



# Molecular Systems group

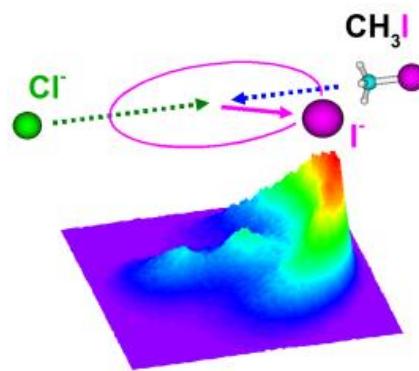


**Our research focus:  
Understand the Dynamics and Spectroscopy  
of Charged Molecular Systems**

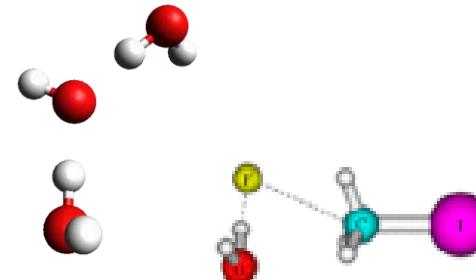


# Dynamics and Spectroscopy of Charged Molecular Systems

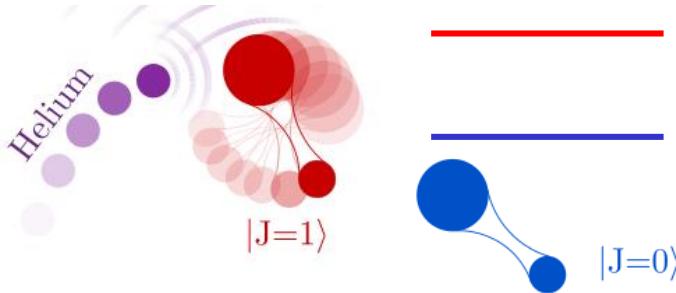
## Ion-molecule reaction dynamics



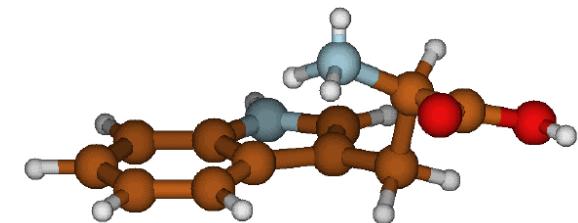
## Micro-hydration effects



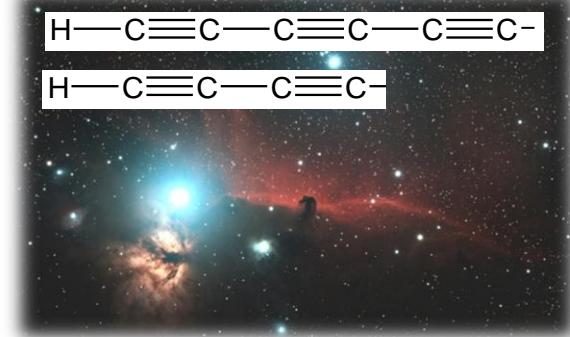
## Cold and state-controlled ions



## Biomolecular ions



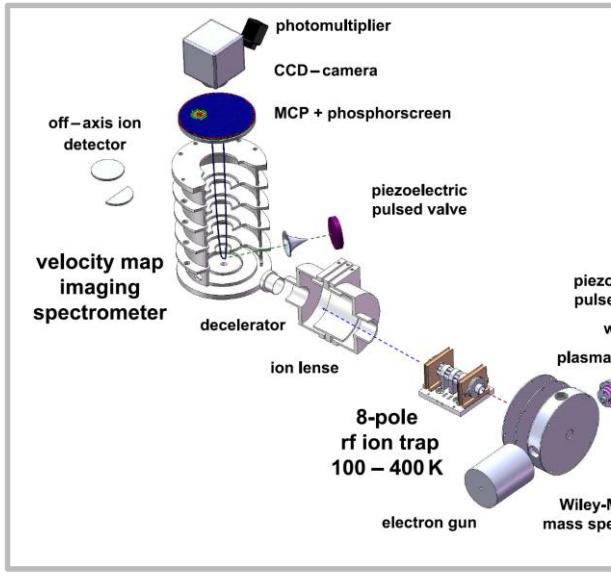
## Interstellar ion formation



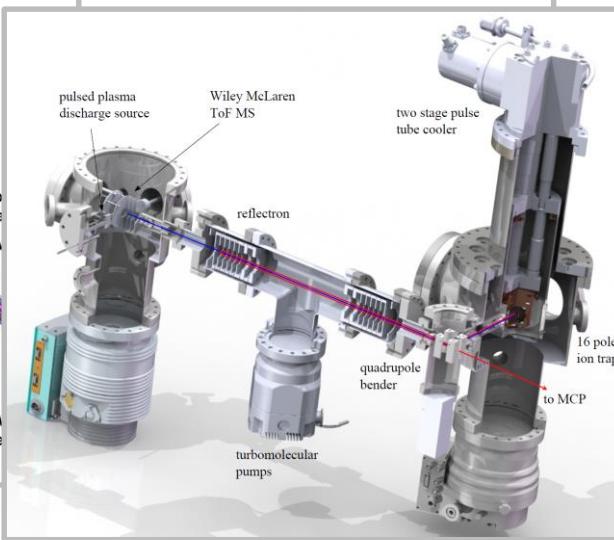


# Dynamics and Spectroscopy of Charged Molecular Systems

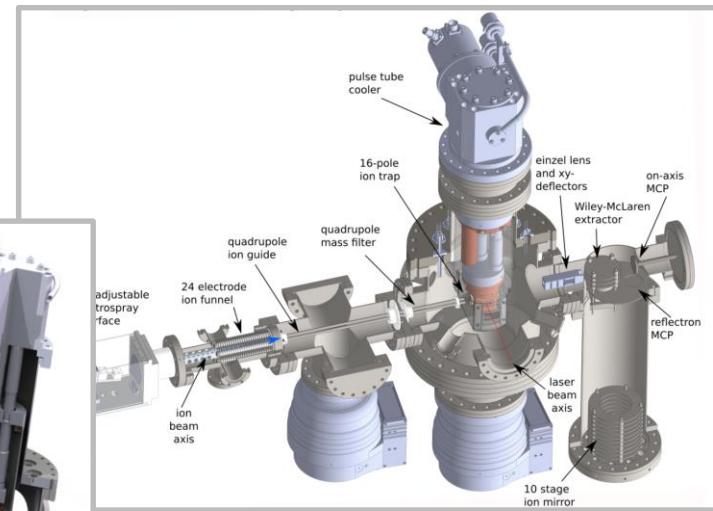
## Experimentelle Aufbauten



Kreuzstrahlspektrometer  
für Ionen-Molekül-  
Reaktionsdynamik



4 Kelvin Ionenfalle  
für Laborastrophysik an  
interstellarer Ionen



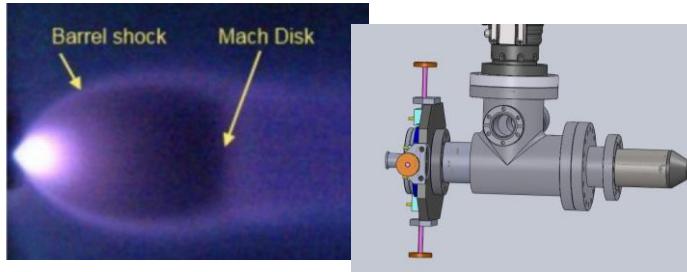
4 Kelvin Elektrospray-  
Ionenfalle für Spektroskopie an  
Biomolekülen und Clustern



# Dynamics and Spectroscopy of Charged Molecular Systems

## Themen für Bachelorarbeiten 2020

Test einer neuen Überschallstrahlquelle  
für kalte Moleküle



Numerische Modellierung interstellarer  
Molekülwolken

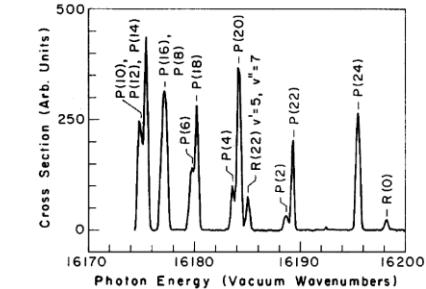
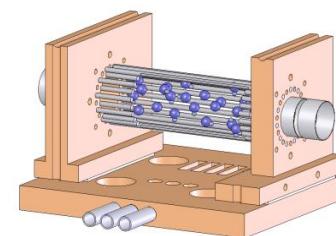
KIDA

KINETIC DATABASE FOR ASTROCHEMISTRY

TERMO MOLECULAR REACTIONS | SURFACE REACTIONS

	$T_f (K)$	Formula	Evaluation
Bimo	$\text{HCN} + \text{OH}$	$\rightarrow \text{H}_2\text{O} + \text{CN}$	1.20E-9    0.00E+0    0.00E+0    10-280    Modified Arrhenius equation
Bimo	$\text{CN} + \text{HCO}^+$	$\rightarrow \text{H} + \text{CN} + \text{CO}$	3.79E-8    -5.00E-1    0.00E+0    10-280    Modified Arrhenius equation
Bimo	$\text{CN} + \text{H}_3\text{O}^+$	$\rightarrow \text{H} + \text{CN} + \text{H}_2\text{O}$	3.79E-8    -5.00E-1    0.00E+0    10-280    Modified Arrhenius equation
Bimo	$\text{CN} + \text{H}_2\text{O}^+$	$\rightarrow \text{H} + \text{CN} + \text{H}_2$	7.51E-8    -5.00E-1    0.00E+0    10-280    Modified Arrhenius equation
Bimo	$\text{CN} + \text{H}_2\text{O}^+$	$\rightarrow \text{H} + \text{CN} + \text{H}_2$	7.51E-8    -5.00E-1    0.00E+0    10-280    Modified Arrhenius equation
Bimo	$\text{C}_2 + \text{N}_2$	$\rightarrow \text{C}_2 + \text{CN}$	9.00E-11    0.00E+0    0.00E+0    300-300    Modified Arrhenius equation
Bimo	$\text{C}_2 + \text{N}_2$	$\rightarrow \text{C}_2 + \text{CN}$	9.00E-11    0.00E+0    0.00E+0    300-300    Modified Arrhenius equation
Bimo	$\text{C}_2 + \text{C}_2$	$\rightarrow \text{C}_2 + \text{C}_2$	0.00E+0    0.00E+0    0.00E+0    300-300    Modified Arrhenius equation

Hochauflösende Spektroskopie an kalten  
gefangenen Molekülionen



Erzeugung von VUV Laserstrahlung  
mittels Frequenzvervielfachung





# Dynamics and Spectroscopy of Charged Molecular Systems

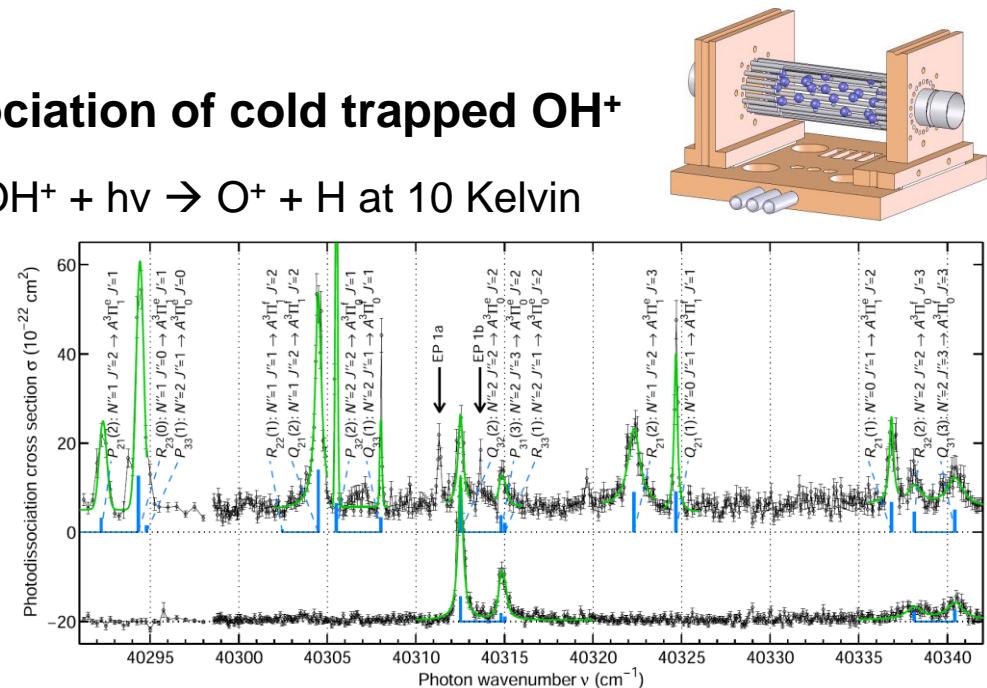
## Master thesis

### Quantum state-resolved photodissociation of cold trapped OH<sup>+</sup>

*Goal:* Investigate the photodissociation of OH<sup>+</sup> + hν → O<sup>+</sup> + H at 10 Kelvin

#### Tasks:

- Learn to experiment with the cryogenic ion trap
- Prepare and investigate OH<sup>+</sup> cooled by Helium
- Analyse photodissociation spectra and determine rotational temperatures



**Big Goal:** Quantum control of rotational states and state-resolved ion-molecule reactions for better understanding of water formation in the universe



# Dynamics and Spectroscopy of Charged Molecular Systems

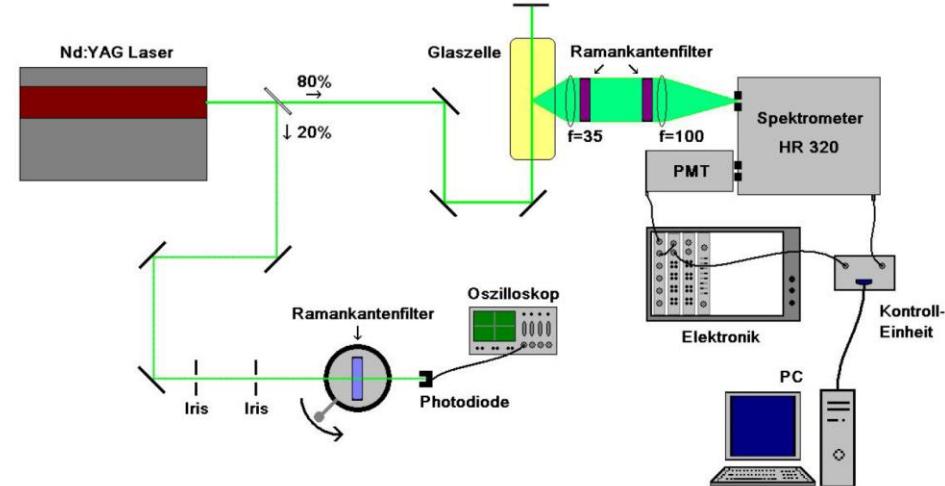
Master thesis

Raman spectroscopy of gas cavities in 3D-printed glass

Goal: Non-destructive identification of molecular species in gas cavities using Raman spectroscopy

Tasks:

- Assemble the laser spectroscopy setup
- Gain understanding of molecular spectroscopy
- Perform measurements on gas cavities in glass



Collaboration with physicists and engineers at Swarovski, Wattens  
Big Goal: The world's first scalable 3D-glass printer technology



# Dynamics and Spectroscopy of Charged Molecular Systems

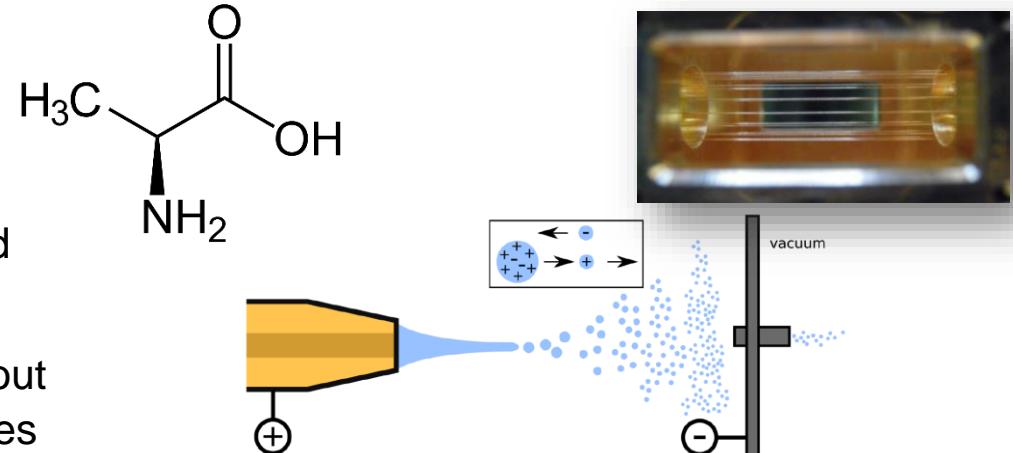
## Master thesis

### High resolution spectroscopy of a protonated amino acid

*Goal:* Investigate vibrational transitions in cold AlaninH<sup>+</sup> and analyze the rotational profiles

*Tasks:*

- Learn to experiment with electrospray ionization and a cryogenic ion trap
- Prepare and mass analyze protonated ions tagged with rare gas atoms
- Analyse the line profiles and learn about the structure of the biological molecules



*Big Goal:* Full rotational resolution for large biomolecular ions and clusters to obtain new and better insight into their spatial structures