Analysis of PAH content in Cosmic Dust Analogues : The AROMA Set-up

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Supervisors : Christine Joblin, Hassan Sabbah


I DON'T ALWAYS FINISH LAB REPORTS EARLY
BUT WHEN I DO, I'TS AT 4 AM
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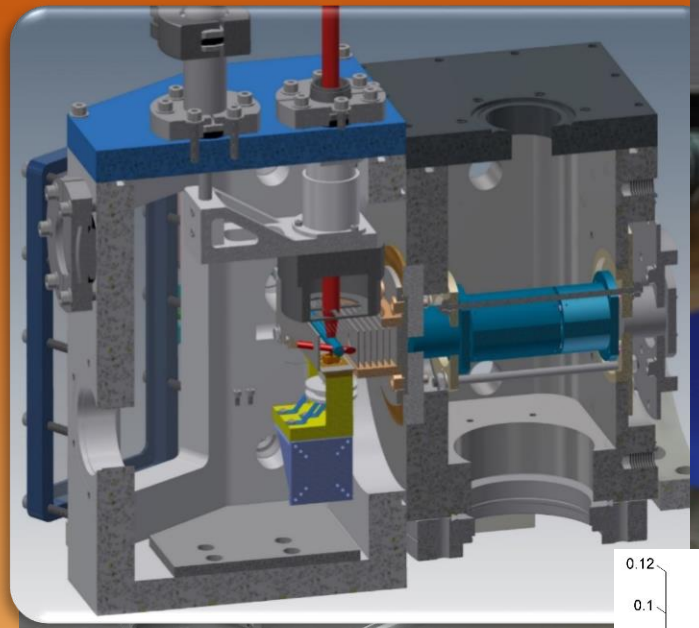
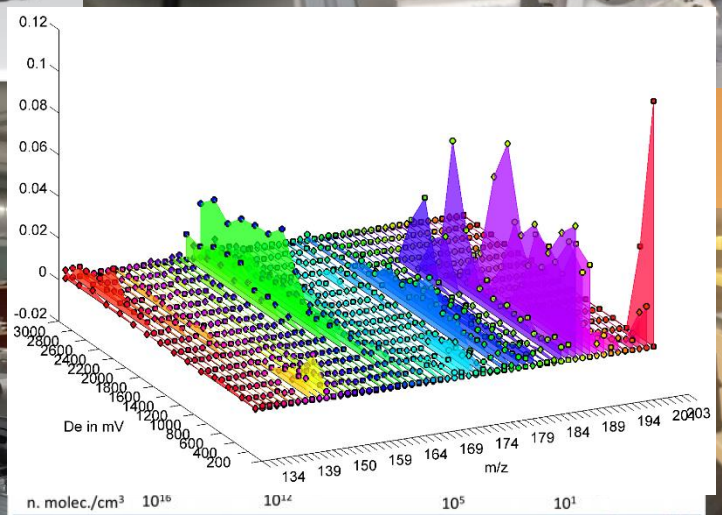
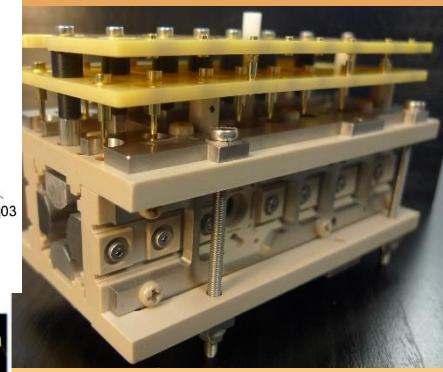
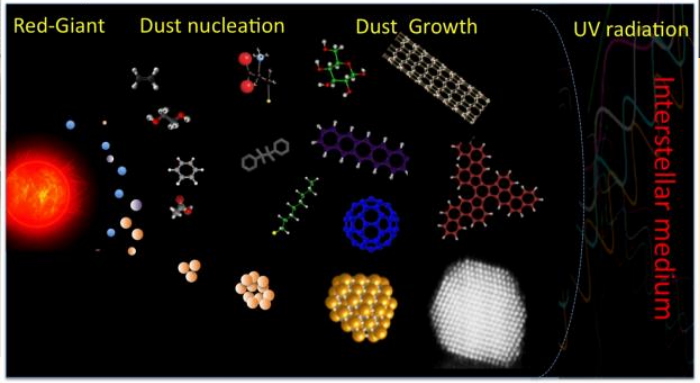
- Introduction
  - Project Nanocosmos
  - My PhD Subject
- AROMA
- CID
- Simulations
- Imaging Source







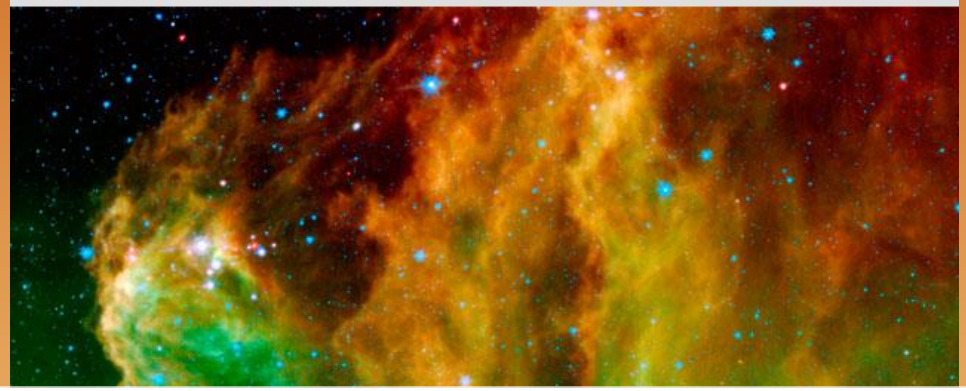


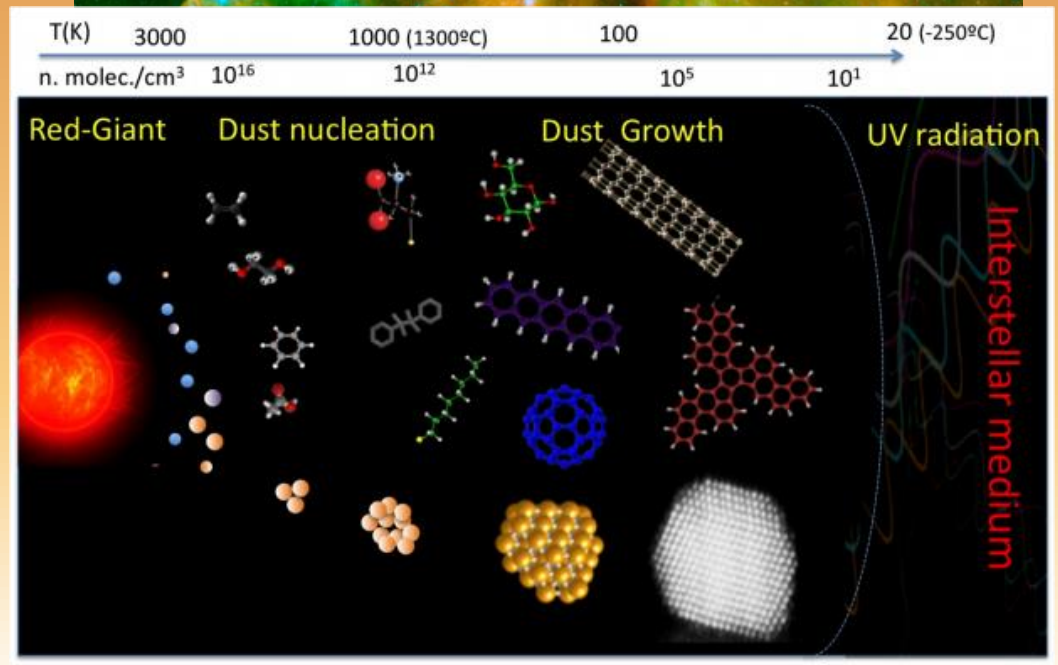
Introduction

- Nanocosmos Project
  - ERC synergy project
  - Understanding physical and chemical processes leading to cosmic dust formation
- PhD Project
  - Motivations
    - Emission bands of Polycyclic aromatic hydrocarbons (PAHs) are observed in interstellar medium (ISM)
    - 20% of Carbon in ISM
  - Work
    - Simulation of ion dynamics in ion traps
    - Characterization of specific PAH structures by CID and photo-dissociation
    - Development of an Imaging Source for complex sample analysis
    - Analysis of both synthetic and extraterrestrial samples by direct injection in AROMA or via the Imaging Source

nanocosmos

Gas and dust from the Stars to the Laboratory: Exploring the Nanocosmos



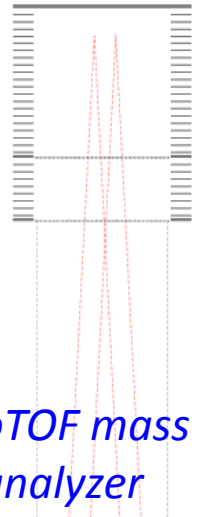


AROMA (Astrochemical Research of Organics using Molecular Analyzer)

- Molecular analyzer that combines laser techniques to produce the ions,
  - Desorption 1064 nm
  - Ionization 266 nm
- Ion Trap to perform dissociation studies or/and guide ions
- oTOF (Orthogonal Time of Flight) to record mass spectra

Performances of AROMA:

- Mass range : 20 to 10^4 amu
- Mass resolution: 8000 to 10000 @ 300 amu
- Mass accuracy : 10 ppm
- Isolation: 1 amu resolution
- MS/MS experiments
- Photodissociation and kinetics studies

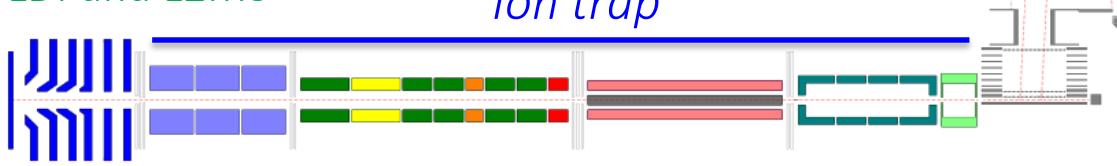


oTOF mass analyzer

Ion source:

LDI and L2MS

Ion trap



L2MS technique used

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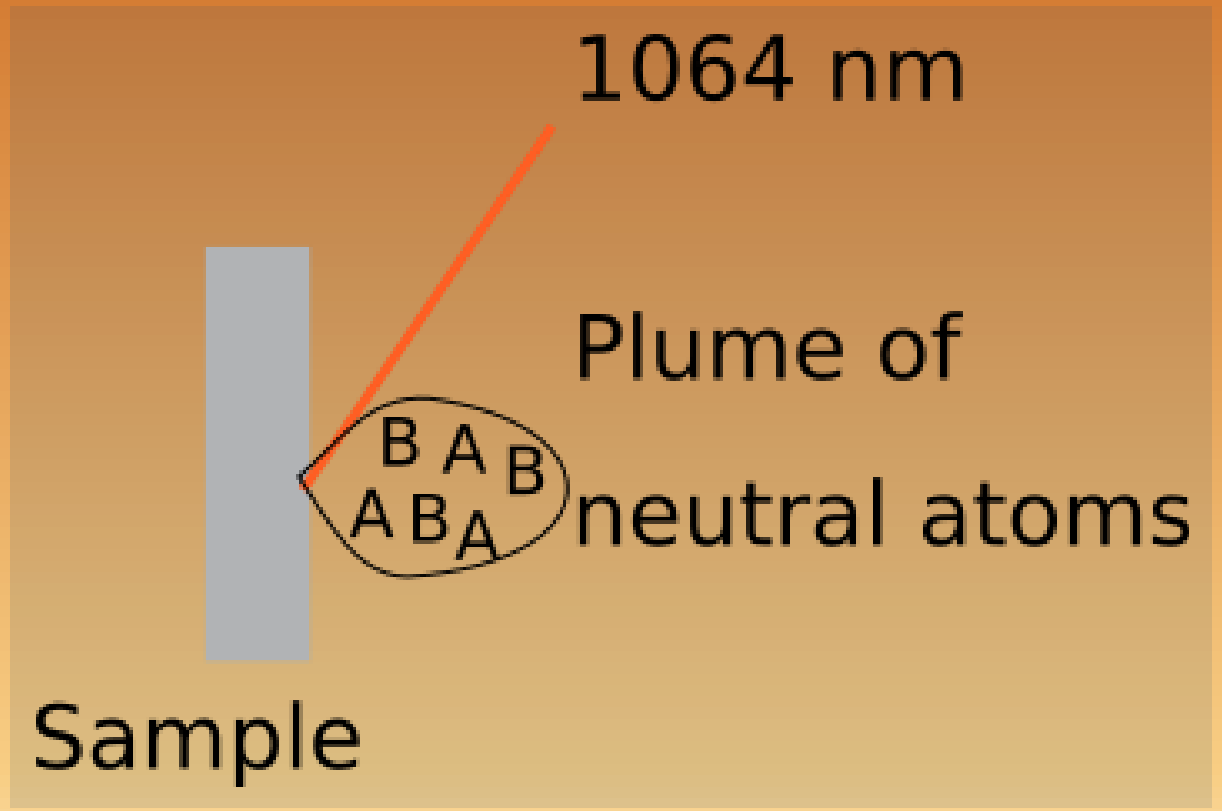

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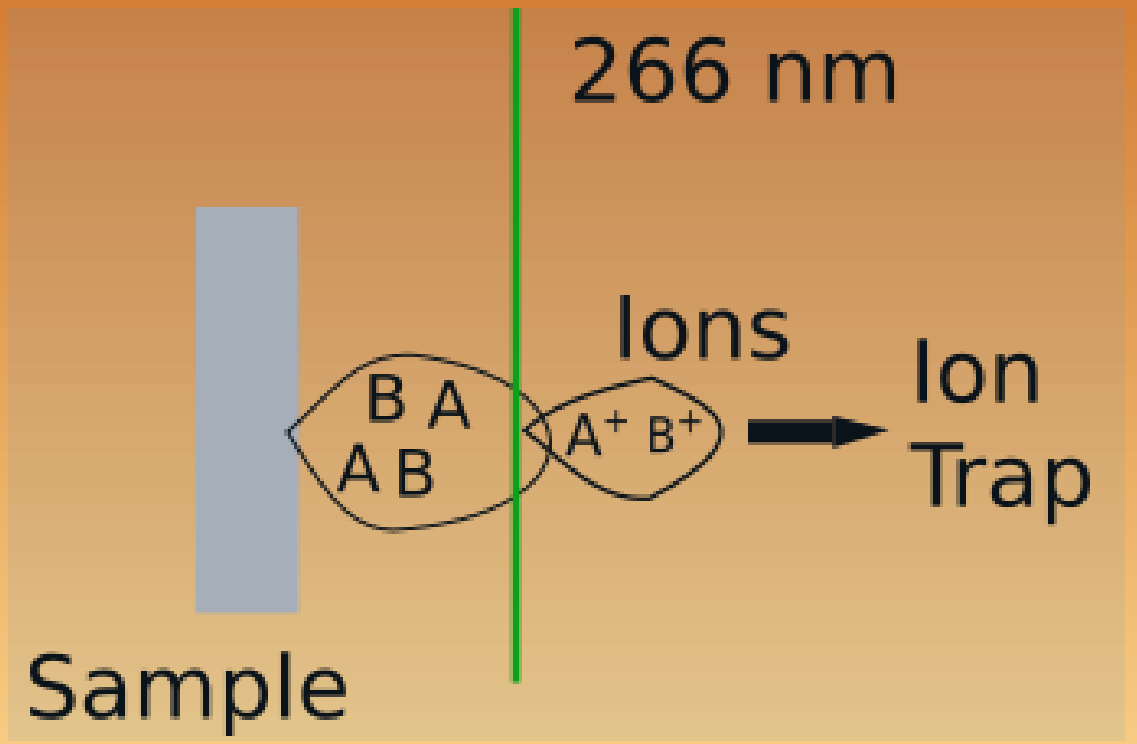

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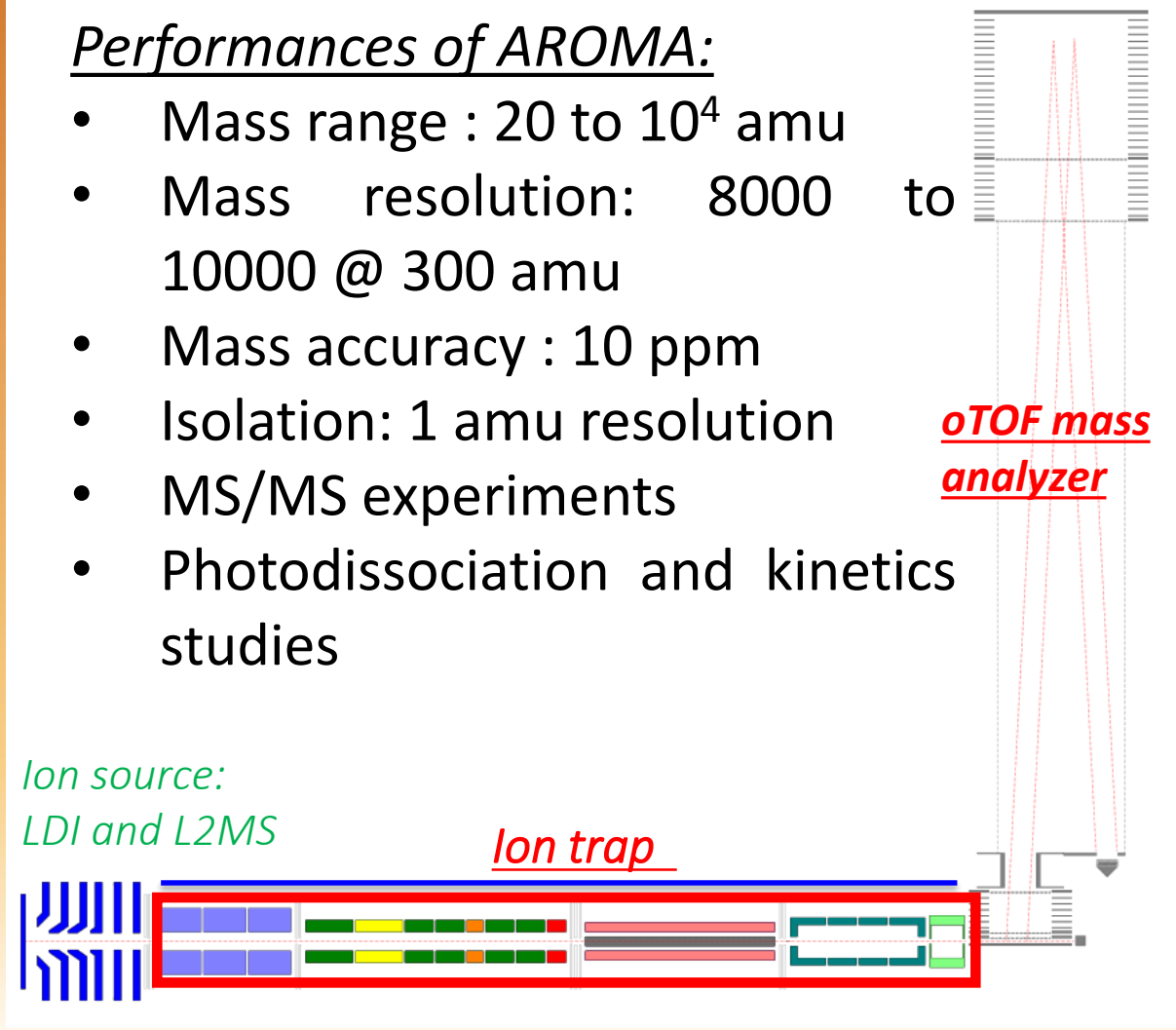

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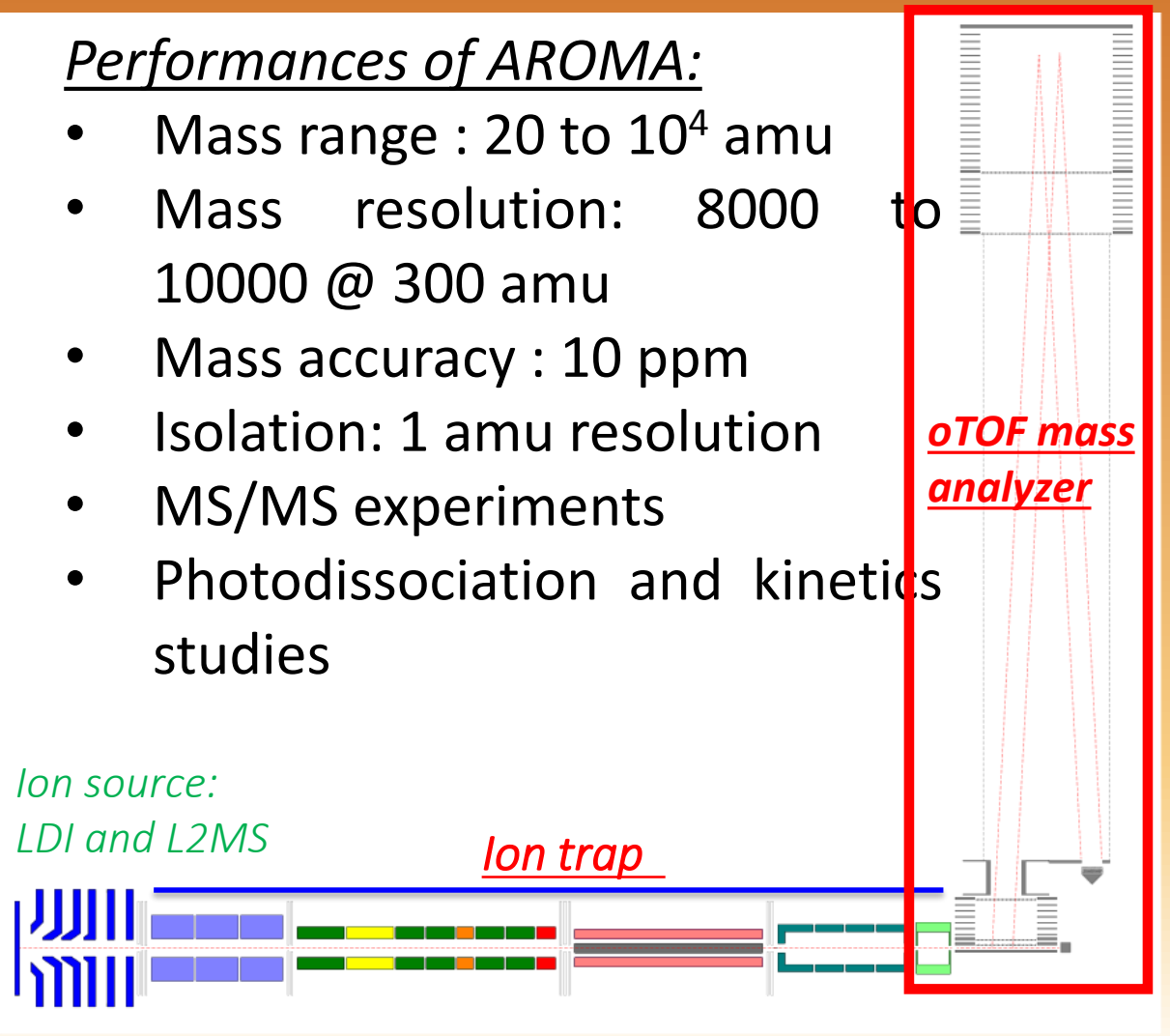
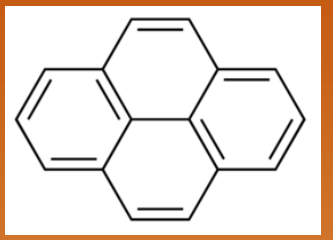
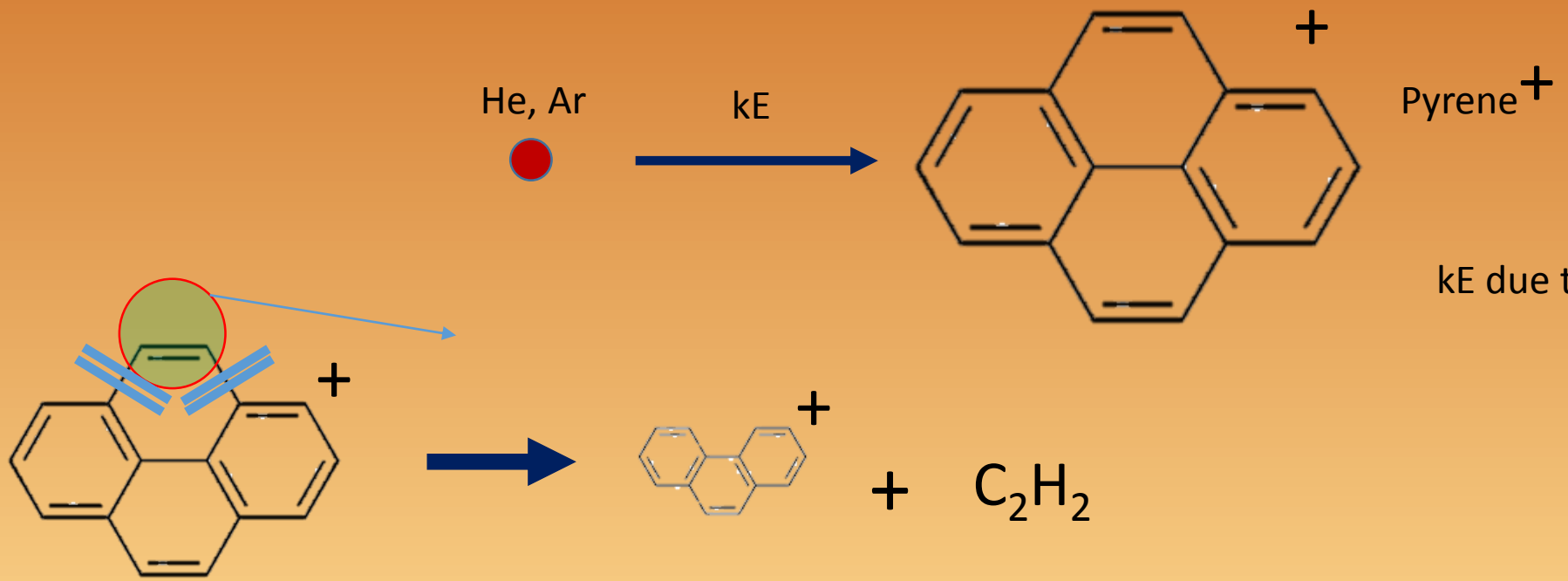


CID : Collision Induced Dissociation

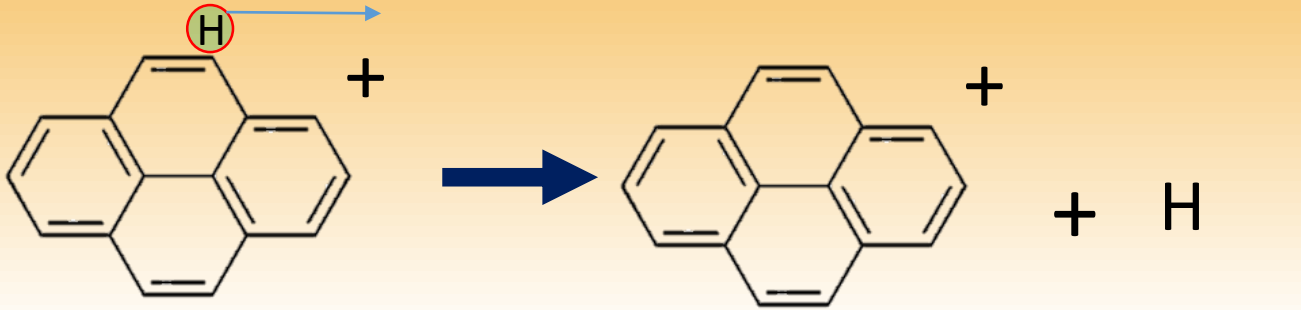


$C_{16}H_{10}$

Examples of CID:



kE due to DE (Dipolar Excitation)



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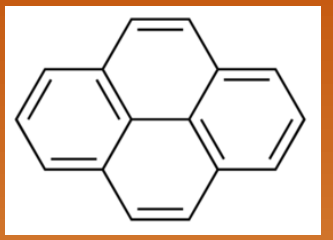
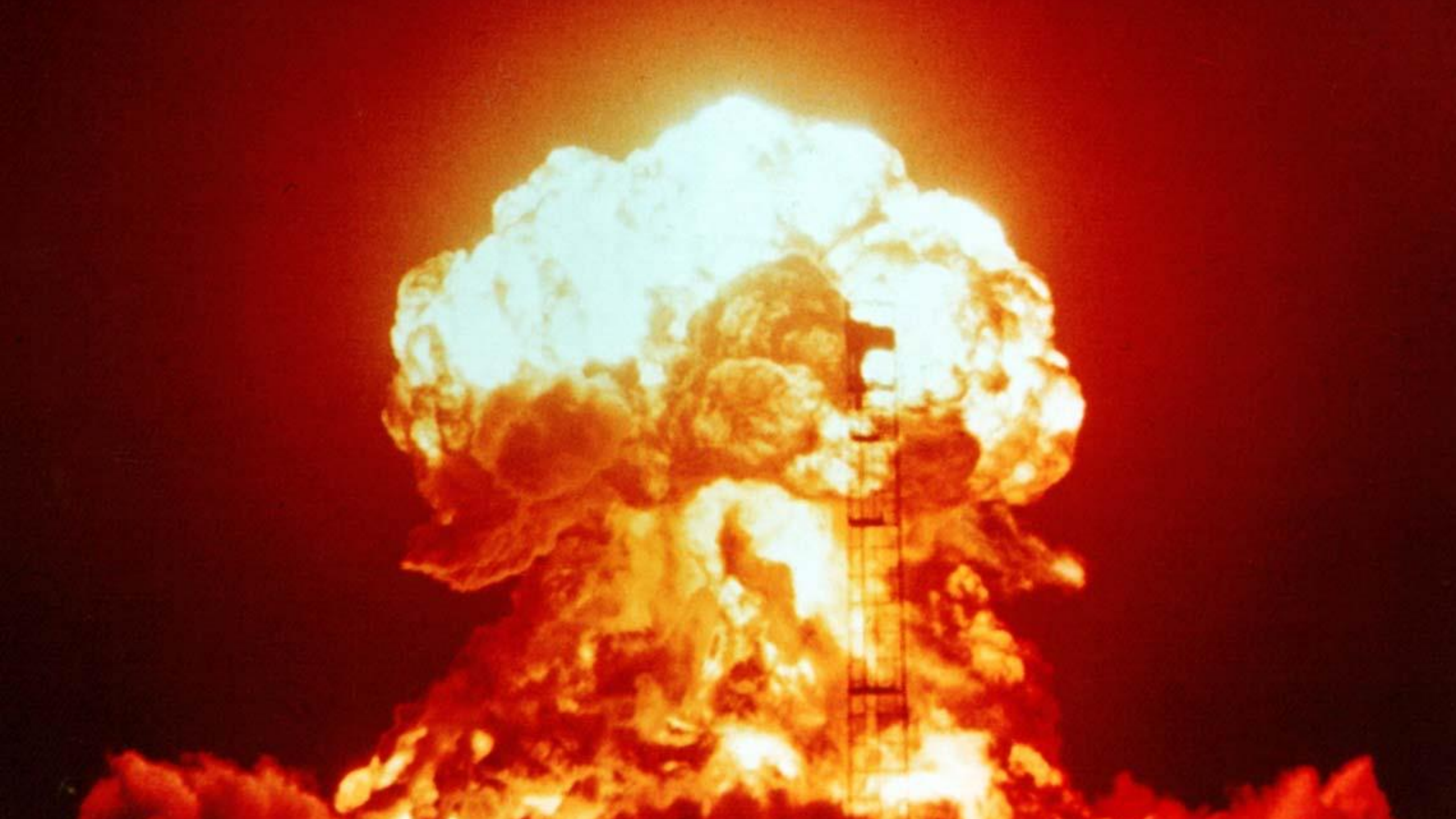


$C_{16}H_{10}$

Examples of CID:

+



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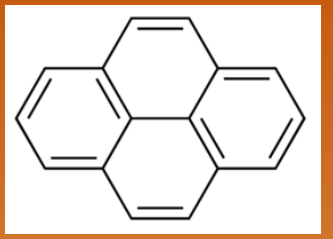

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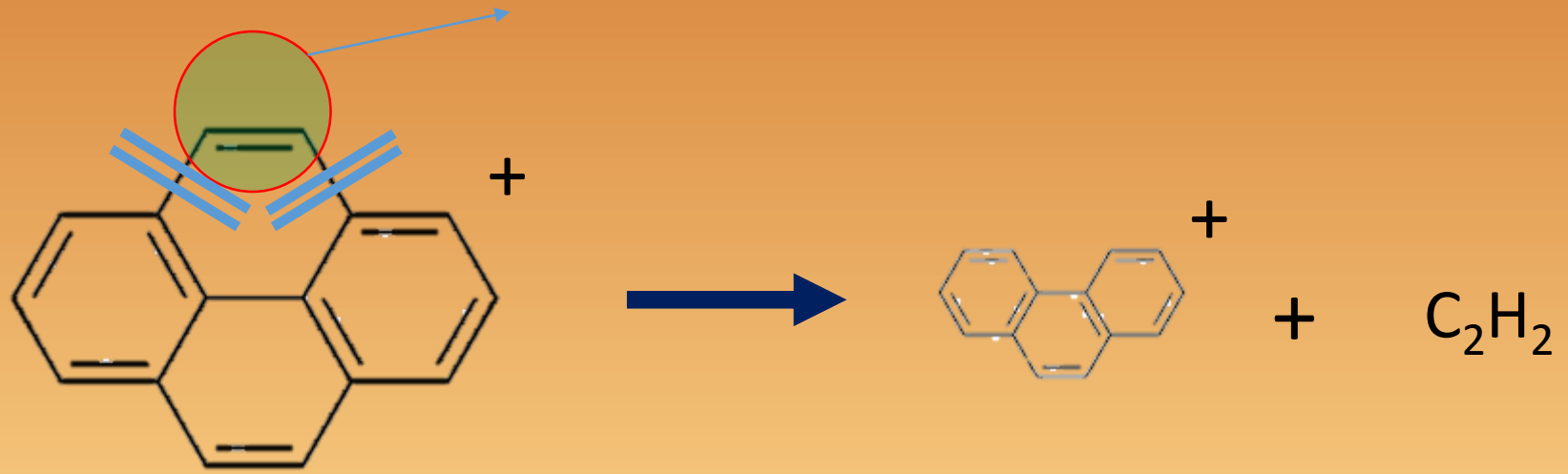
Examples of CID



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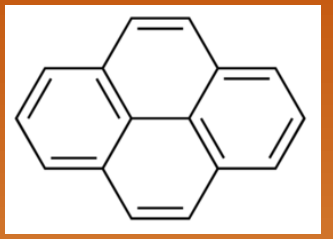

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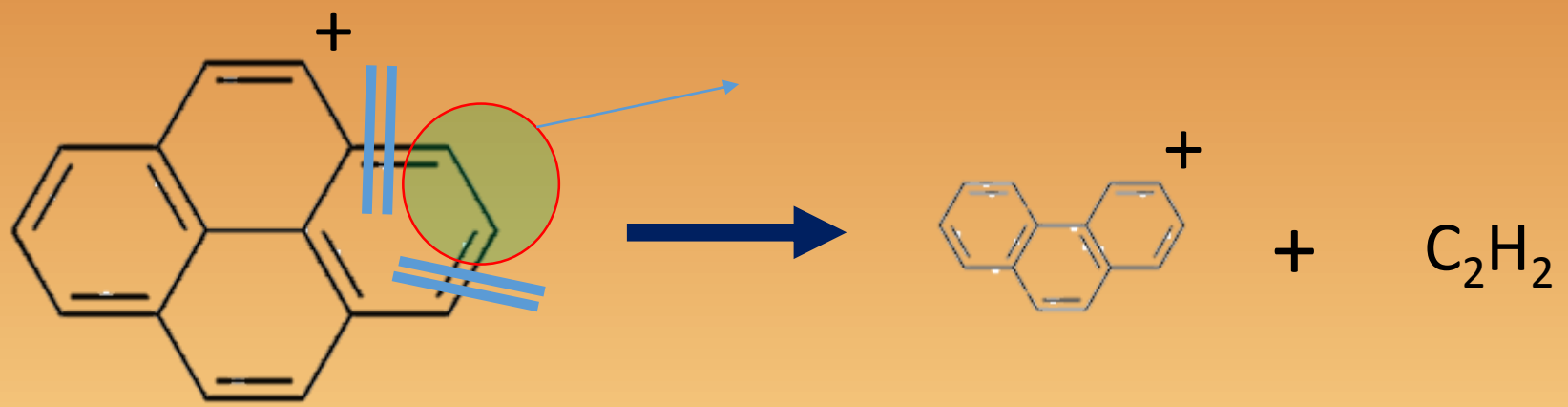

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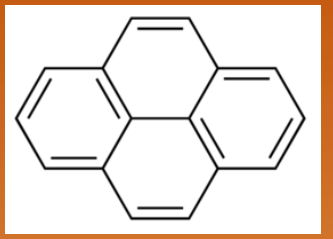

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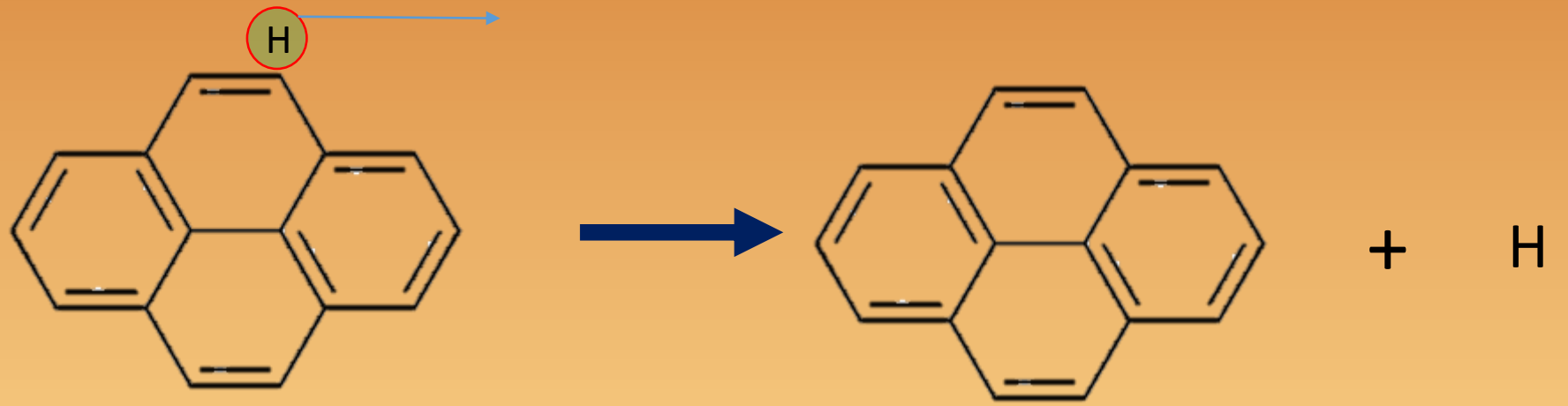
Examples of CID

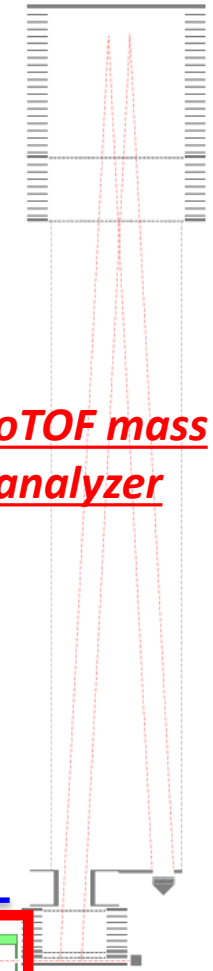


Simulations

Aroma

Ion Dynamics in Trap
- motion/trajectory of ions in trap,
- Electrostatic and electrodynamics properties of traps,
- Gas in trap, Collisions, cooling…

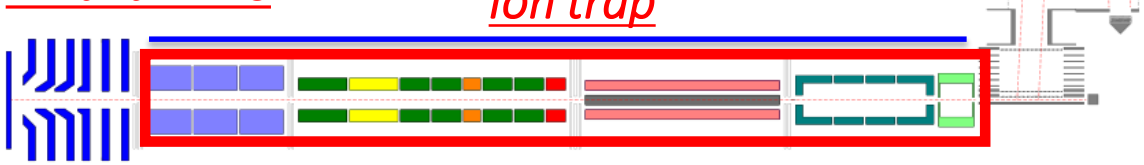
Very important to understand and calculate collision energies.

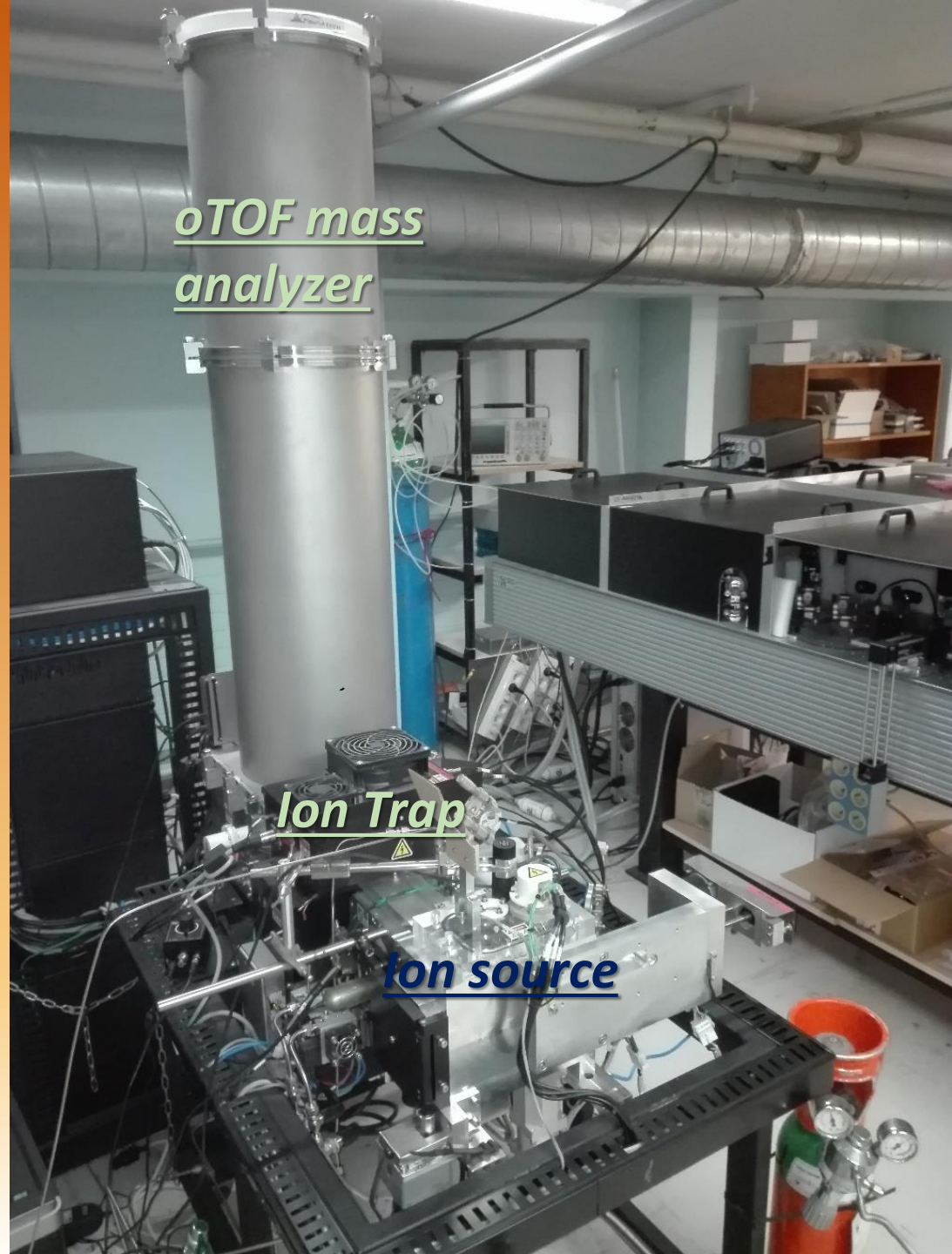


oTOF mass analyzer

Ion source:
LDI and L2MS

Ion trap

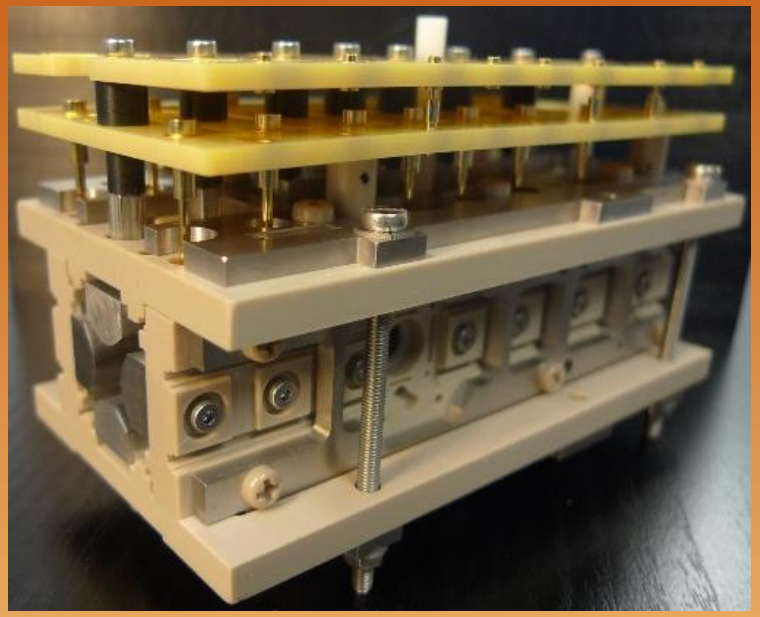




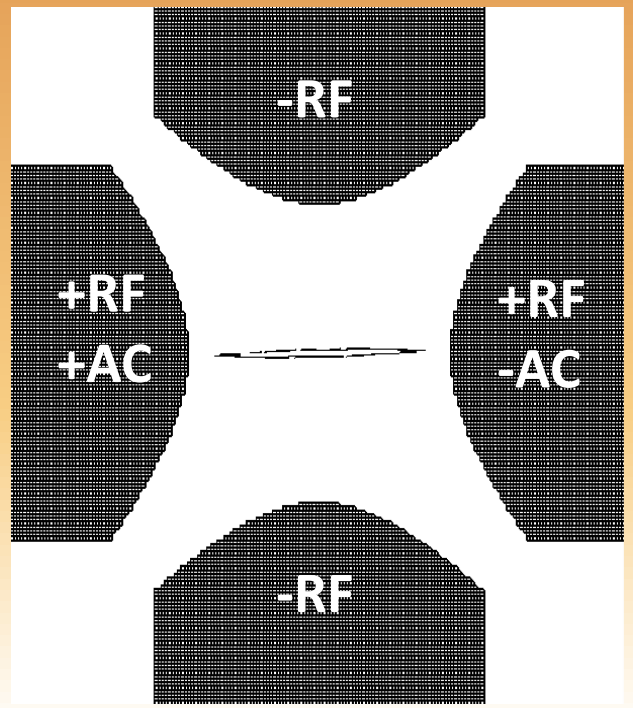
AROMA Simulations

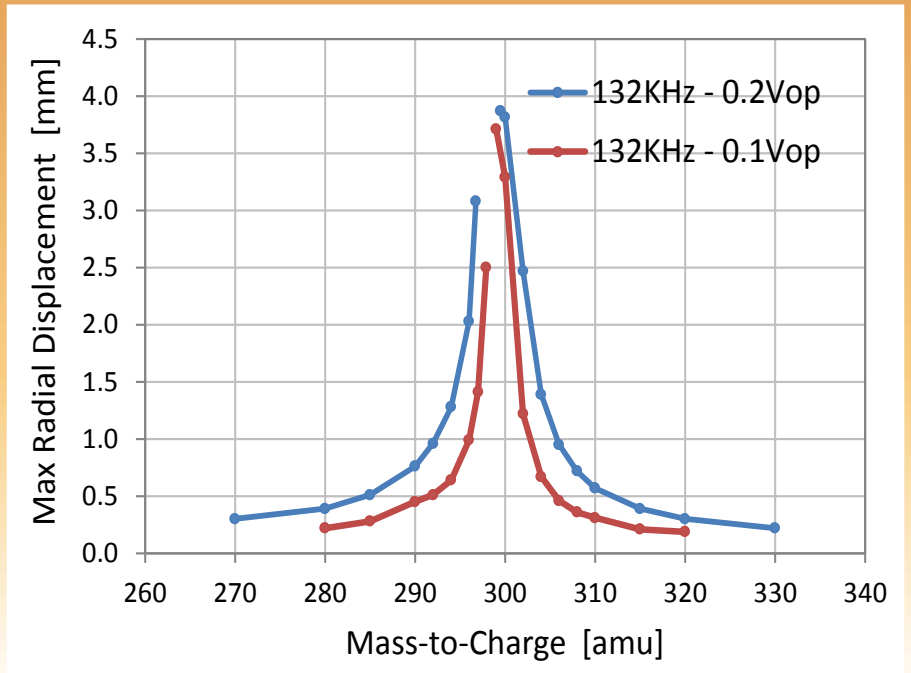
As an example, here I present:

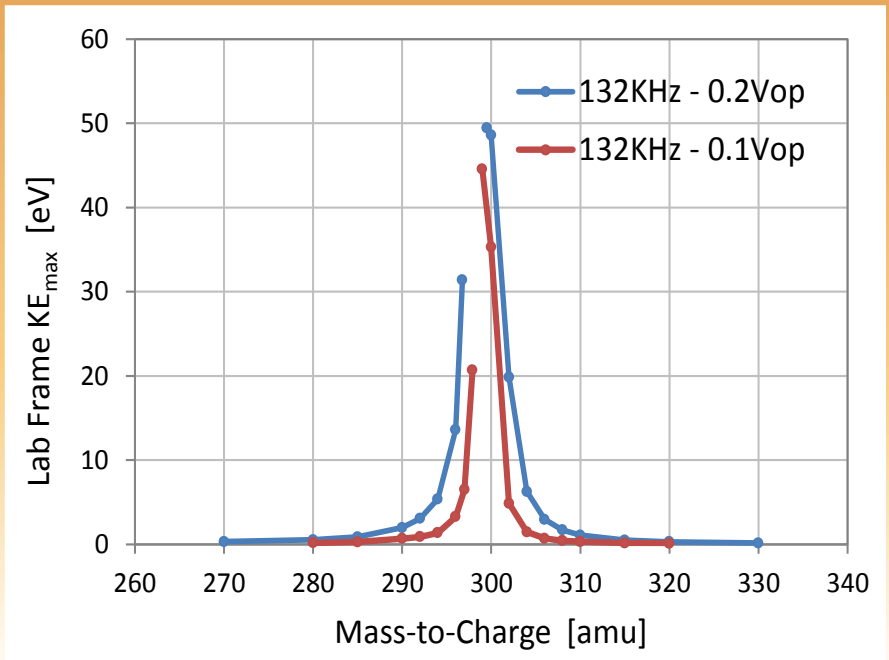
- The trajectory of ions in the trap,
- The maximum displacement from the center as a function of the masses,
- The maximum energy of the ions as a function of the masses.



Dipolar excitation to tune the colliding energy



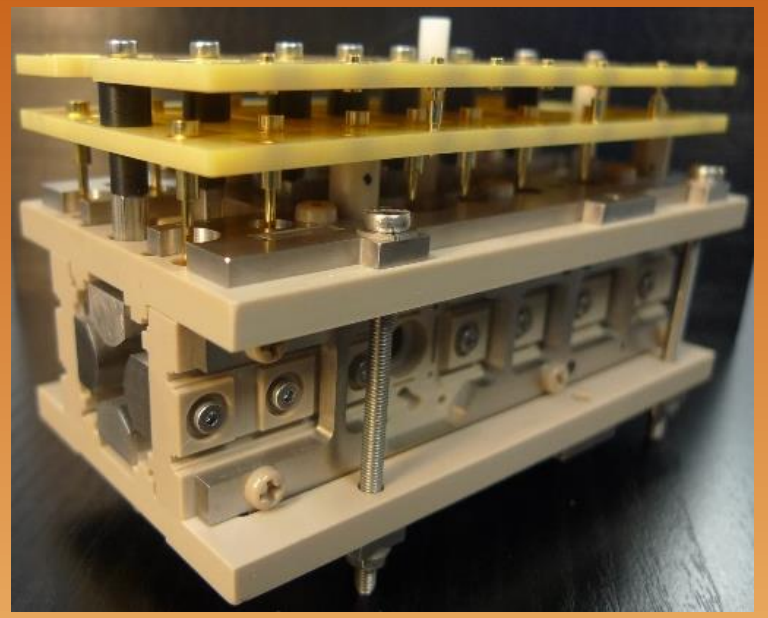


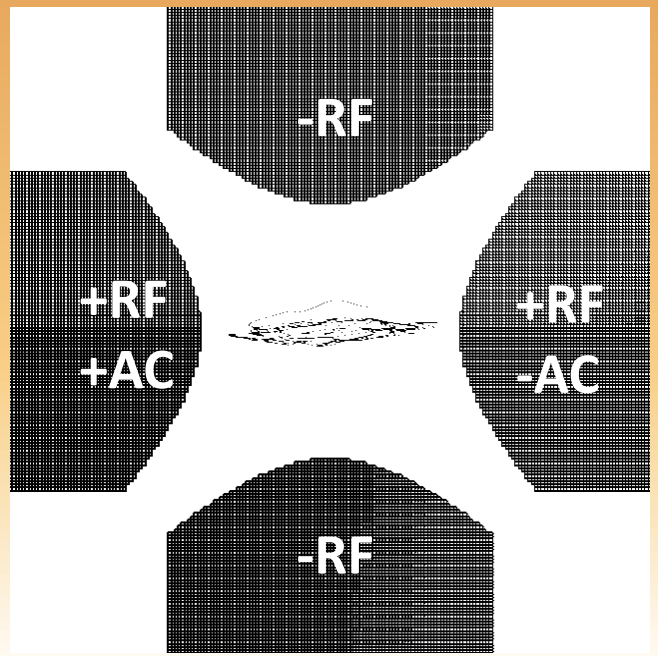


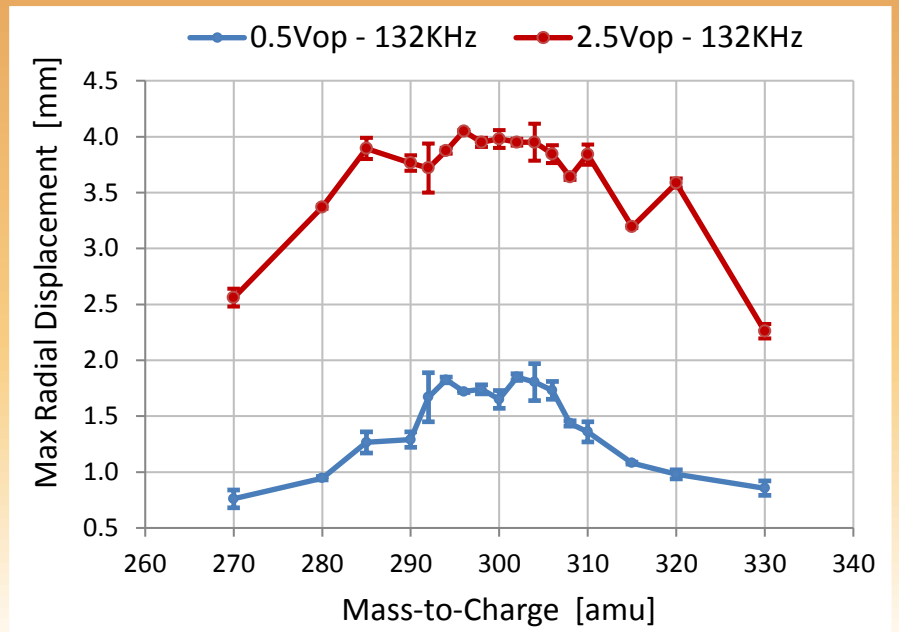
AROMA Simulations

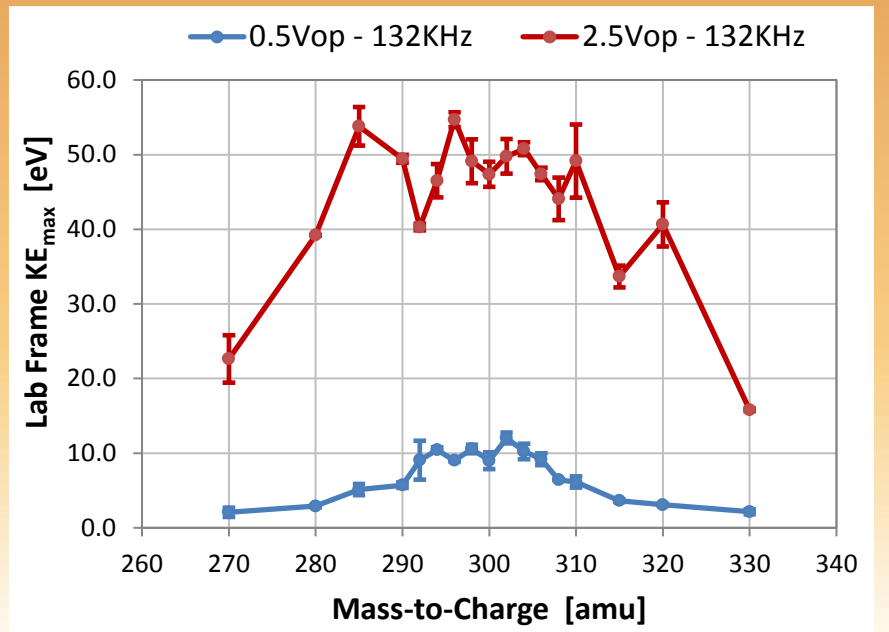
Same simulations as above but with 10^{-2} mbar of Ar, corresponding to the instaneous pressure when we incorporate colliding gas.

This shows the effect of pressure and gas type in the trap. My aim is to perform a full study of these parameters and others.

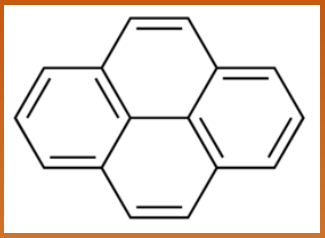








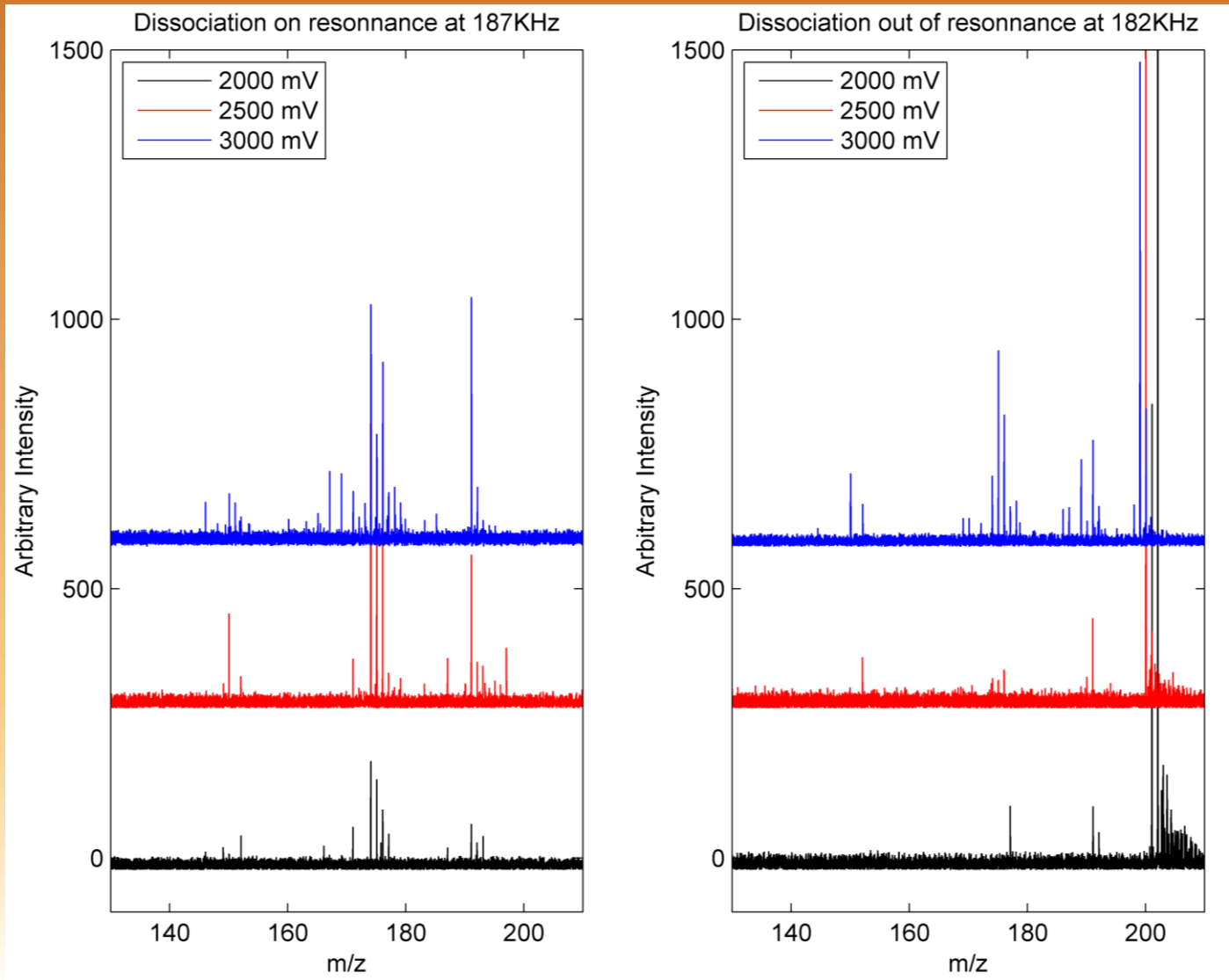
CID : Experiments and analysis



$C_{16}H_{10}$

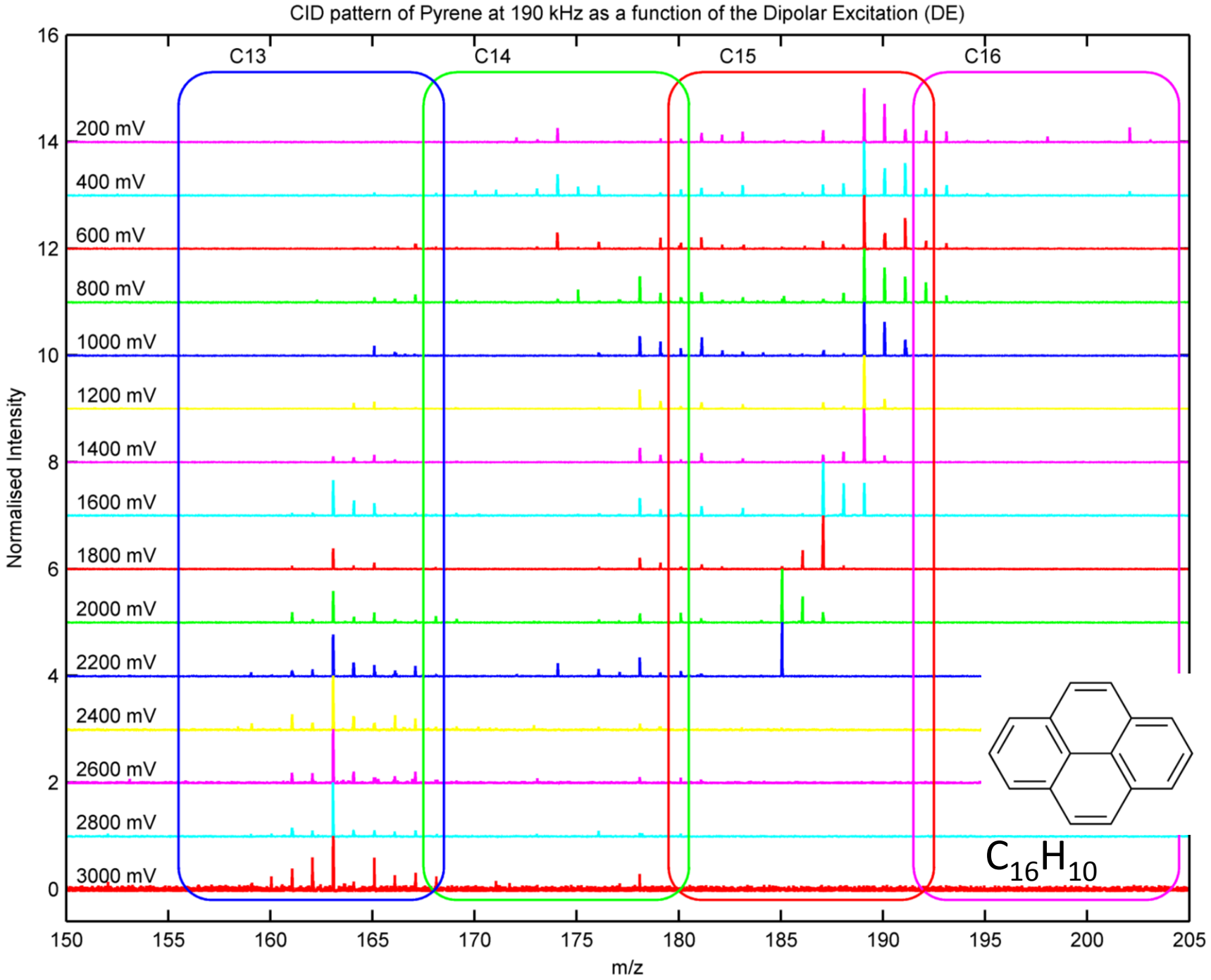
- Study of Pyrene cation m/z = 202.078

- CID = Collision induced dissociation
  - Collisions of the ions with rare gas atoms
  - We can tune the collision energy by changing the excitation of the ions.
  - We can address here 3 very important parameters which are the V_{app}, the frequency of the excitation and the duration of application of the DE
    - V_{app} is directly linked to the Voltage applied to the electrodes for the DE



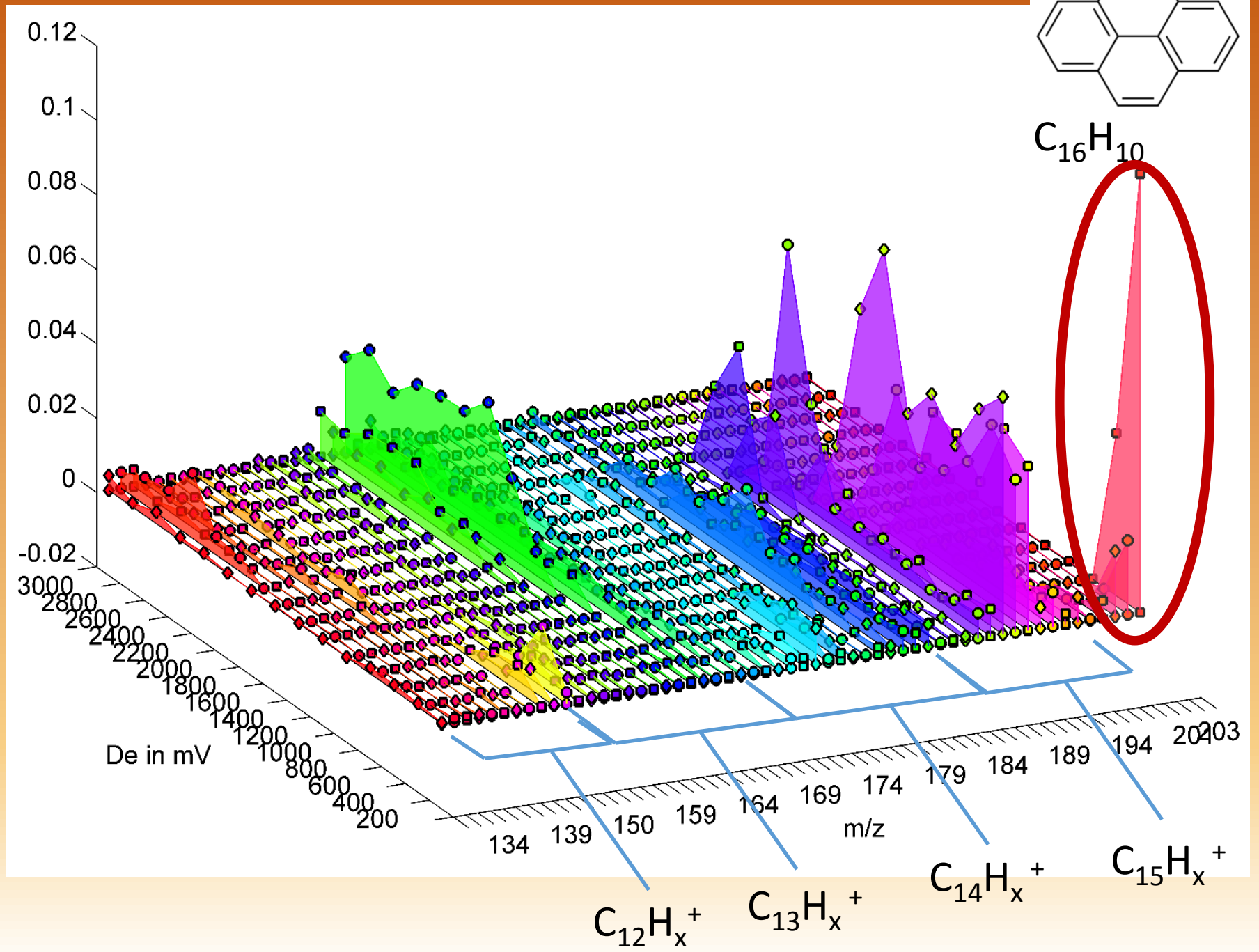
First Results

- We present CID results performed with off resonance (190kHz) excitation.



First Results

- From previous work we know that **two main channels** are involved in the dissociation of PAHs:
  - losses of H/H_2.
  - losses of C_2H_2.
- Abundance of fragments as a function V_{app} for a duration of 20 ms



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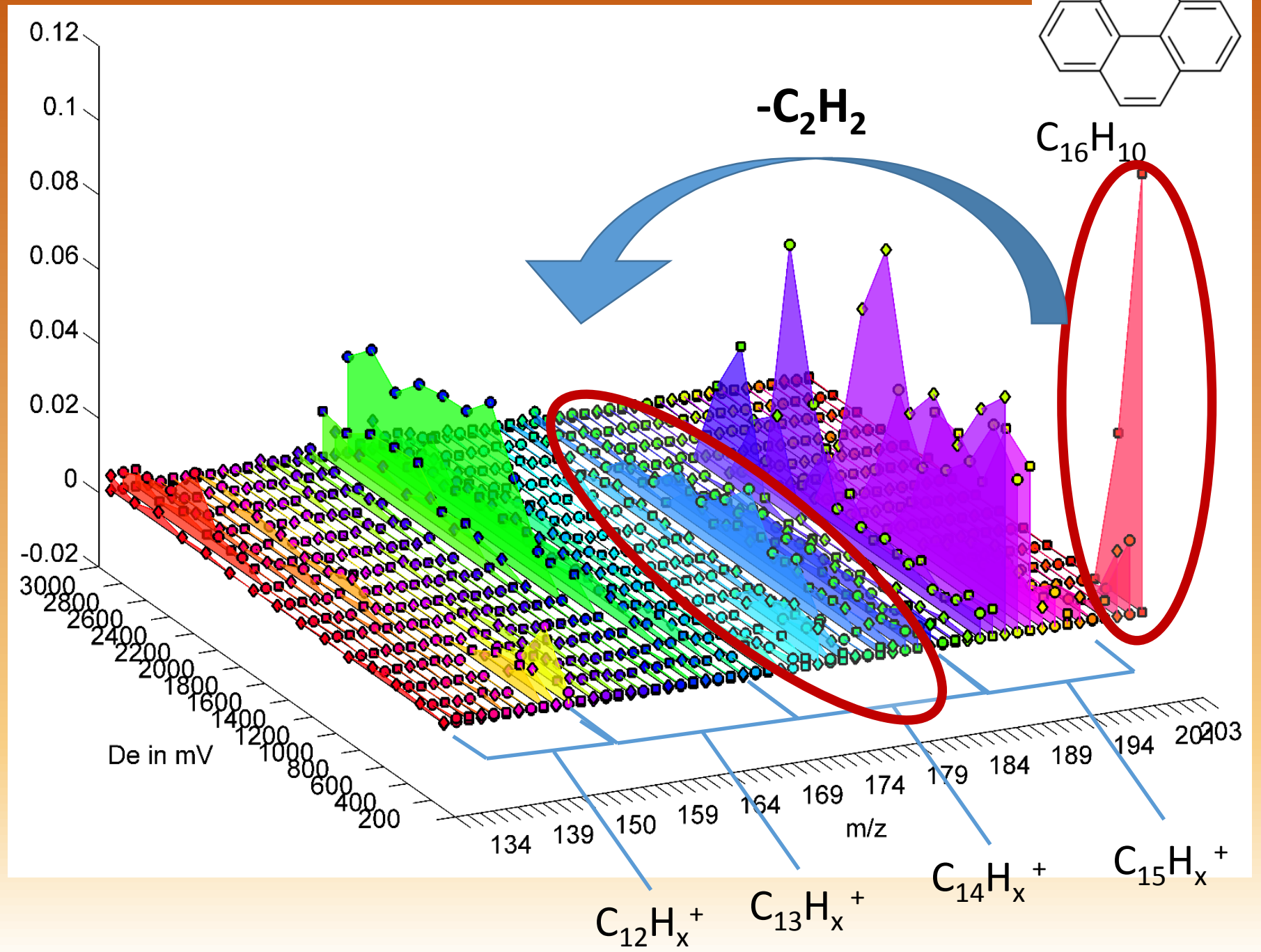

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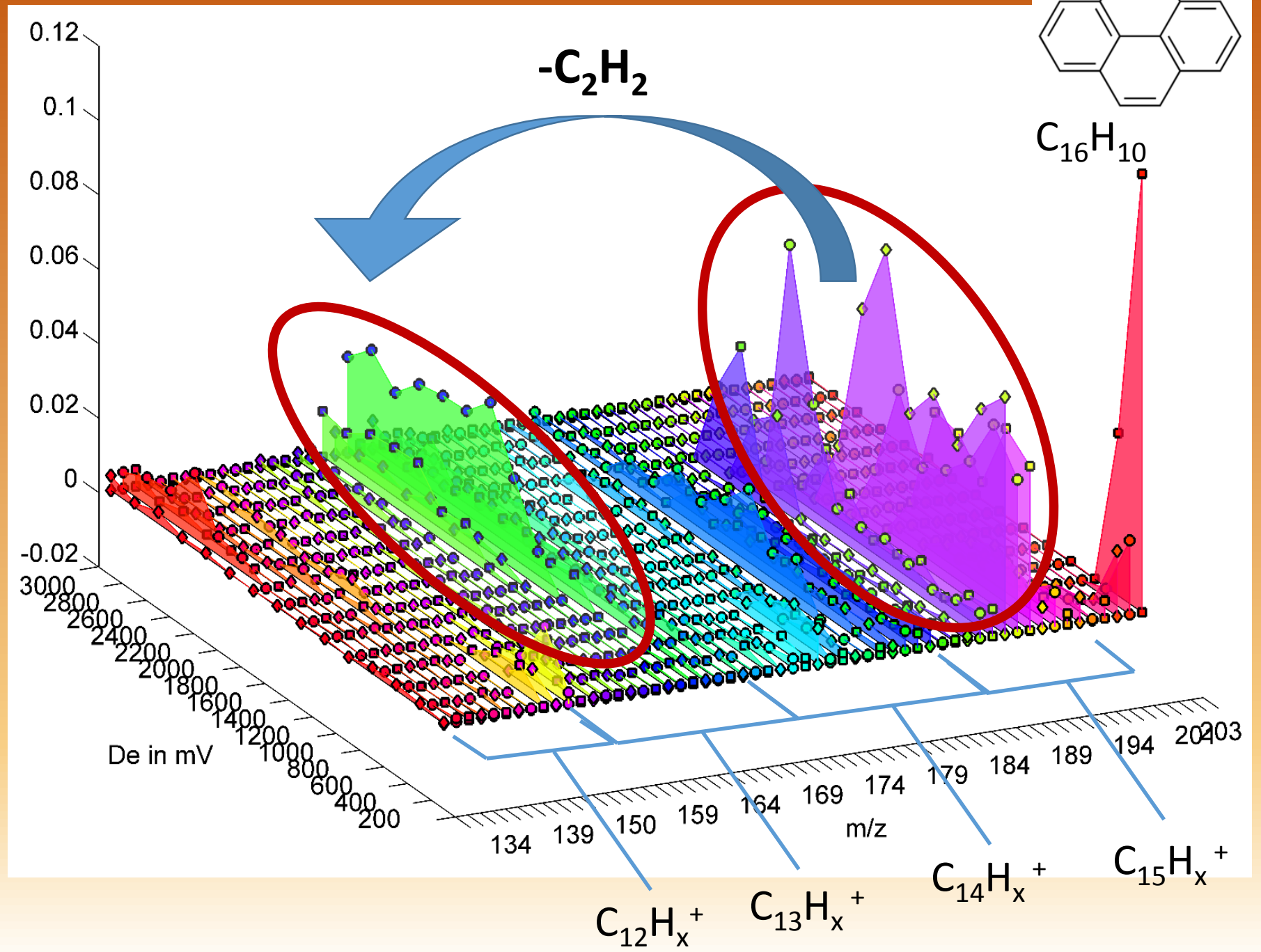
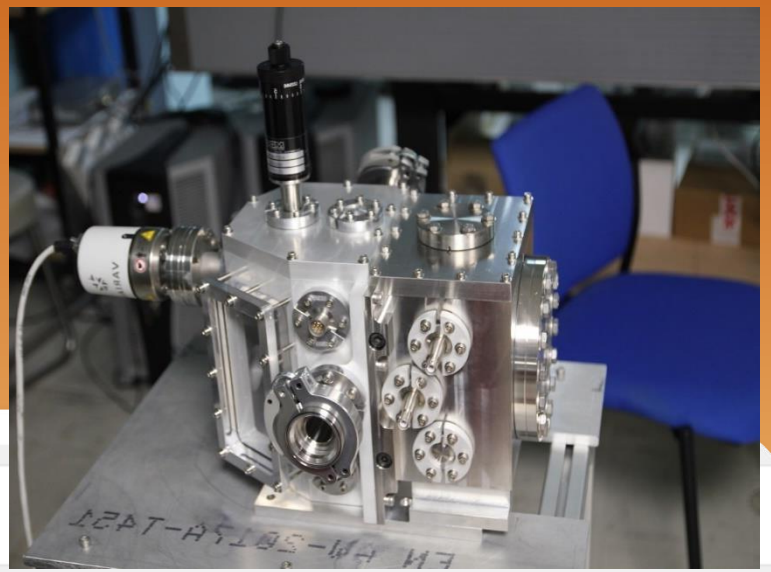
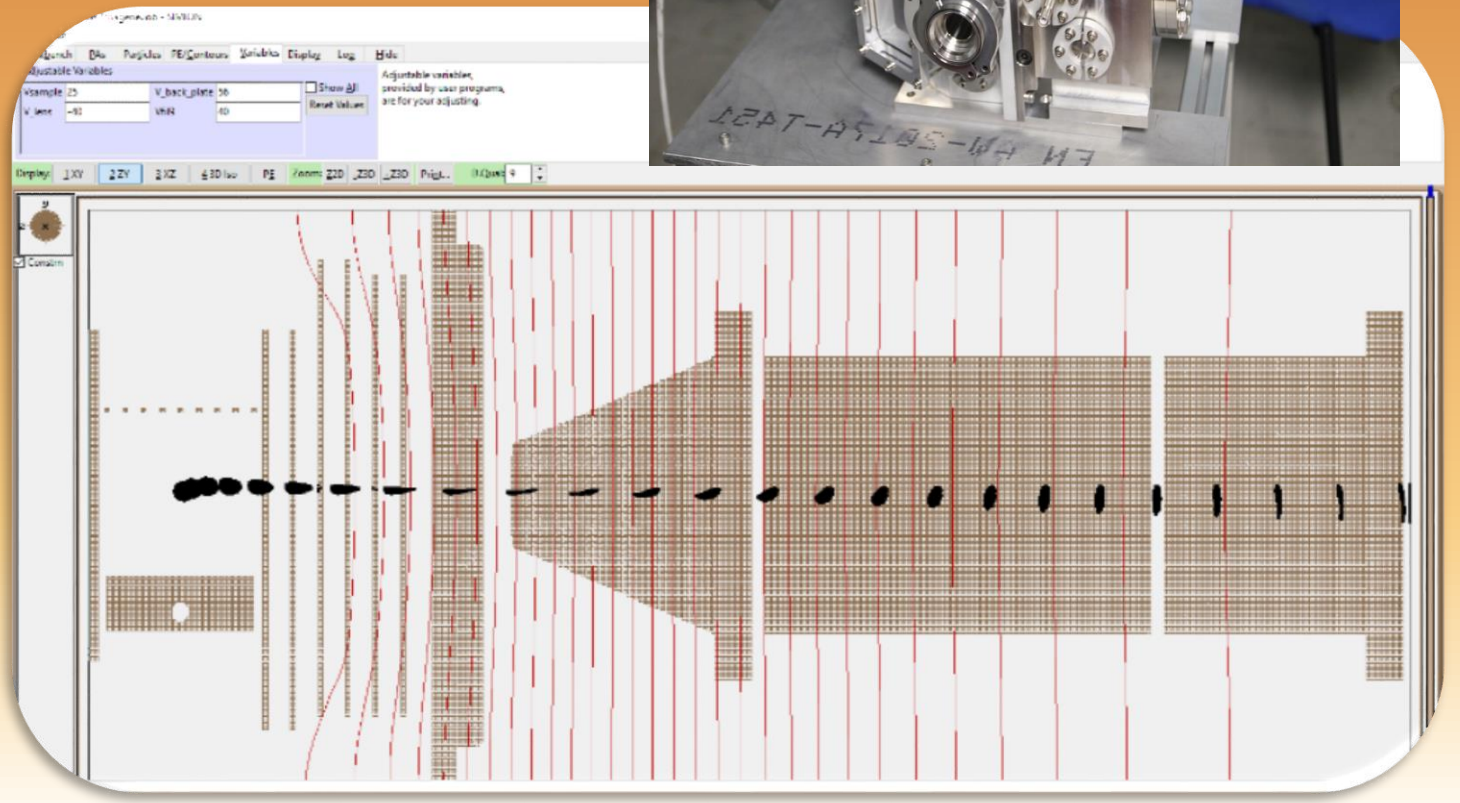


The Imaging Source and Ion Dynamics

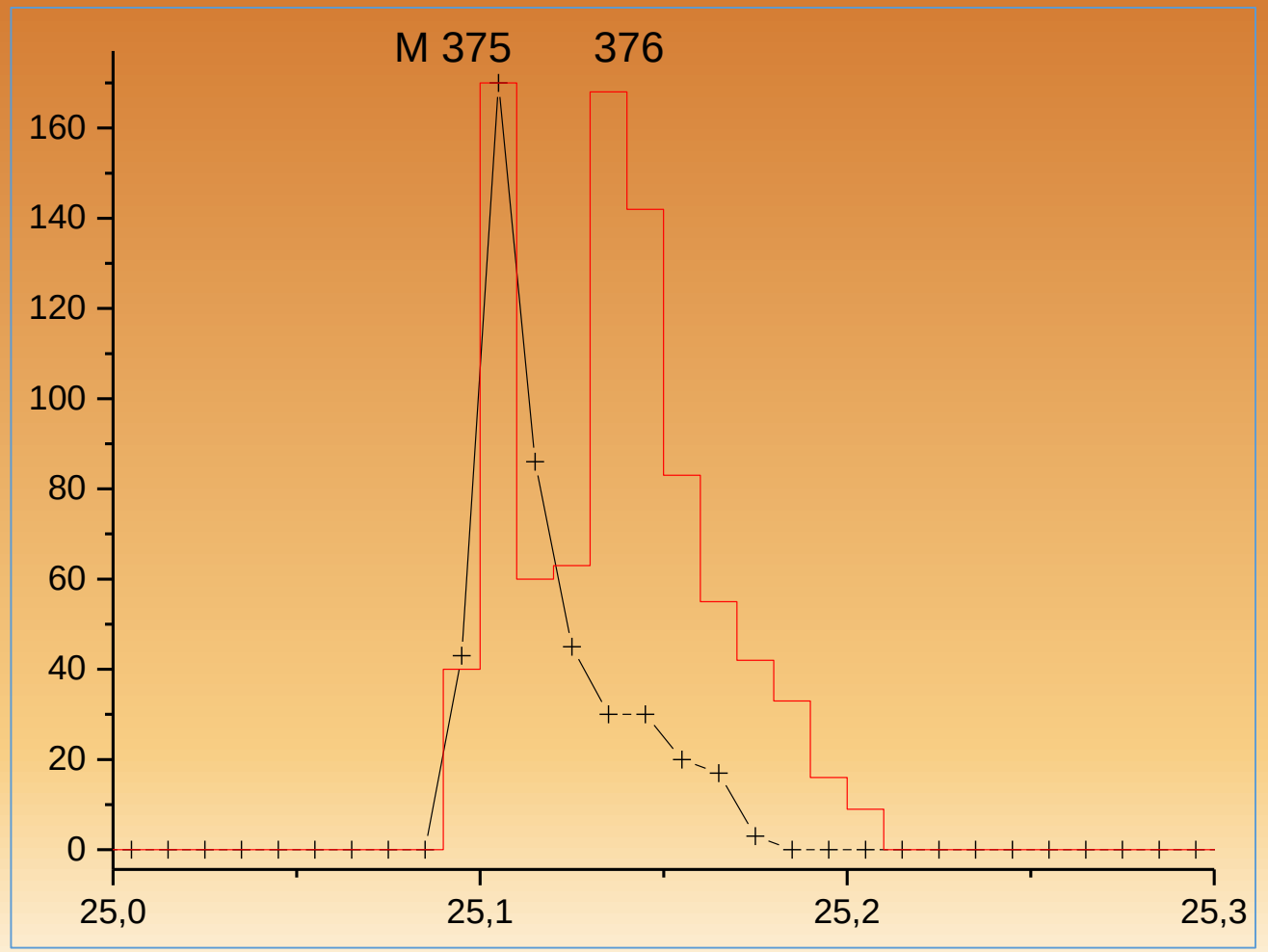
- The ion source uses L2MS technique.
- It will be tested on a home-made TOF and then coupled with the AROMA setup.
- Laser desorption with a spatial resolution of 5 µm on the sample.
- Direct analysis of the sample.
- Distinction of ions with 1m/z mass difference despite the small TOF.
- Scan of a surface
- Mapping the presence of a specific species.





Ion Dynamics in Imaging Source

- We sent a population of 2 different masses.
- Voltages on the electrodes are optimized.
- We obtain the time resolution needed to distinguish ions separated by 1 m/z.



Conclusion

- We succeeded to observe the main channels of dissociation of pyrene (C_2H_2 and H/H_2 loss) using the CID in the LQIT

- We are in the phase of testing the vacuum on the Imaging Source

Perspective

- Analyzing CID results on PAH cations by coupling experiments and ion dynamic simulations.
- Continue developing the ionization source
- Photo-dissociation studies