Mobile High-Resolution Multiple-Reflection Time-of-Flight Mass Spectrometer for in-Situ Analytics

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Agenda:

- **Motivation**
- **MR-TOF-MS**
- **Applications**
- **Conclusion**

Motivation

- Mobile MS is a promising field with important applications – however current instruments are limited to low or medium resolution

- **(Ultra-) high resolution** ($m/\Delta m > 10^5$) offers fundamental advantages
  - ➔ Resolving isobars
  - ➔ Isotopic resolution at very high mass
- **Accurate Mass** ($\delta m/m < 1$ ppm)
  - ➔ Determination of composition and structure

- Our goal is to develop a **mobile high-resolution mass spectrometer**
  - Here: transportable device
  - Future: portable device (?)

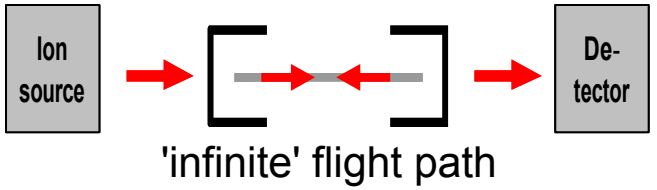
Multiple-Reflection Time-of-Flight MS (MR-TOF-MS)

Time-of-Flight Mass Spectrometry:

- No magnet → low weight → mobility
- Short flight time → reduced vacuum requirements → low weight compared to other HR-MS
- No principle high mass limit
- Mass resolving power and mass accuracy almost mass-independent
- Short cycle time → compatibility with chromatography / MS

- Single-reflecting: m/Δm not large enough →

Multiple-Reflection



Mass resolution ~ overall time-of-flight

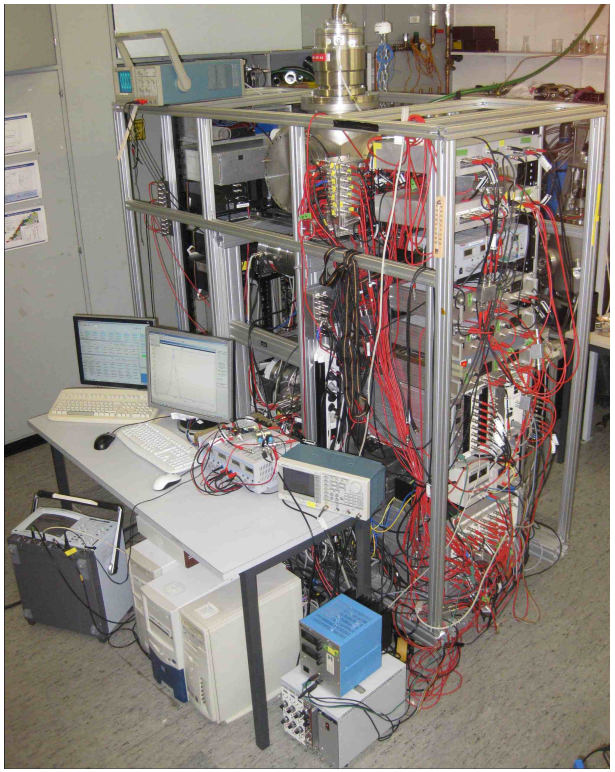
$$R_m = \frac{m}{\Delta m} = \frac{T}{2\Delta T} = \frac{NT_{turn}}{2\sqrt{(N\Delta T_{turn})^2 + \Delta T_{initial}^2}} = \frac{T_{turn}}{2\sqrt{(\Delta T_{turn})^2 + (\Delta T_{initial}/N)^2}}$$

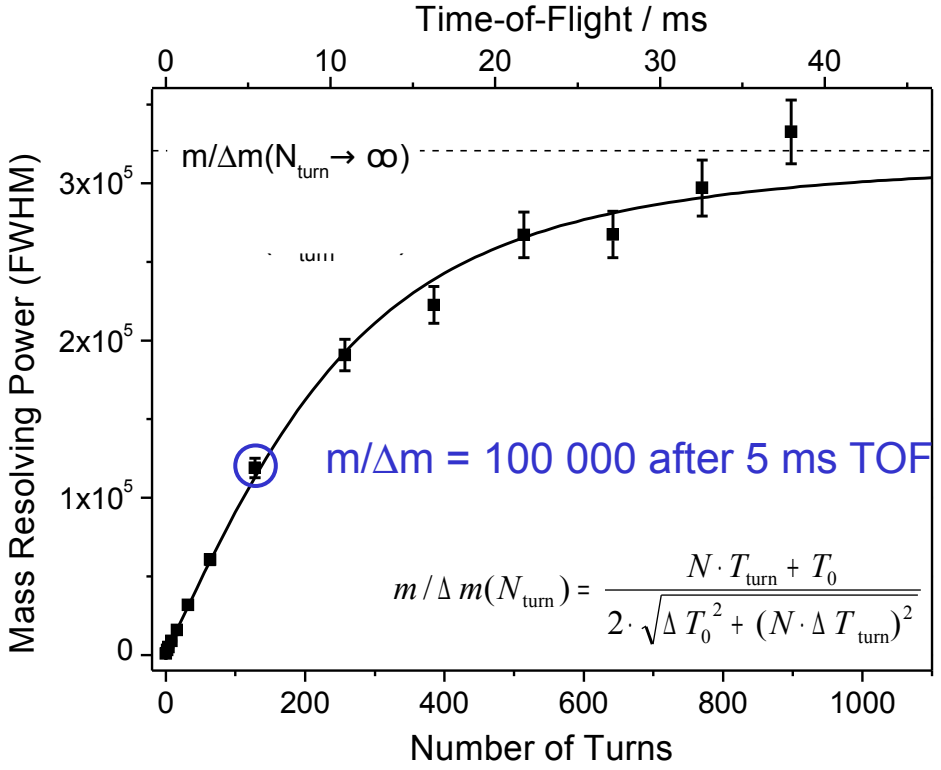
Increasing TOF → increasing resolution

Unambiguous mass range

$$\frac{m_{max}}{m_{min}} = \left(\frac{N}{N-1}\right)^2$$

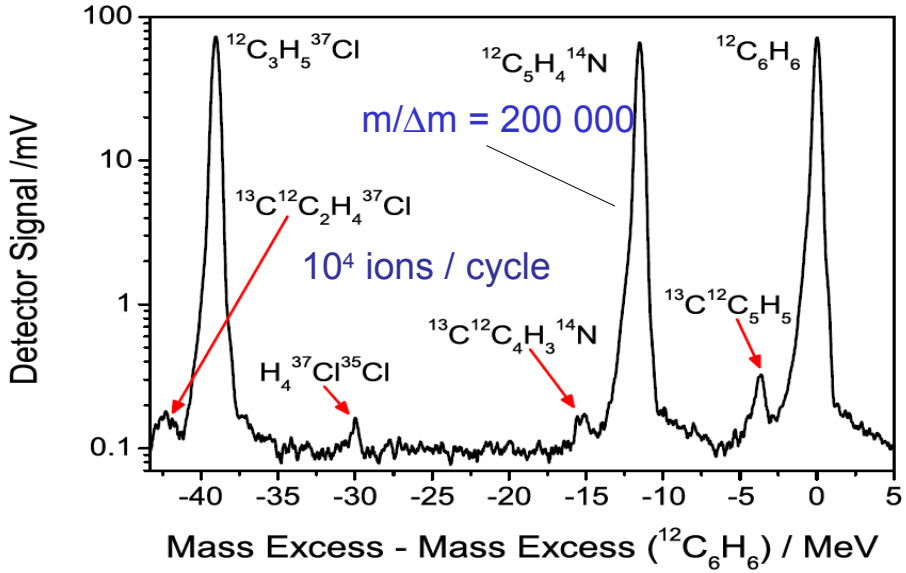
MR-TOF-MS in Nuclear Physics





Prototype for applications in nuclear physics

- Mass resolving power: 600 000
- Mass accuracy ~ 10^{-7}
- Single ion sensitivity
- Ion capacity ~ 10^6/s
- Measurement duration ~ 10 ms
- Isobar separator



W.R. Plaß et al., Nucl. Instrum. Methods B 266 (2008) 4560
T.Dickel, PhD thesis, JLU Gießen, 2010

AmbiProbe: In-Situ Analytics

Ion Sources

Ion Transport

MS

Applications

Research project AmbiProbe

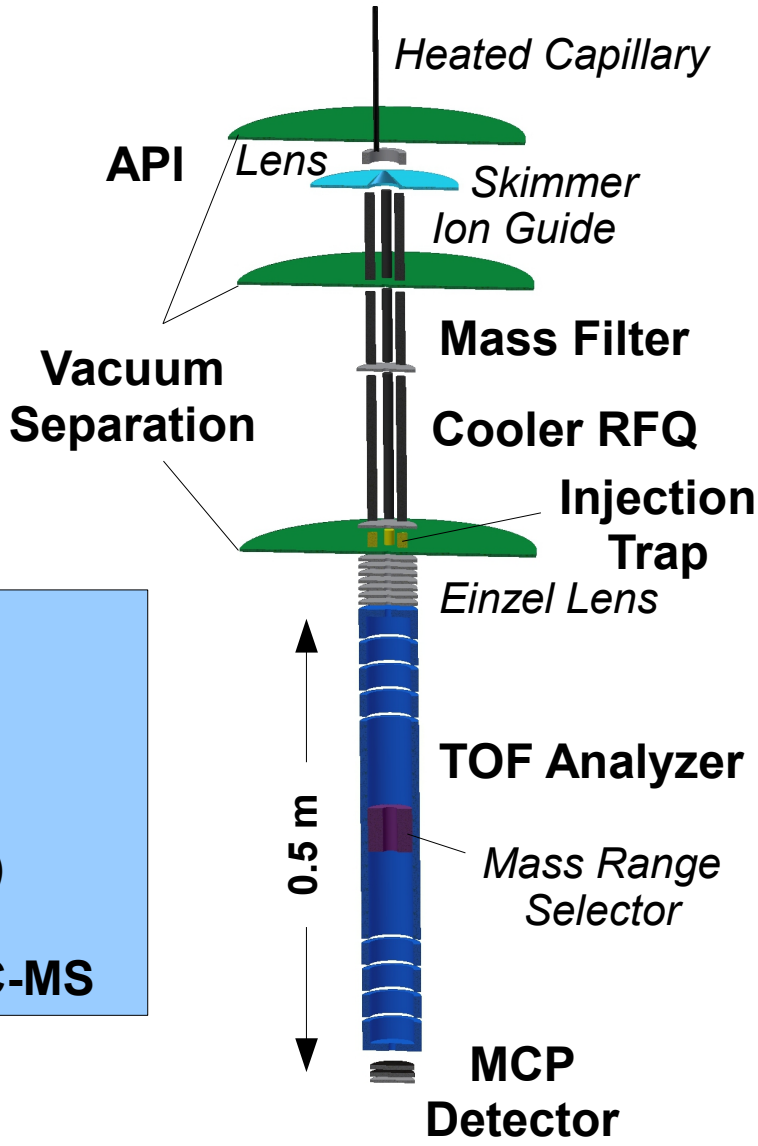
- 'LOEWE' exellence initative by State of Hesse, Germany
- Meassurement 'in situ' and online
- No sample preparation
- Opens up new investigation fields
- Interdisciplinary: chemistry, biology, geology, pharmacy & physics
- Applications in:
  - Health
  - Environmental research
  - Climate research
  - Security

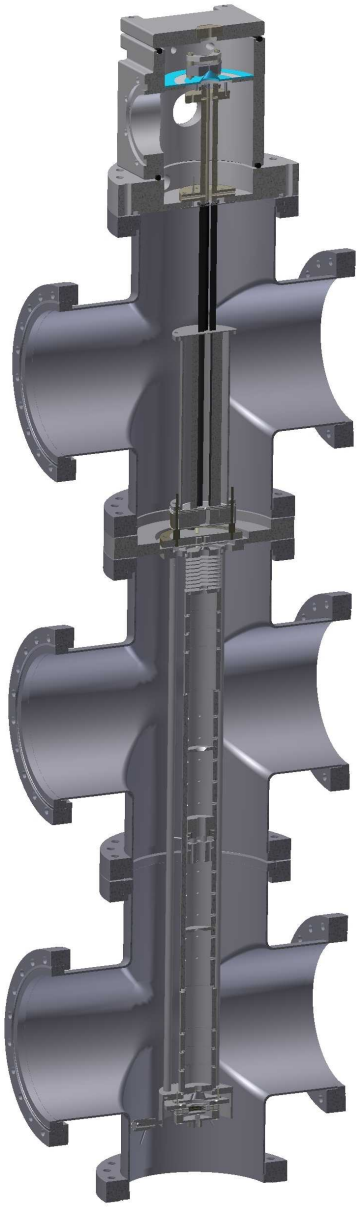



MR-TOF-MS: Design

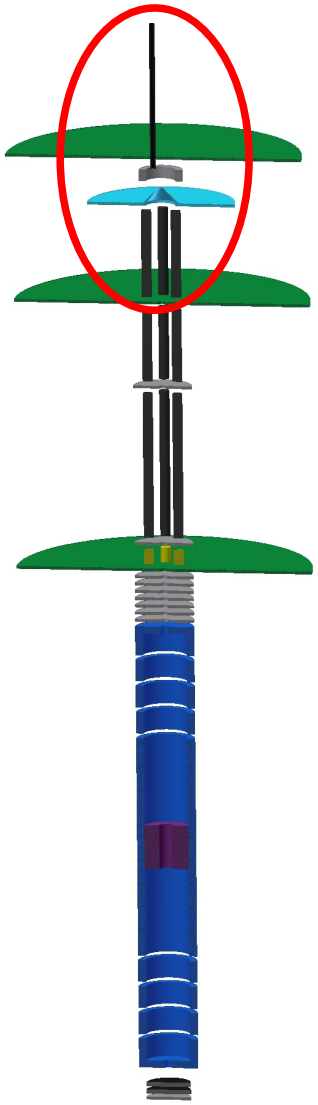
Design goals

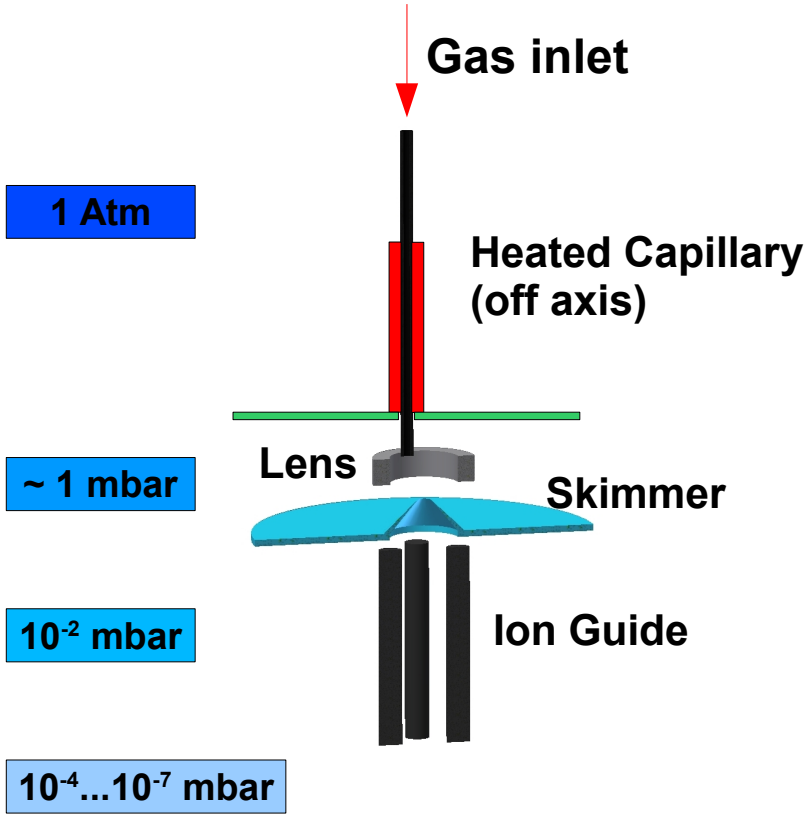
- **Mobile**
- **m/Δm > 100 000**
- **δm/m < 1 ppm**
- **High masses (>>1000)**
- **Repetition rate ~ kHz**
  → potential for LC/GC-MS

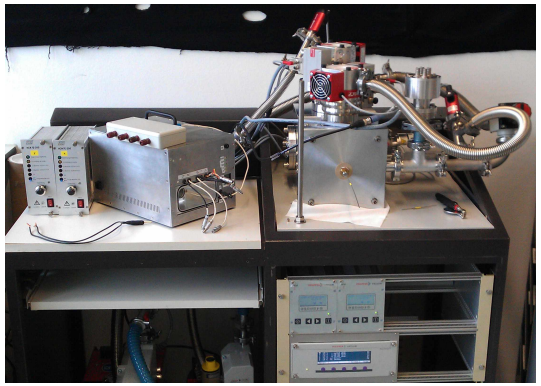


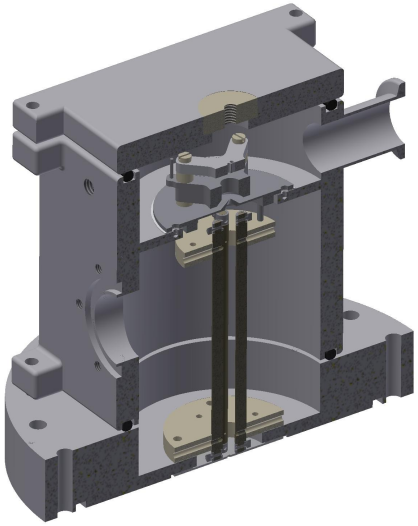


Atmospheric Pressure Interface (API)





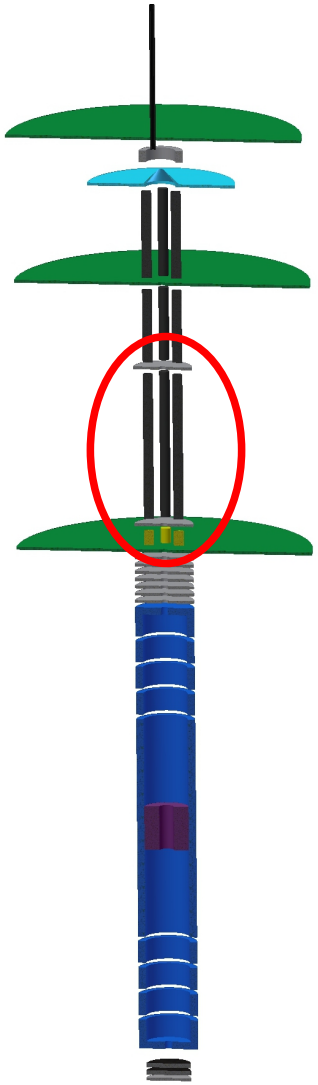


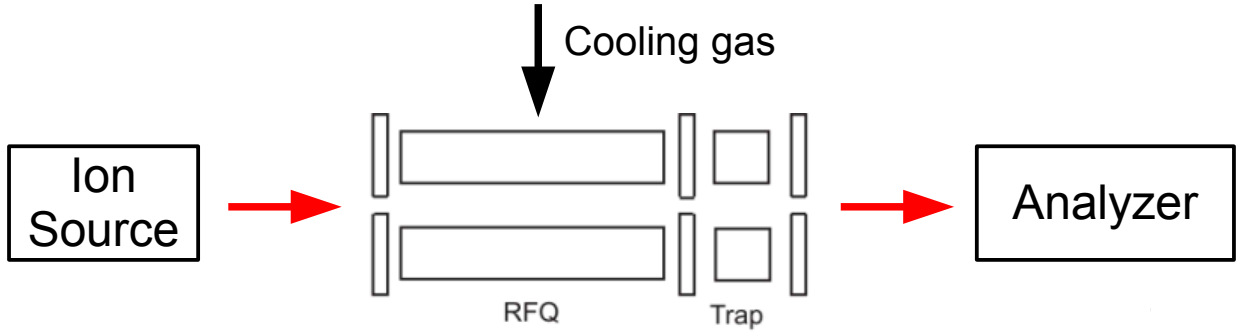


- Sample introduction
  10^{3}mbar ⟶ 10^{-4}...10^{-7}mbar
- Compatible with various ion sources
  ESI, DESI, REIMS, …
- Coupling to LC/GC
- Under commissioning

Collaboration with Z.Takats et al.

Trap System





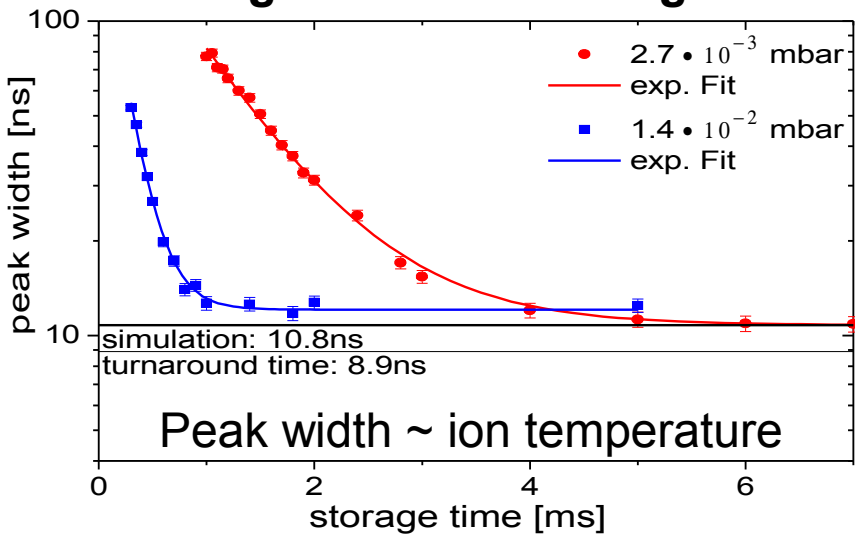
Cooler RFQ

- Encapsulated
- Cooling gas inlet
- Adjustable pressure (10^{-2} – 10^{-4} mbar)

Injection Trap

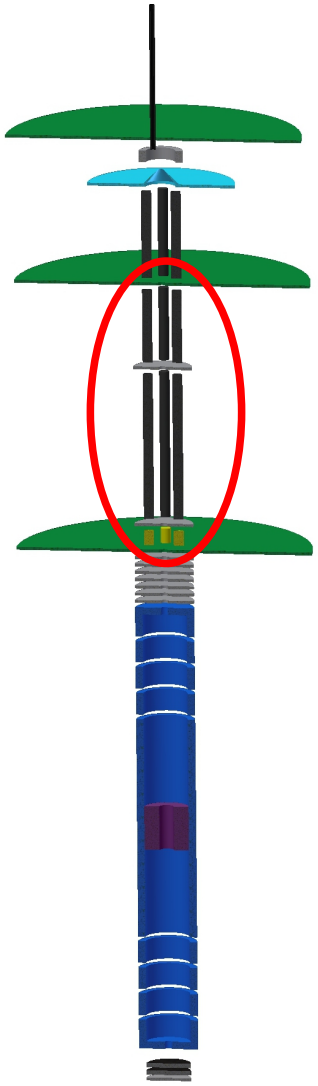
- Ion capacity ~ 10^5 ions/cycle
- RF switch-off for extraction

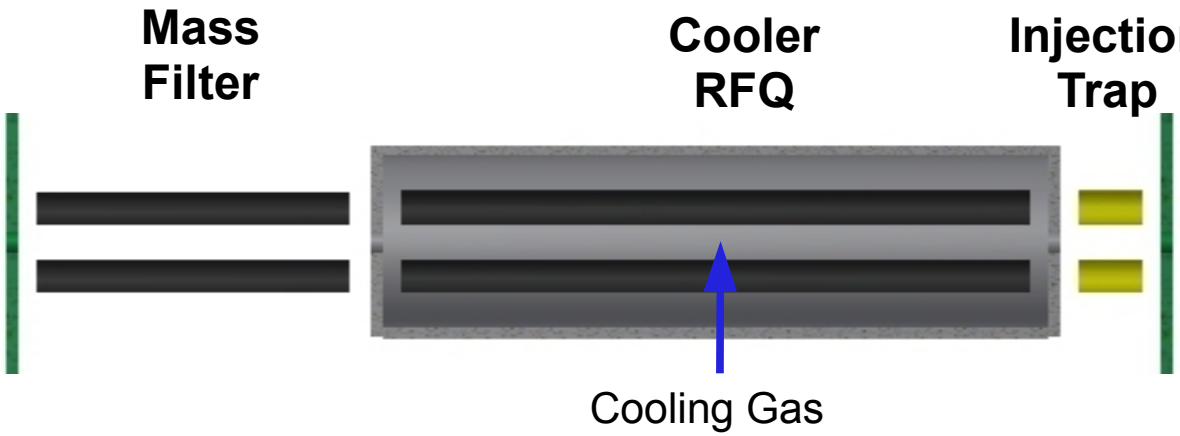
Cooling of ^{133}Cs vs Storage Time



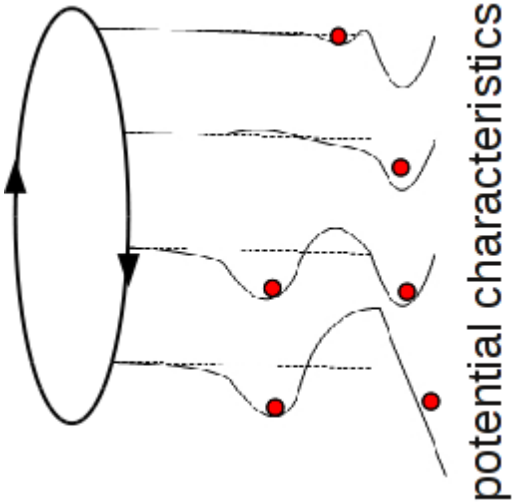
K.Reinheimer, Diploma thesis, JLU Giessen, 2008

Advanced RFQ Beam Preparation System



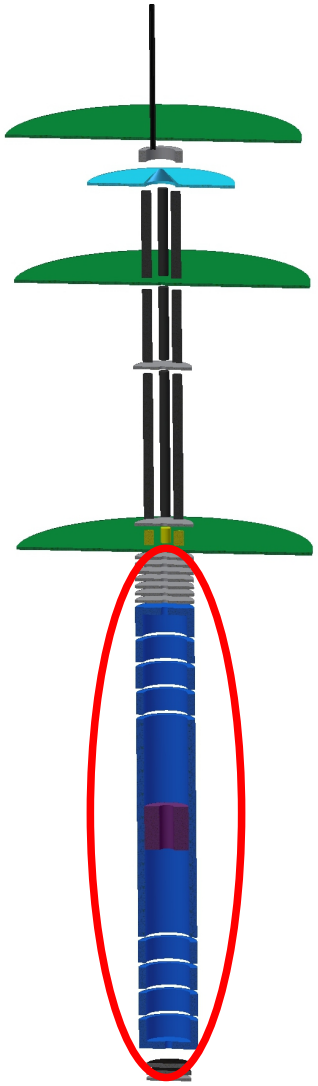


1. Capture of cooled ions
2. Transfer to injection trap
3. Cooling in injection trap & pre-capturing
4. Injection to analyzer & pre-capturing

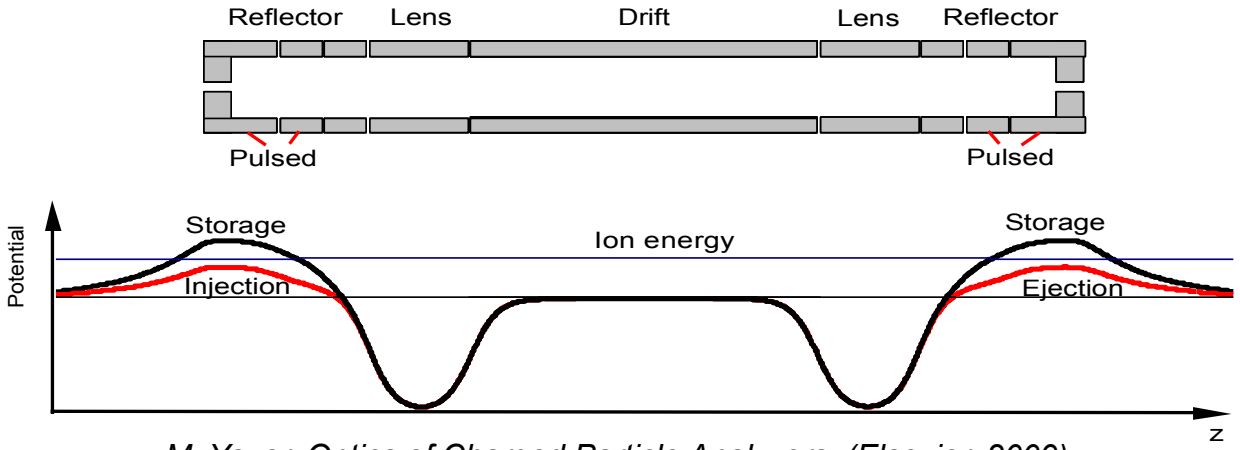


- Connection to API
- Full duty cycle
- Mass filter resolution ~ 100
- MS/MS capability
- Status: design & simulations underway (SIMION, ITSIM)

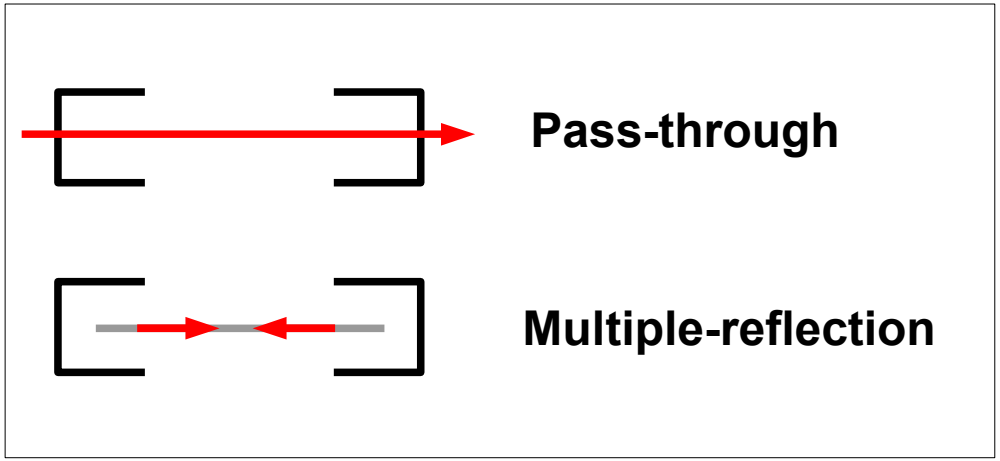
Time-of-Flight Analyzer



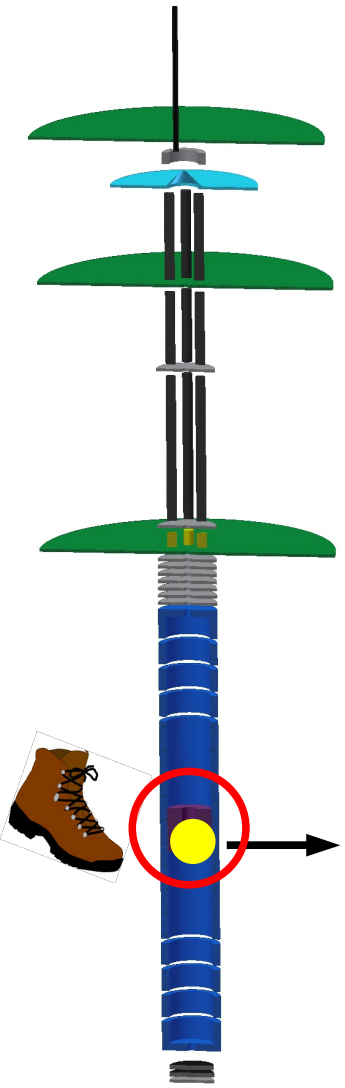
Analyzer with gridless electrostatic reflectors based on a four electrode design



M. Yavor, Optics of Charged Particle Analyzers, (Elsevier, 2009)



Mass Range Selector



Ions can overtake → Ions with different mass (and turn number *N*) can have same TOF:

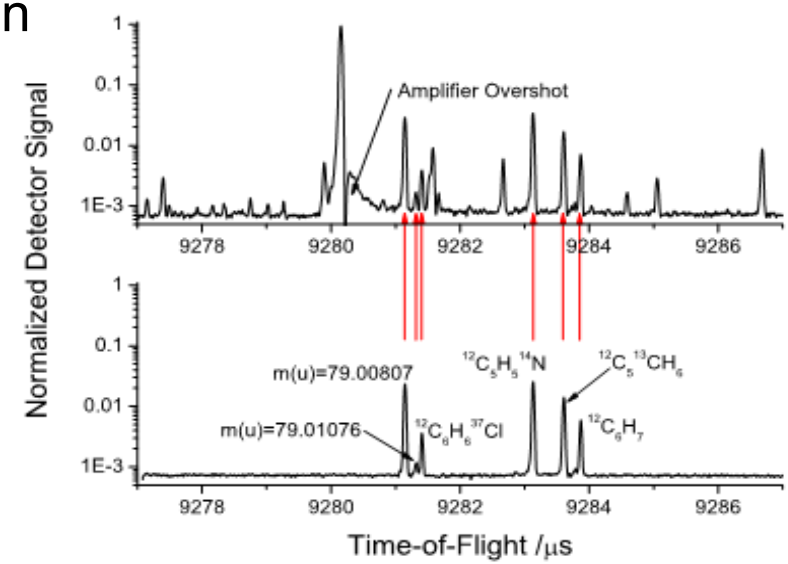
$$T_{m1}(N) = T_{m2}(N \pm x) \quad \rightarrow \quad \frac{m_{max}}{m_{min}} = \left(\frac{N}{N-1}\right)^2$$

Mass Range Extension

- Software disentanglement
- Single turn (m_{max}/m_{min} ~ 4, m/Δm > 2000)
- Zoom mode
- Scan mode
- Ion optical mass range extension

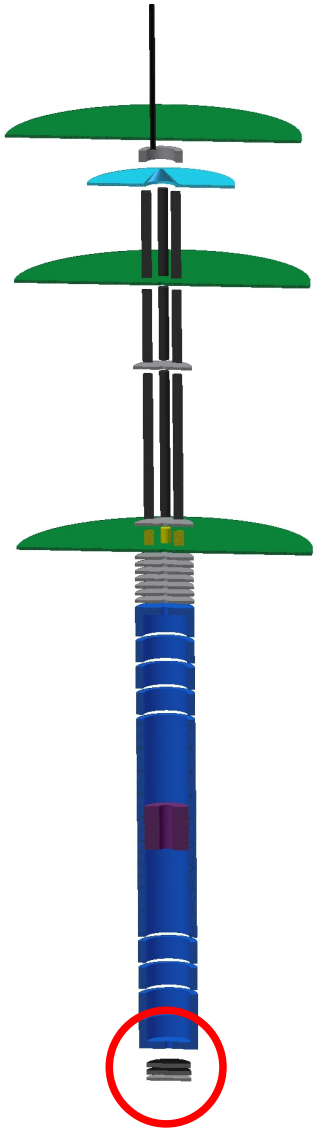
Mass Range Selector (MRS)

- Purifies spectrum
- Makes spectrum unambiguous
- Tool for mass range investigations

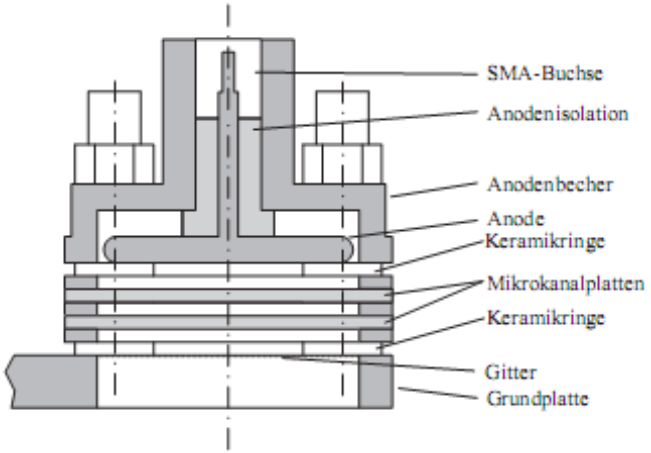


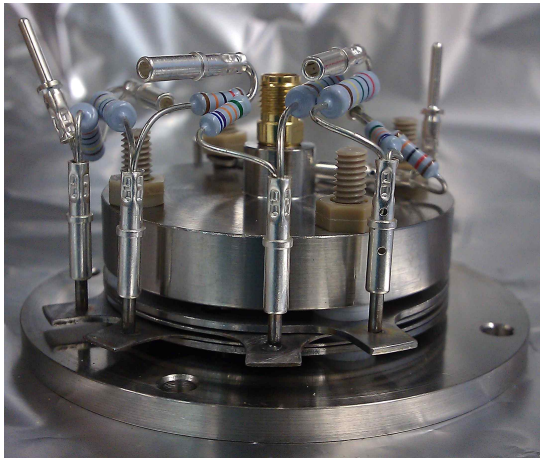
T.Dickel, PhD thesis, JLU Gießen, 2010

Detector



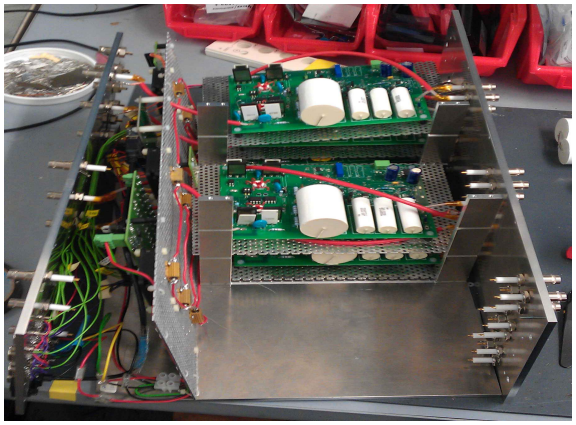
Chevron arrangement of Micro-Channel-Plates (MCP)



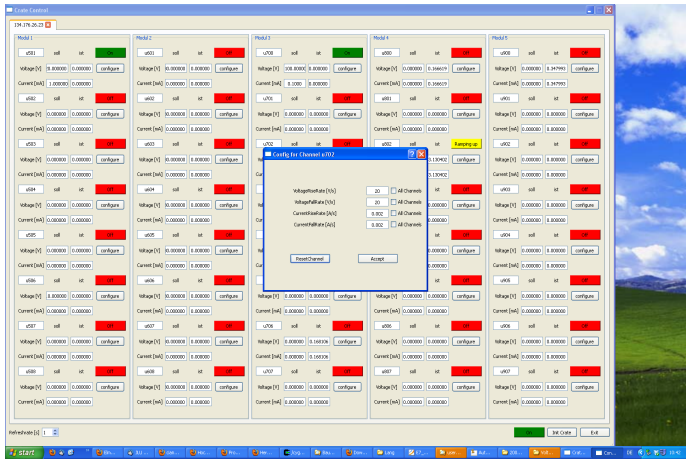


- Single ion pulse ~ 15mV
- High dynamic range
- Robust design
- Optional AC coupling → independent operating potential
  ➔ Post-acceleration for optimal high mass efficiency

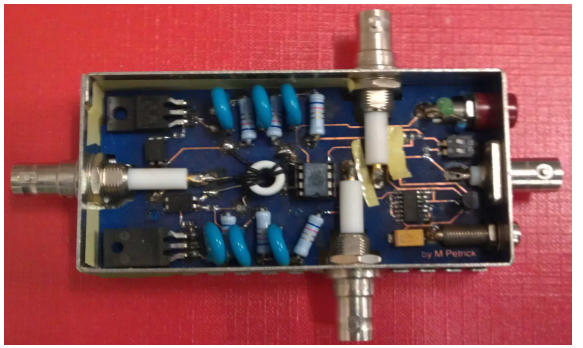
Technical Developments



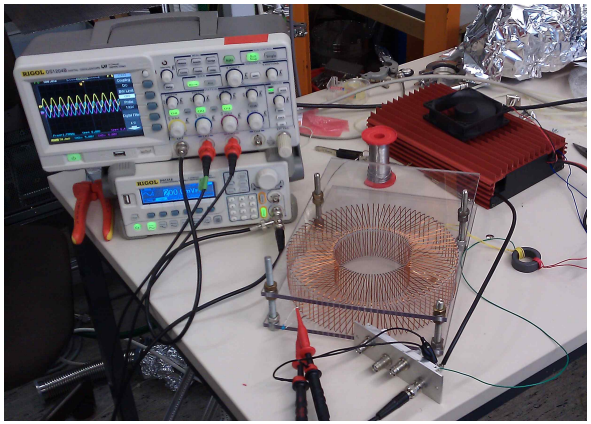
Voltage stabilization



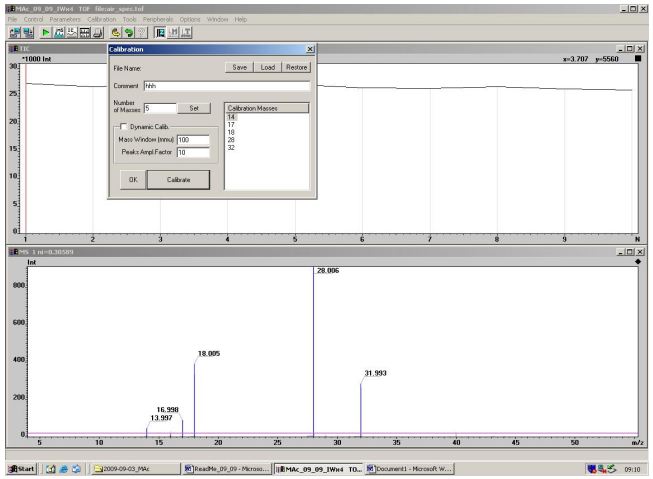
Voltage control software



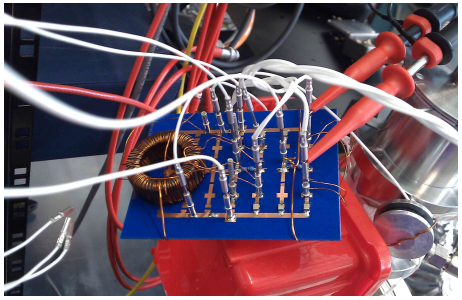
(Fast) high voltage switching

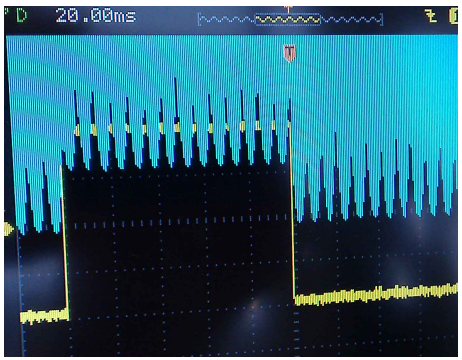


RF generation



DAQ software development

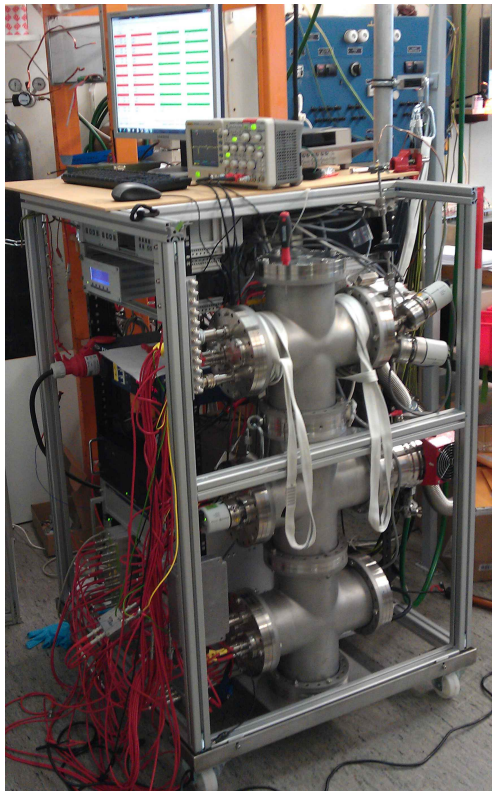


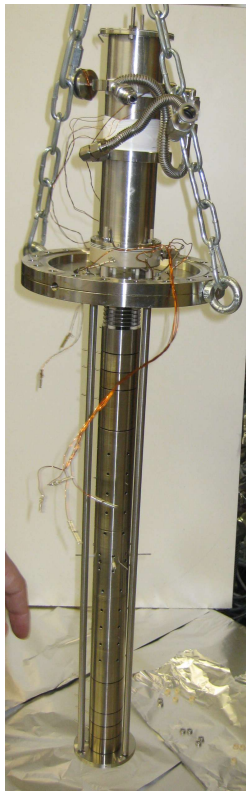


RF offset switching

Mobile MR-TOF-MS: Setup

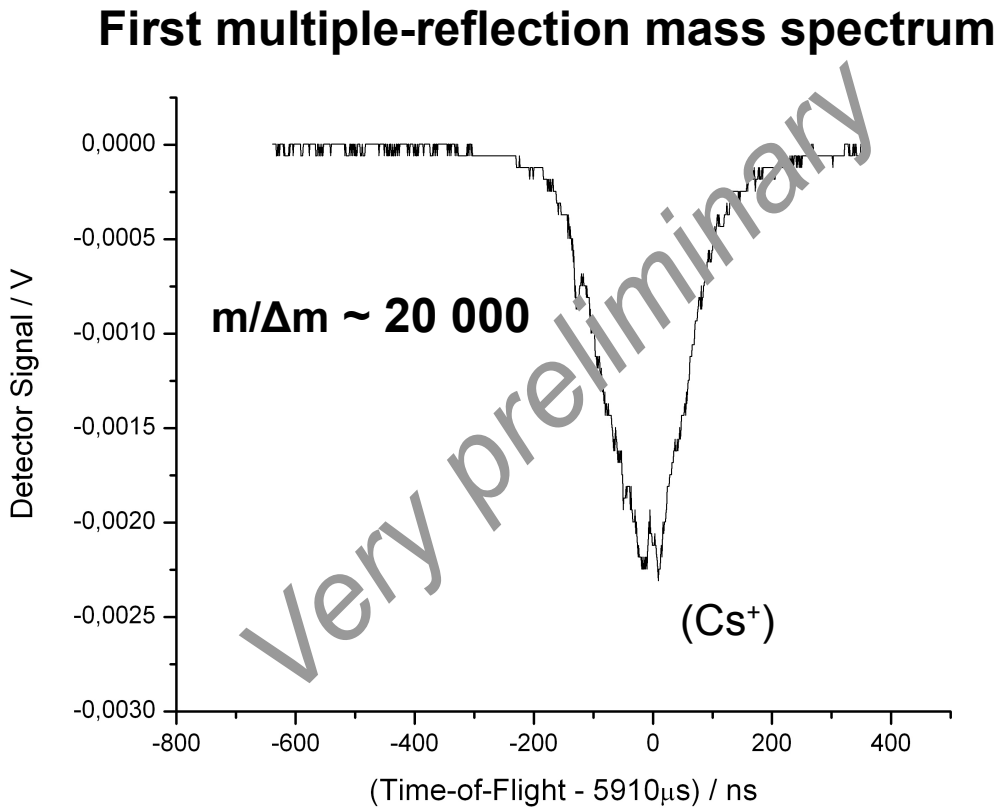
- Transportable, compact and robust setup
- Fits into a van
- No further infrastracture needed
- 3 stacked DN150CF crosses as recipient
- 30m^3/h rough pump integrated
- 80 x 84 x 120 cm^3 ~ 0.8 m^3
- Power consumption < 1,5 kW
- Remote controle (via LAN / WLAN)
- Ruggedization
  - Special construction preventing influence of mechanical forces
  - Stable custom-made Al frame
  - Arbitrary robust enclosure possible (shielding, hygenienic reasons, ...)
  - Electrode material (Invar) insensitive to temperature changes
  - Custom-tailored system control and data acquisition software





Commissioning

- Commissioning in progress (with internal ion source)
- First result: Works!



- Next steps
  - Optimization
  - Install voltage stabilization
  - Increase kinetic energy

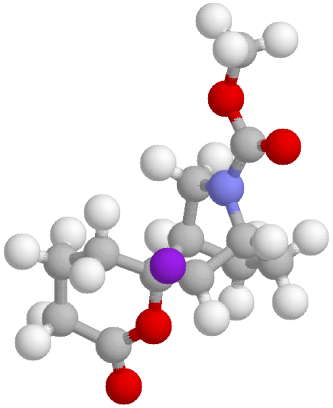
Envisaged in-situ Applications

Realtime tissue recognition

Identification of mycotoxins

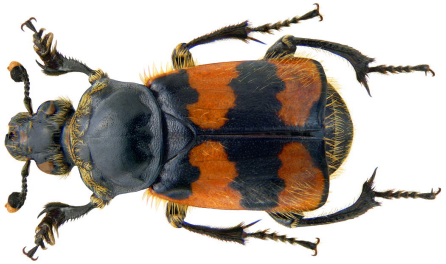
Water monitoring at 'hot spots'

LC/MS in soil science

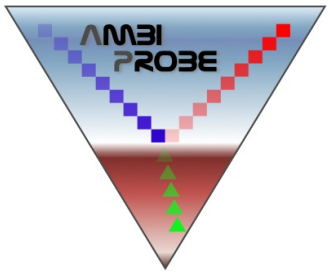


Structure and composition of biomolecules

Climate impact research



Combination with electro-antennography



Future Harsh-Environment Application !?

- Next generation device: portable (?)
- Standard components → use customized components → saving in size, weight, power, ...

- High-Resolution MS in Space Science (Planets, Comets)

Questions:

- Is there life in outer space?
- Chiral symmetry?
- Transport of biological matter
- Cell damages by cosmic rays

Comments welcome !

Conclusion

- Motivation: high resolving mobile MS
- Method: MR-TOF-MS
- Device performance goal:

  $m/\Delta m > 100\,000$, $\delta m/m < 1$ ppm
- Commissioning underway:
  - ➔ Works! First results in multiple-reflection mode.
  - Further performance enhancement coming soon
- Various in-situ applications envisaged
- Next generation device: portable, space missions (?)

Special thanks to:

S. Ayet, U. Czok, C. Horbach, W. Kinsel, C. Lotze, T. Schäfer, M. Petrick, A. Pikhtelev,

precision mechanics workshop of our institute and to the whole **IONAS group**

Many thanks for your attention !

Comments and questions welcome !

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