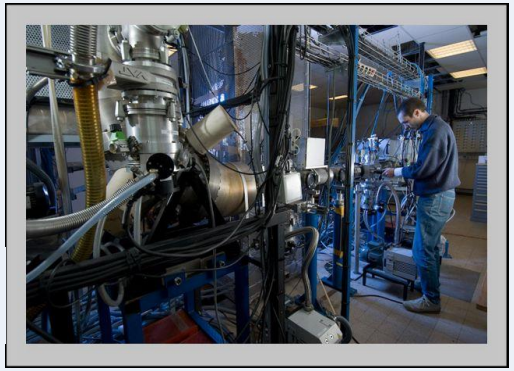
APP_02 project : Study of biomolecular ion stability in the gas-phase by two complementary approaches: A RICE-ring RIKEN and DIAM-IPNL

Introduction: The goals

IPN Lyon, France

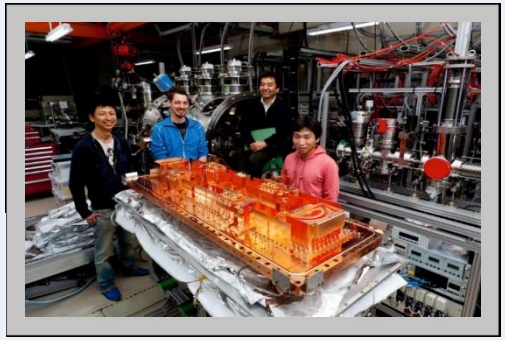
DIAM device for irradiation of nanosystem
First Results with the COINTOF-VMI Technique



Prof. Farizon M, Ass. Prof. Dr. Abdoul-Carime H, Dr Farizon B, Dr. Feketeová L, PhD Bertier P

RIKEN, Japan

RIKEN Cryogenic Electrostatic ring (RICE)
The experimental status



Prof. Azuma T, Prof. Shiromaru H, Prof. Tanuma H, Dr. Nakano Y, Dr. Kuma, Assistant Prof. Furukawa T, Assistant Prof. Matsumoto J, Ph.D. Bertier P

Motivation

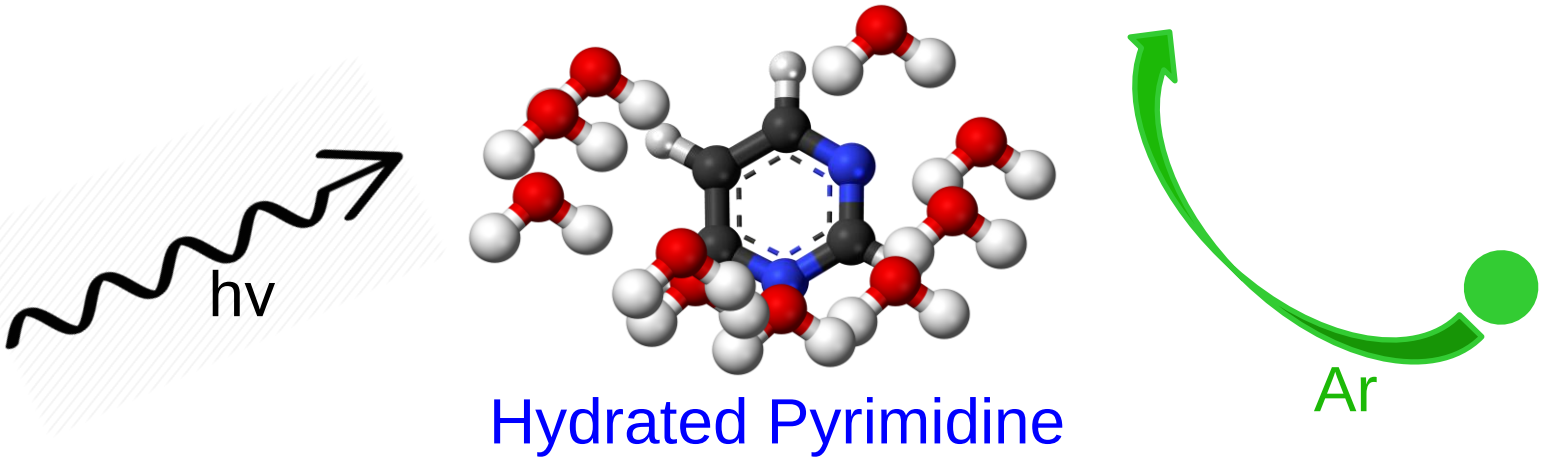
Water is known for its exceptional ability to absorb and hold heat at the macroscopic level, while at the sub-microscopic level the intermolecular transfer of vibrational energy was reported to be ultrafast due to strong interactions between the O-H oscillators.

Zhang Z., Piatkowski L., Bakker H.J. and Bonn M., Ultrafast vibrational energy transfer at the water/air interface revealed by two-dimensional surface vibrational spectroscopy, *Nature Chemistry* **3**, 888-893 (2011)

Quantitative description of the energy transfer in hydrogen bonded molecular systems after local electronic excitation is particularly challenging.

Scientific goal of the collaboration

We address the thermalizing ability of water molecules surrounding a biomolecule after a sudden electronic excitation

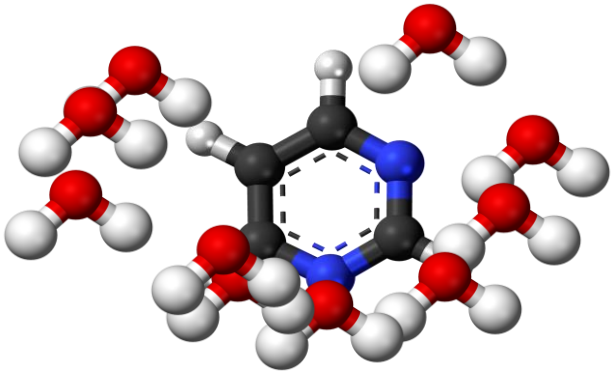


The electronic excitation is induced by
a laser pulse (RIKEN) or collision with an argon atom (IPNLyon)

Why Pyrimidine and water?

Pyrimidine as a model biomolecule to study radiation-induced damage at the molecular scale

- a ring-shaped molecule made up of carbon and nitrogen
- prototypical structure for the RNA/DNA bases thymine, cytosine and uracil
- In living cells DNA biomolecules are surrounded by water molecules



Radiation action at the nanoscale

Astrochemistry

DIAM@IPNLyon

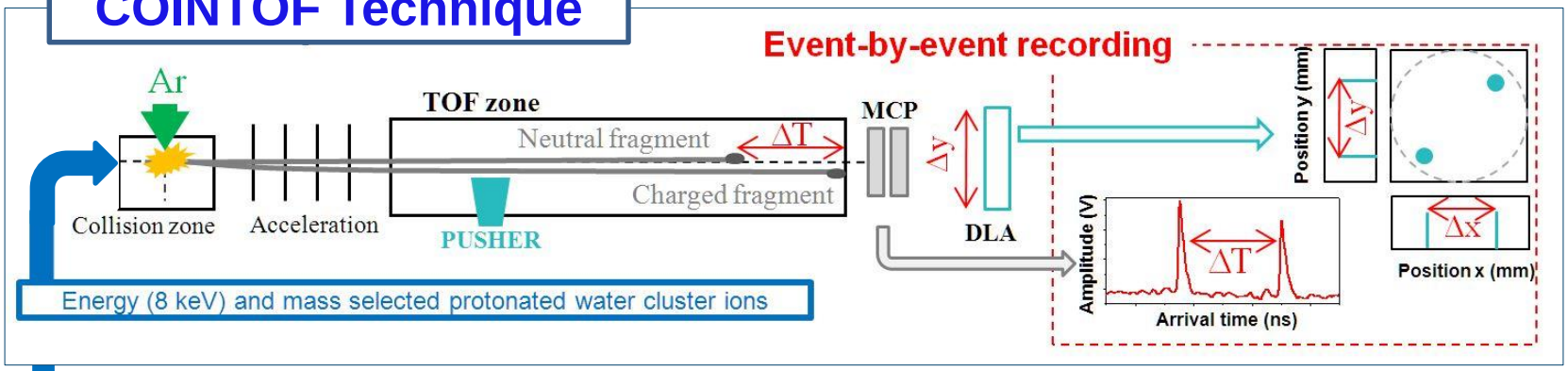
Device for Irradiation of Nanosystem

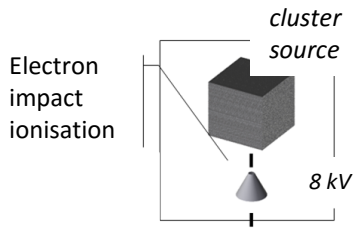
IPN Lyon set-up : DIAM

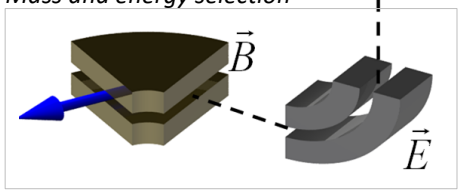
COINTOF technique in combination with velocity map imaging

A **single high-velocity collision with an Ar atom** leads to energy deposition in the droplet via electronic excitation. (fs time-scale)
Such high-velocity collisions probe **a broad range of energy deposition** from 0 to 12 eV.

COINTOF Technique





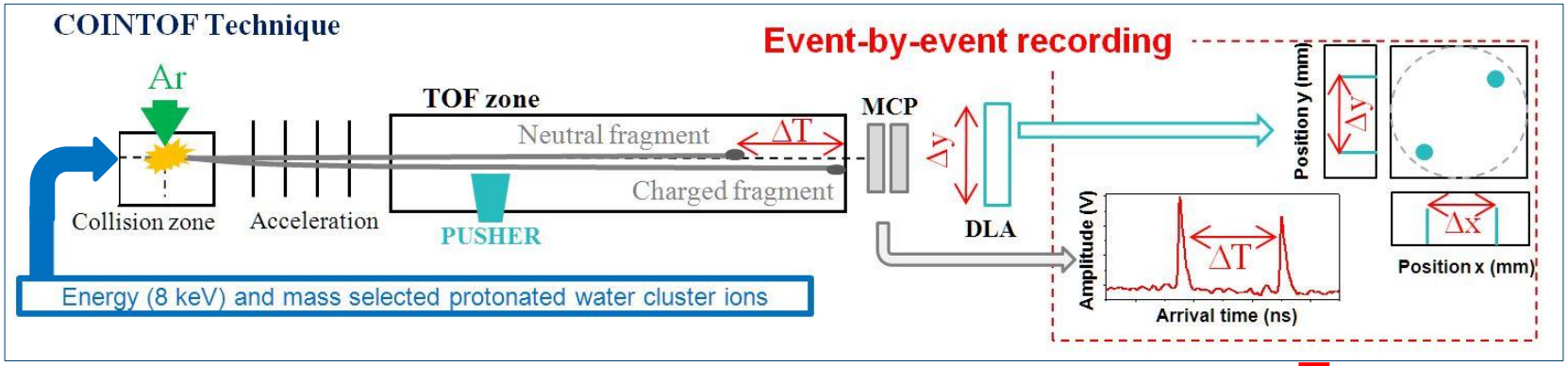


- Supersonic expansion followed by electron impact ionization.
- **8keV-$H^+(H_2O)_n$** : Velocity in the laboratory reference frame ranging from 10^5 to 2.10^5 ms^{-1}
- Clusters are mass- and velocity-selected more than 1 µs after being formed.
- The binding energy of a molecule in the droplet : typically 1.37 eV for n=2, 0.85 eV for n=3, 0.78 eV for n=4, and 0.55 eV for n>4.

IPN Lyon set-up : DIAM

COINTOF technique in combination with velocity map imaging

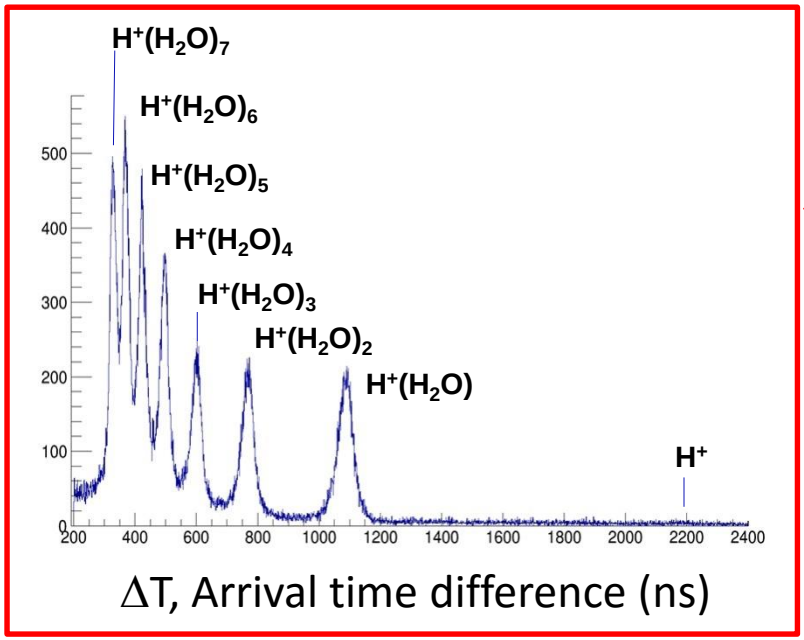
COrrelated Ion and Neutral Time-Of-Flight



8keV-$H^+(H_2O)_8$ -> Ar

Protonated octamer

Histogram of the arrival time difference for the recorded dissociation events



The protonated fragment is mass analyzed at least 80 ns after the collision

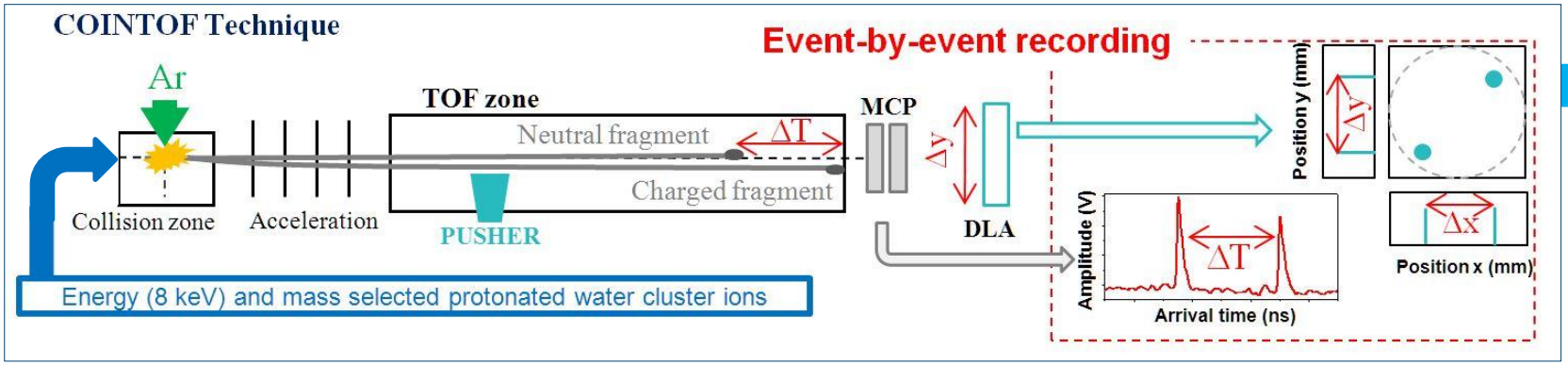
G. Bruny et al. *Rev. Sci. Instrum.* **2012**, *83*, 013305

C. Teyssier et al. *Rev. Sci. Instrum.* **2014**, *85*, 015118

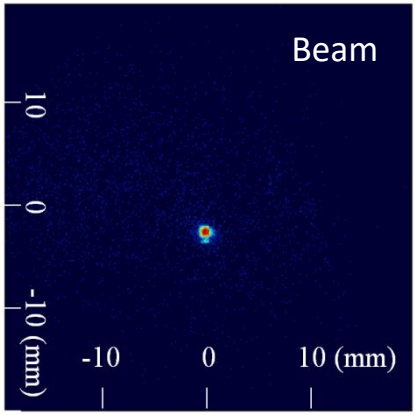
B. Farizon, project APP_02, workshop Seoul May 2016

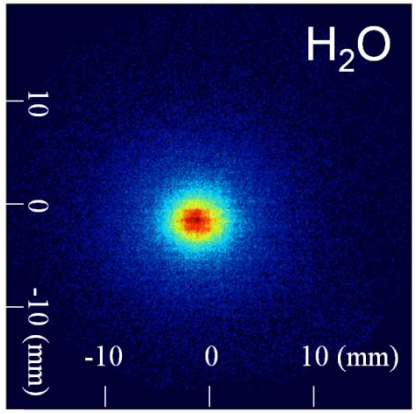
IPN Lyon set-up : DIAM

COINTOF technique in combination with velocity map imaging



Impacts of the incident cluster beam

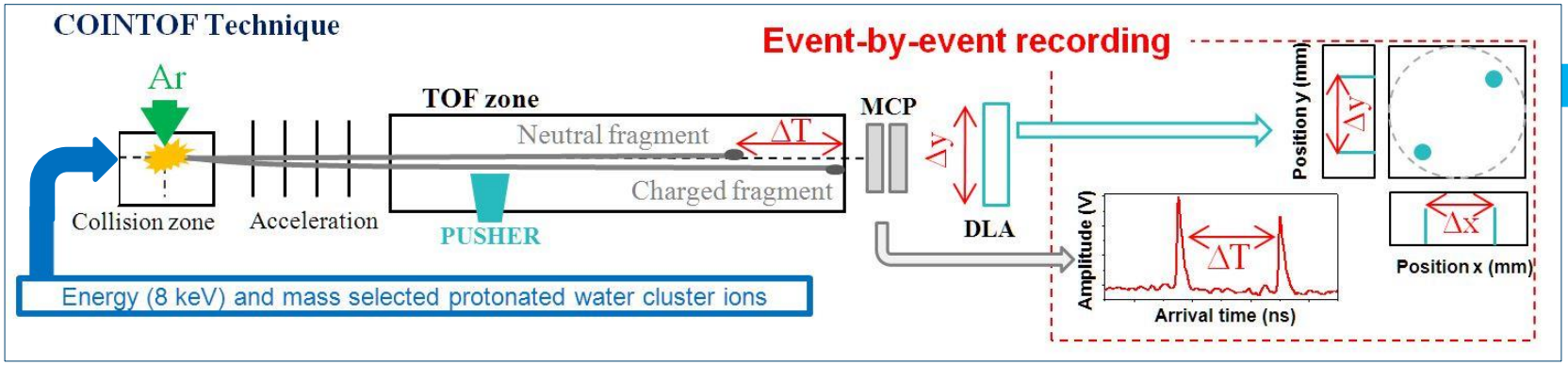




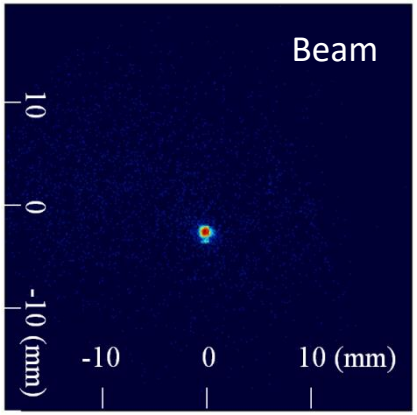
Impacts of the evaporated molecules (all dissociation channels)

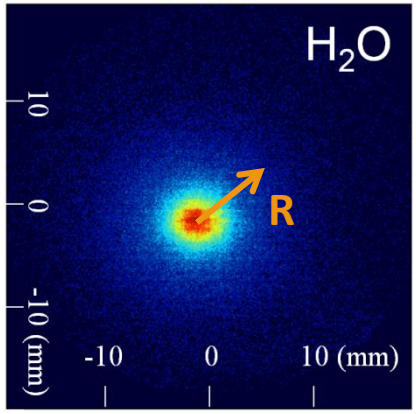
IPN Lyon set-up : DIAM

COINTOF technique in combination with velocity map imaging

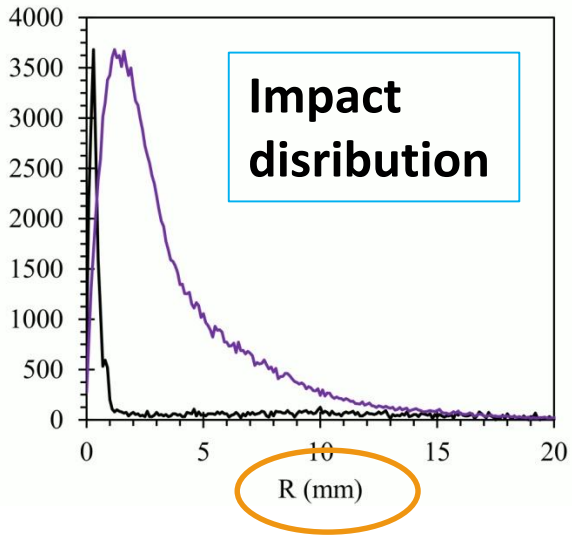


Impacts of the incident cluster beam



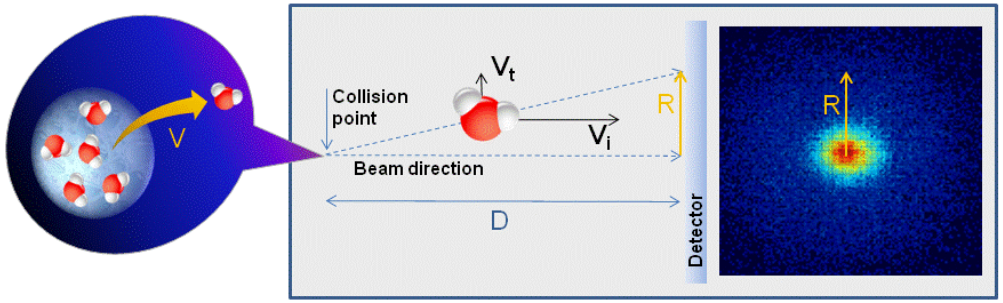


Impacts of the evaporated molecules (all dissociation channels)



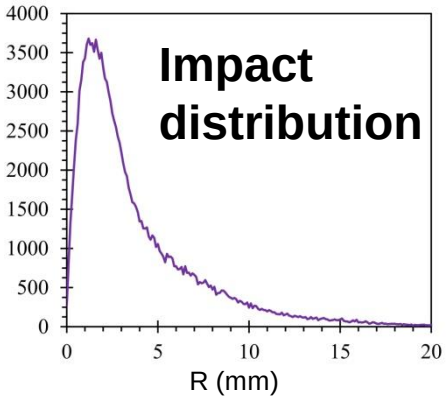
IPN Lyon set-up : DIAM
COINTOF technique in combination with velocity map imaging

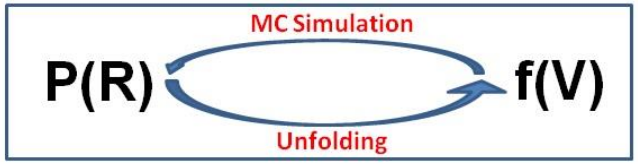
From impact distribution to velocity distribution



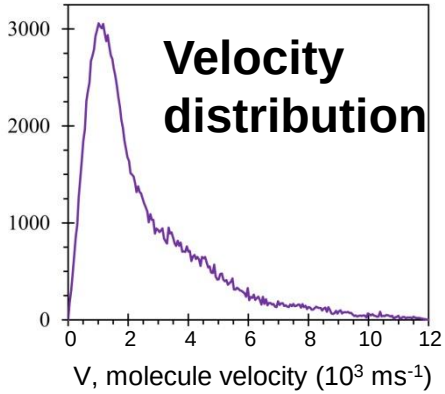
P(R)
impact distribution

The evaporated molecule acquires an additional velocity randomly oriented in the center-of-mass reference frame of the parent droplet.

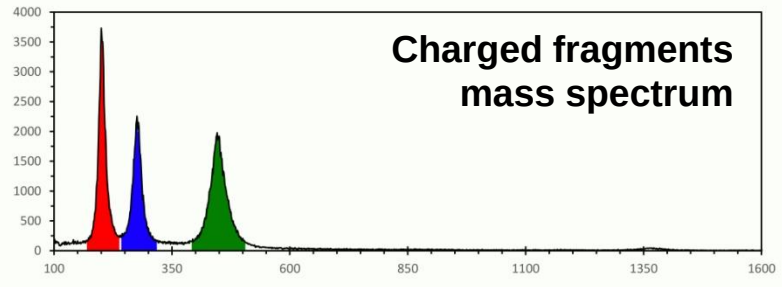




I. Antcheva et al. *Comput. Phys. Commun.* **2009**, *180*, 2499-2512



Results on water nanodroplets



Impact and velocity distributions of the evaporated molecules for a selected dissociation channel

$H^+(H_2O)_4 \rightarrow H^+(H_2O)_{4-m} + mH_2O$

m=1

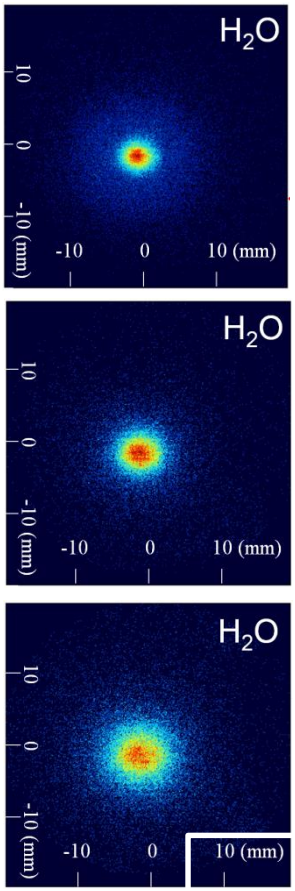
$H^+(H_2O)_3$

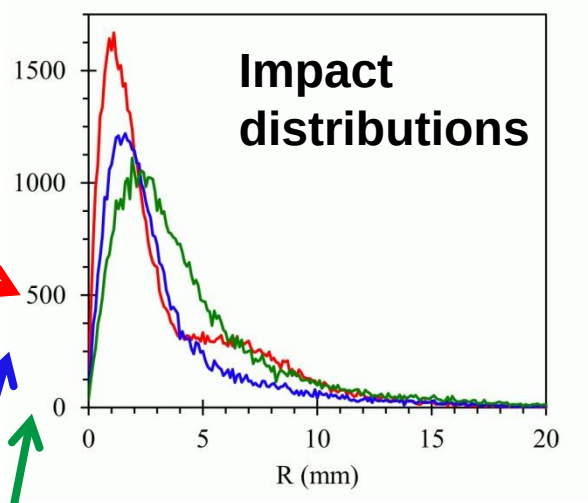
m=2

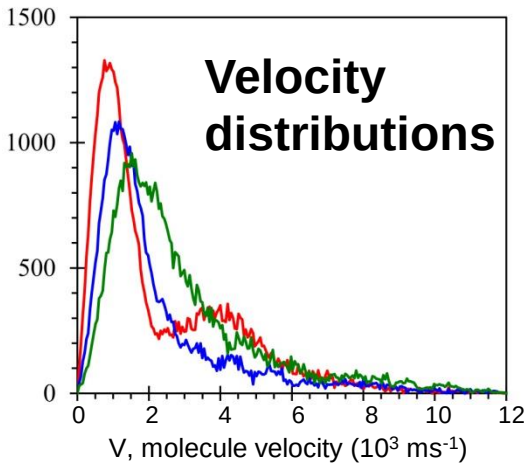
$H^+(H_2O)_2$

m=3

$H^+(H_2O)$

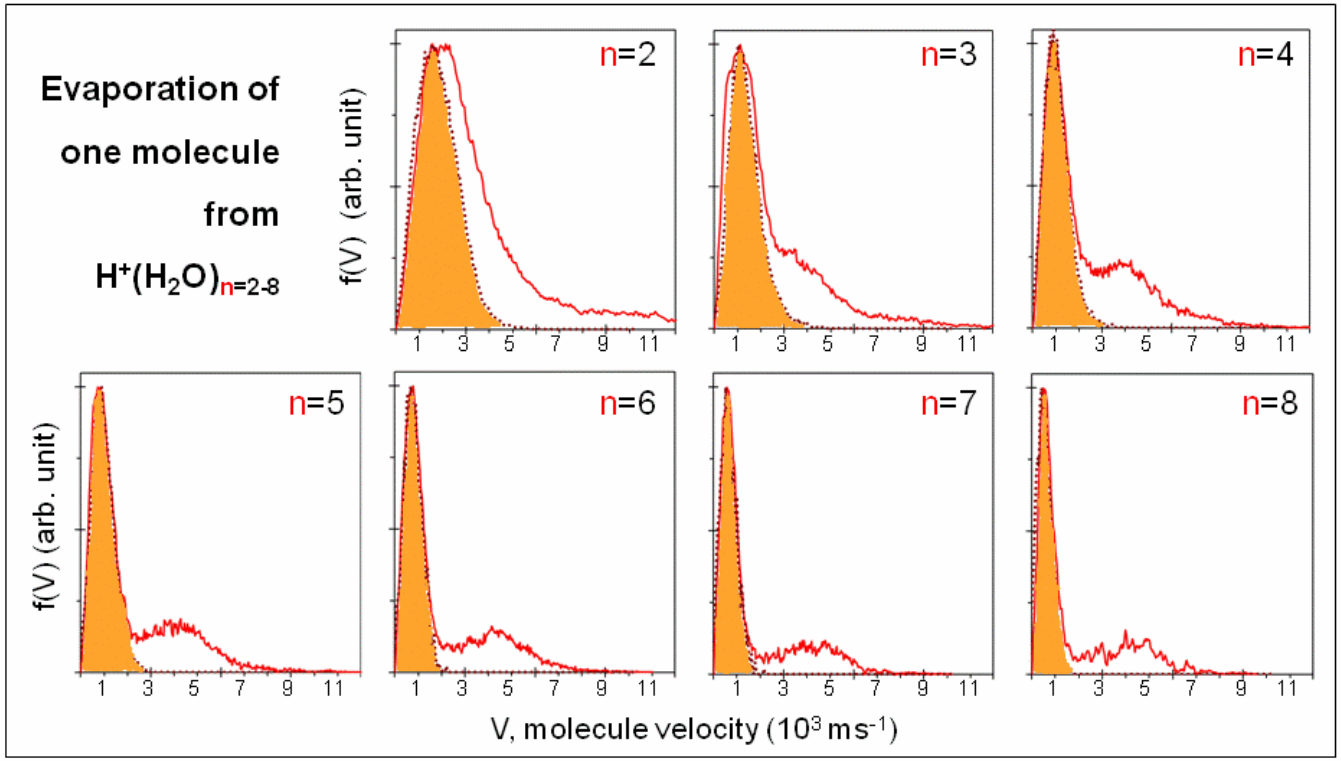


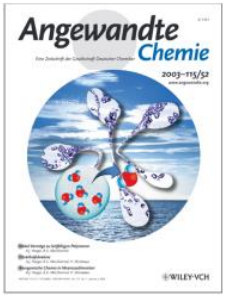




Results on water nanodroplets

Maxwell Boltzmann statistics





H. Abdoul-Carime et al. Angew. Chem. 2015 DOI: 10.1002/anie.201505890R1

versus non-ergodic events

The velocity distributions allow probing energy redistribution before evaporation

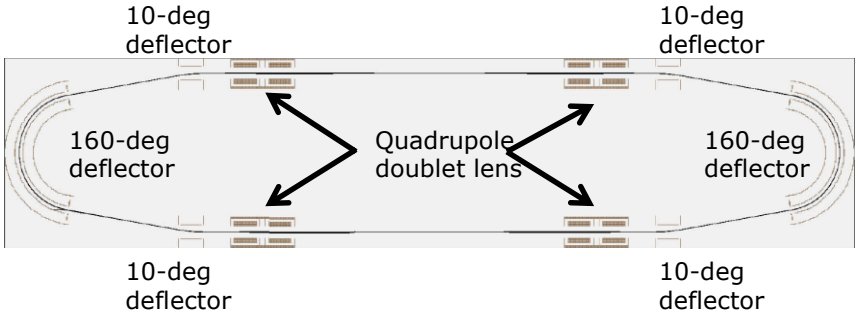
Current status at IPNL

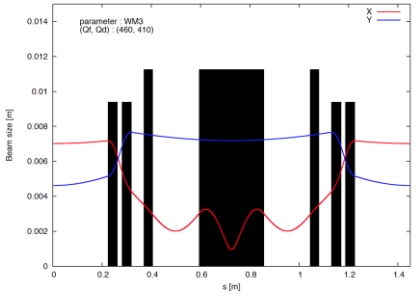
- Runs with hydrated pyrimidine $PyrH^+(H_2O)_n$ from n= 0 up to n=6
- Measurements of the velocity distributions of the neutral fragments for all dissociation channels with the COINTOF-VMI technique

RICE@RIKEN

RIKEN Cryogenic Electrostatic ring

Electrostatic Storage Ring



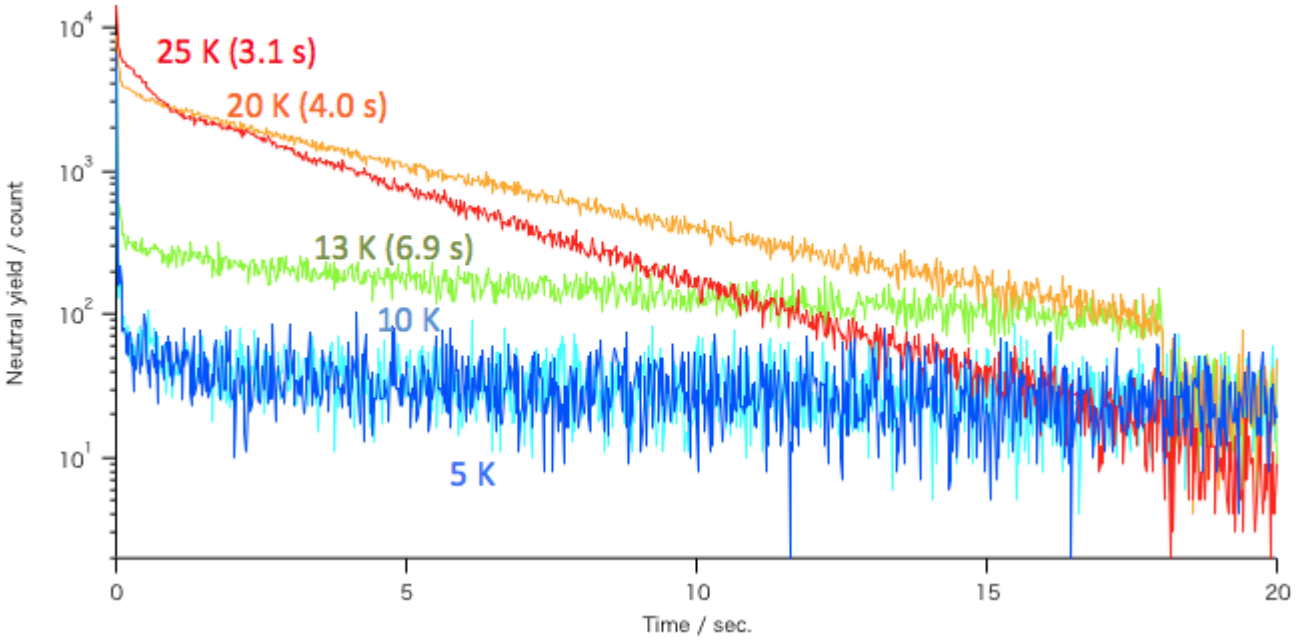


Compact-size (low-cost)
No hysteresis effects (easy tuning)
No limitation in mass (suitable to study biomolecules)

Design parameters of the RICE.
stored ion energy 20 keV
circumference 2965 mm
environmental temperature ≤ 5 K
background pressure ≤ 10^{-13}Torr

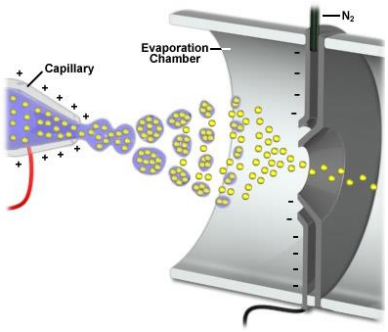
6th International Workshop on
Electrostatic Storage Devices
June 6-11, Tokyo

Current status

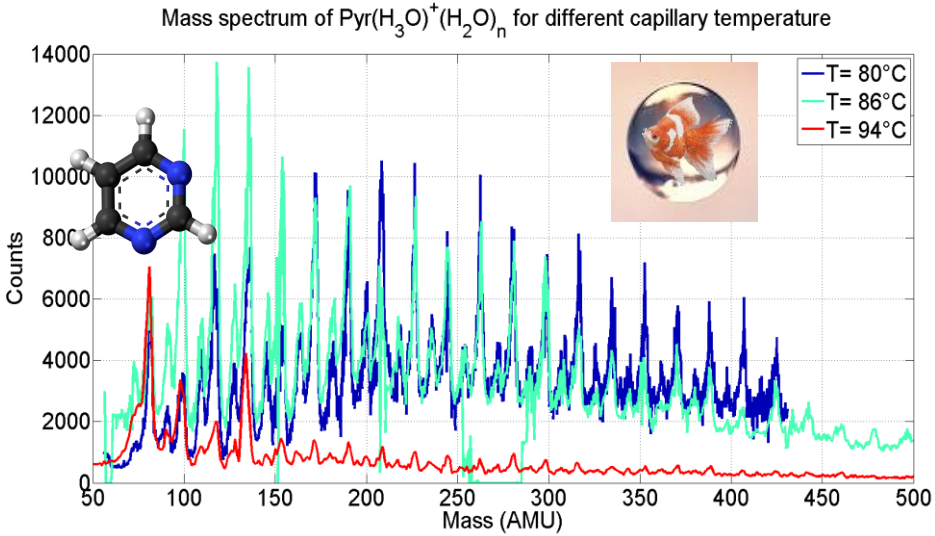


Temperature dependence of the storage lifetime of 10 keV Ne^+ beam

ESI source



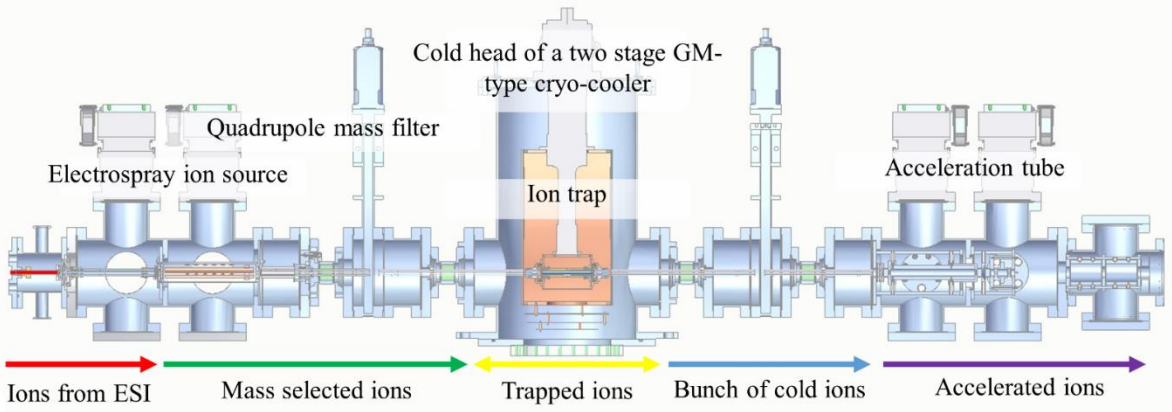
https://nationalmaglab.org/



Pyrimidine water clusters are successfully produced.

The ion trap injection beam line

Goal: produce a bunch of cold molecular ion with high kinetic energy for injection to the ring or photo dissociation experiment.



Current status

The ion beam line is now under operation and preliminary experiment have been carried out.

Methylene blue was chosen as a molecule test:

- easy to produce
- high photon absorbance
- absorption spectrum already measured in solution

Production of a ion bunch of 10-20 keV in energy and a few 10 µs in width.

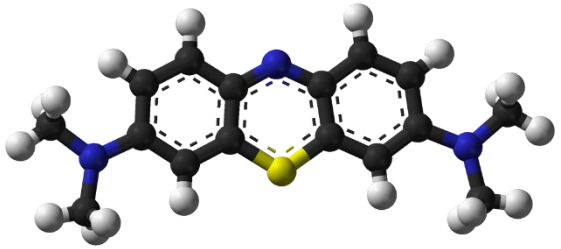


Photo dissociation experiment

A tunable visible OPO laser beam (pulsation duration ~1µs) crosses the extracted ion beam (~15 µs).

The produced neutral fragments are detected by a Micro Channel Plate MCP detector after deflecting the ion components by an electric field.

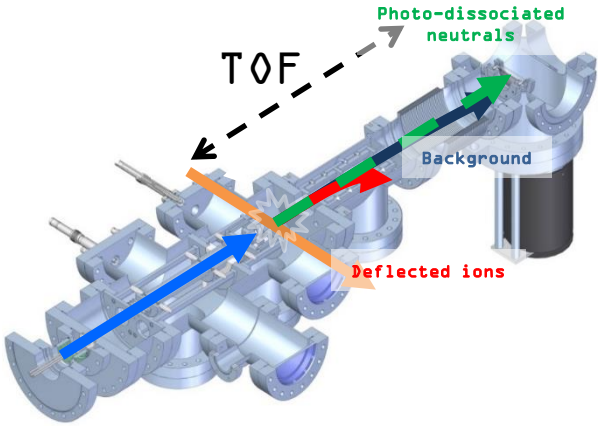
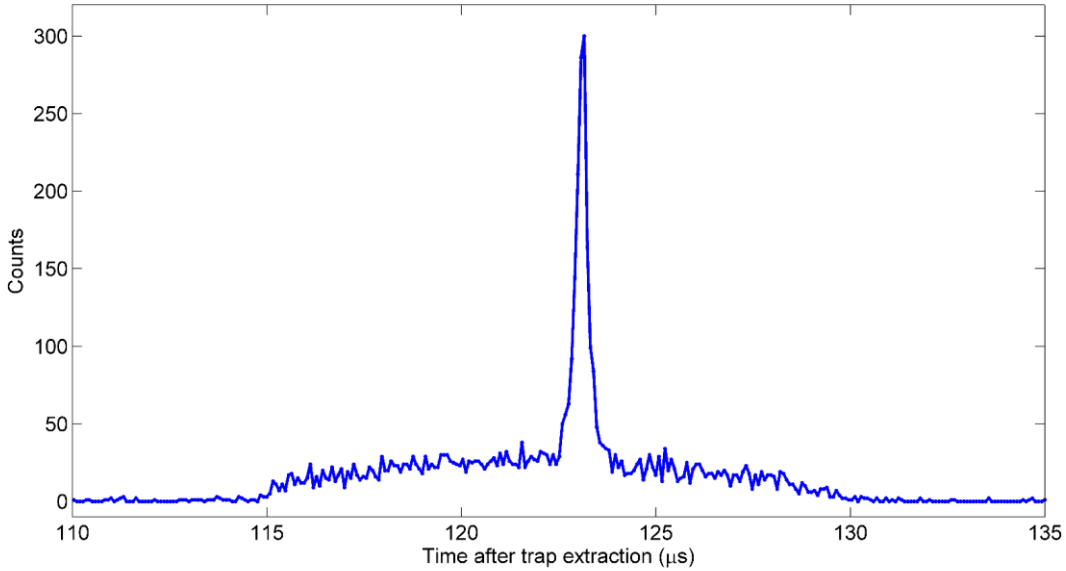


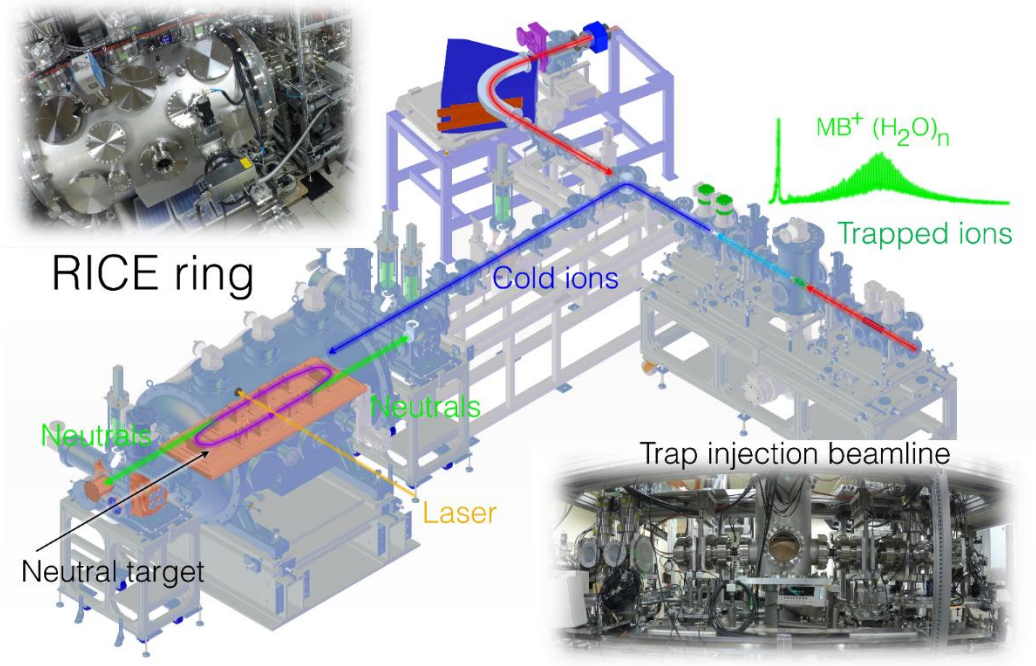
Photo dissociation experiment

$MBH_3O^+(H_2O)_n$ dissociation for 1000 bunches with a laser at 600nm, 11mJ



A sharp peak of less than 1μs in width corresponding to the component made by the laser irradiation is clearly observed in addition to the bunch component of about 15 μs in width resulting from collision with residual gas.

Next step: inject in the storage ring



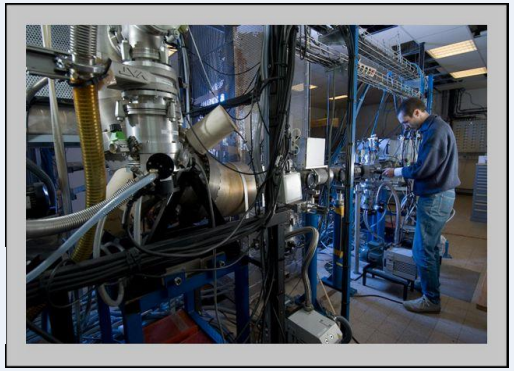
APP_02 project : Study of biomolecular ion stability in the gas-phase by two complementary approaches: A RICE-ring RIKEN and DIAM-IPNL

Introduction: The goals

IPN Lyon, France

DIAM device for irradiation of nanosystem
First Results with the COINTOF-VMI Technique

Prof. Farizon M, Ass. Prof. Dr. Abdoul-Carime H, Dr Farizon B, Dr. Feketeová L, PhD Bertier P



RIKEN, Japan

RIKEN Cryogenic Electrostatic ring (RICE)
The experimental status

Prof. Azuma T, Prof. Shiromaru H, Prof. Tanuma H, Dr. Nakano Y, Dr. Kuma, Assistant Prof. Furukawa T, Assistant Prof. Matsumoto J, Ph.D. Bertier P