Ionenmobilitätsspektrometrie: Grundlagen und Anwendungen

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Mäuseburger Sommer-Kolloquien

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D-02763 Zittau

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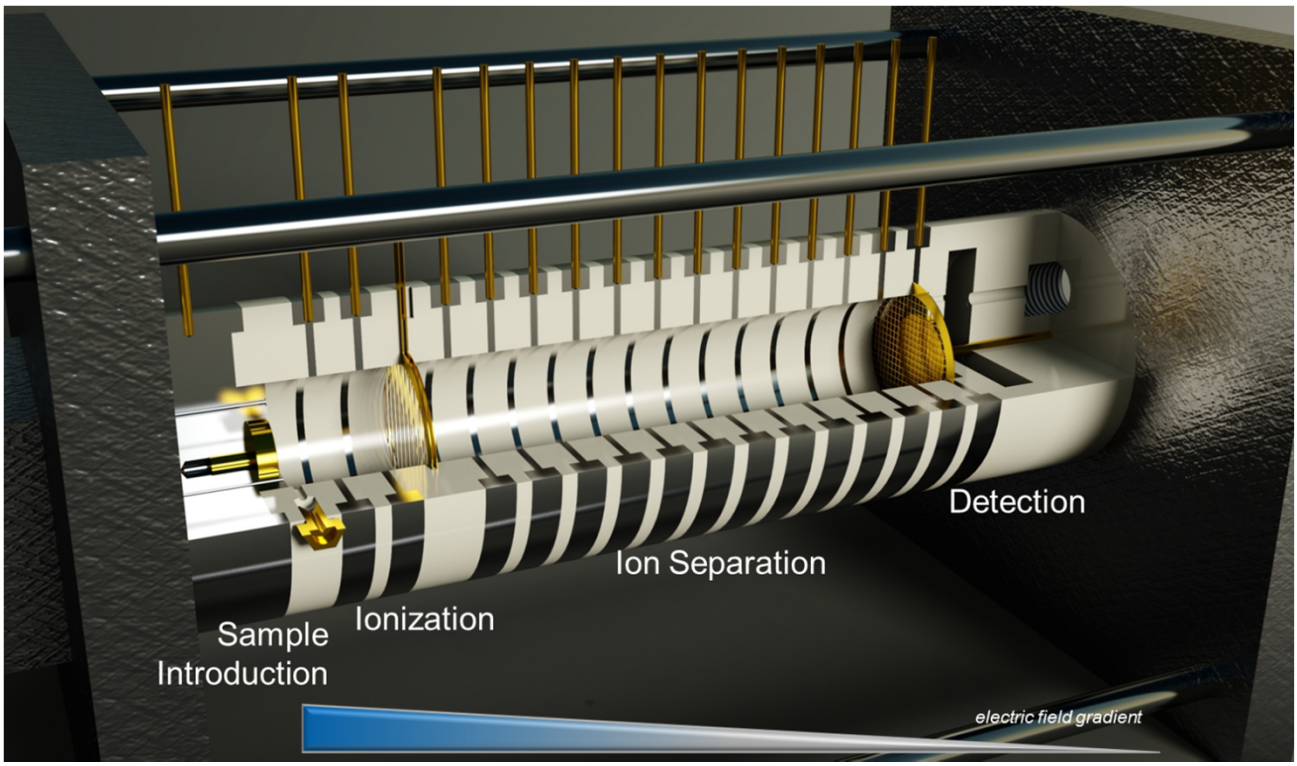
Helmholtz-Zentrum, UFZ Leipzig

Montag, 08. Mai 2017, 18.00 Uhr

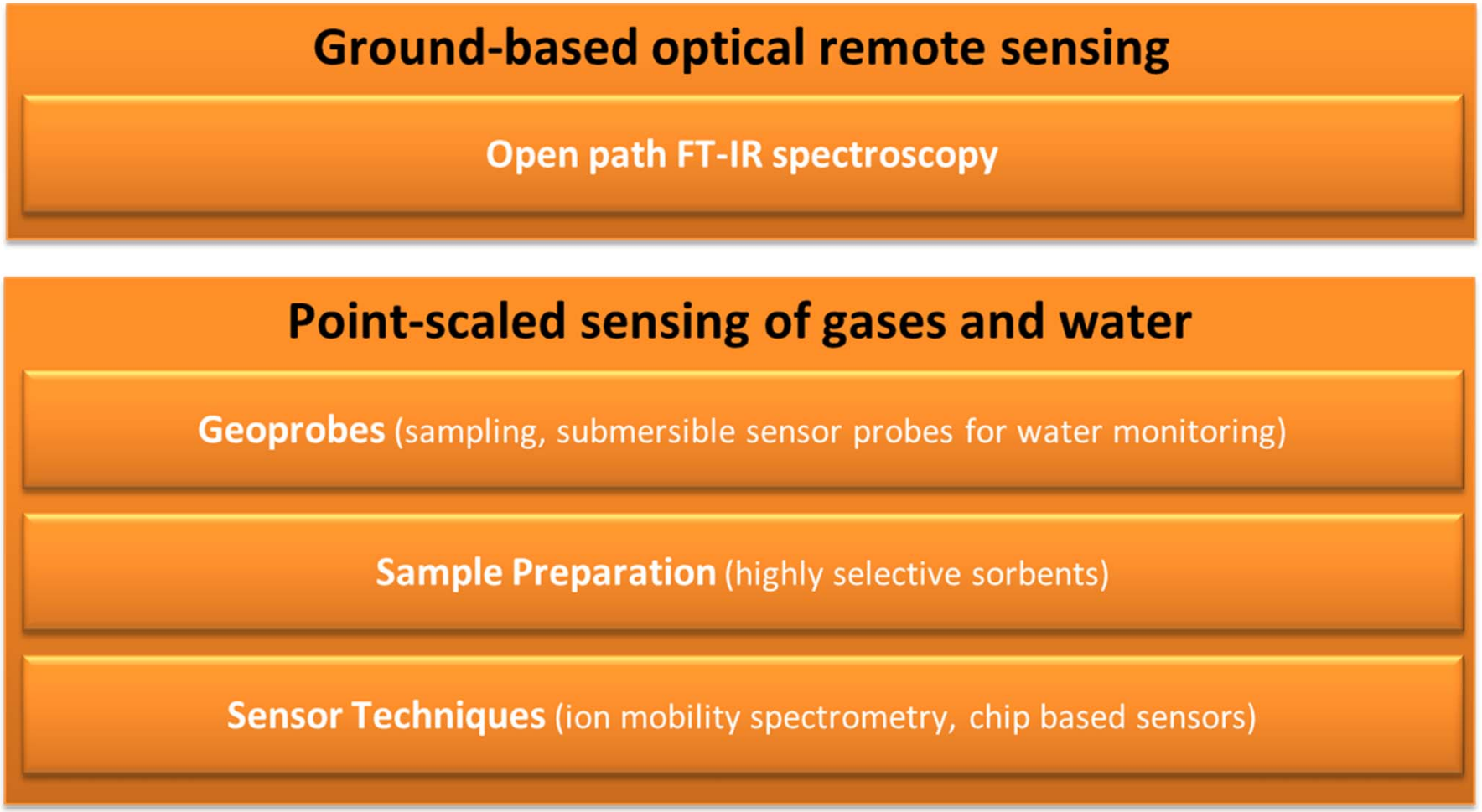
„Ionenmobilitätsspektrometrie: Grundlagen und Anwendungen“



Prof. Dr. Manfred Gey

Mitarbeiter und Studenten sind wie immer sehr herzlich willkommen!

Arbeitsgruppe Vor-Ort Analytik



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IMS aus den frühen 70igern

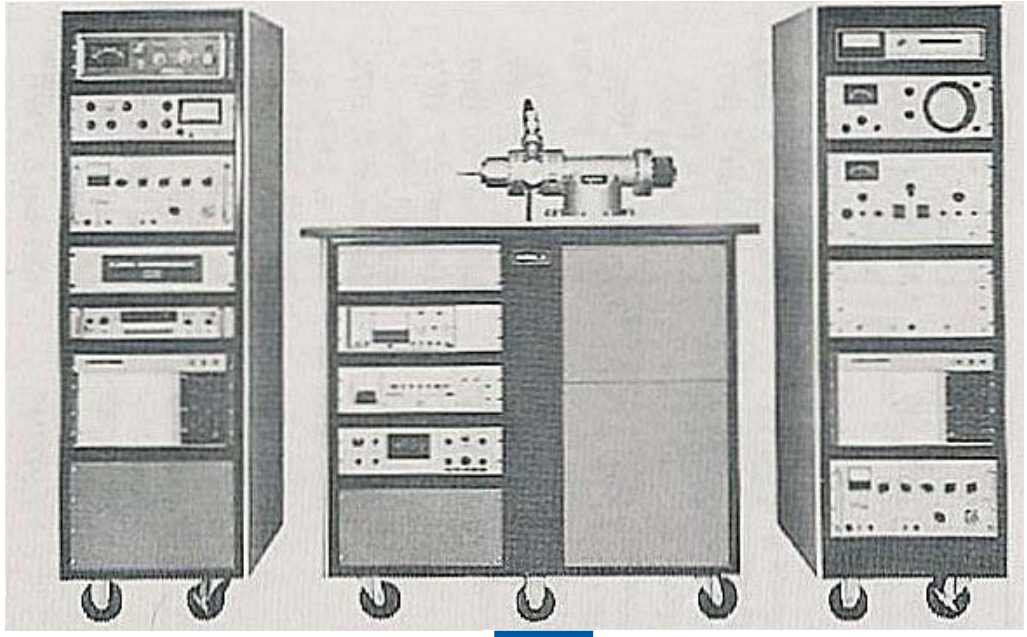

Abbildung aus
Eiceman / Karpas / Hill, Jr.
Ion Mobility Spectrometry, Third Edition
CRC Press, Taylor & Francis Group, Boca Raton, FL, USA
December 2013
ISBN 978-1-4398-5997-1

IMS basierte
handgehaltene Sensoren

- Ankopplung von ESI Quellen zur Ionisierung flüssiger Proben
- Verbesserung der Elektronik
- Verbesserung der Auflösung
- Neue Trennmethoden

Neue Applikationen:

- Klinische Diagnostik
- Pharmazeutische Analyse
- Analytik von Biomolekülen
- Umweltanalytik
- Prozess-Monitoring

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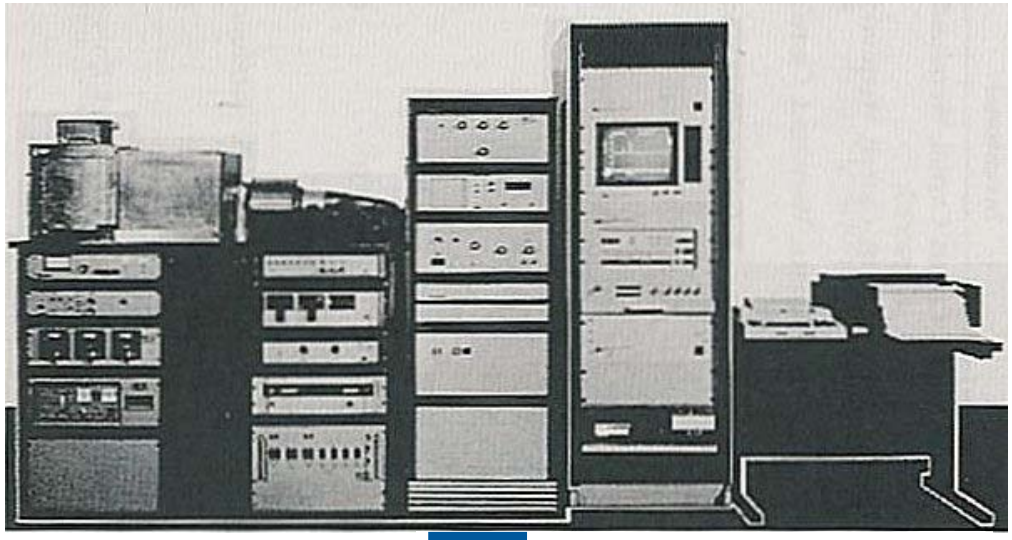
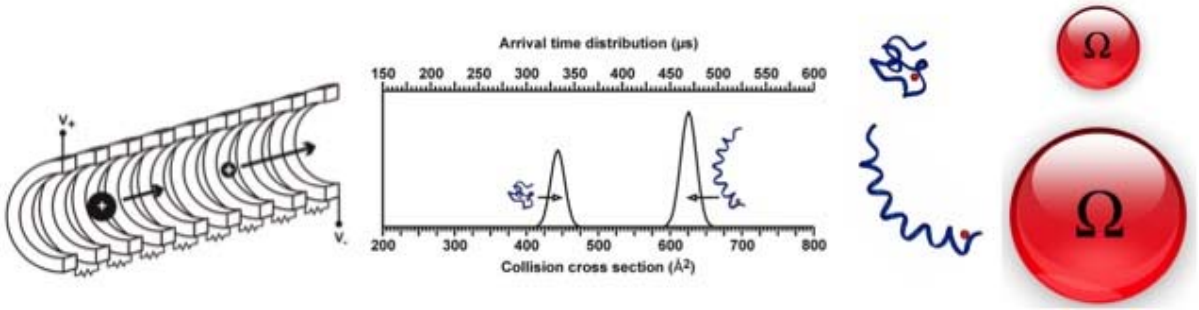
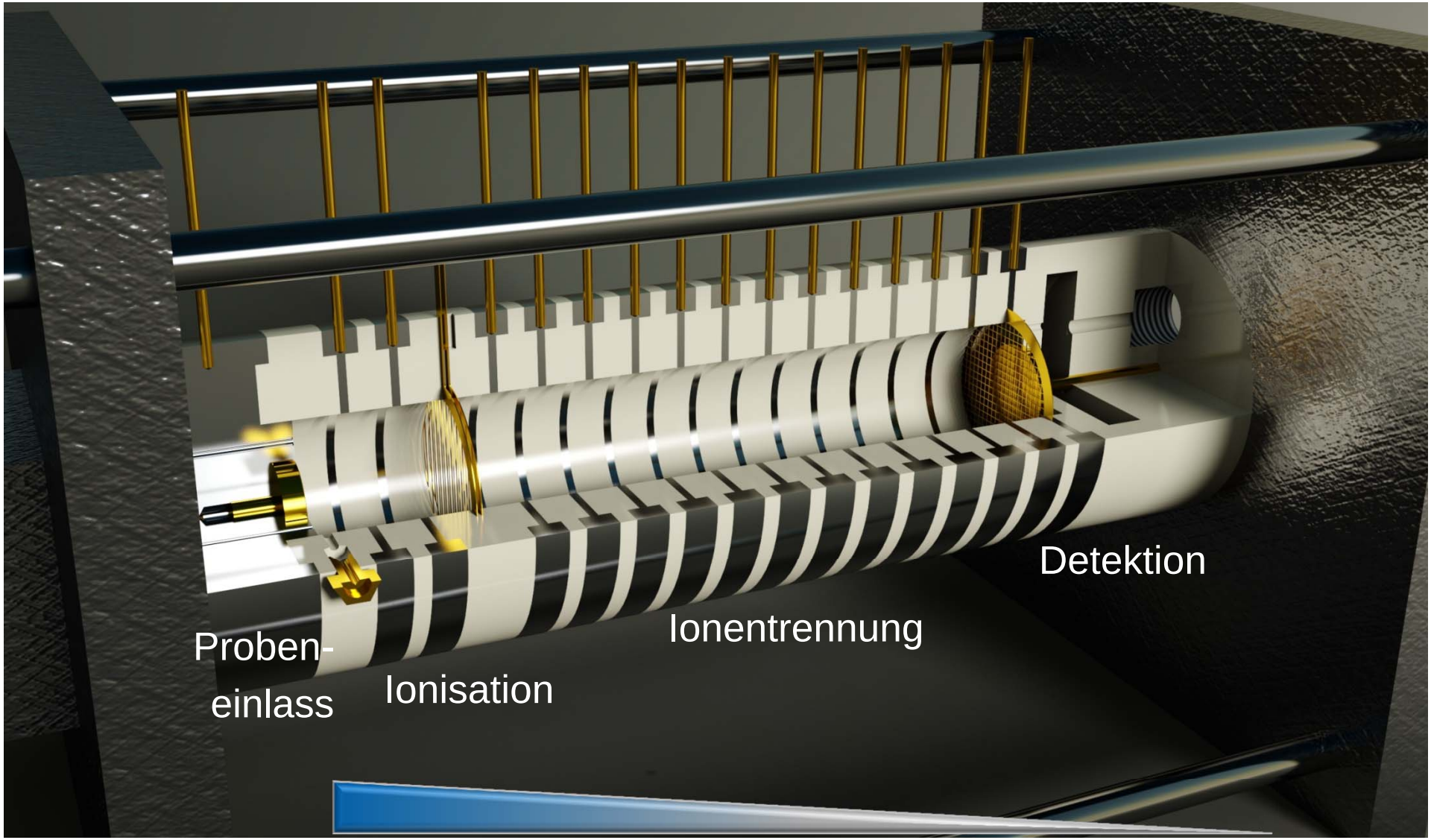
IMS-MS aus den frühen 80igern



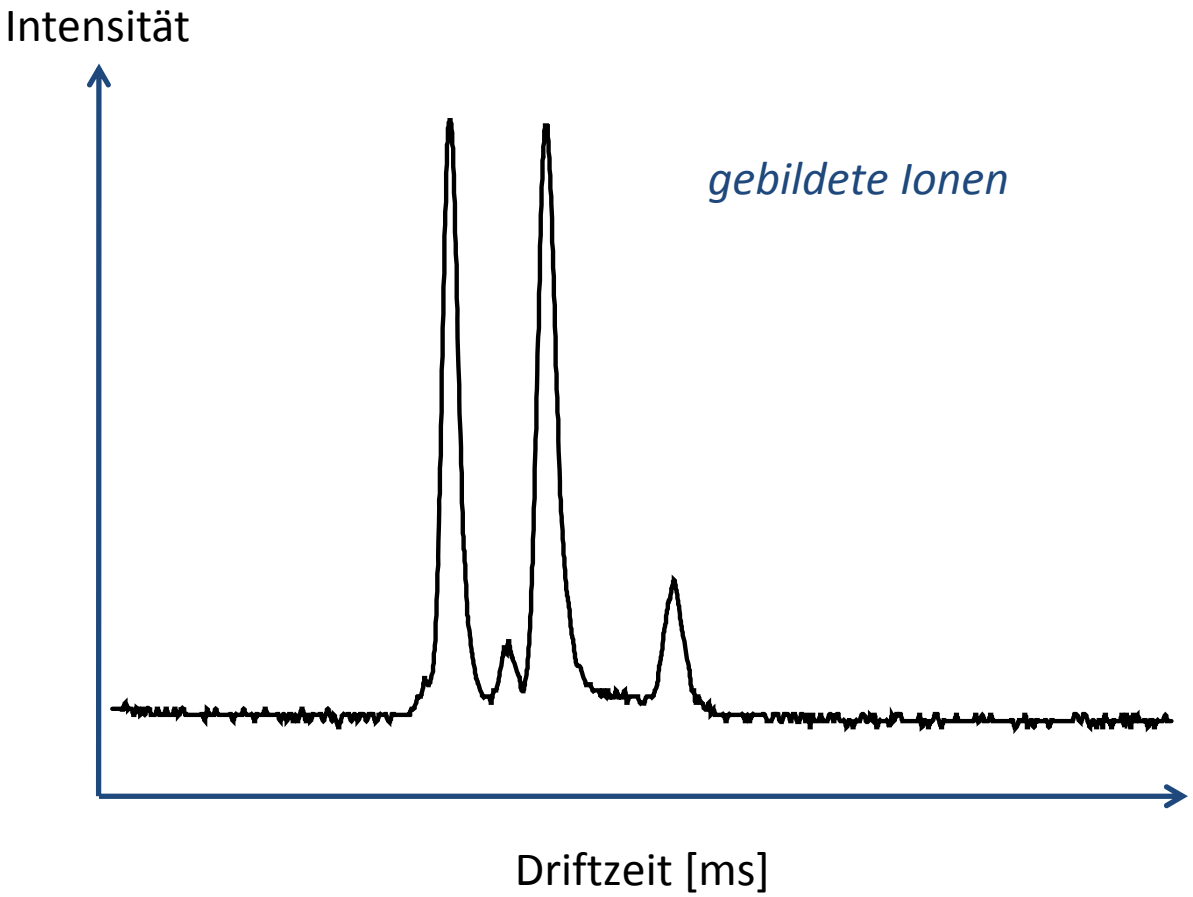
IMS als schnelle Trenntechnik für die Massenspektrometrie

- Schnelle Trennung von Ionen (innerhalb von ms)
- Trennung von Isomeren, Isobaren, Konformeren und strukturell ähnlichen Ionen
- Messung der Ionengröße
- Verbesserung des Signal-Rausch-Verhältnisses





Elektrischer Feldgradient


Intensität
gebildete Ionen
Driftzeit [ms]

$$v = \frac{d}{t}$$

$$K = \frac{v}{E}$$

$$K_0 = K * \left(\frac{p_{Driftröhre}}{p_0} \right) * \left(\frac{T_0}{T_{Driftröhre}} \right)$$

$$K = \left(\frac{3q}{16N}\right) * \left(\frac{2\pi}{\mu kT}\right)^{\frac{1}{2}} * \left(\frac{(1+\alpha)}{\Omega_D}\right)$$

Mason-Schamp (1958)

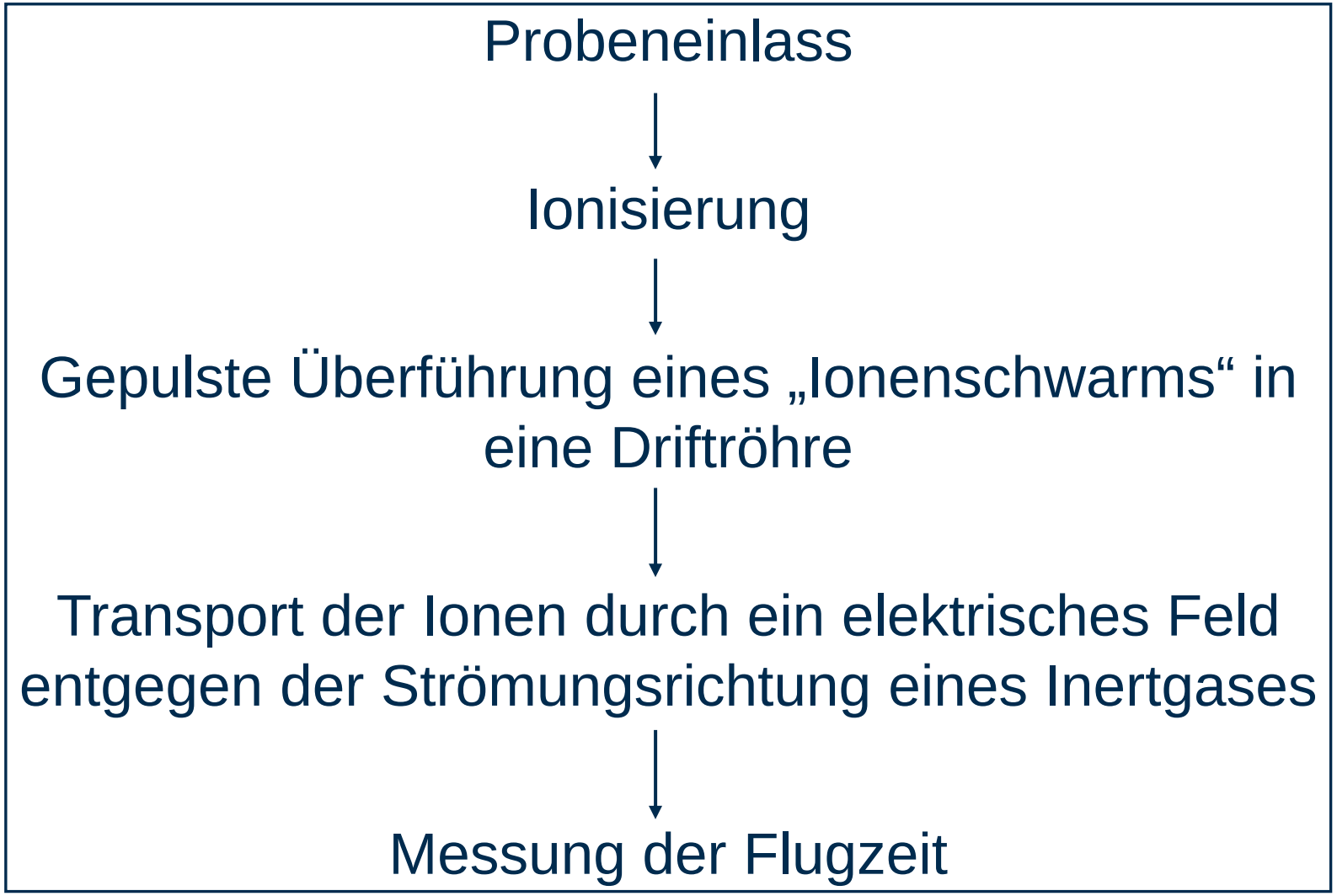
$$K = \left(\frac{3q}{16N}\right) * \left(\frac{2\pi}{\mu kT}\right)^{\frac{1}{2}} * \left(\frac{(1+\alpha)}{\Omega_D}\right)$$

Reduzierte Masse

Struktur

$$\mu = \frac{m_{Ion} * M_{DG}}{m_{Ion} + M_{DG}}$$

- Geometrie (räumliche Ausdehnung und Form)
- Elektronische Faktoren, die die Wechselwirkung zwischen Ionen und Neutralteilchen beschreiben



Atmosphärendruck

Chemische Ionisation mit beta-Strahlern

$$RH^+ + M \rightarrow R + MH^+$$

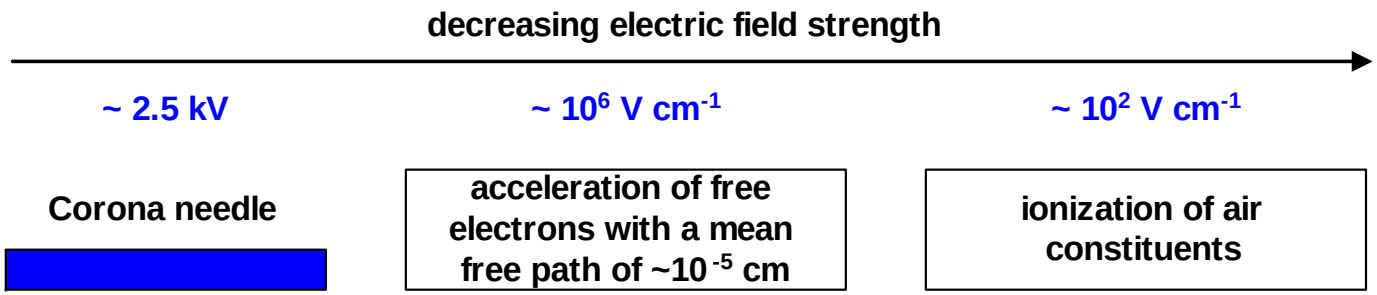
$$MH^+ + M \rightarrow M_2H^+$$

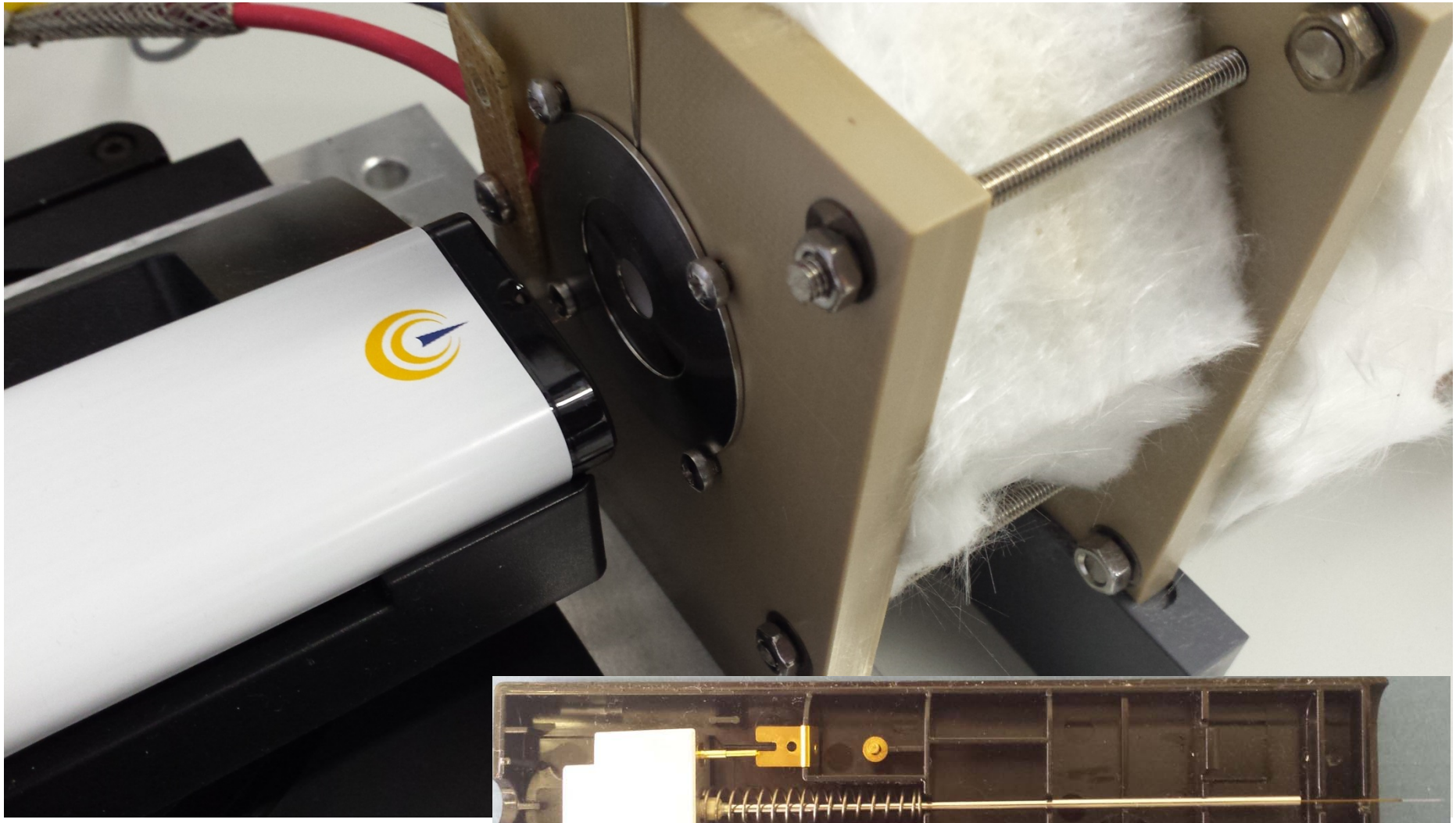
if proton affinity (M) > (H_2O or NH_4^+)

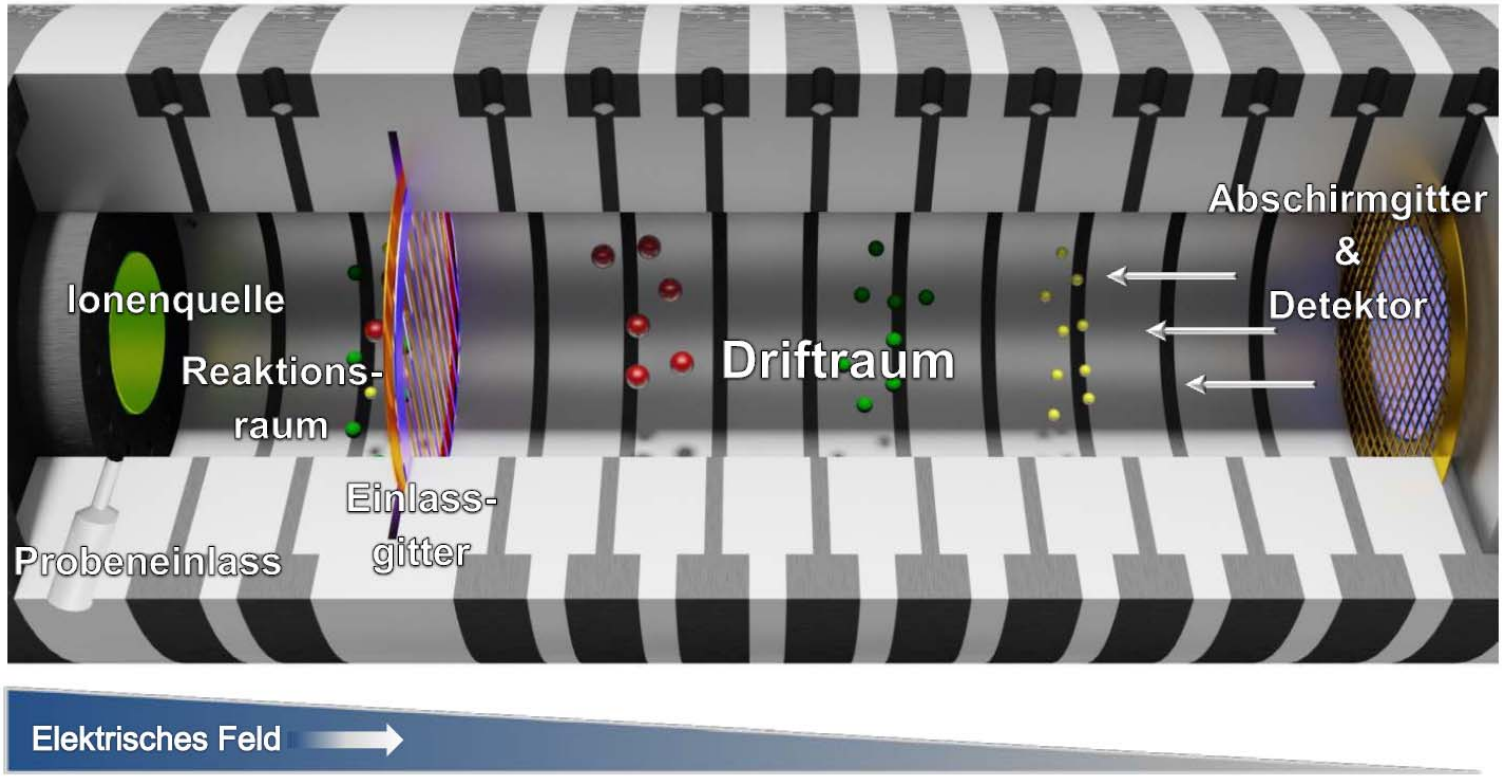
Photoionisation (APPI)

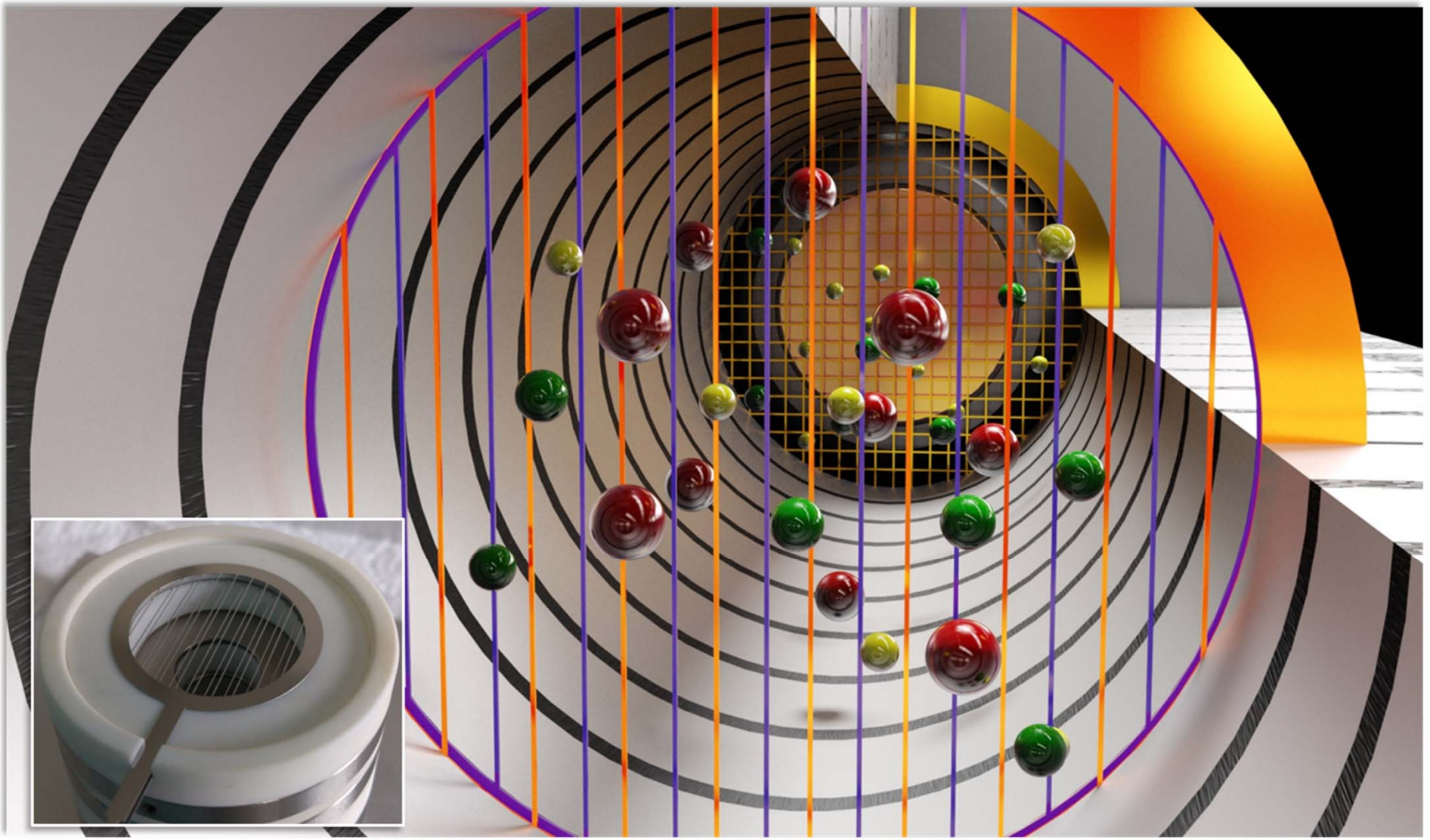
$$M + h\nu \rightarrow \mathbf{M^+} + e^-$$

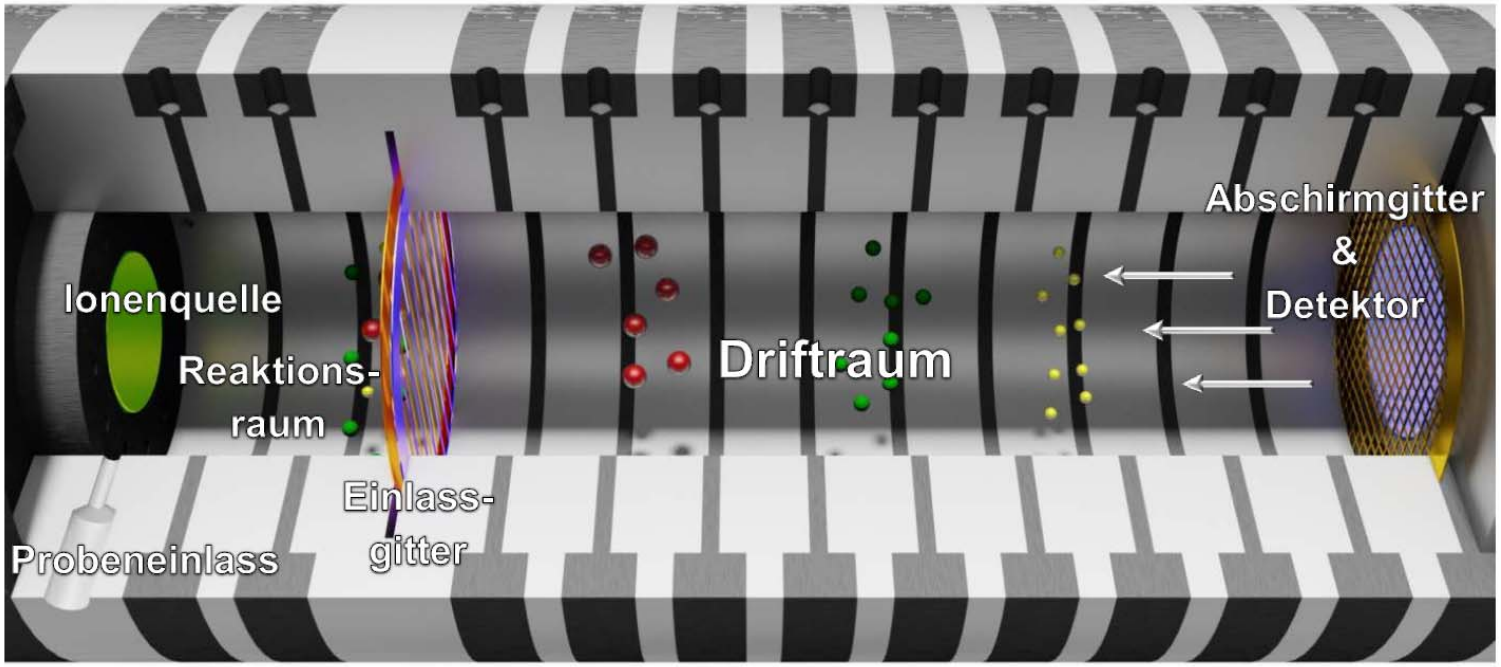
Corona Discharge Ionisierung

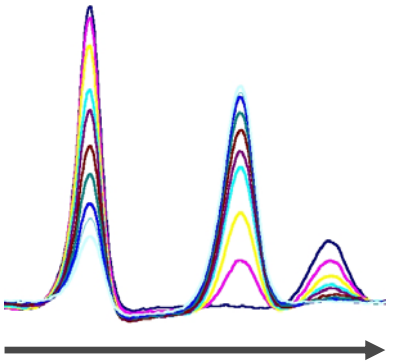




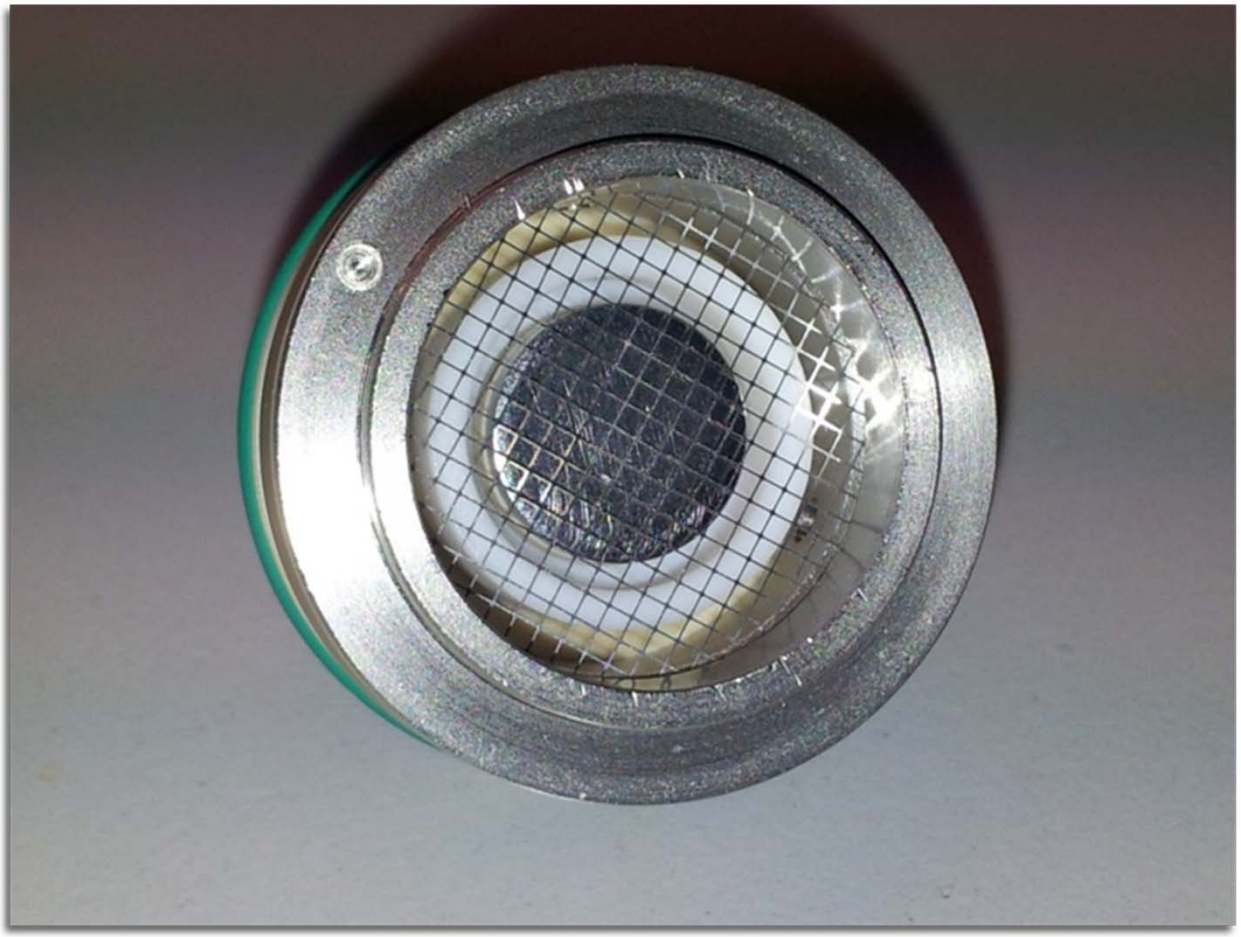

Abschirmgitter
&
Detektor
Ionenquelle
Reaktions-
raum
Driftraum
Einlass-
gitter
Probeneinlass
Elektrisches Feld

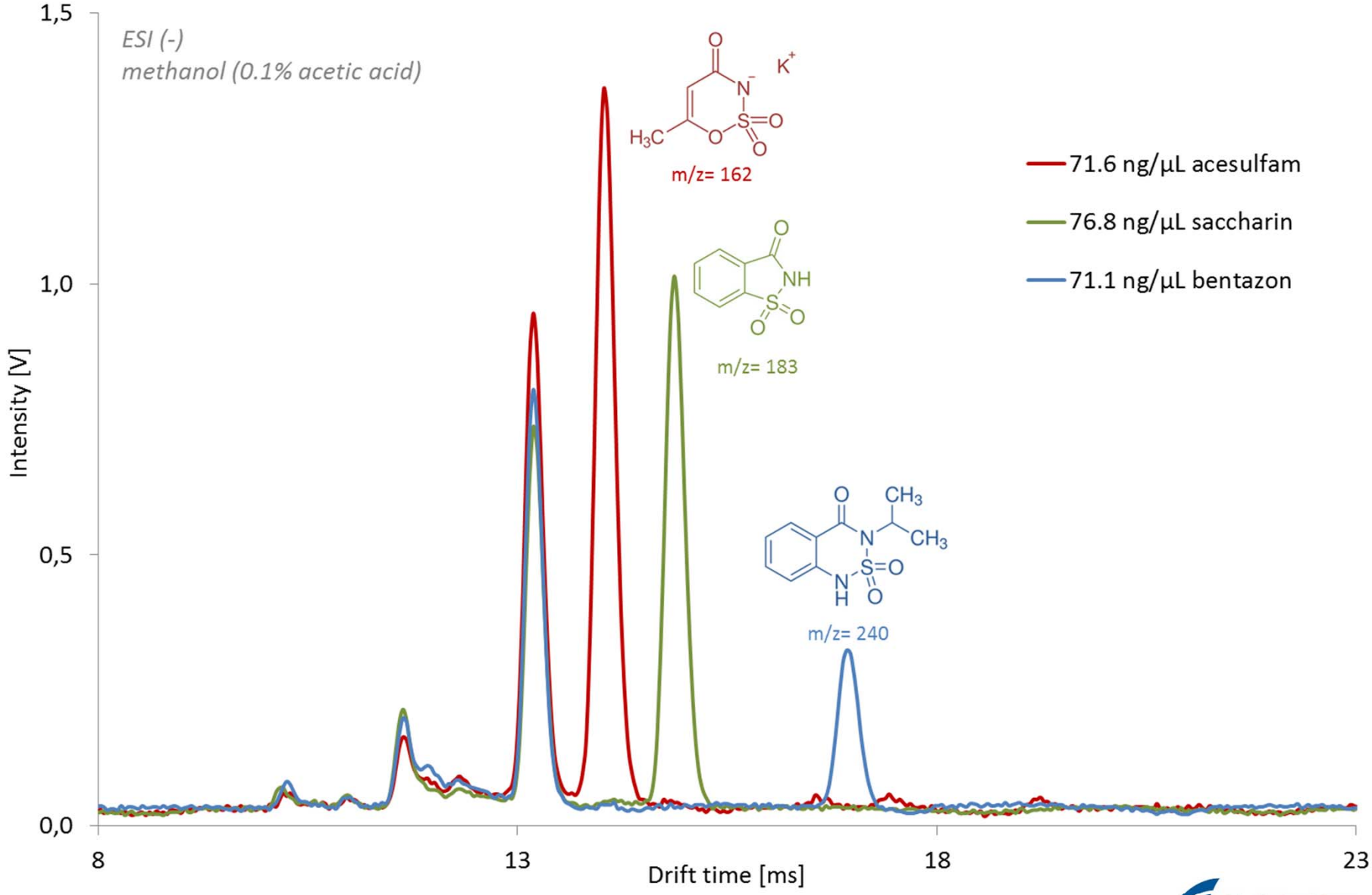


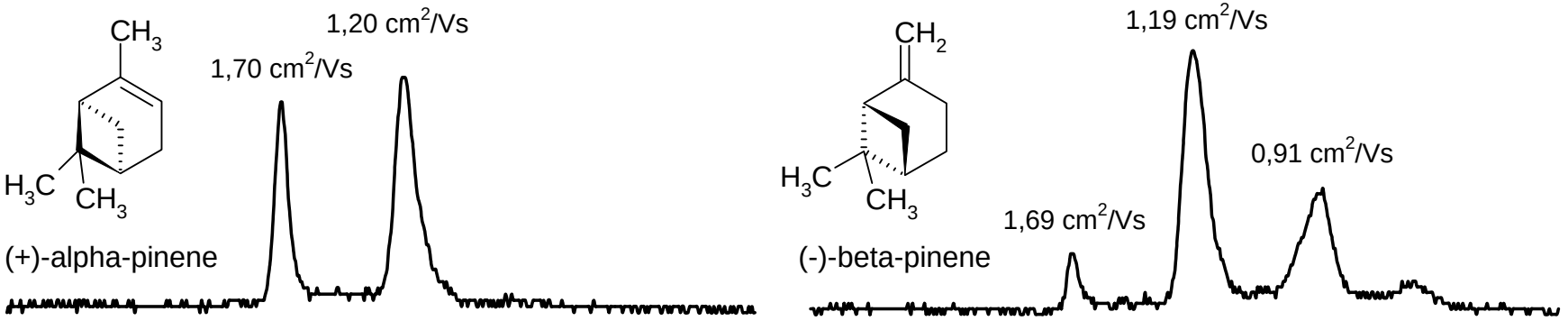




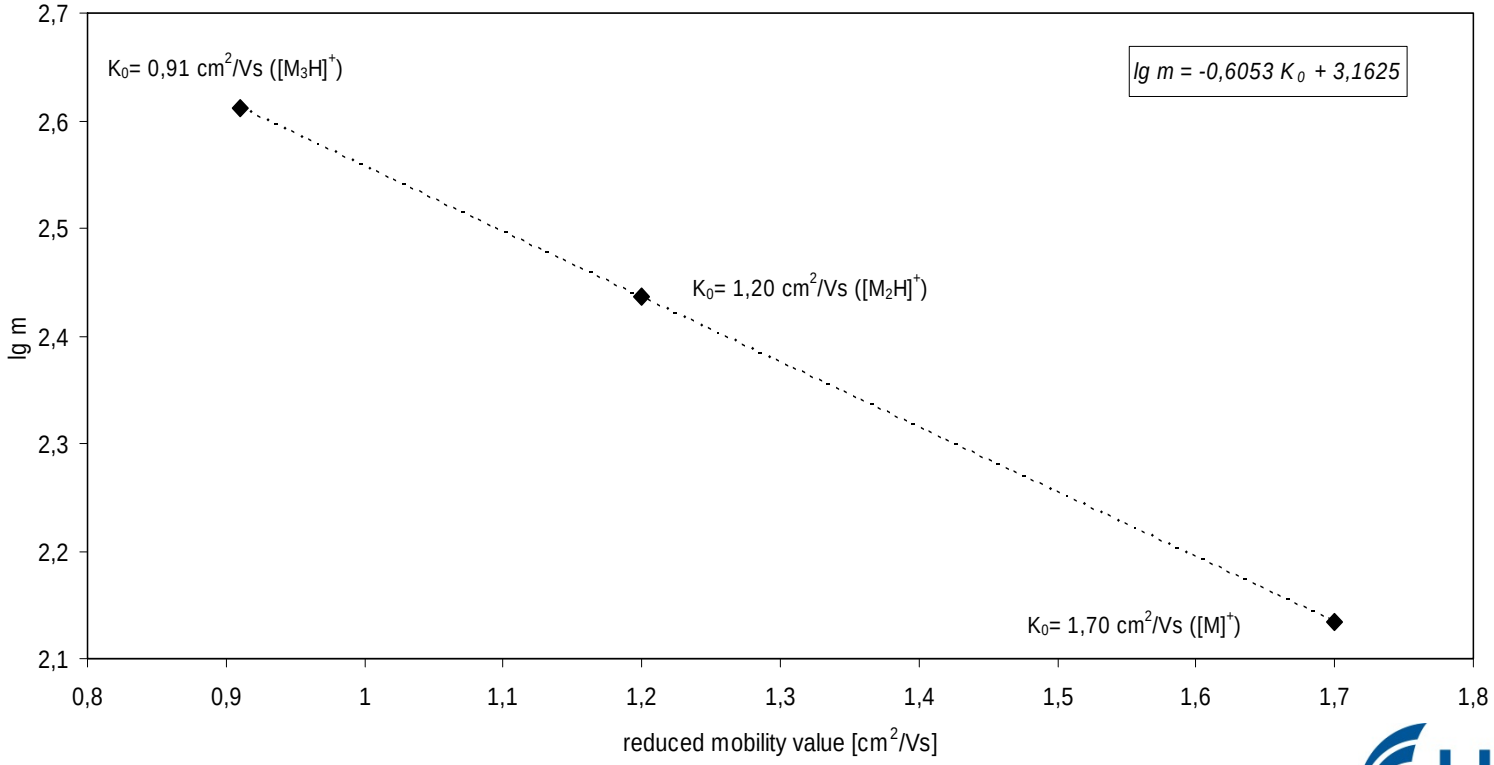
Driftzeit 3-15 ms



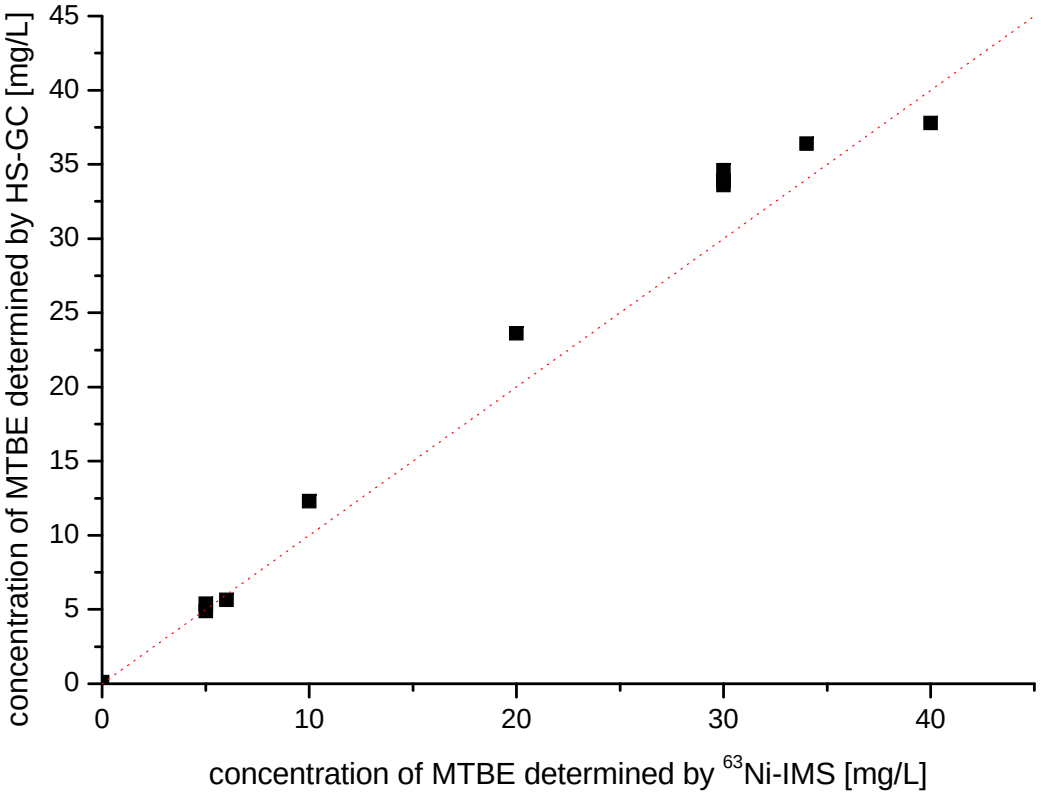

ESI (-)
methanol (0.1% acetic acid)
m/z= 162
m/z= 183
m/z= 240
71.6 ng/µL acesulfam
76.8 ng/µL saccharin
71.1 ng/µL bentazon
Intensity [V]
1,5
1,0
0,5
0,0
8
13
18
23
Drift time [ms]

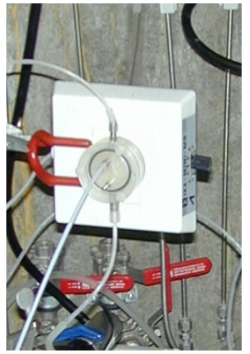


Mass-to-mobility correlation curve for isomers of pinene



Comparison of analytical results (HS-GC vs. ^{63}Ni IMS)





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Geruchsquelle (Emission)
Geruchsstoffkonzentrationen

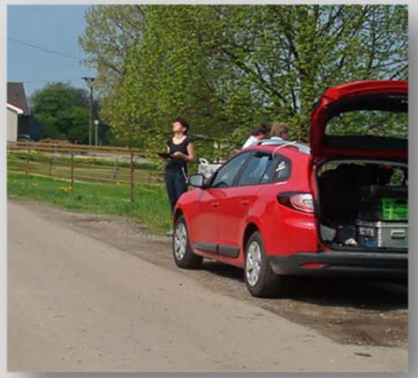
BImSchV (Bundes-Immissionsschutzverordnung)
TA Luft (Technische Anleitung zur Reinhaltung der Luft):
definierte GE/m^3 für Emissionsbegrenzung und Genehmigungsbescheide

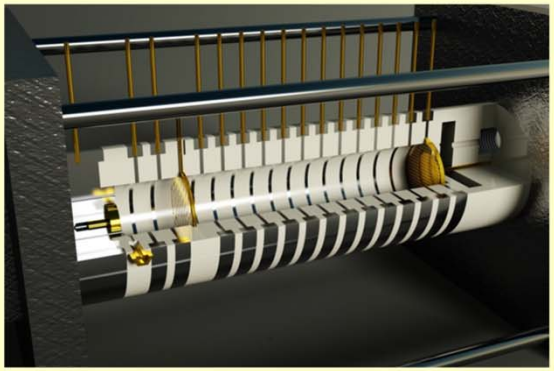
Bestimmungsmethode: Olfaktometrie

Geruchsbelästigung (Immission)
Geruchshäufigkeiten

GIRL (Geruchsimmissions-Richtlinie):
Erhebliche Geruchsbelästigung, wenn an 10% der Jahresstunden (876 h) ein Geruch wahrnehmbar ist (Wohngebiete) ohne Berücksichtigung von Intensität und Geruchscharakteristik

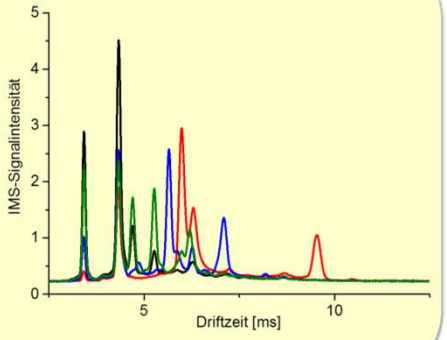
Bestimmungsmethode: Begehung



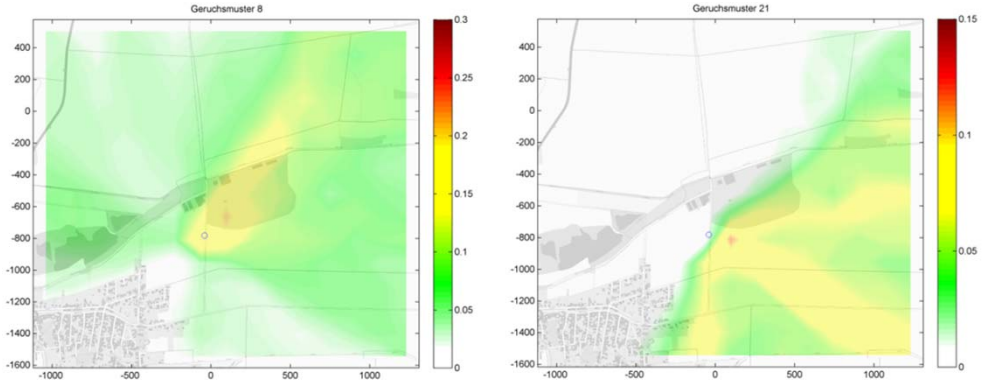


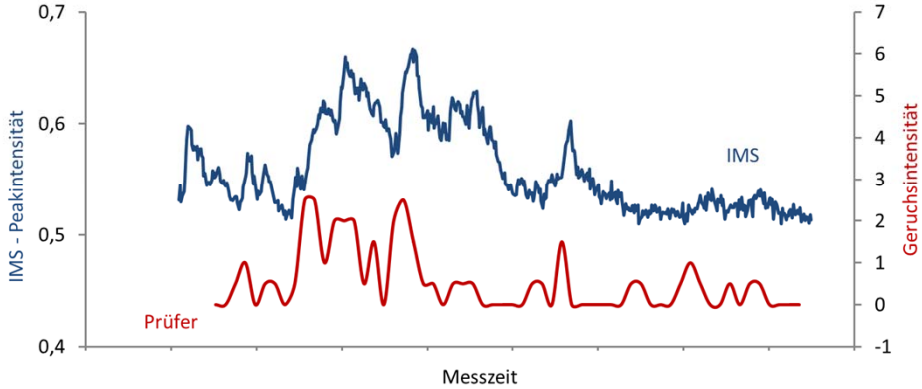
Ionenmobilitätsspektrometrie (IMS)

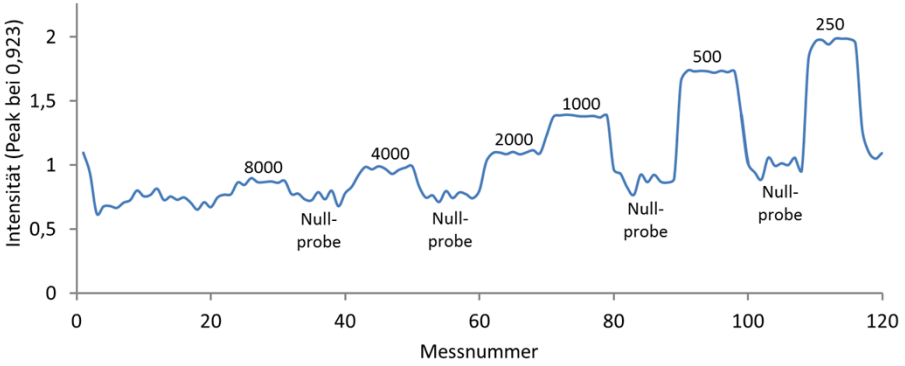
- Rein physikalisches Messprinzip (keine Oberflächenreaktionen)
- Uneingeschränkt feldtaugliche Geräte
- Langzeitstabil
- Sehr empfindliche Methode
- Aufnahme substanzspezifischer Spektren
- Preiswert
- Schnell (Millisekunden)



- ✓ **Anwendung: Geruchsradar**
- ✓ **Anwendung: Geruchwahr-nehmungshäufigkeiten**
- ✓ **Kalibrierung: Olfaktometrie**







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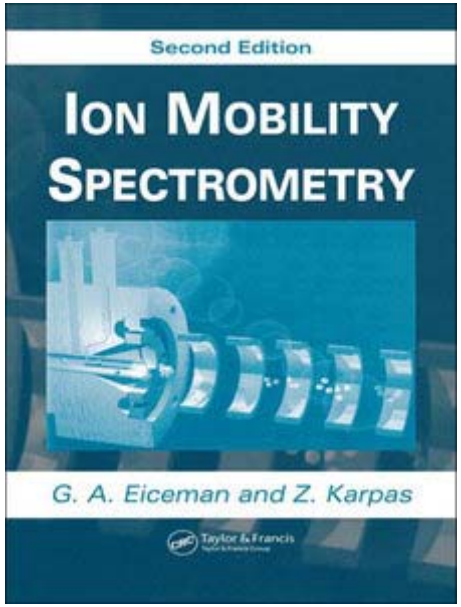

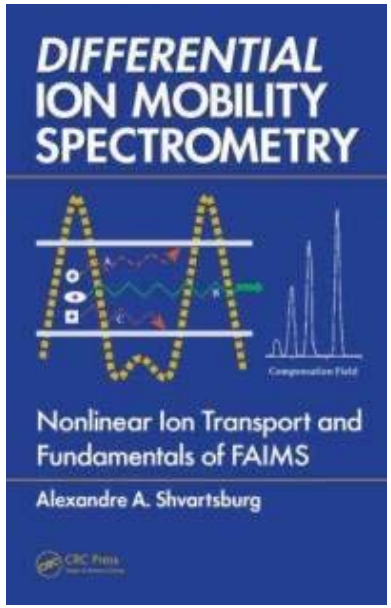

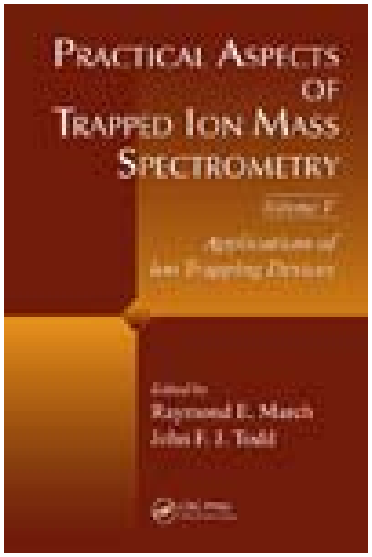

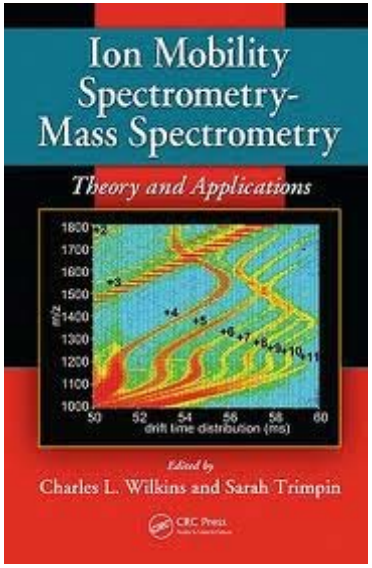

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Ion Mobility Spectrometry: Principles and Applications

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Department of Chemistry and Biochemistry, New Mexico State University, Las Cruces, New Mexico, USA

Abstract: General principles are reviewed for ion mobility spectrometry including new methods for ion separation through field dependent mobilities in strong electric fields with high frequency asymmetric waveform. Additionally, recent advances in the instrumentation for the characterization of ion mobilities in air at ambient pressure are described and critically reviewed. Advances in instrumentation, understanding of principles of measurements by IMS, and the development of hyphenated technologies have resulted in an increase in the number of applications in recent years.

Keywords: Ion mobility spectrometry, differential mobility spectrometry, high-field asymmetric waveform ion mobility spectrometry

INTRODUCTION

Ion mobility spectrometry (IMS) was developed over the past few decades as a method for detecting and identifying volatile and semi-volatile organic compounds, principally in security and military venues. This technique is based on the determination of mobilities in electric fields of gas phase ions derived from constituents in a sample.

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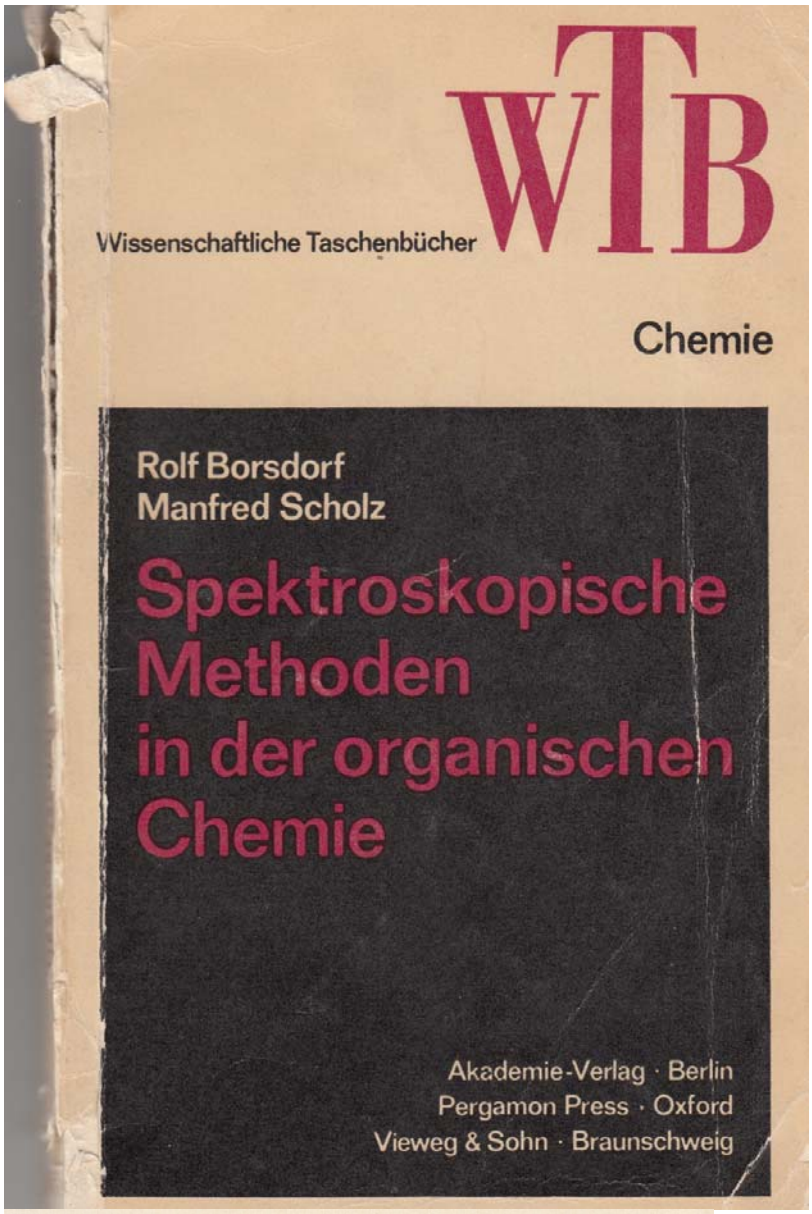

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