	1.39E-5	0.2	10%	0
NH3	$^{14}N^{1}H_3$	17.0	P	1.39E-7	1.39E-7	7.7	10%	8
Ar	^{36}Ar	36.0	P	5.37E-6	1.81E-8	21.1	10%	0
Ar	^{38}Ar	38.0	38Ar	5.37E-6	3.41E-9	111.7	10%	0
C2H6	$^{12}C_2{}^{1}H_6$	30.0	P	3.34E-8	3.27E-8	2219.5	1%	3
C2H6	$^{12}C^{13}C^{1}H_6$	31.1	13C	3.34E-8	7.38E-10	98205.	1%	16
Kr	^{80}Kr	79.9	80Kr	3.04E-9	6.89E-11	13948.3	10%	3
Kr	^{82}Kr	81.9	82Kr	3.04E-9	3.51E-10	2734.5	10%	0
Kr	^{83}Kr	82.9	83Kr	3.04E-9	3.49E-10	2748.1	10%	0
Kr	^{84}Kr	83.9	P	3.04E-9	1.74E-9	552.4	10%	0
Kr	^{86}Kr	85.9	86Kr	3.04E-9	5.25E-10	1829.	10%	0
Xe	^{128}Xe	127.9	128Xe	3.04E-10	2.18E-12	229818.6	10%	0
Xe	^{129}Xe	128.9	P	3.04E-10	2.21E-10	2269.6	10%	0
Xe	^{130}Xe	129.9	130Xe	3.04E-10	4.61E-12	108669.6	10%	0
Xe	^{131}Xe	130.9	131Xe	3.04E-10	2.41E-11	20797.4	10%	0
Xe	^{132}Xe	131.9	132Xe	3.04E-10	3.05E-11	16409.1	10%	0
Xe	^{134}Xe	133.9	134Xe	3.04E-10	1.19E-11	42291.8	10%	0
Xe	^{136}Xe	135.9	136Xe	3.04E-10	1.E-11	49875.7	10%	0

Orbitrap

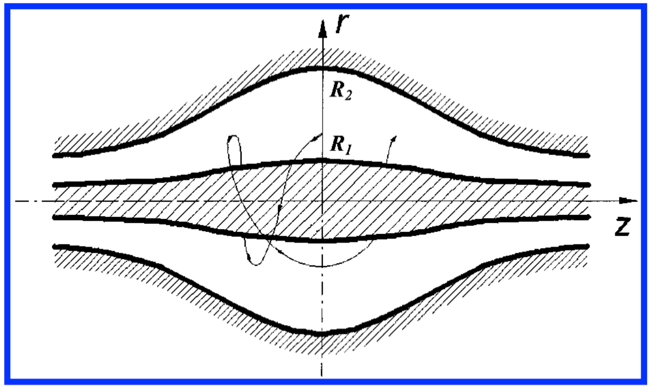


Figure 1. Equipotentials of the quadro-logarithmic field and an example of a stable ion trajectory

$$U(r,z) = \frac{k}{2}\left(z^2 - \frac{r^2}{2}\right) + \frac{k}{2}(R_m)^2 \ln\left[\frac{r}{R_m}\right] + C$$

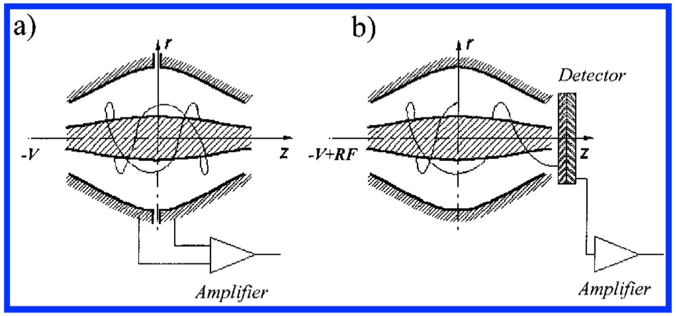


Figure 2. Modes of mass analysis in the orbitrap: (a) Fourier transform mass spectrometry (image current detection); (b) mass-selective instability (detection using secondary electron multiplier).

- Early work
  - A. Makarov, Electrostatic axially harmonic orbital trapping: a highperformance technique of mass analysis. Anal. Chem. 72, (2000) 1156–1162
  - Qizhi Hu, Robert J. Noll, Hongyan Li, Alexander Makarov, Mark Hardman, and R. Graham Cooks, The Orbitrap: a new mass spectrometer, J. Mass Spectrom. 2005; 40: 430–443
- Theory
  - Andriy Kharchenko, Gleb Vladimirov, Ron M. A. Heeren, Eugene N. Nikolaev, Performance of Orbitrap Mass Analyzer at Various Space Charge and Non-Ideal Field Conditions: Simulation Approach, J. Am. Soc. Mass Spectrom. (2012) 23:977–987
- Multiple MS (MS^M)
  - Robert Cho, Yingying Huang, Jae C. Schwartz, Yan Chen, Timothy J. Carlson, Ji Ma, MS^M, an Efficient Workflow for Metabolite Identification Using Hybrid Linear Ion Trap Orbitrap Mass Spectrometer, J. Am. Soc. Mass Spectrom. (2012) 23:880–888

Orbitrap

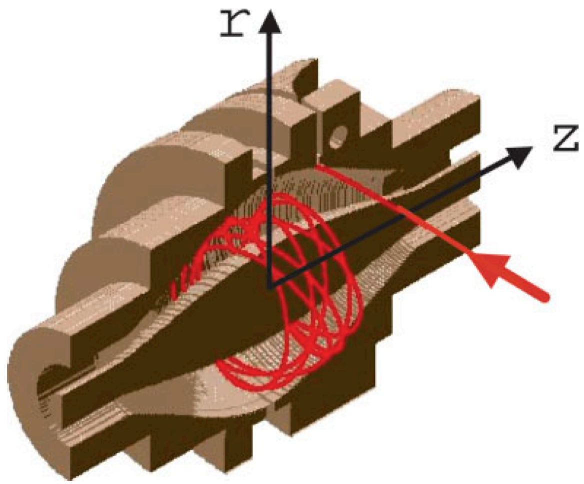


Figure 1. Cutaway view of the Orbitrap mass analyzer. Ions are injected into the Orbitrap at the point indicated by the red arrow. The ions are injected with a velocity perpendicular to the long axis of the Orbitrap (the z-axis). Injection at a point displaced from $z = 0$ gives the ions potential energy in the z-direction. Ion injection at this point on the z-potential is analogous to pulling back a pendulum bob and then releasing it to oscillate.

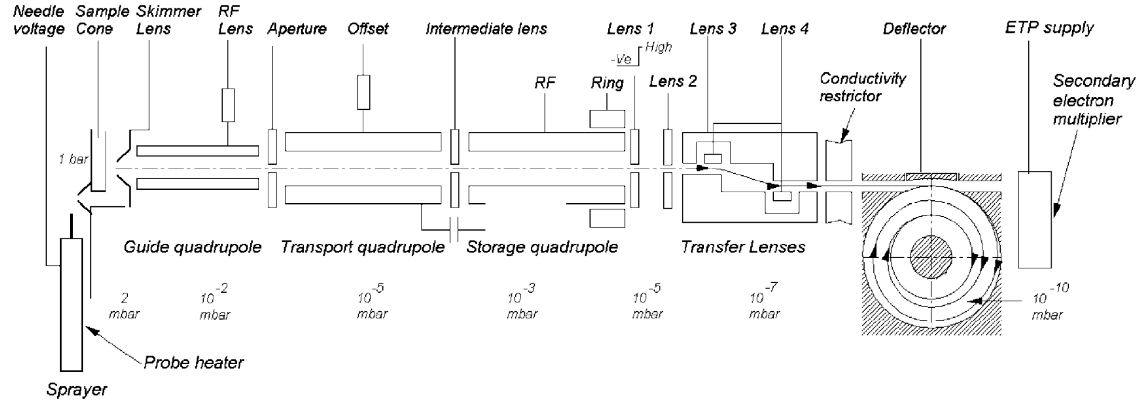


Figure 2. The experimental Orbitrap mass spectrometer. Ions are produced by the electrospray ion source at the extreme left. Ions then proceed through the source, collision quadrupole, selection quadrupole and then pass into the storage quadrupole. The storage quadrupole serves as an ion accumulator and buncher, allowing a pulsed mass analyzer such as the Orbitrap to be coupled to a continuous source like an electrospray ionization source. After accumulation and bunching in the storage quadrupole, the exit lens ('Lens 1') is pulsed low, the ion bunches traverse the ion transfer lens system and are injected into the Orbitrap mass analyzer (shown end-on).

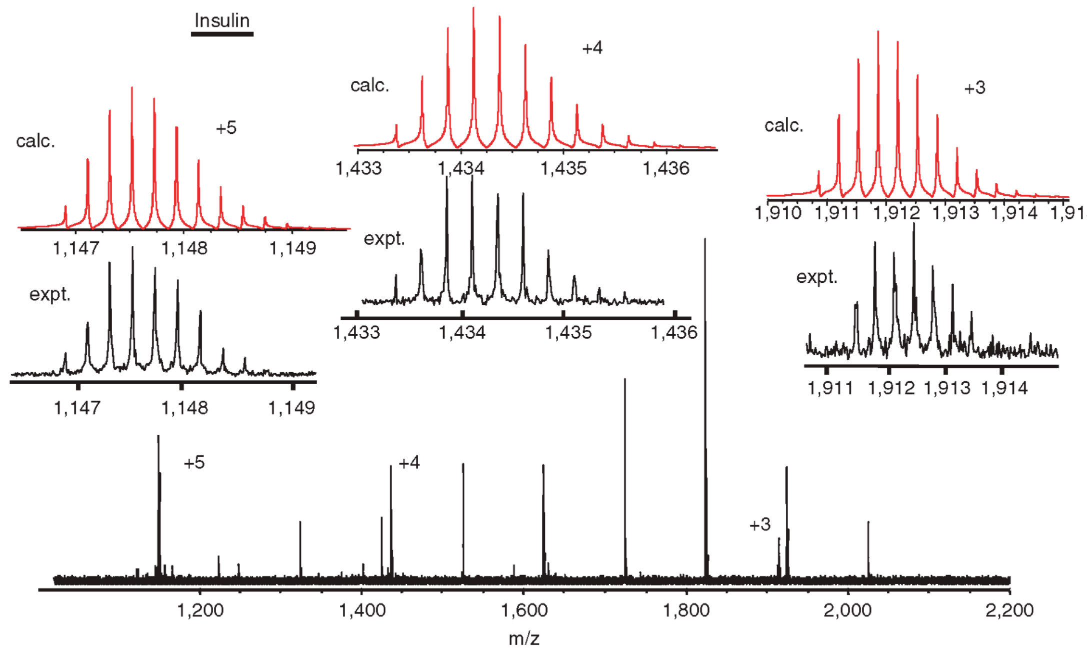


Figure 8. ESI mass spectrum of bovine insulin. Data acquisition parameters include a data sampling rate of 5 MHz, record length was 8 million data points, and the Fourier transform was performed with no apodization function or zero-filling. The lower spectrum shows a wide range mass spectrum including the internal mass calibrant Ultramark 1621 whose oligomers are spaced by 100 mass/charge unit intervals. Lower traces in the close-ups show experimentally obtained isotopic distributions for each charge state. Upper traces in the close-ups show the theoretically expected isotopic distributions. The calculated isotope distributions were obtained from IsoPro 3.0 using Gussian peak shapes with resolution of 100 000.

Qizhi Hu, Robert J. Noll, Hongyan Li, Alexander Makarov, Mark Hardman, and Graham R. Cooks, The Orbitrap: a new mass spectrometer, J. Mass Spectrom. 2005; 40: 430–443

Reduced instrument resources

Micro-Gas Chromatography Systems

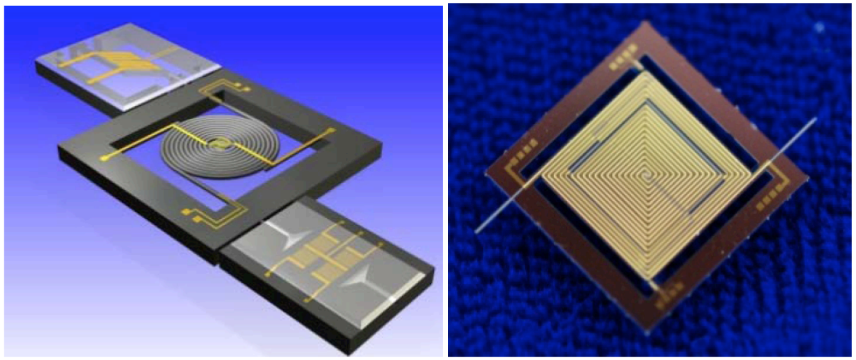


Figure 1: Left: Drawing of complete µGC analysis system. Right: A 25cm-long separation column with built-in fluidic interconnects.

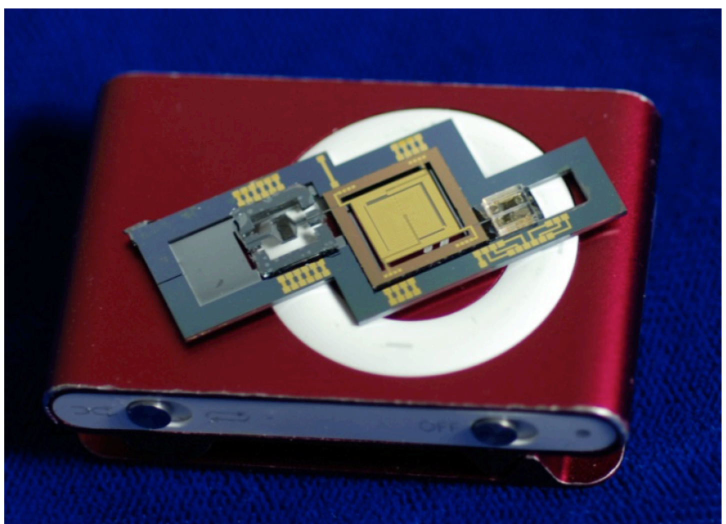


Figure 9: A 25cm separation column, single-bed preconcentrator, and chemi-resistive detector on a 2nd generation Apple iPod Shuffle about the size of the intended µGC system. The outer circle is about the size of a U.S. quarter.

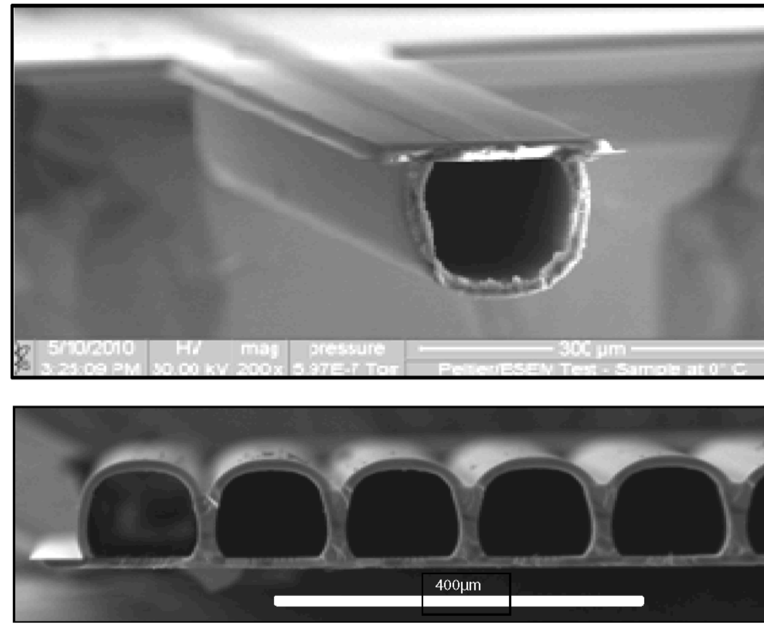


Figure 3: Cross-sections of the laser-cut fluidic interconnects and the column cross-section. The flow channel is 120µm across and 90µm deep.

K.T.M. Beach, S.M. Reidy, R.J.M. Gordenker, and K.D. Wise, A low-mass high-speed µGC separation column with built-in fluidic chip-to-chip interconnects, IEEE proc. 2011

Micro-Gas Chromatography Systems (GC-GC)

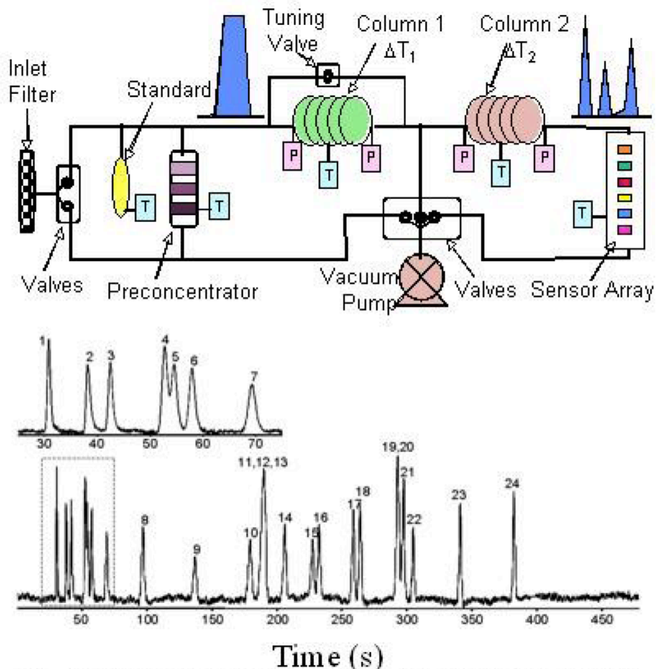
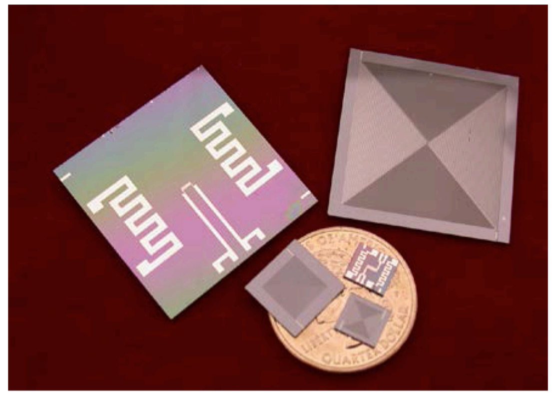


Fig. 1: Block diagram of a microfabricated chromatography-based gas analyzer (above), with a chromatogram on the separation of air-phase petroleum hydrocarbons.



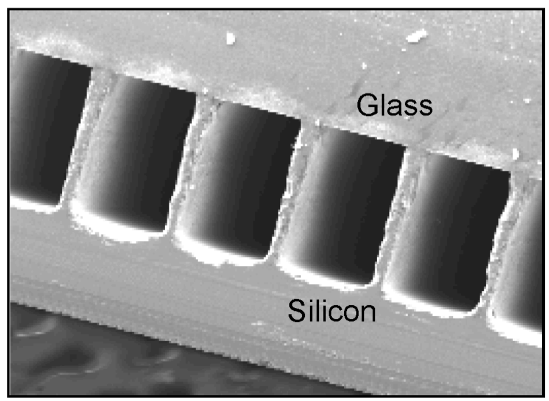


Fig. 4: 2D-GC columns (3m, 25cm, and 10cm) having optimized dimensions on a U.S. quarter, with heaters and sensors to allow closed-loop temperature program on their back surfaces.

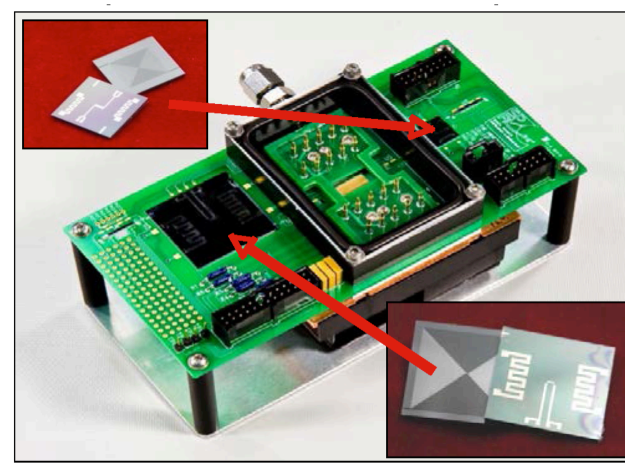


Fig. 6: The GCxGC system, with insets of the first-dimension column (bottom right) and the second-dimension column (top left).

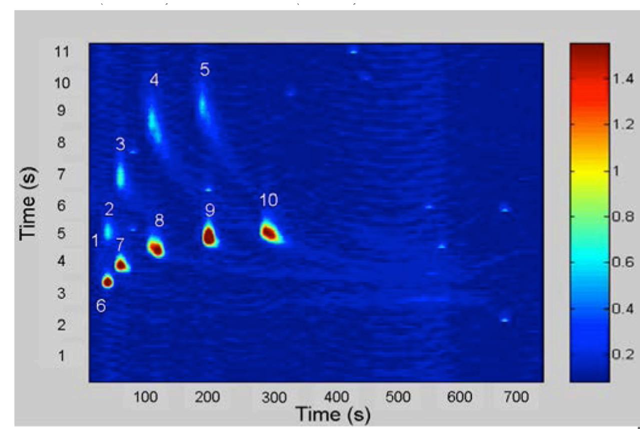


Fig. 7: A two-dimensional contour plot of a 10-component GCxGC separation using 3m- and 0.25m-long microcolumns and a two-stage thermal modulator. Alkanes are separated primarily by the first column (x-axis) and the ketones are separated primarily by the second column (y-axis). Color reflects peak height on the FID.

S. Reidy, S.-J. Kim, K. Beach, B. Block, E.T. Zellers, K. Kurabayashi, and K.D. Wise, A micro-fabricated two-dimensional gas chromatography system, 2010

Summary

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Possible Future Developments

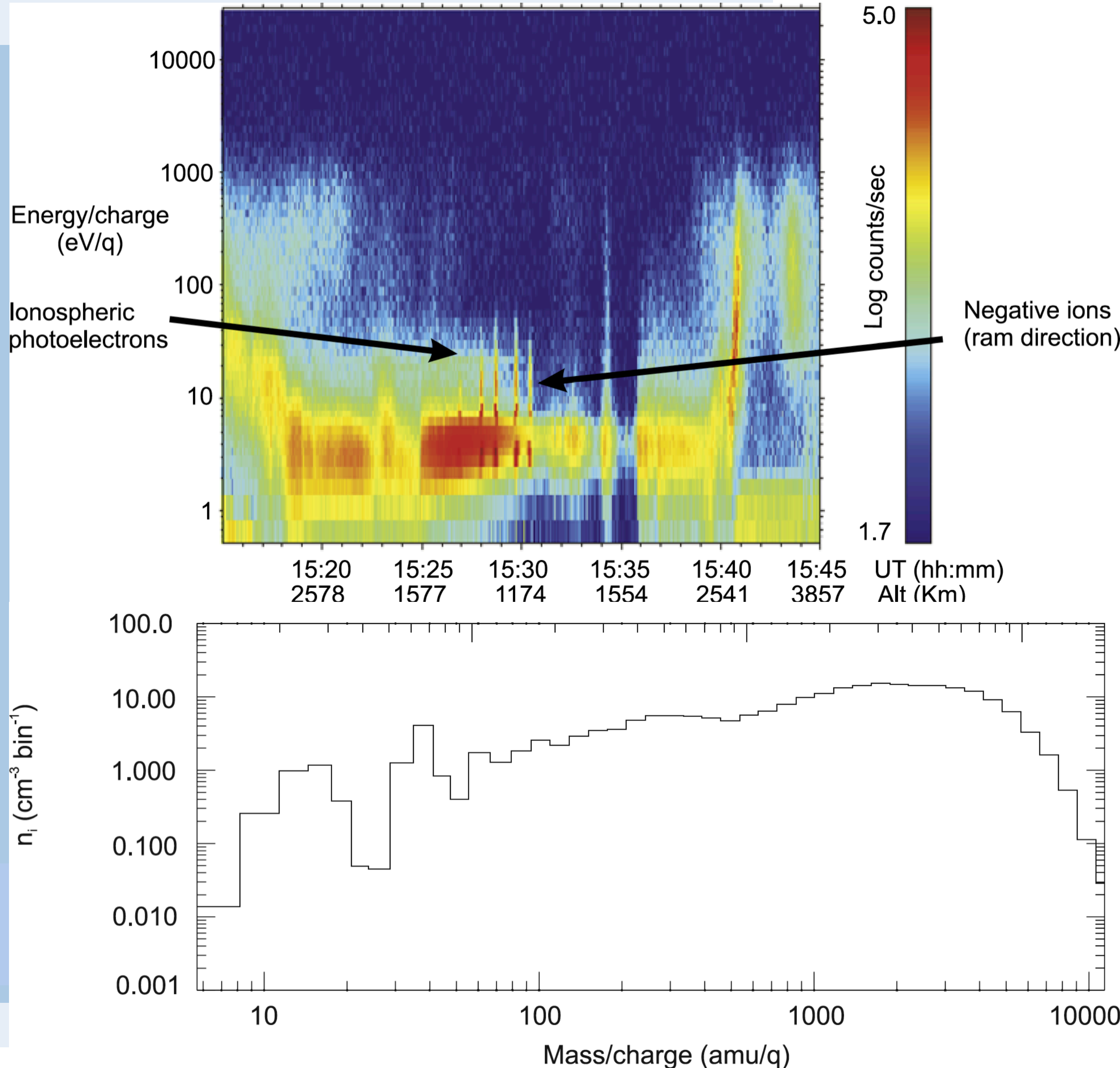
- Increase in sensitivity
  - Non-scanning instruments
    - Time of flight MS
  - Cryo trap
- Increased mass range
  - Time-of-flight MS
  - Orbitrap MS
- Increase in mass resolution
  - ROSINA instrument package
    - DFMS: Double focusing mass spectrometer
    - RTOF: Time-of-flight mass spectrometer
  - Multi-bounce TOF
  - Orbitrap MS
- Reduced complexity
- Reduced instrument resources
  - Micro-GC systems
  - TOF
  - Orbitrap

septembre 4, 2012

Negative Ions in Titan's Upper Atmosphere

- Negative ions in the upper atmosphere
- Typical mass groups
  - M: 10–30, 30–50, 50–80, 80–110, and 110–200 amu
- Ions with very high masses
  - M < 10'000 amu
- Important for the formation of organic-rich aerosols (tholins) eventually falling to the surface

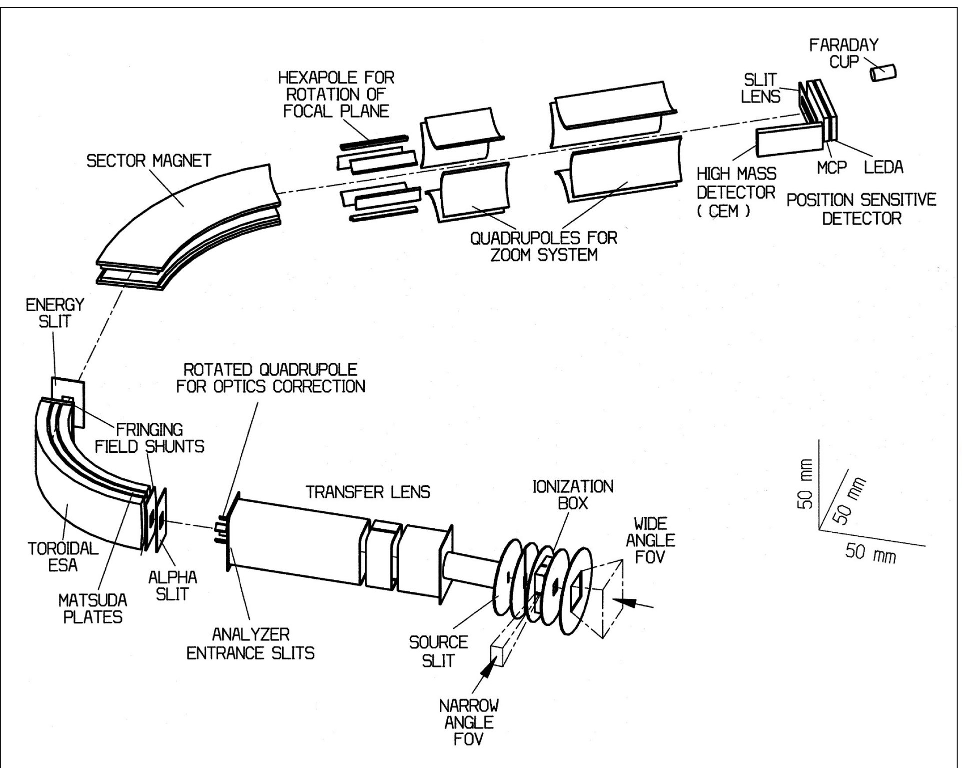
A. Coates et al., Geophys. Res. Lett. 34 (2007) L22103

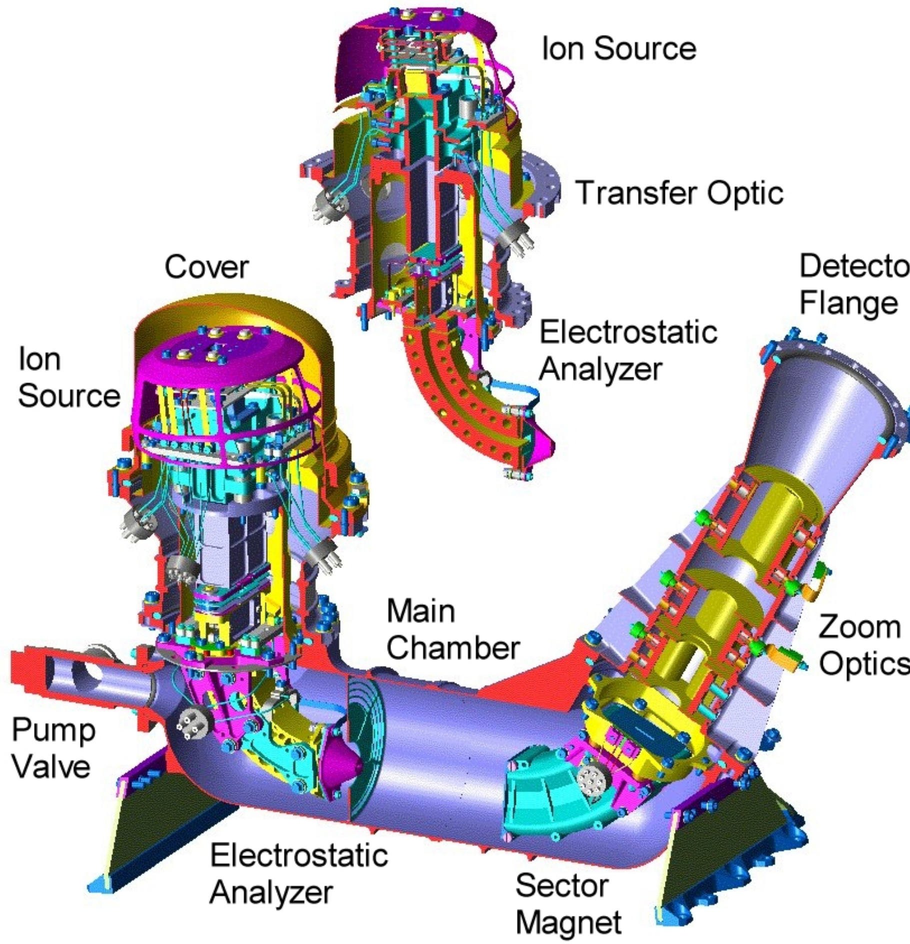


Reduced Complexity

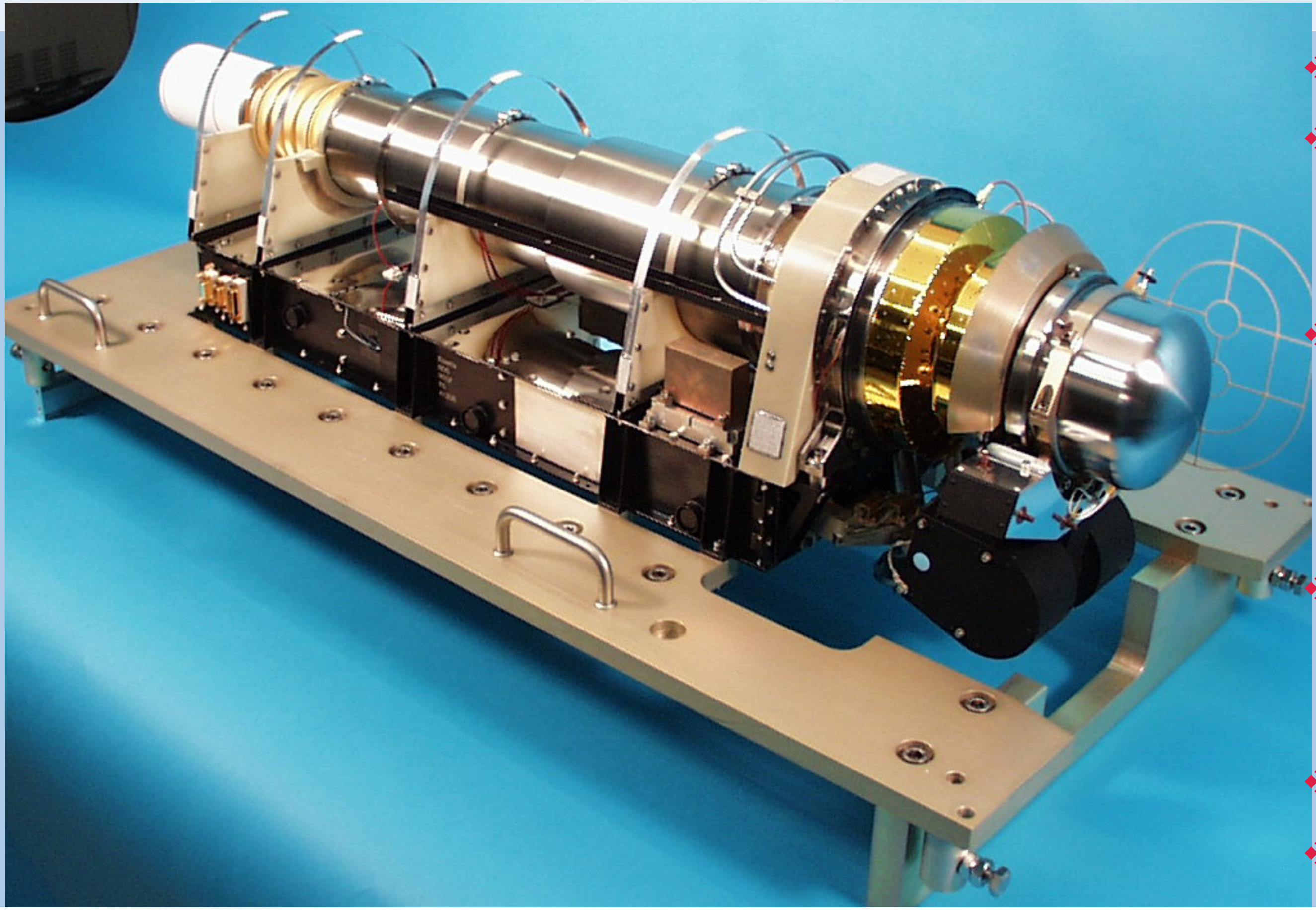
Reduced Complexity

Rosetta / ROSINA / DFMS Sensor





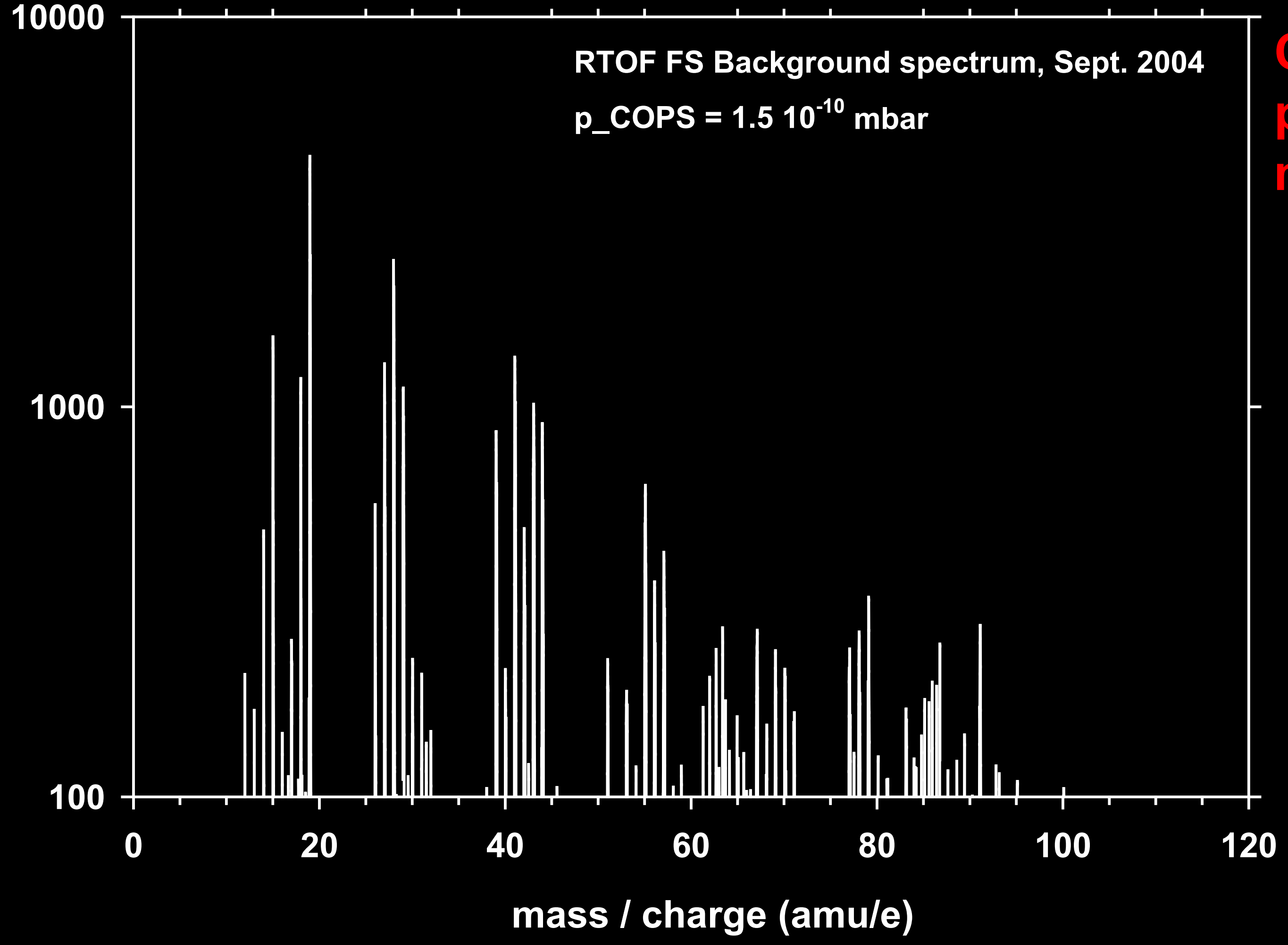
RTOF / ROSINA on Rosetta Mission



- RTOF design: 1996
- Mass resolution: m/ Δm = 1500 ... 4500 (depending on mode)
- Mass range: 1 ... 500 amu (in principle unlimited, because TOF instrument)
- Sensitivity: 10^{-4}... 10^{-3} A/mbar (depending on mode)
- Mass: 14.7 kg
- Power: 28 W

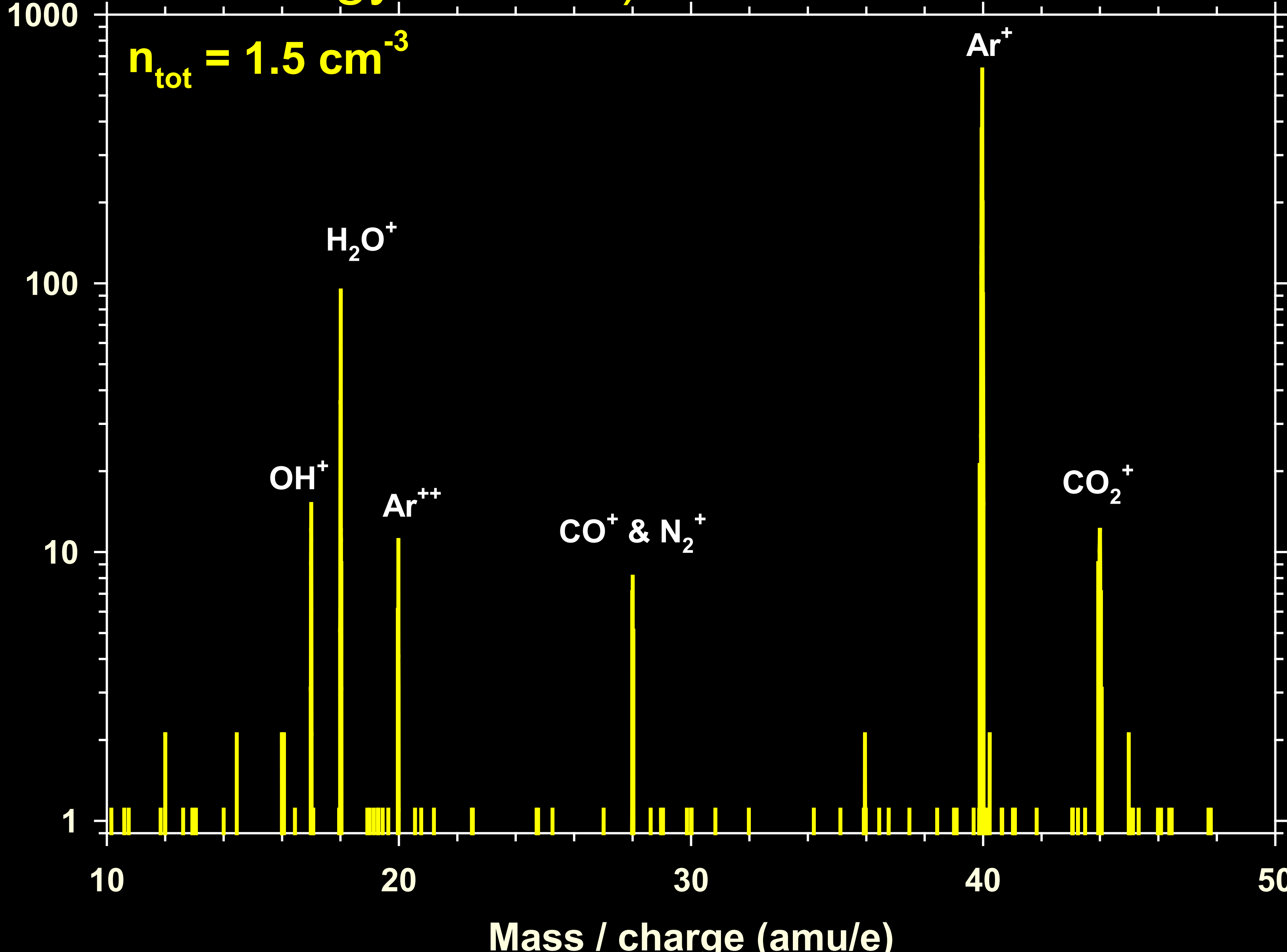
H. Balsiger, et al., "ROSINA - Rosetta Orbiter Spectrometer for Ion and Neutral Analysis," Space Science Review 128 (2007), 745–801.
S. Scherer, K. Altwegg, H. Balsiger, J. Fischer, A. Jäckel, A. Korth, M. Mildner, D. Piazza, H. Rème, and P. Wurz, A novel principle for an ion mirror design in time-of-flight mass spectrometry, Int. Jou. Mass Spectr. 251 (2006) 73–81.

RTOF / ROSINA on Rosetta mission



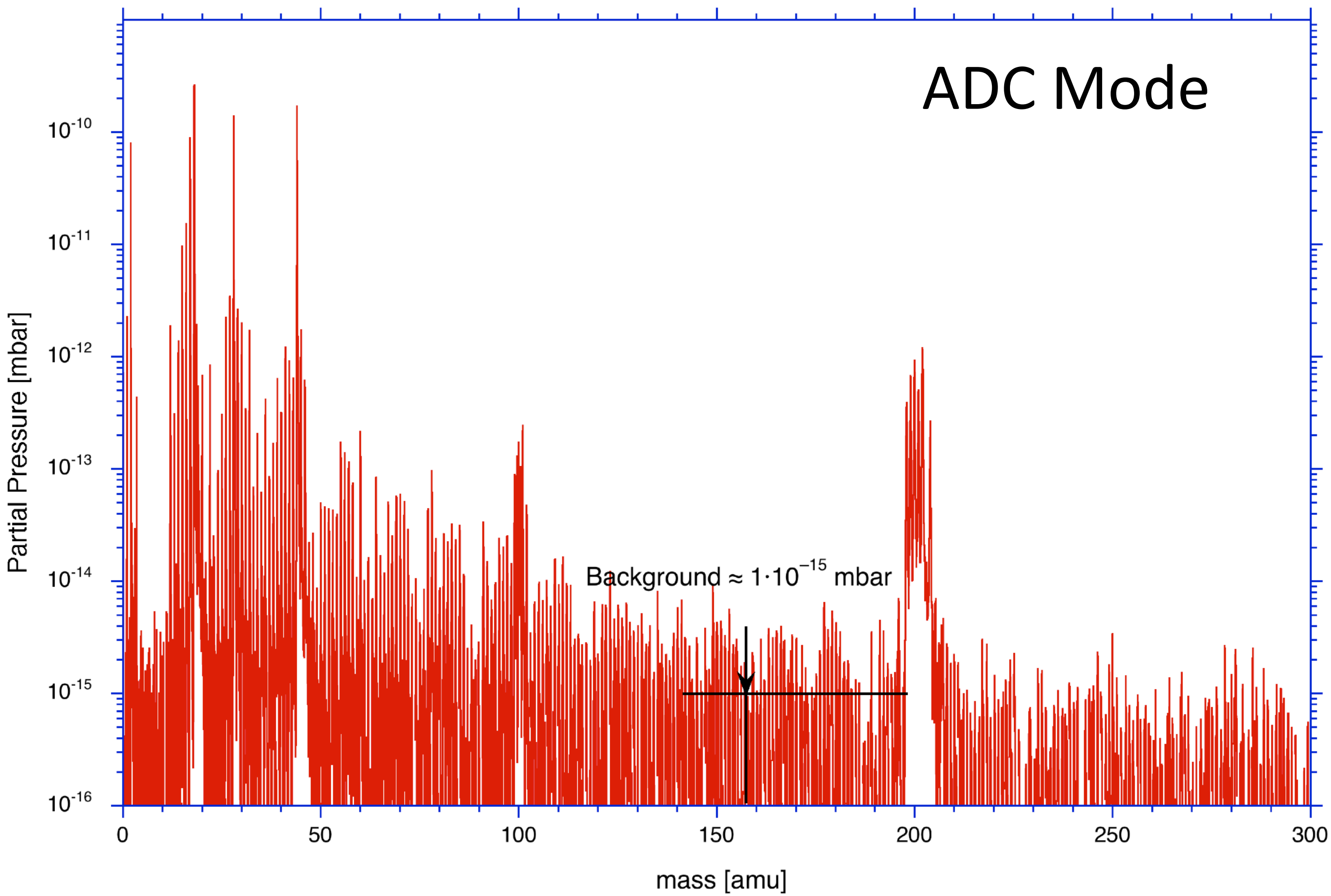
Cruise phase data:
$p_{COPS} = 1.5 \cdot 10^{-11}$ mbar

RTOF/ ROSINA ion spectrum
Ion energy < 15 eV)



Prototype Results: Sensitivity

NGMS Sensitivity, static, ADC Mode



Prototype Results: Sensitivity

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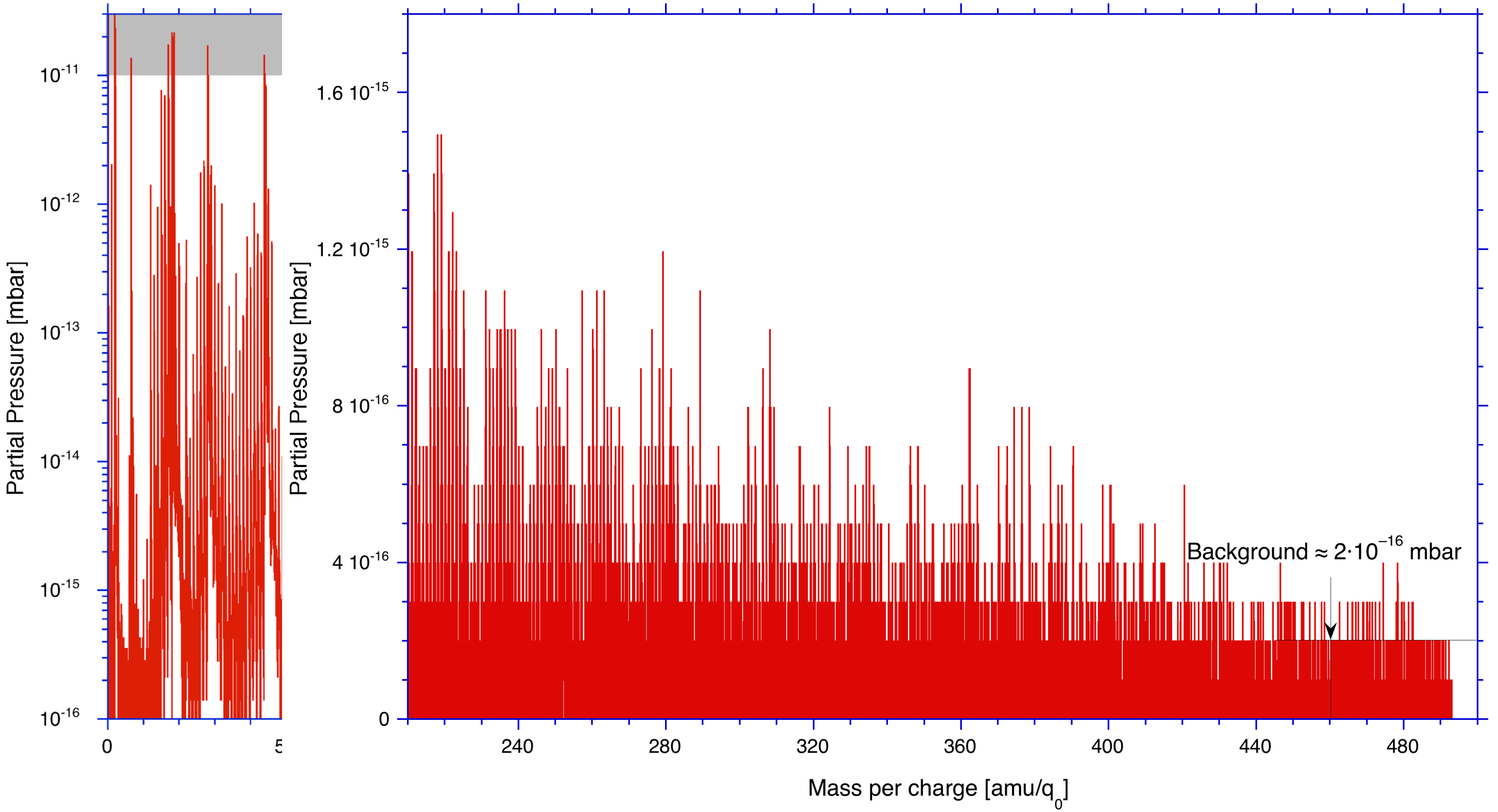
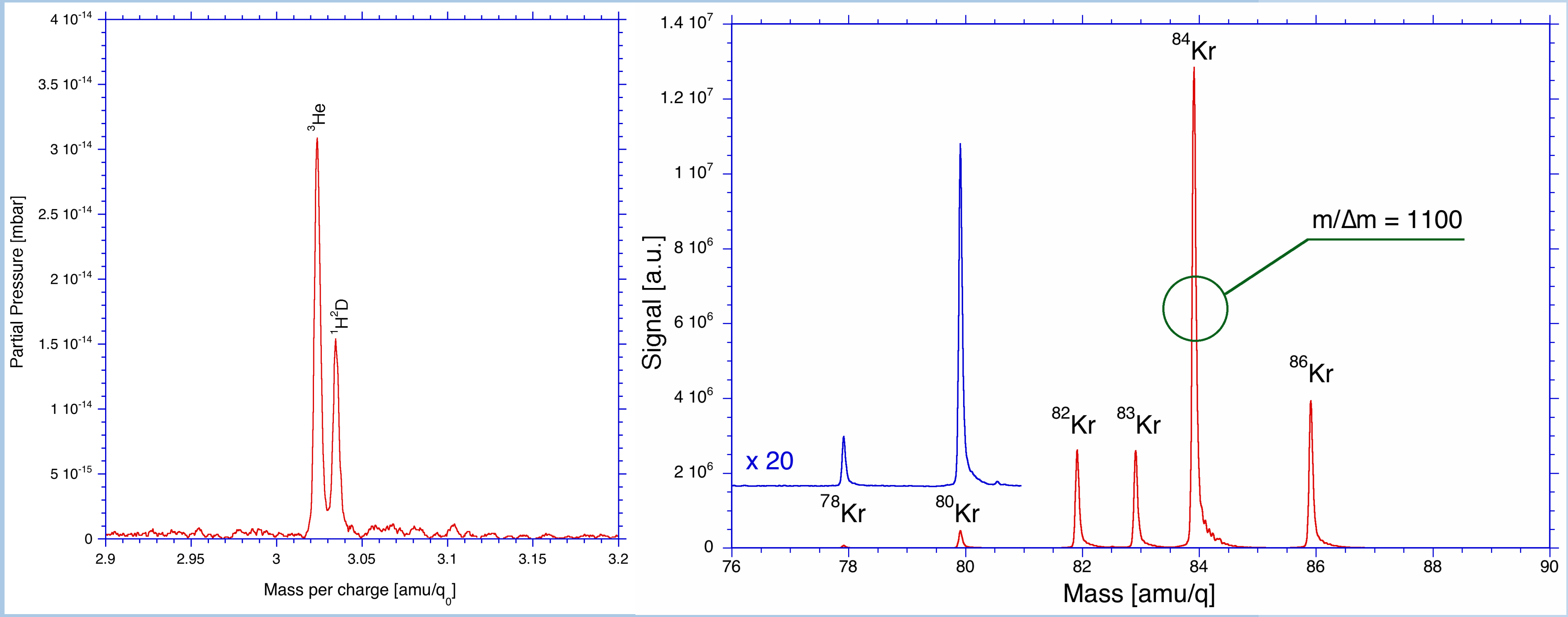
NGMS Sensitivity, static, TDC Mode



Prototype Results: Mass Resolution

Neutral Gas mass Spectrometer (NGMS)



P. Wurz, D. Abplanalp, M. Tulej, and H. Lammer, **"A Neutral Gas Mass Spectrometer for the Investigation of Lunar Volatiles,"** Planet. Sp. Science (2012) in print.

Neutral Gas Mass Spectrometer
Luna-Resurs / Luna-Glob

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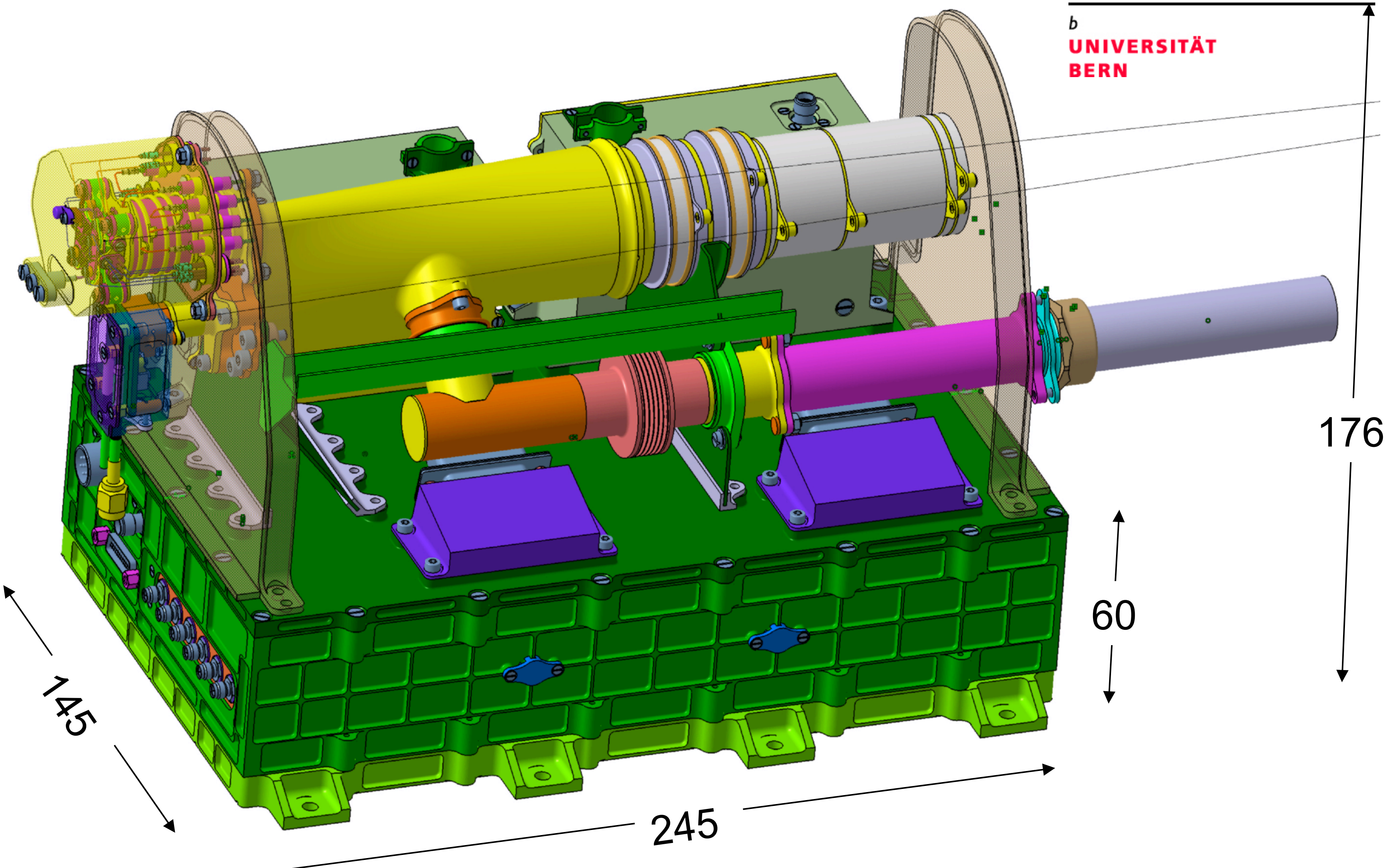

P. Wurz, D. Abplanalp, M. Tulej, and H. Lammer, "A Neutral Gas Mass Spectrometer for the Investigation of Lunar Volatiles," Planet. Sp. Science (2012) in print.

Summary

- We developed a mass spectrometer for gas analysis of atmospheres and exospheres
  - Mass range 1 – 1000 amu
  - Sensitivity ≈ 1 cm^{-3} in 10 s integration
  - Prototype successfully used for stratospheric research
    - Abplanalp et al. Adv. Sp. Res. 2010, Wieser et al. Adv. Sp. Res. 2010
  - Flight design for Luna-Resurs
    - Mass 3.5 kg, power 17W
- Luna-Resurs: GC-MS
  - Investigation of the volatiles contained in the soil by GC-MS analysis
  - Investigation of the lunar exosphere
    - Contamination by spacecraft
    - The Rosetta experience: Schläppi et al. JGR 2010

PEP-NU Design

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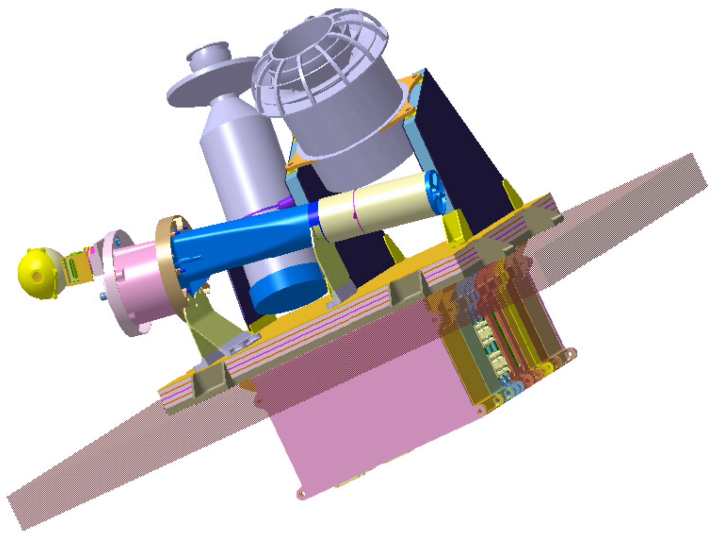

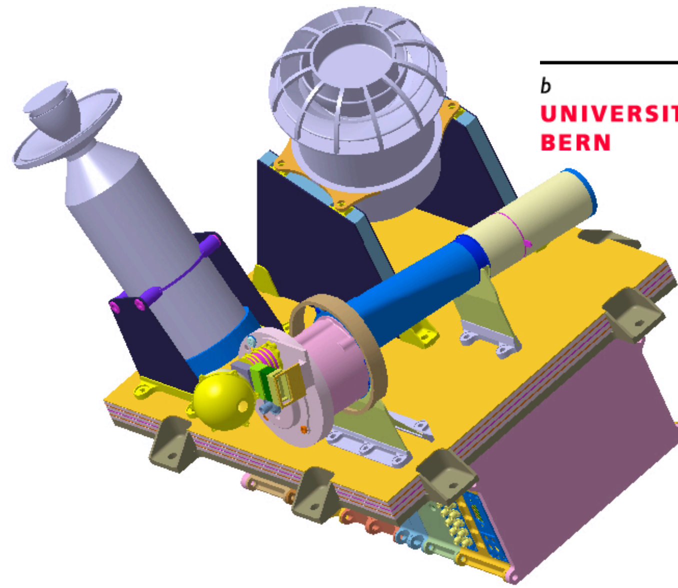

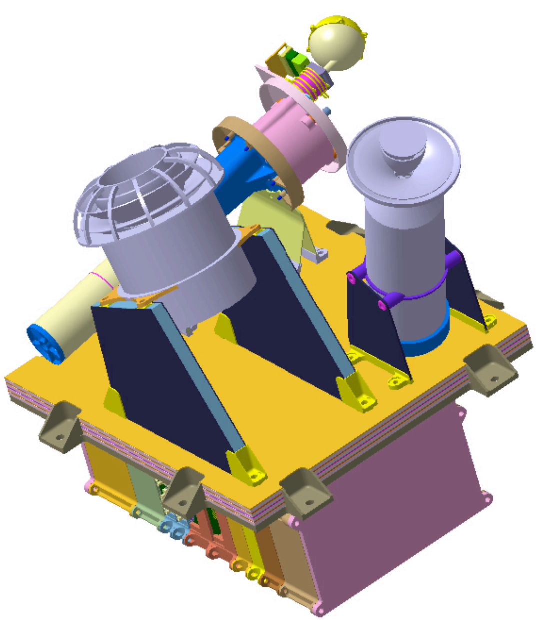

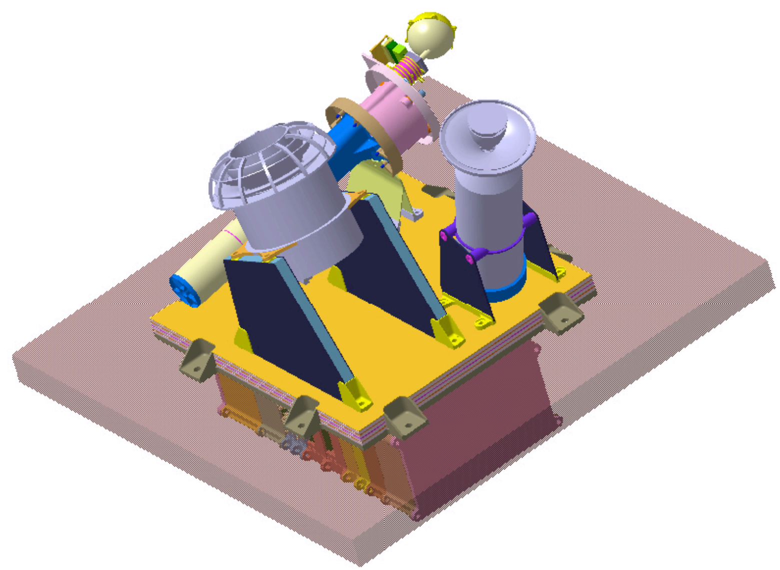

Summary

- PEP-NU Design overview
  - NIM progress since PM #5
    - Luna-Resurs / Luna-Globe design
    - Prototype measurements
  - PEP-NU no progress
    - Wait for input on LEN and ELS
    - Decide on instrument placement
- Radiation shielding
  - Detailed radiation analysis for PEP-NU on JGO
    - JGO-PEP-TN-0901-I1R0 (Radiation Analysis PEP-NU).pdf
  - Total dose increase
    - From 38 to 50 krad Si behind 20 mm Al equivalent.
  - Assessment of Europa flybys

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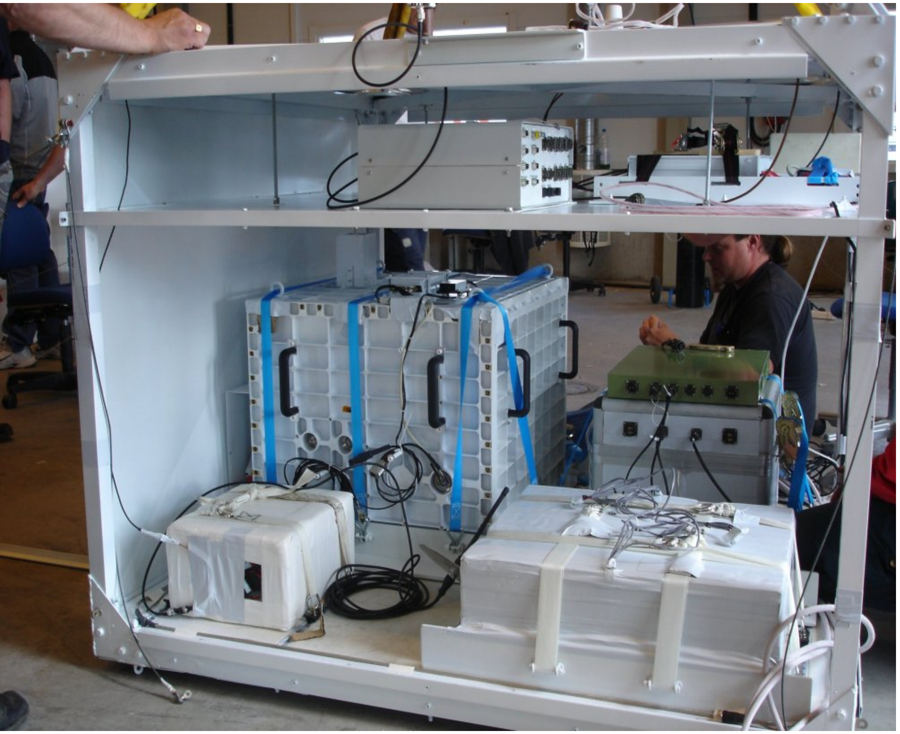
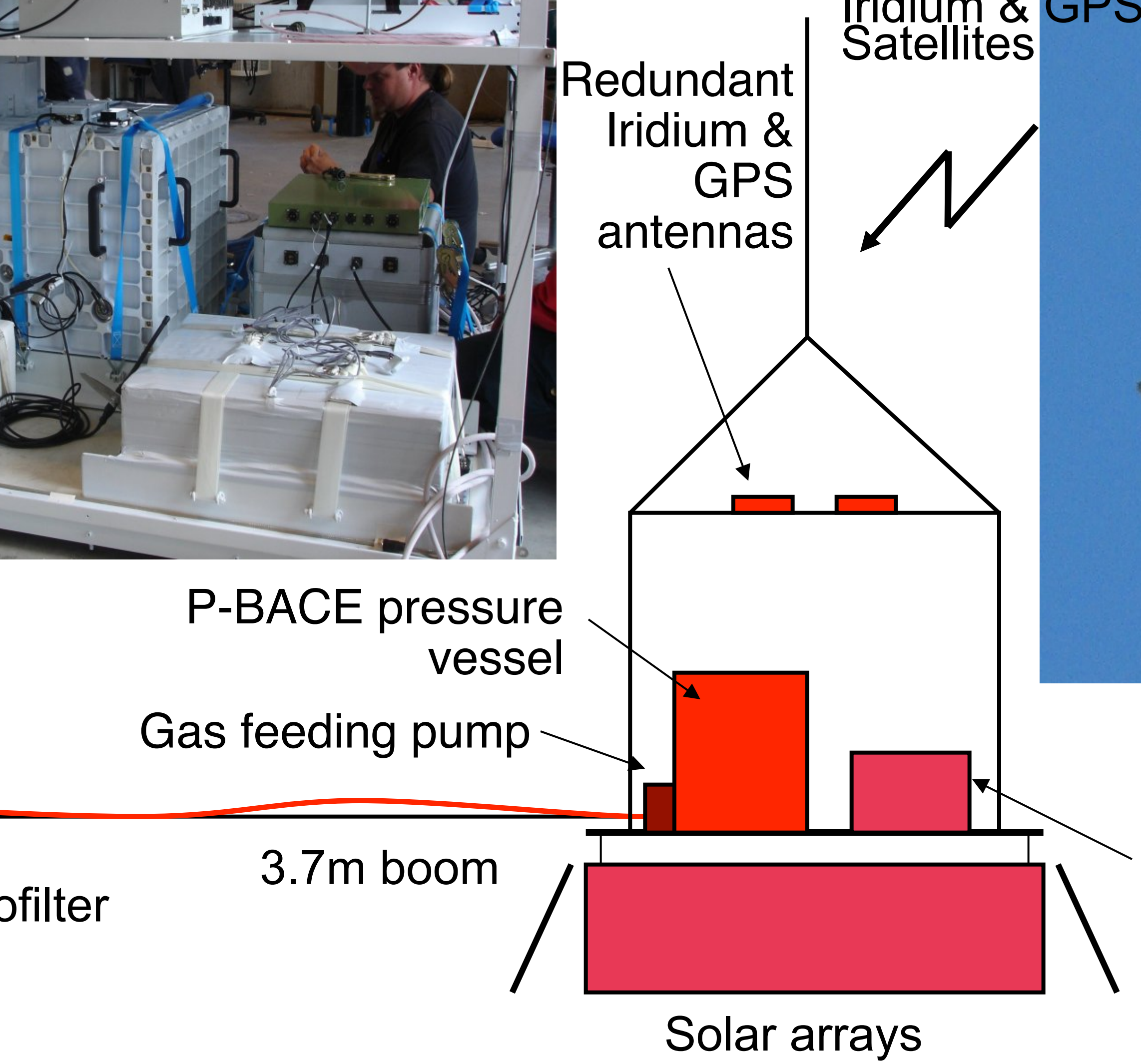
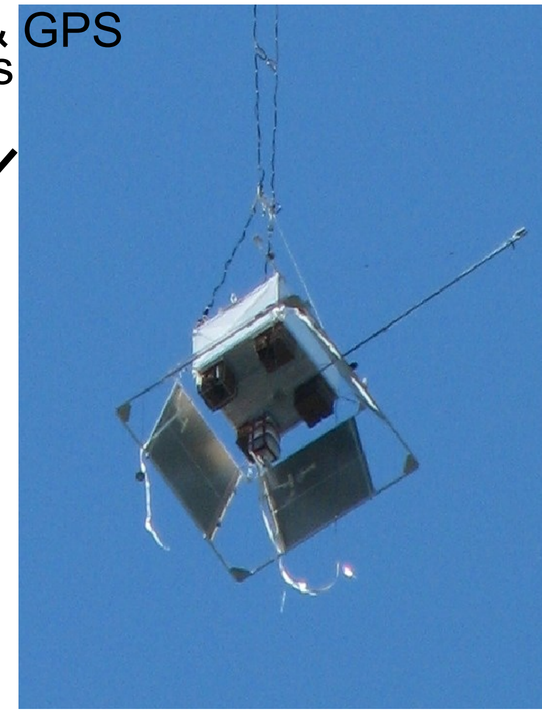
P-BACE on the MEAP platform







MEAP flight path

- Balloon provided by Esrange Space Center to test beyond line of sight flight
- Semicircular flight following the summer polar vortex
- Launched from Esrange, Sweden on 28 June 2008
- 116 hours flight time
- Altitude 33 ... 38 km
- Landed in Canada, near Umingmaktok, on 3 July 2008.
- Recorded ~ 4500 mass spectra in stratosphere

Background image: NASA, http://visibleearth.nasa.gov/

P-BACE quicklook data, dynamic range

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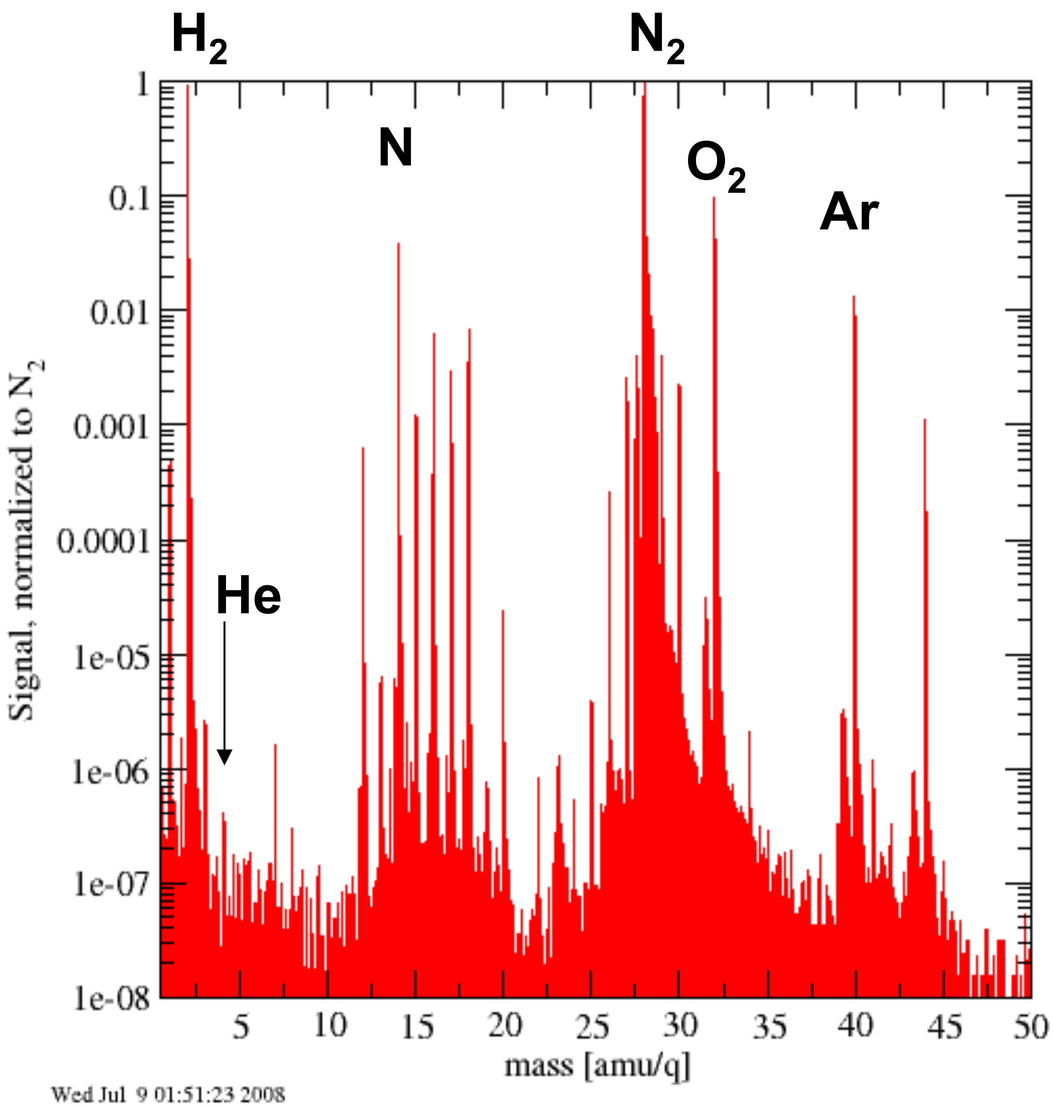

- Raw data
- No background subtracted

- Dynamic range: 6–7 orders of magnitude per spectrum
- Mass range: 1–1000 amu/q

- D. Abplanalp, P. Wurz, L. Huber, I. Leya, E. Kopp, U. Rohner, M. Wieser, L. Kalla, and S. Barabash, Adv. Space Res. 44 (2009) 870-878.