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# Chemical Ionisation in a High Resolution Mass Spectrometer for Real Time Analysis

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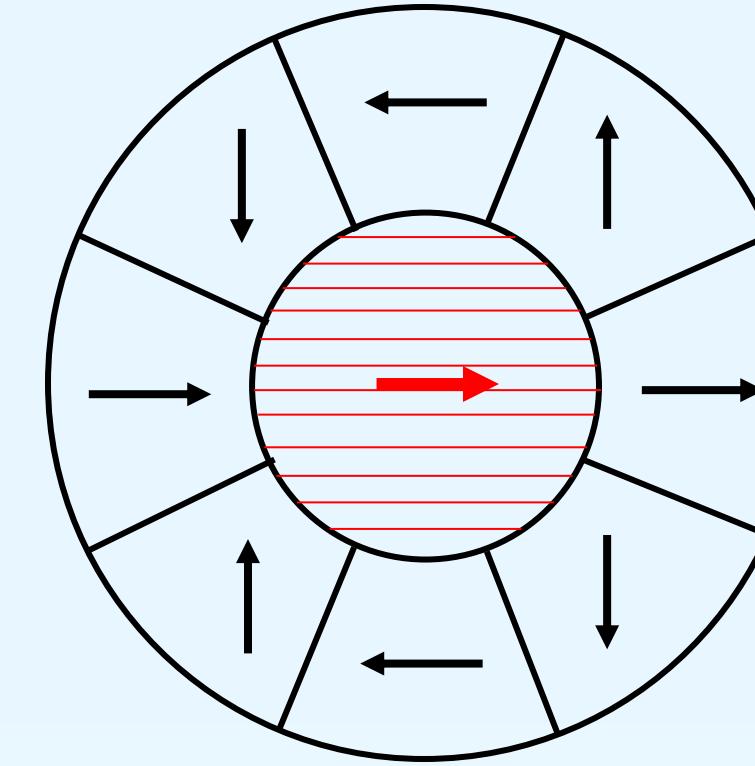
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## Compact FTICR instrument

The use of a **permanent magnet** to generate a constant magnetic field in an FTICR mass spectrometer has many advantages :

- compacity : (60 x 80 x 120) cm - reasonable weight : less than 150 kg - transportability
- no power supply required for the magnet, no expensive cooling fluids,
- maintenance free



### Magnet design : Halbach cylinders

- nominal magnetic field : 1.1 Tesla
- good magnetic field homogeneity : variation < 10<sup>-3</sup> in the ICR cell volume

Mass resolution of 70000 @ 131 umu was obtained with this configuration.

BTrap

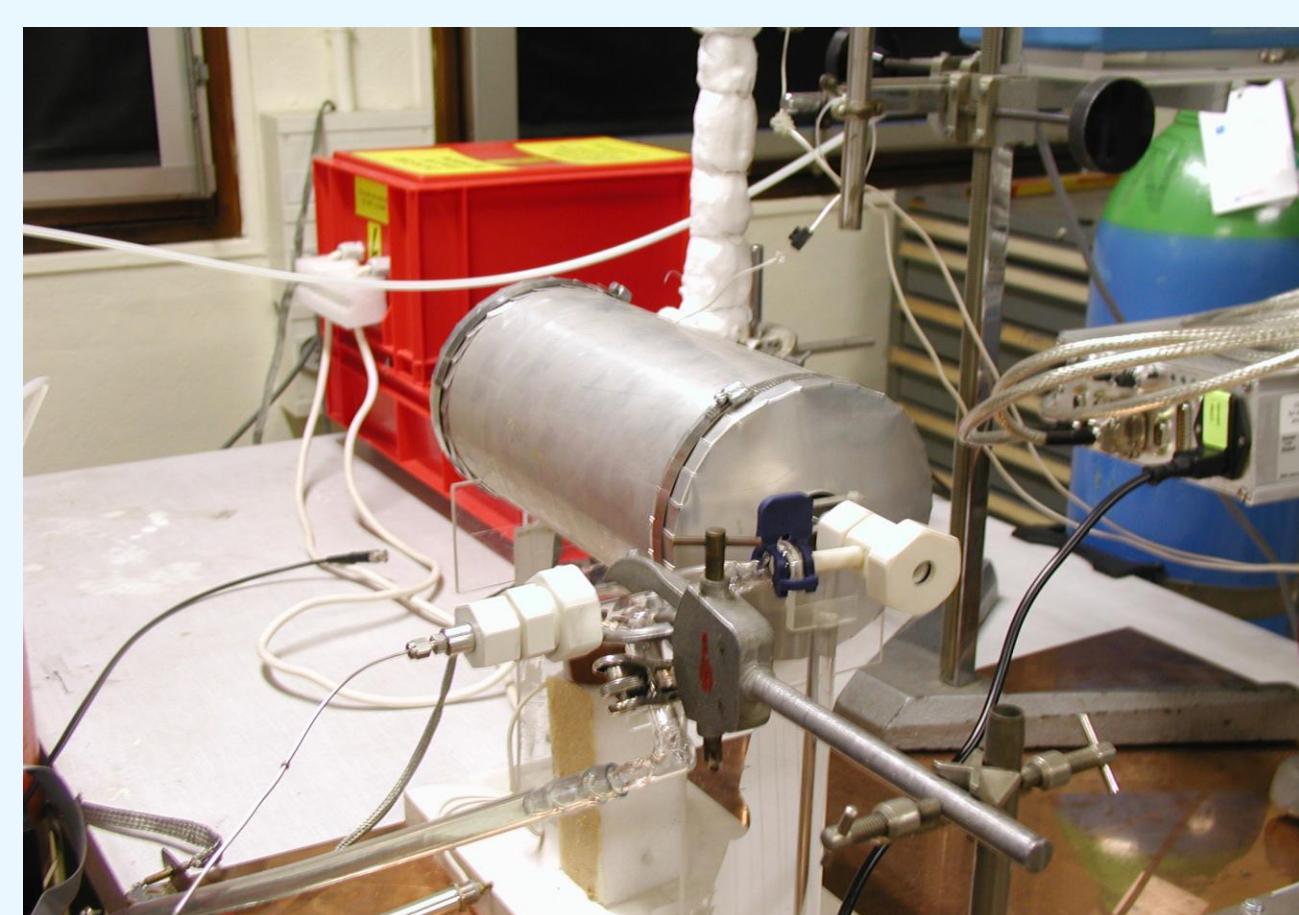
compact FTICR prototype  
for mixture analysis



## Monitoring the removal of pollutants by plasma catalytic process

### Non-thermal plasma discharge

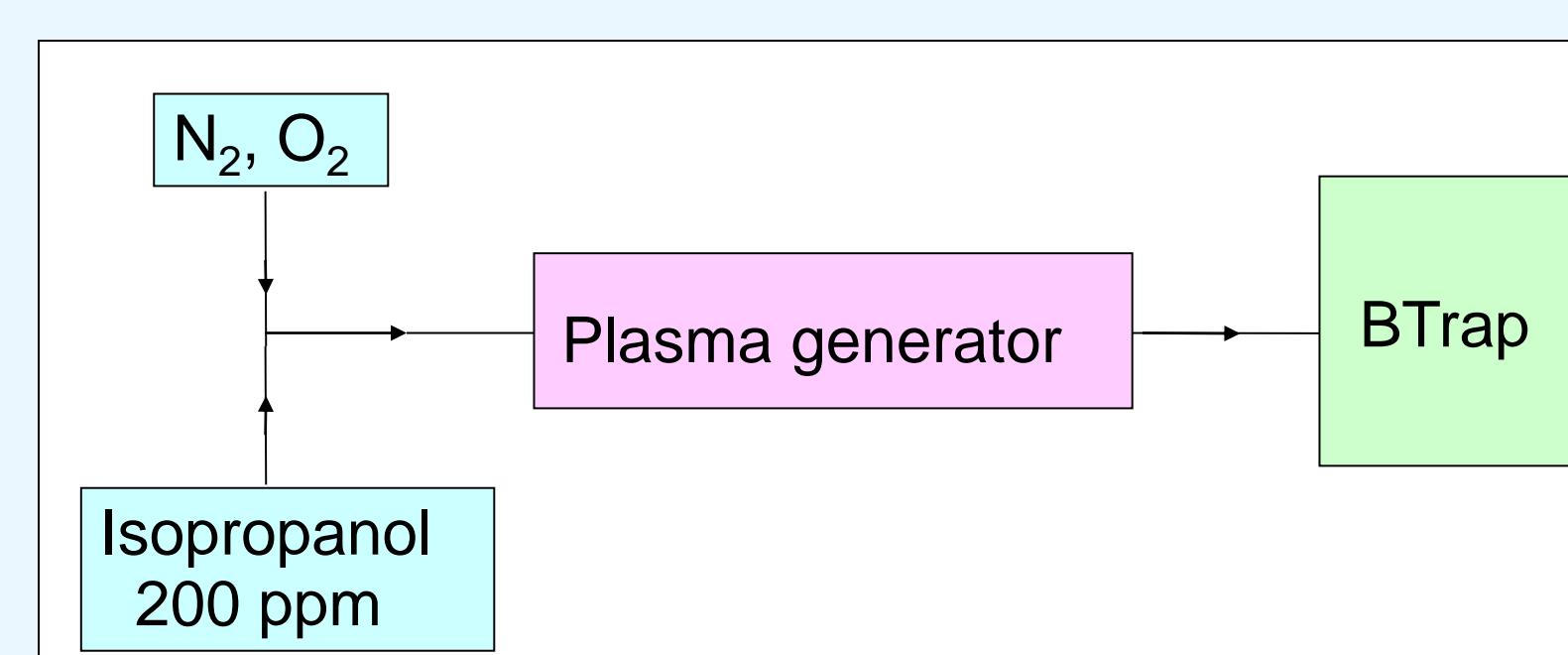
Dielectric Barrier Discharge (DBD)  
Sinusoidal applied voltage



Non-thermal plasmas are known as powerful means to eliminate Volatile Organic Compounds (VOCs) from the ambient air. However complete oxidation of the undesirable molecules is not yet achieved by this method. Further investigations involve plasma+ catalyst combination.

A detailed understanding of the discharge effluent composition is therefore needed. Real-time monitoring with compact ICR mass spectrometer is a promising tool for this purpose. FTICR study of the plasma degradation of two representative molecules is presented below : 2-propanol and 2-heptanone.

### Coupling of BTrap to the plasma discharge



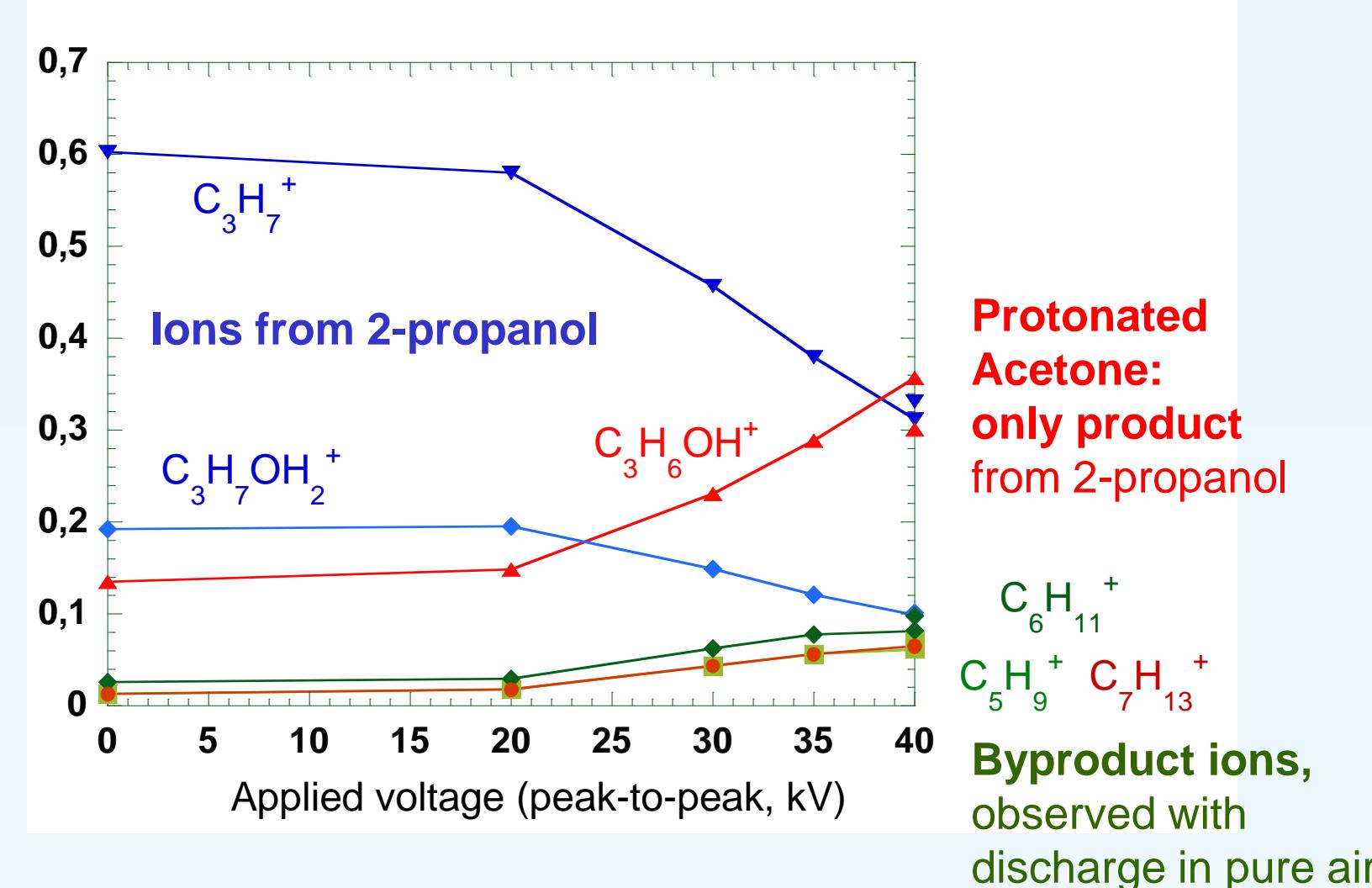
Chemical ionisation method used: PTRMS  
 $\text{H}_3\text{O}^+ + \text{COV} \rightarrow (\text{COV})\text{H}^+ + \text{H}_2\text{O}$

Owing to mass resolution, molecular formulae of the protonated species were determined without ambiguity.

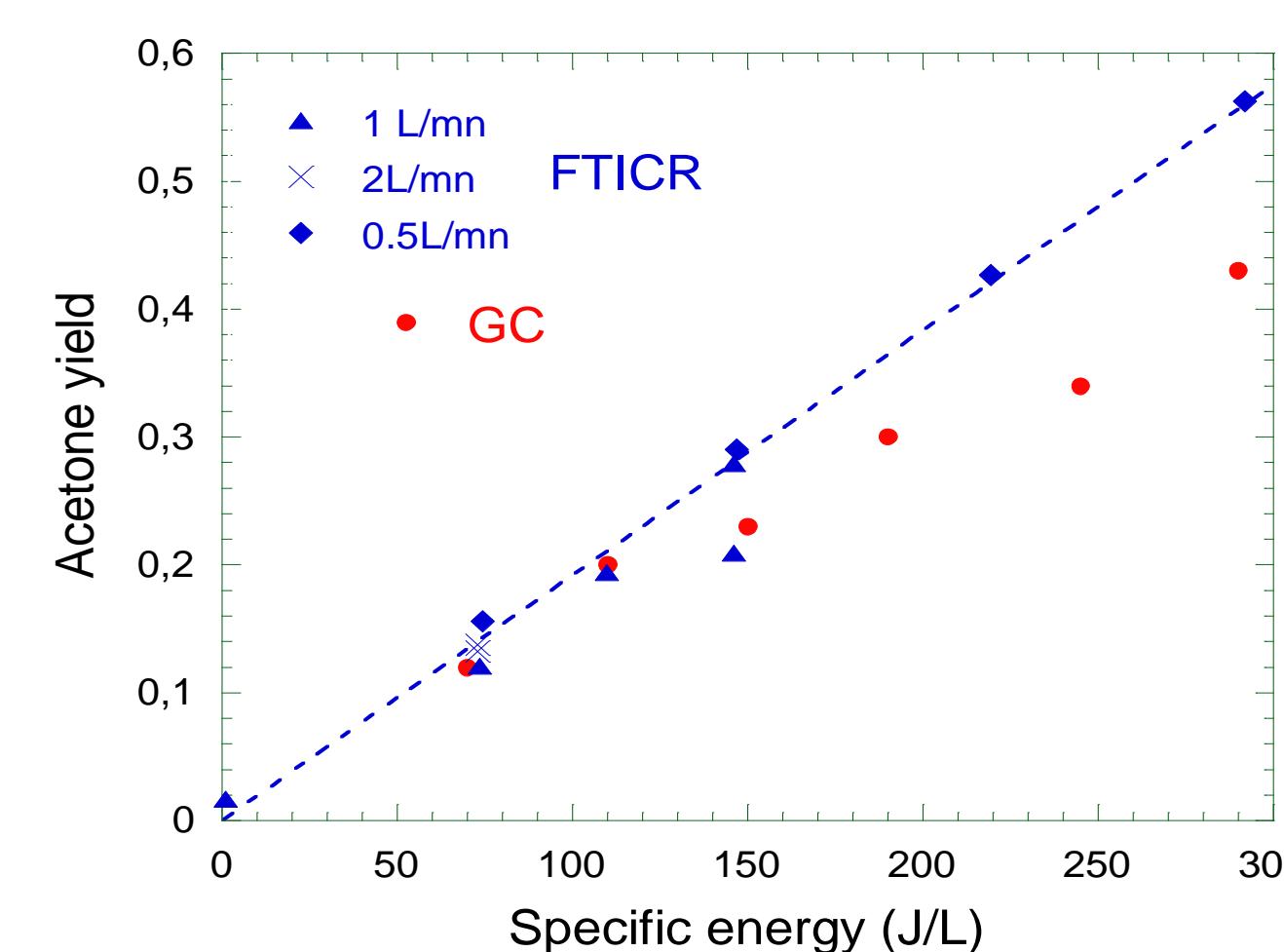
### 2-propanol

A common VOC : its plasma degradation, already studied by GC, yields mainly one product : acetone

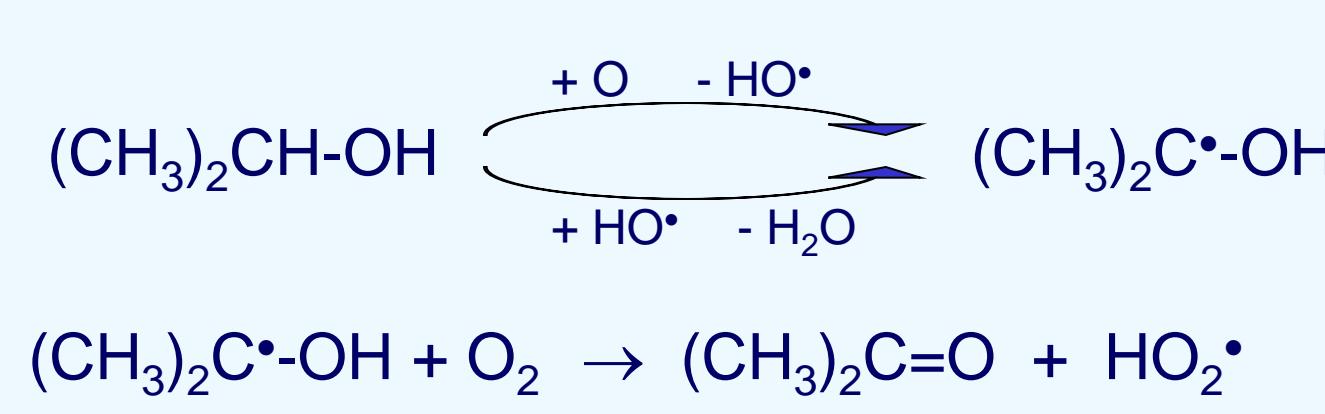
Dependence of product amount with applied voltage



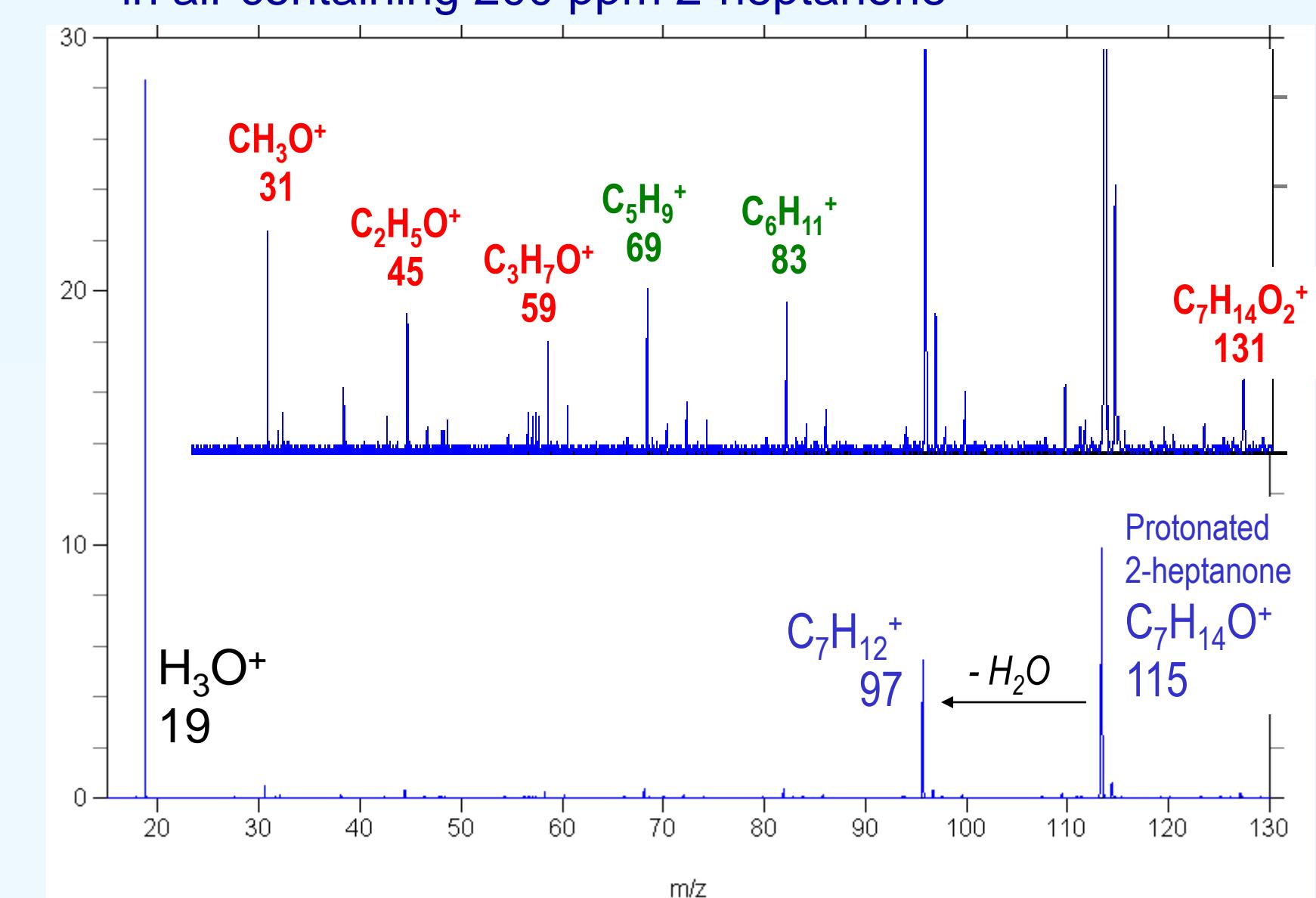
Acetone yield as a function of energy deposited in the discharge for different values of the gas flow. Comparison with GC measurements.



Tentative mechanism for acetone formation :



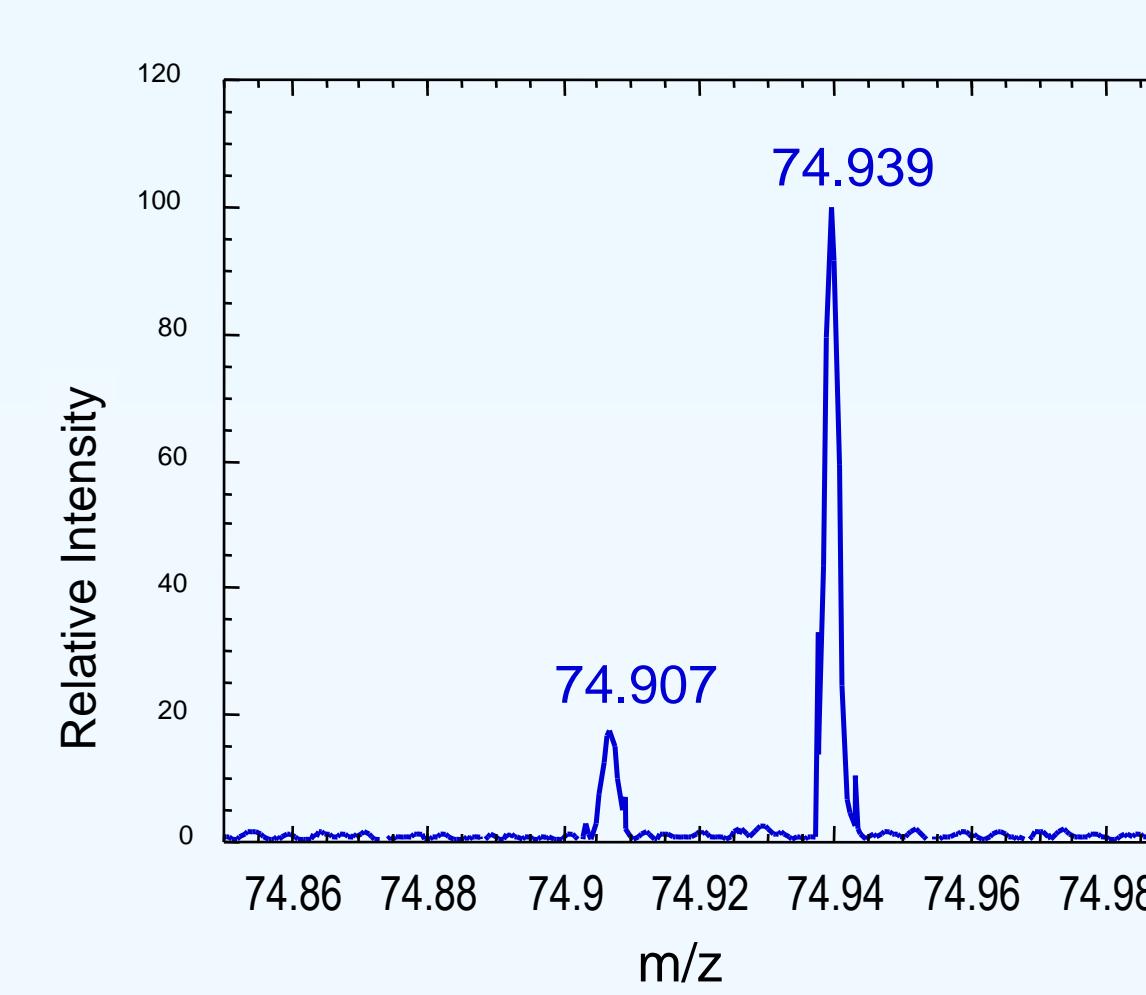
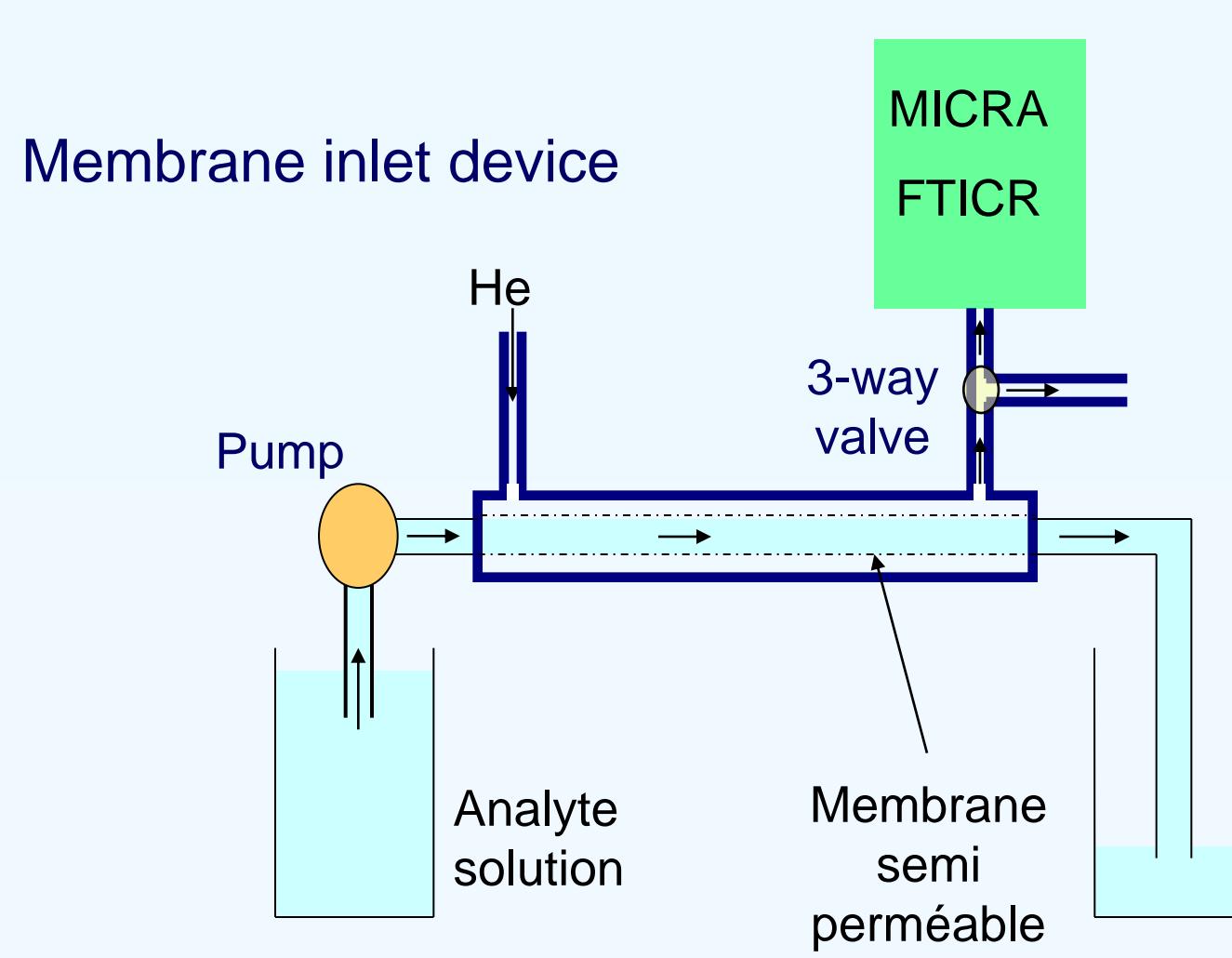
Mass spectrum of the effluent from 20 kV discharge in air containing 200 ppm 2-heptanone



Several products are detected, corresponding to protonated carbonyl compounds with 1-4 C atoms. Determining influence of the vector gas composition : in nitrogen, the products are  $\text{C}_3\text{H}_7\text{O}^+$ ,  $\text{C}_4\text{H}_9^+$ ,  $\text{C}_2\text{H}_5\text{O}^+$ . The reaction mechanisms in the discharge are under investigation.

## MIMS Analysis of an aqueous solution

Mixture of quasi-isobaric compounds :  $\text{C}_2\text{H}_5\text{OC}_2\text{H}_5$  (diethylether) +  $\text{CH}_3\text{COOCH}_3$  (methyl acetate) at ppm concentration



Use of chemical ionisation in the compact FTICR mass spectrometer Btrap allows to perform real-time analysis of the complex effluent mixture from a plasma discharge, as well as MIMS analysis of a dilute aqueous solution. The mass resolution of FTICR allows to differentiate quasi-isobaric species.

New chemical ionisation methods are under investigation. Example : detection of sulfur compounds with reactant ions obtained from Electron Ionisation of dimethylether :

