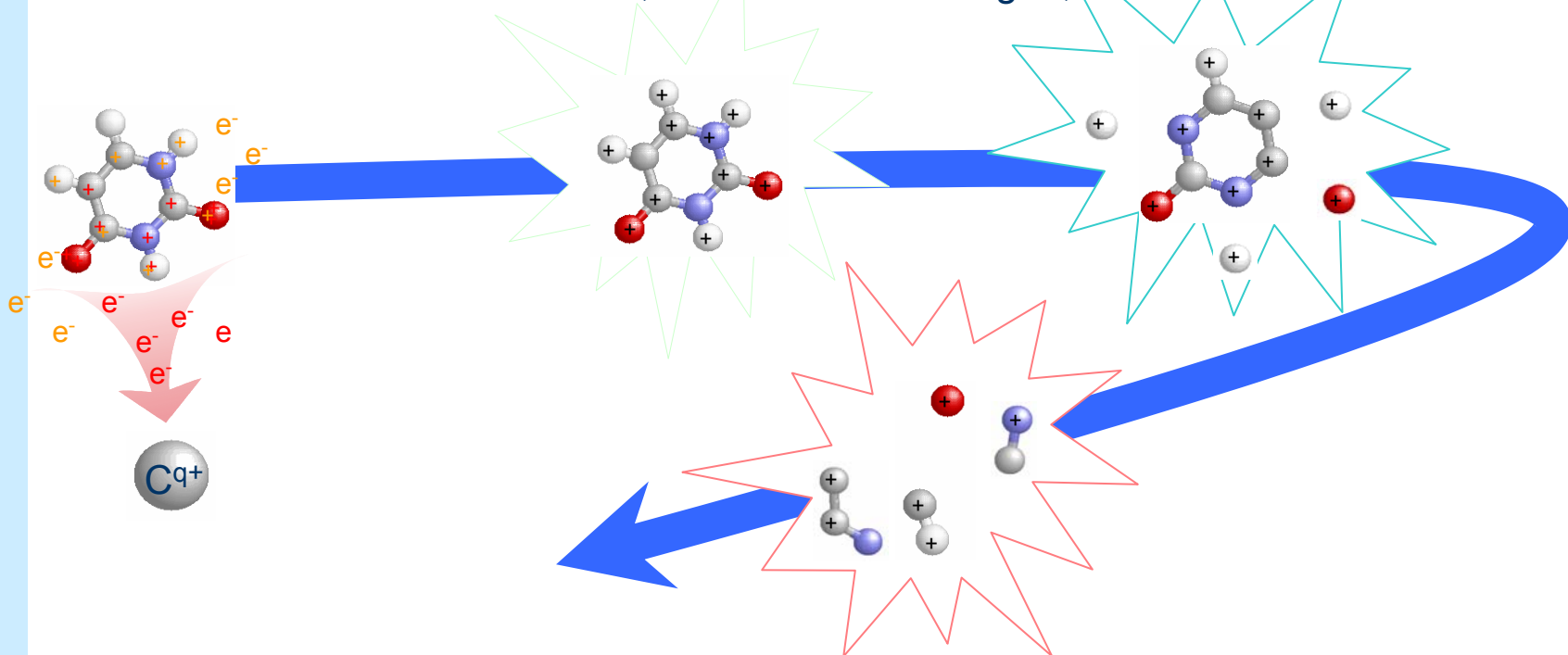


# Ionization, excitation and fragmentation of the isolated nucleobases *uracil* and *thymine* by multiply charged ions

Fresia Alvarado

KVI Atomic Physics, Rijksuniversiteit Groningen,  
Zernikelaan 25, NL-9747AA Groningen, The Netherlands



# Overview

- ➔ What is the role of Multiply Charged Ions (MCI) in Radiation Damage research?
- ➔ How do we study MCI interaction with nucleobases?
- ➔ What is the fragment mass distribution?
- ➔ Are there projectile effects?
- ➔ Are there target effects?
- ➔ What can be learned from fragment kinetic energies?
- ➔ What can be extracted from coincidence plots?
- ➔ Is it possible to identify fragmentation channels?

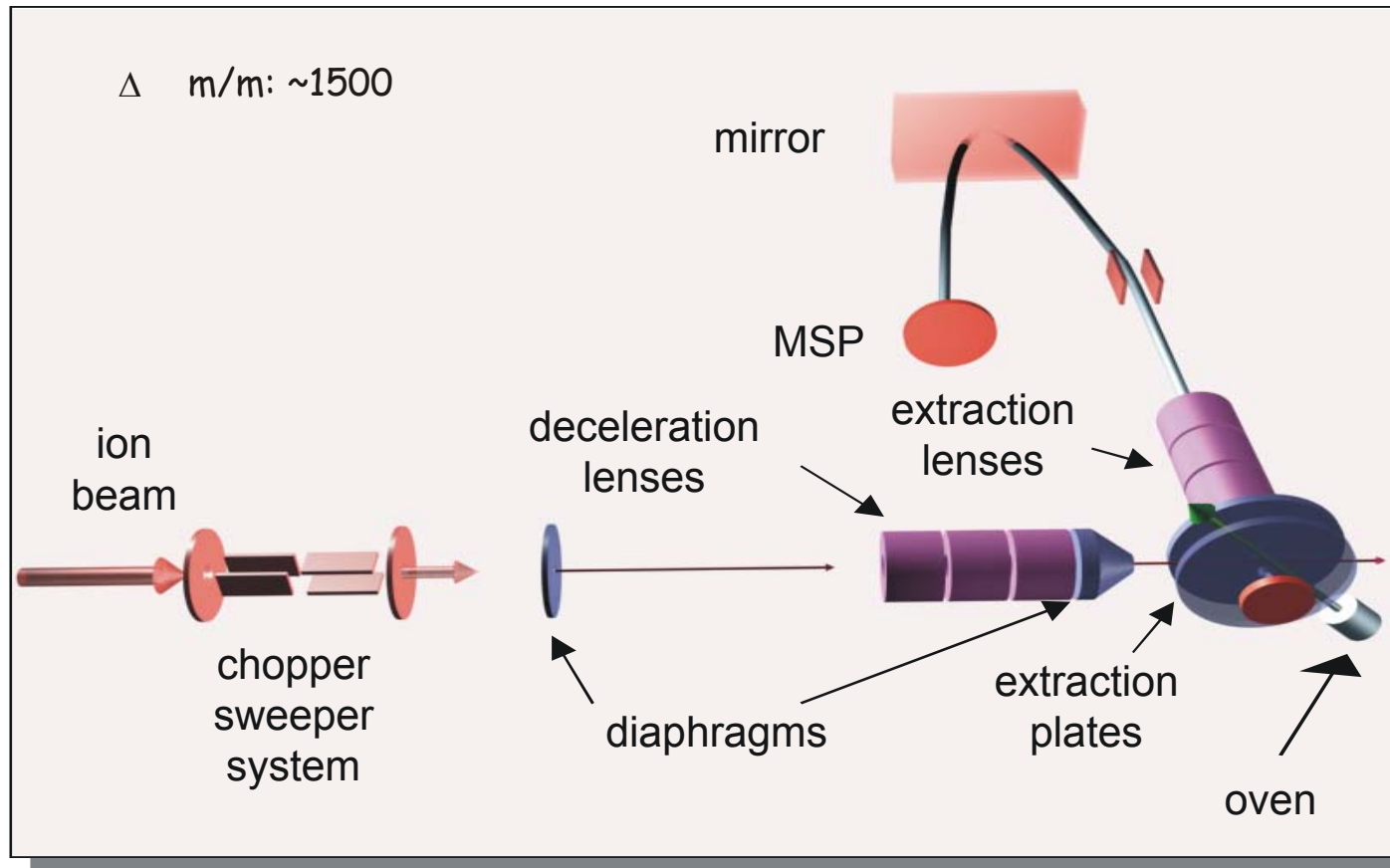
# Multiply charged ions (MCI)

**They are involved in primary or secondary radiation damage!!**

Primary: Heavy ion therapy (C-ions), proton therapy and radiation exposure of biological tissue in space.

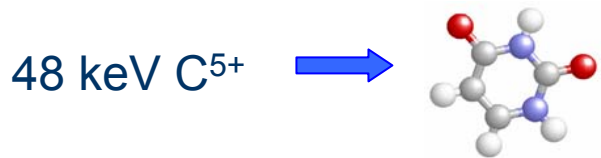
Secondary: They are formed within the track of primary radiation, together with low energy electrons and radicals.

# Our Experimental Setup

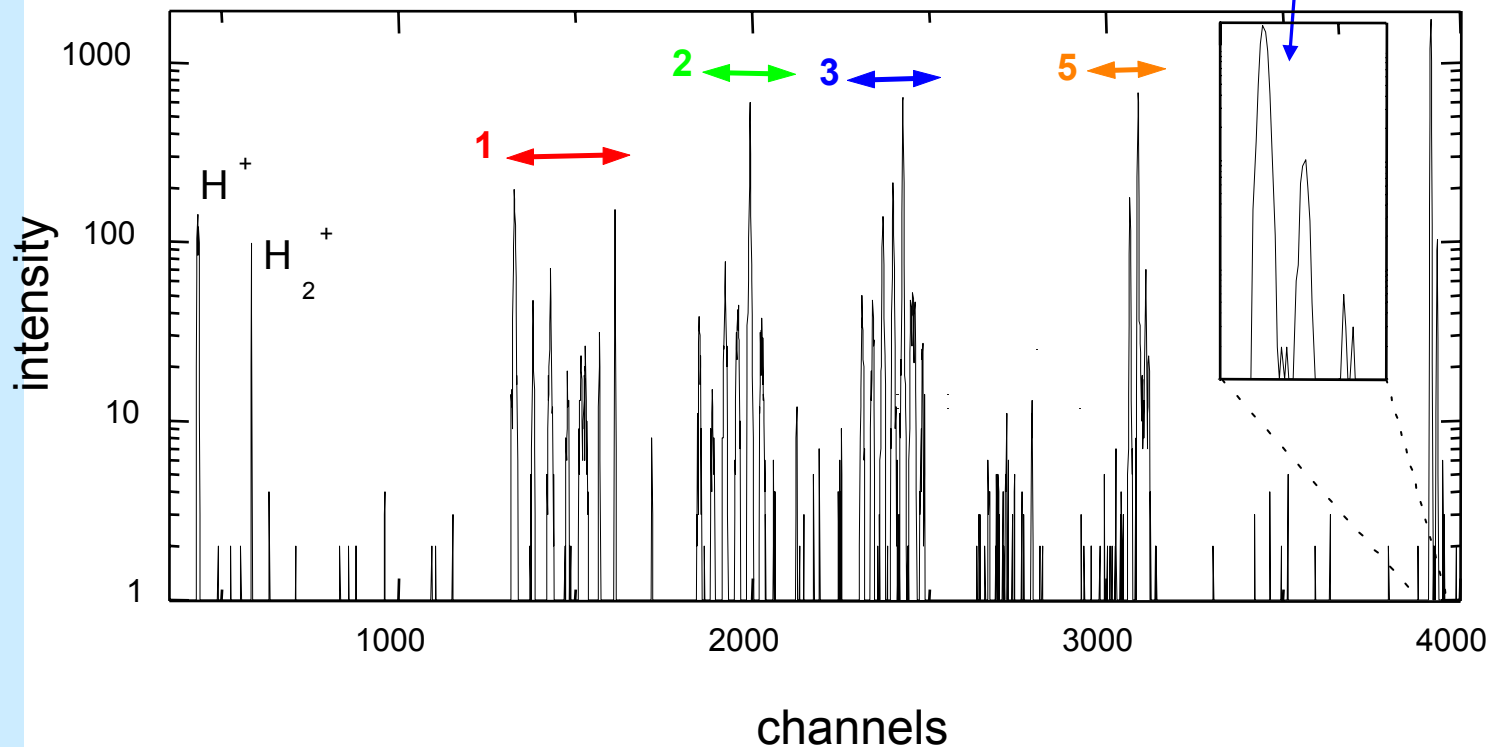


- fragment ion detection in event by event mode (FAST P7888 TDC, 1 ns resolution)
- chopper ion coincidences
- electron-ion coincidences
- electron-ion-ion coincidences

# Uracil TOF spectrum



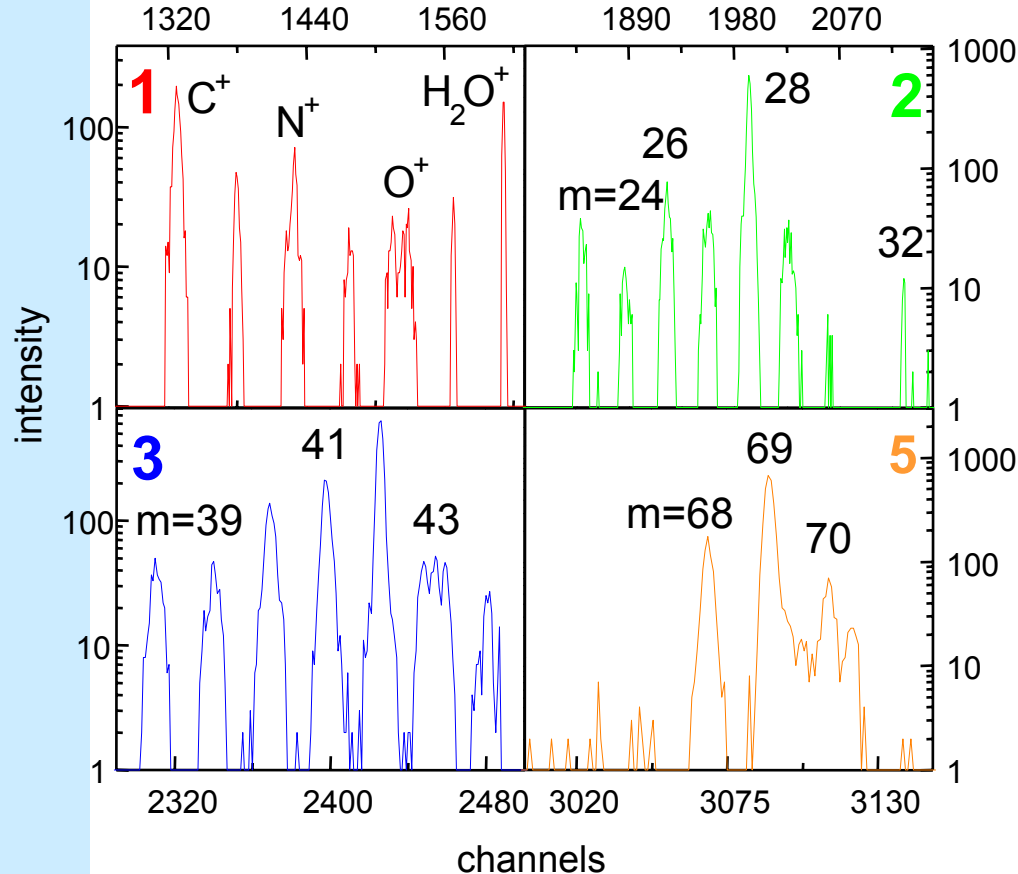
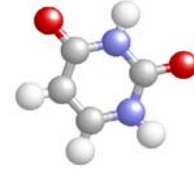
isotope structure of parent resolved



It is difficult to extract information only from the fragment's groups because they are the same for most organic molecules

*J de Vries et al.,  
J. Phys. B. 35,  
4373 (2002)*

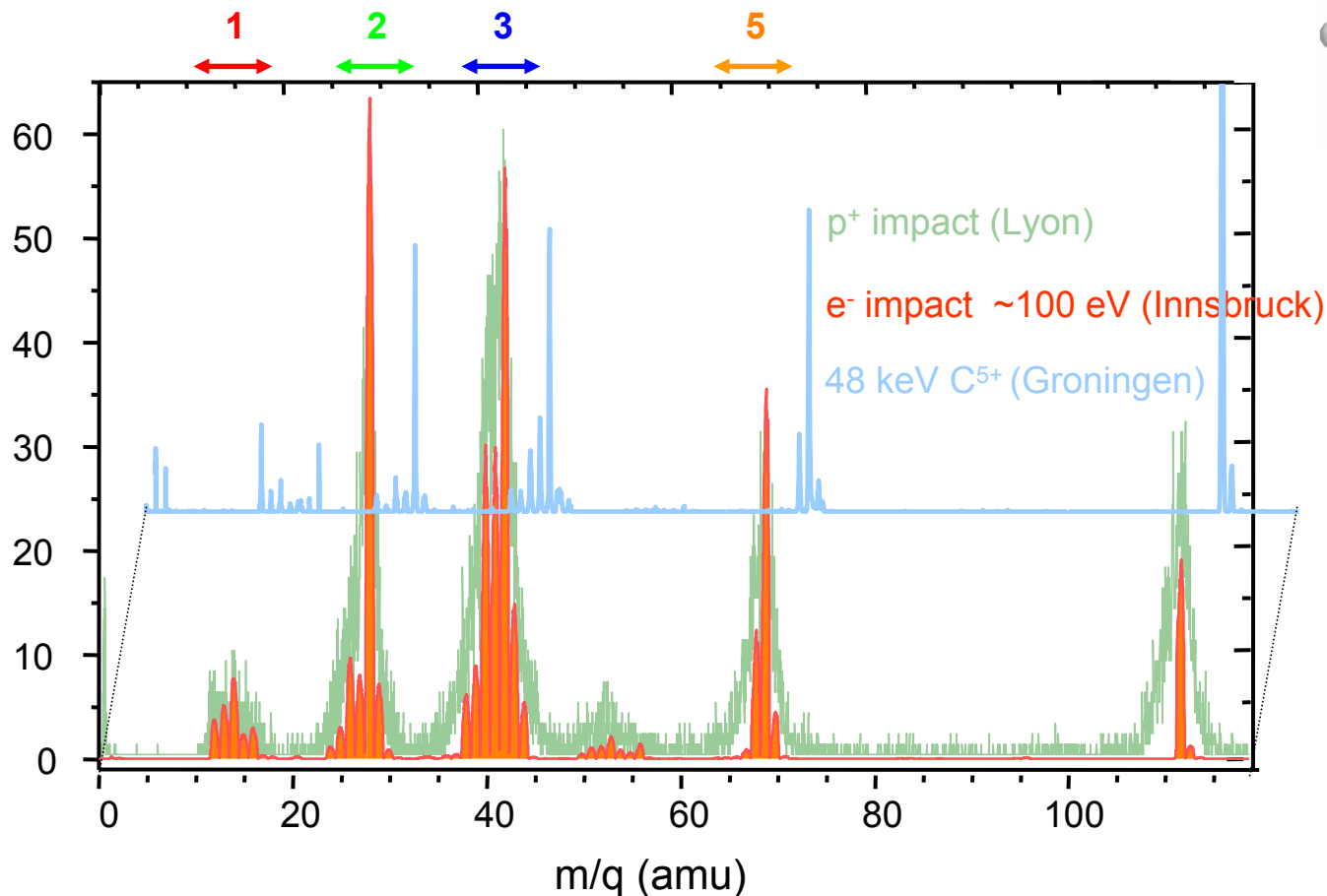
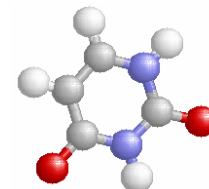
# Zoom into Uracil TOF



- $H_2O^+$ ,  $OH^+$  and  $O_2^+$  are very narrow, they are from the residual gas
- most other peaks of comparable width
- specific fragmentation channels:  $O^+$ ,  $CHNO^+$  and  $m=70$

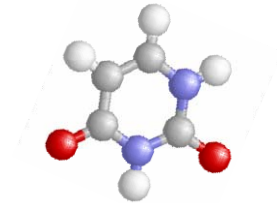
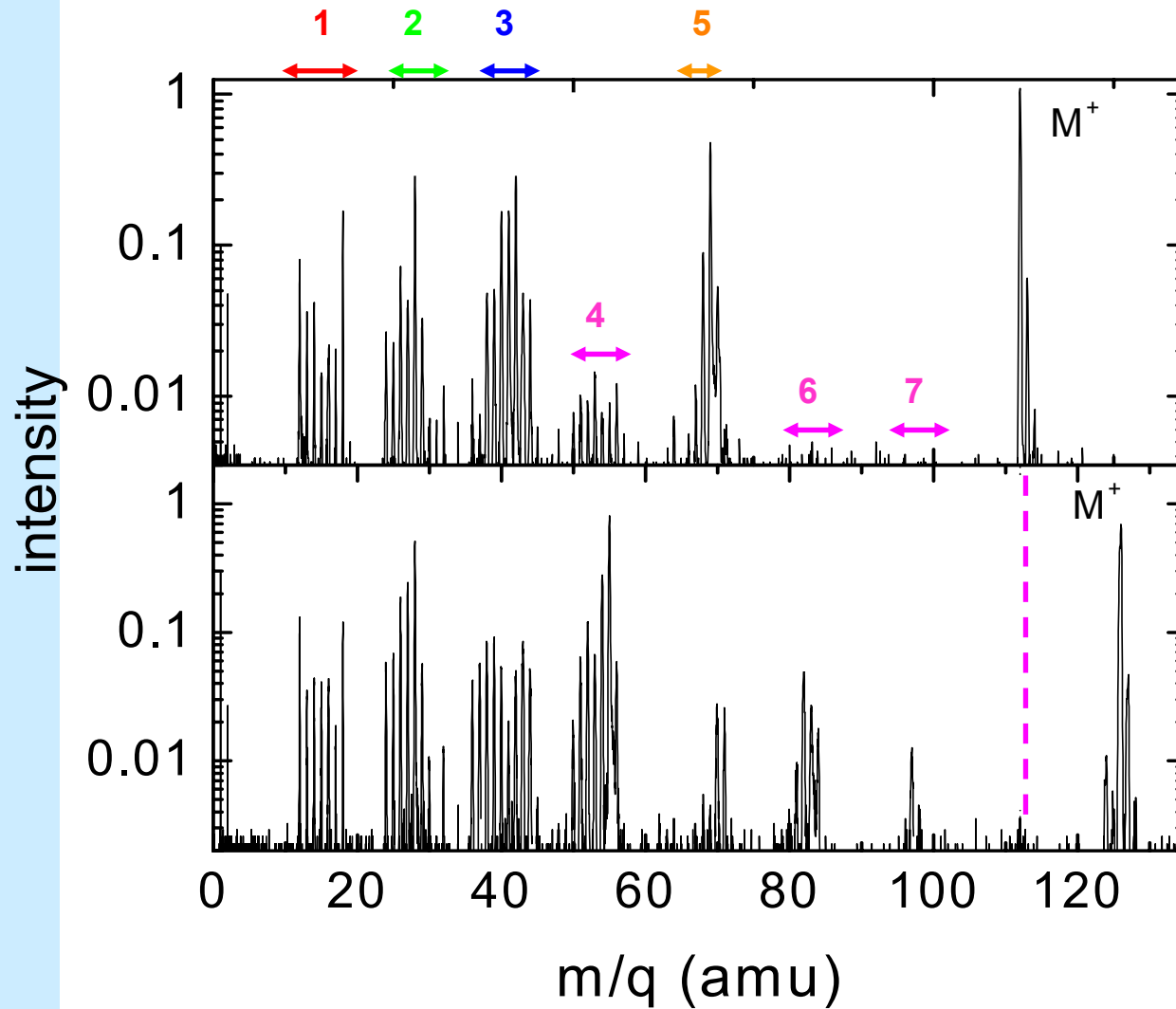
To obtain extra information, kinetic energies can be calculated

# Proton vs. electron vs. ion impact

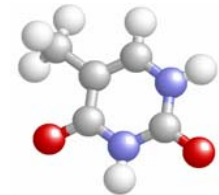


⇒ Similar fragmentation pattern!  
Different fragmentation yield!

# Uracil and Thymine



24 keV C<sup>+</sup>



Fragmentation changes dramatically!!

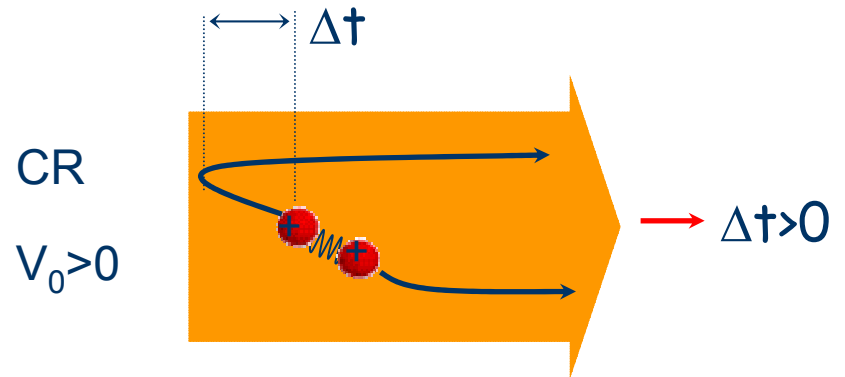
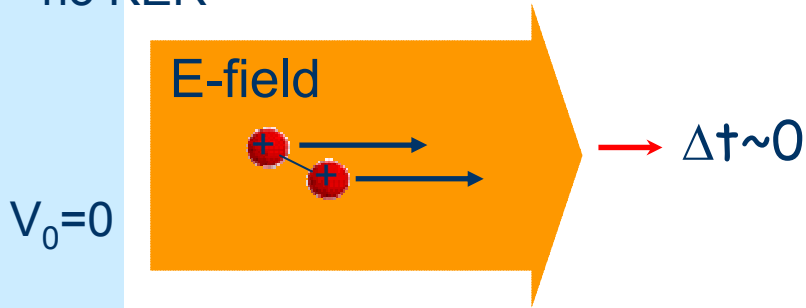
*J de Vries et al., Physica Scripta. (in press, 2004)*



# Kinetic Energy Release (KER)

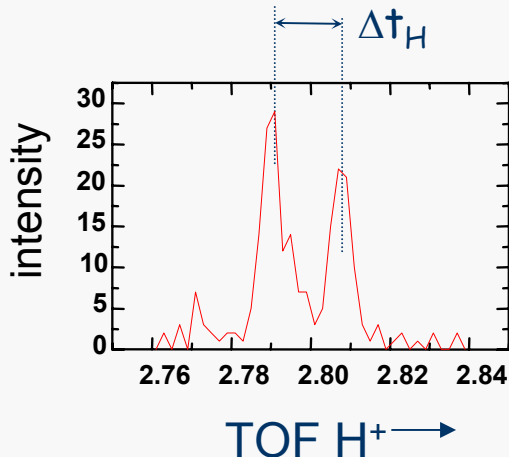
## Simple case – two bodies

no Coulomb Repulsion (CR)  
no KER

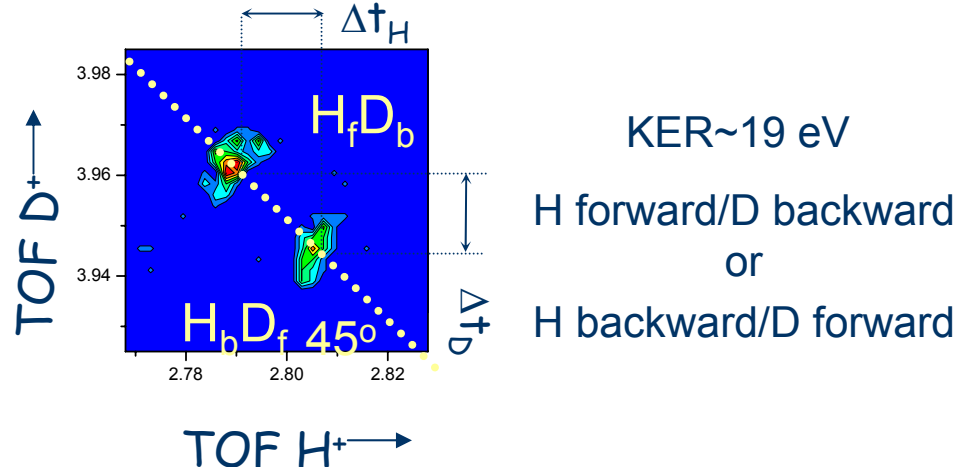


## HD<sup>++</sup> fragmentation

e<sup>-</sup>-ion coincidences

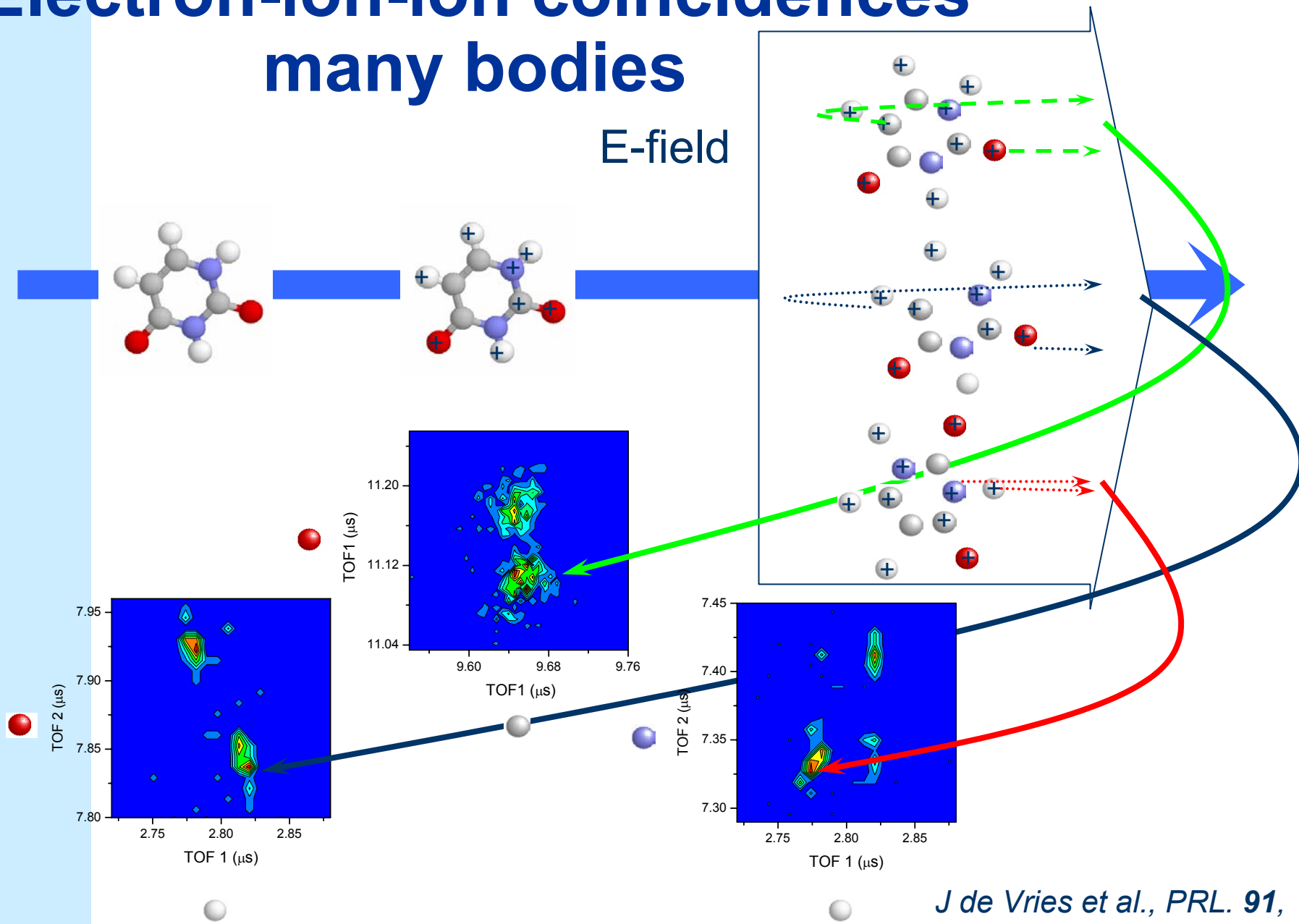


e<sup>-</sup>- ion-ion coincidences



# Electron-ion-ion coincidences many bodies

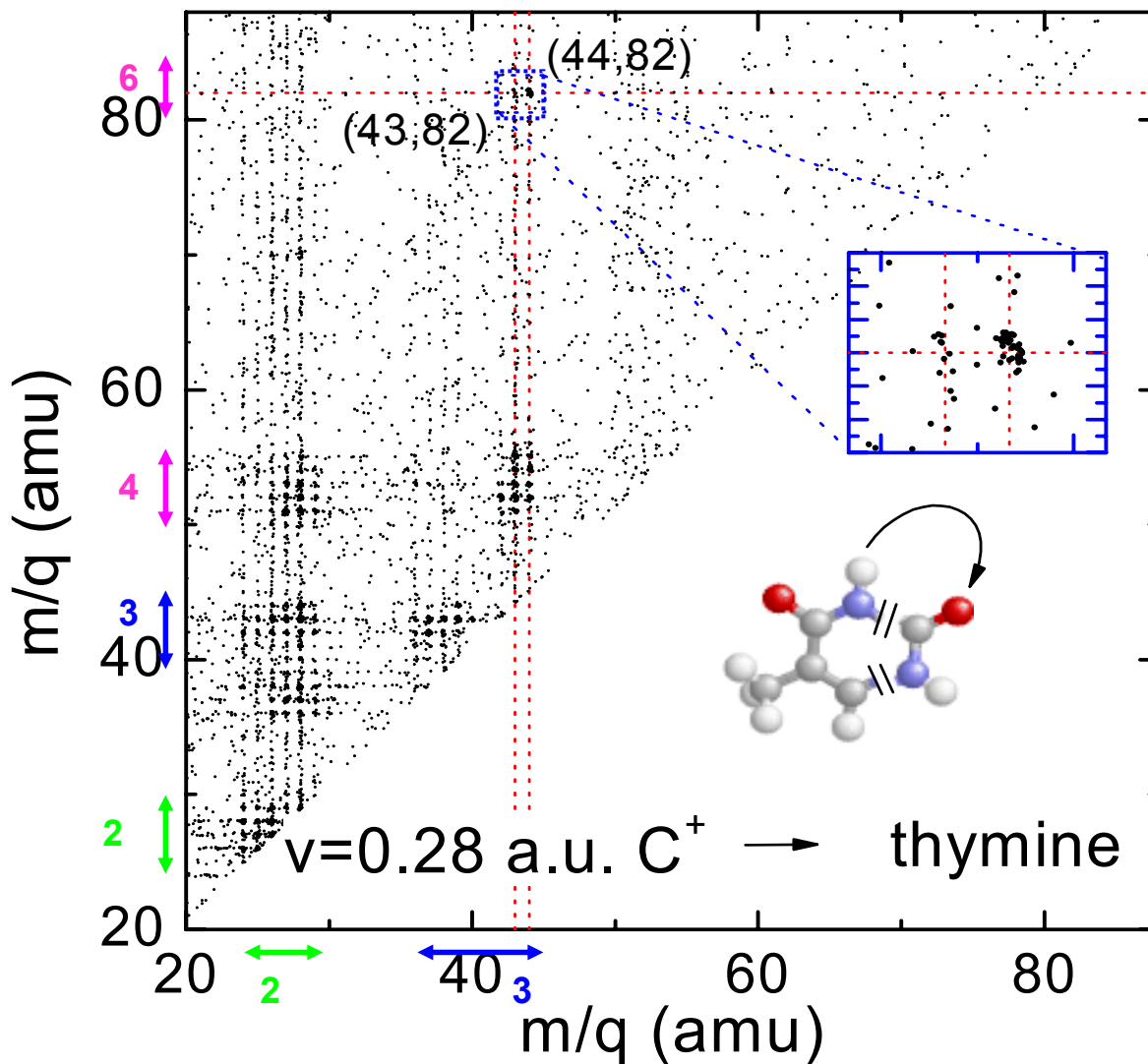
E-field



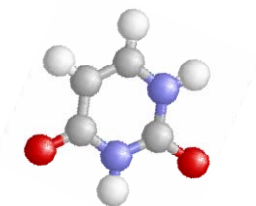
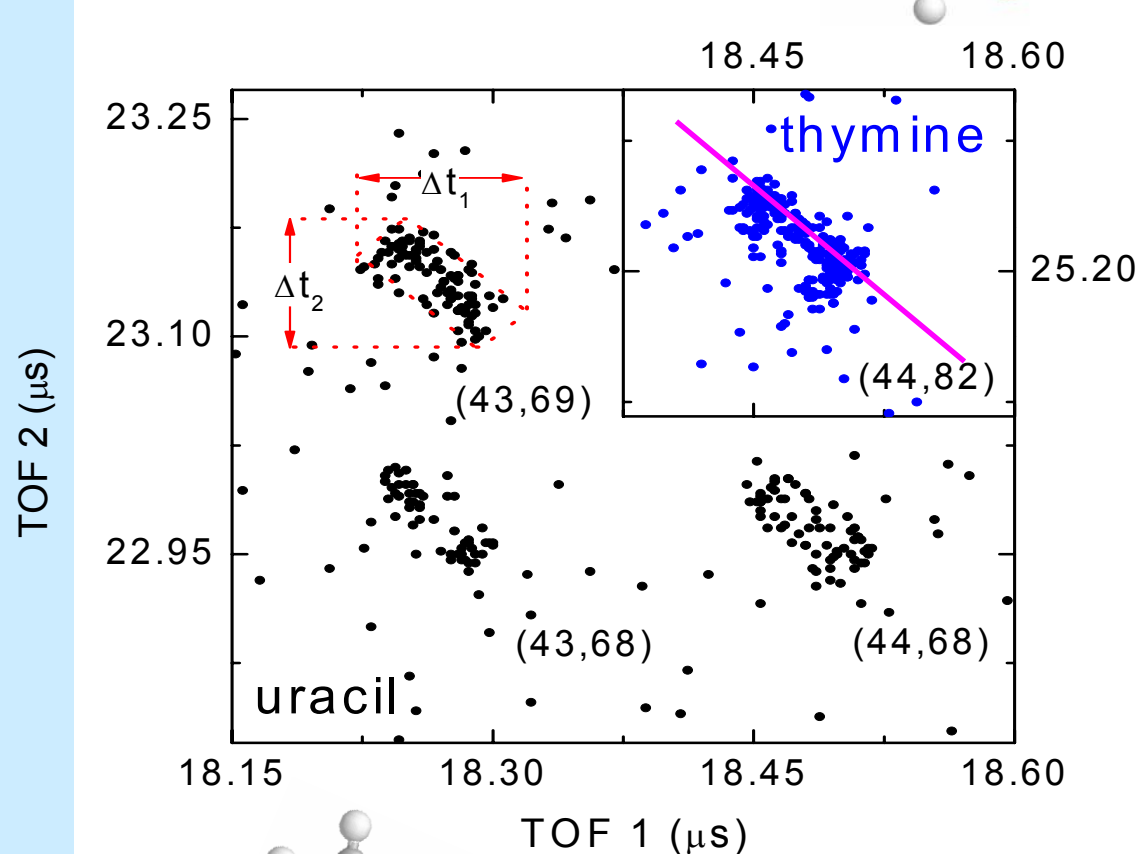
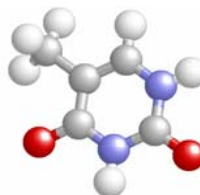
Information about molecular geometry

*J de Vries et al., PRL. 91,  
053401 (2003)*

# Coincidence plot for thymine



# Two body breakup similarities



$$\Delta t_i = \frac{2m_i v_0}{U}$$

$$\Rightarrow E \approx 5.2 \text{ eV}$$

repulsion of two charges



0.28 nm apart  
(ring diameter)

# Summary

- ② Fragment mass distribution for uracil and thymine can be obtained but contains little information
- ② Different projectiles → different fragmentation yields
- ② In spite that thymine and uracil have similar structure → fragmentation changes dramatically
- ② Studies of fragment kinetic energies can give us information about the reaction dynamics and the molecular geometry
- ② Coincidence plots are useful to identify the fragmentation channels, for instance two body breakup

# Thanks



Reinhard Morgenstern



Ronnie Hoekstra

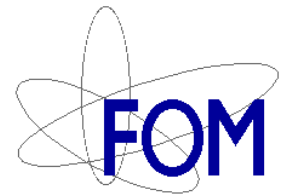


Jur de Vries



Thomas Schlathölter

funding:



Koninklijke  
Nederlandse  
Akademie van  
Wetenschappen