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Broadband gas analysis at high resolution with a small FTICR

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Introduction.

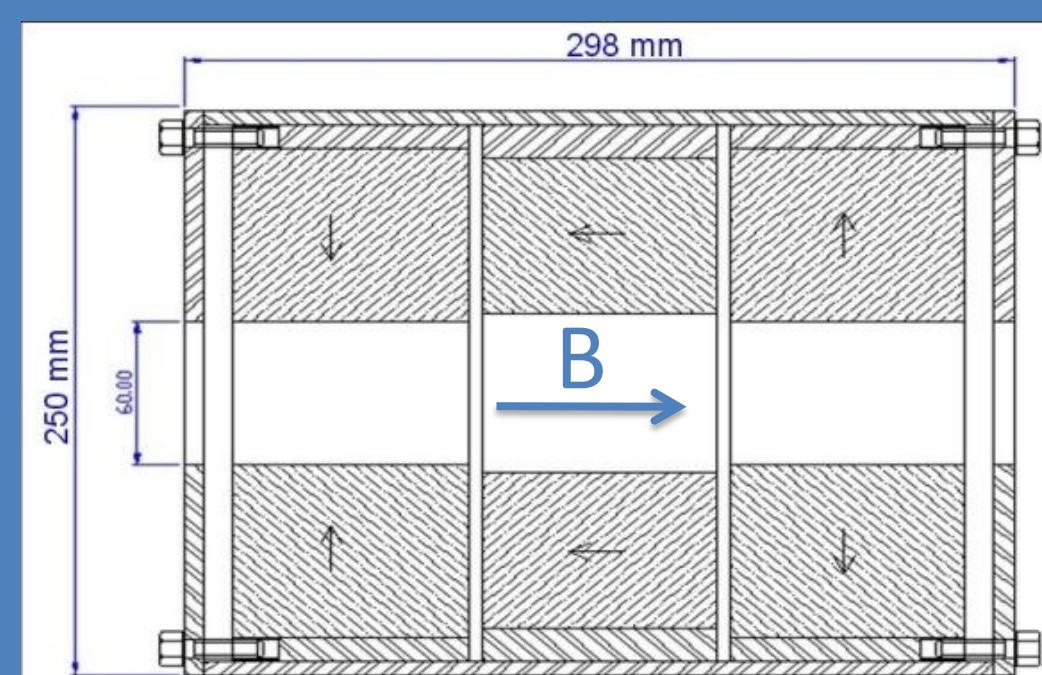
Real time monitoring of gases at high resolution is realized with a small permanent magnet based FTICR mass spectrometer. The mass range of the instrument starts at m/z 2 up to m/z 500 with a resolution higher than 20000 over the whole mass range.

Potential applications are in a wide range of domains : air monitoring, security applications, industrial process control,...

Magnets

Magnetic field strength and homogeneity are key parameters for the good performance of the FTICR instrument.

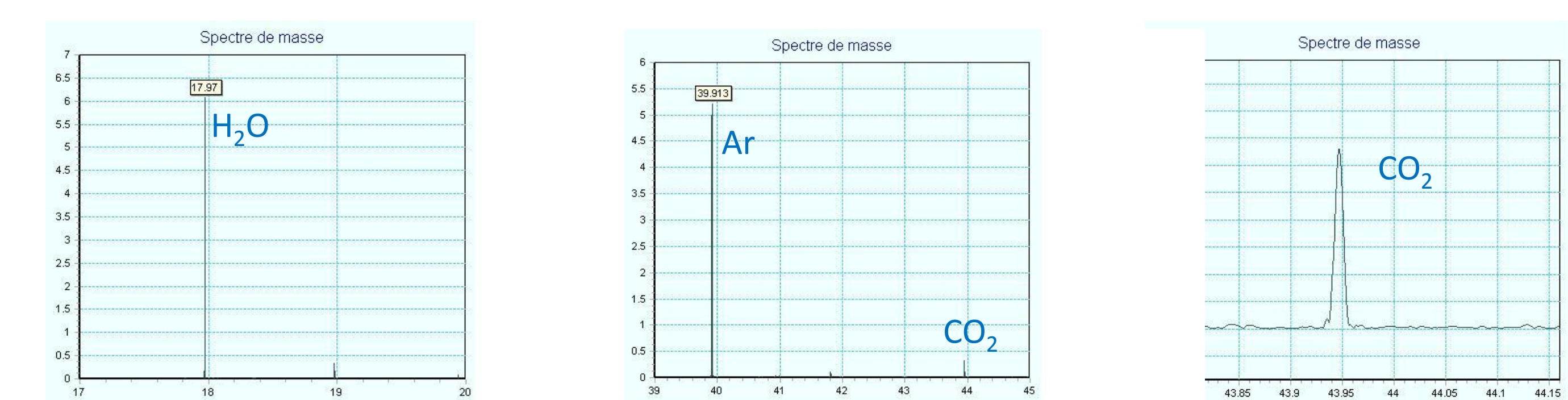
Our structured NdFeB magnets are assembled from several magnetized segments. Two types of configurations are used, one producing a central magnetic field perpendicular to the magnetic cylinder main axis and one producing an axial field.



Example of an axial field magnet configuration. This one is well adapted for coupling with an external ion source

Direct electron impact analysis

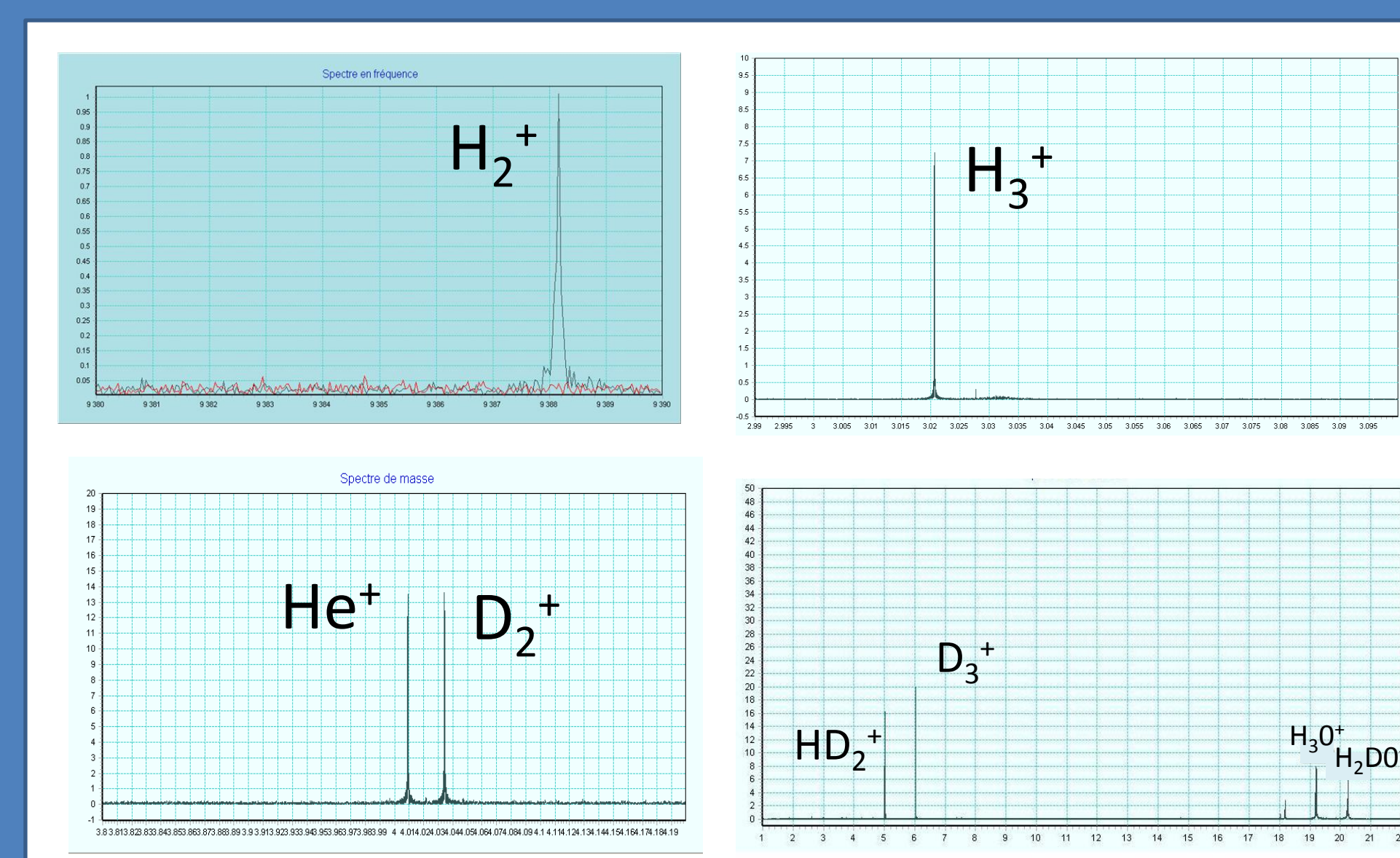
When producing the ions directly by in cell electron impact ionization, the instrument sensitivity is limited by the detection dynamics (number of ions in the smallest detectable peak over the total storage capacity of the trap). This can be partly circumvented by selective ejection of the main ions during the electron pulse.



Here major constituents of air such as H_2O , Ar, CO_2 , are detected using a selective ejection event for N_2^+ and O_2^+

Detection at small masses

The bandwidth of the detection electronics has been extended toward high frequencies so as to be able to detect ions starting from m/z 2, as exemplified below by the detection of H_2^+ . Detection is here always realized in broadband mode and both low and high mass ions can be simultaneously detected.

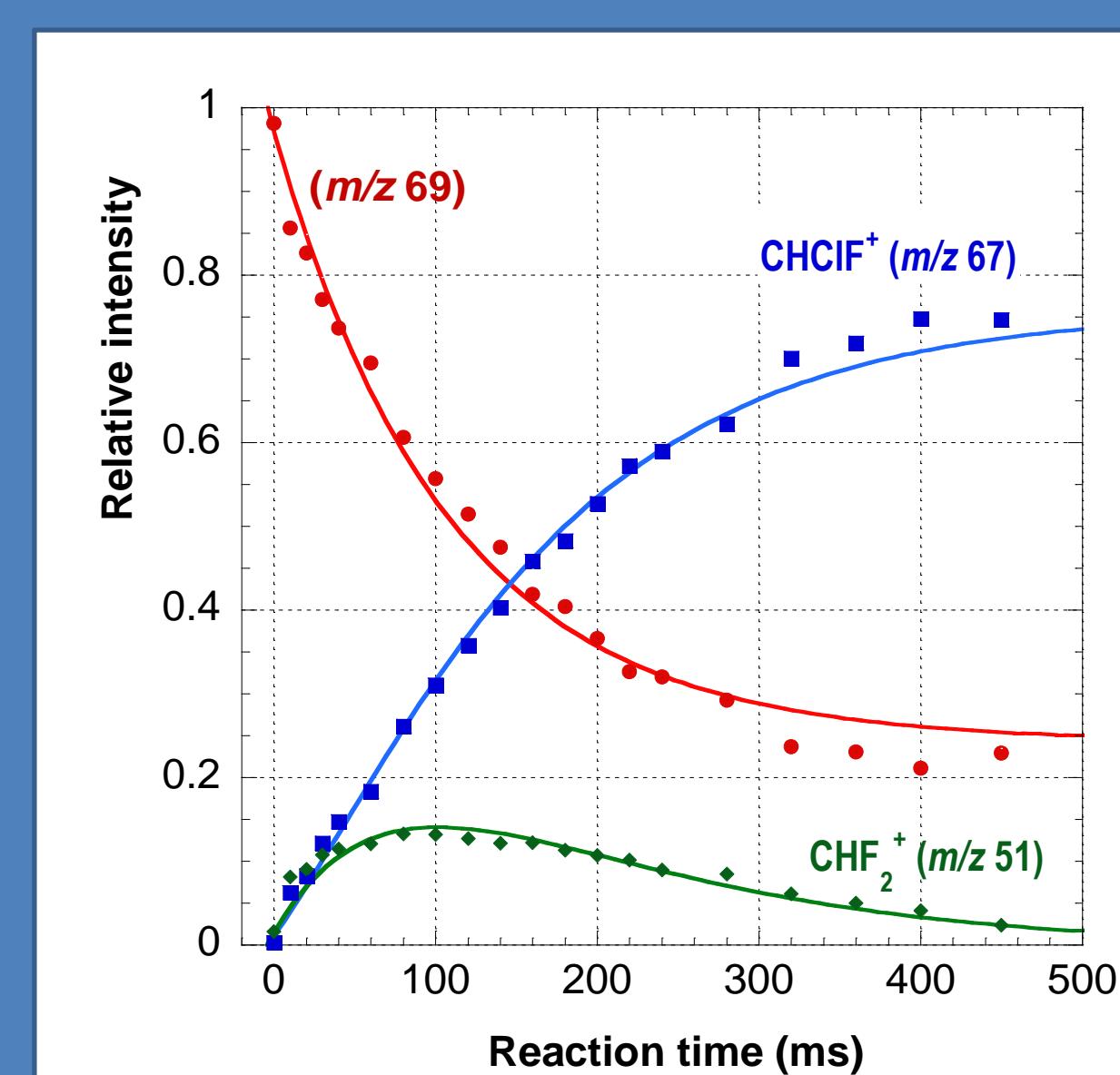


Chemical Ionization

Selective ionization of organic compounds present in air is accomplished using in cell chemical ionization.

The ionic precursor is chosen so that the reaction is soft and selective : major component of air should not be ionized and their should be no or little fragmentation of the analyte. One peak is observed per compound present and identification rely on precise mass measurement.

H_3O^+ and OH^+ are used as generalist precursors ionizing almost all VOCs.

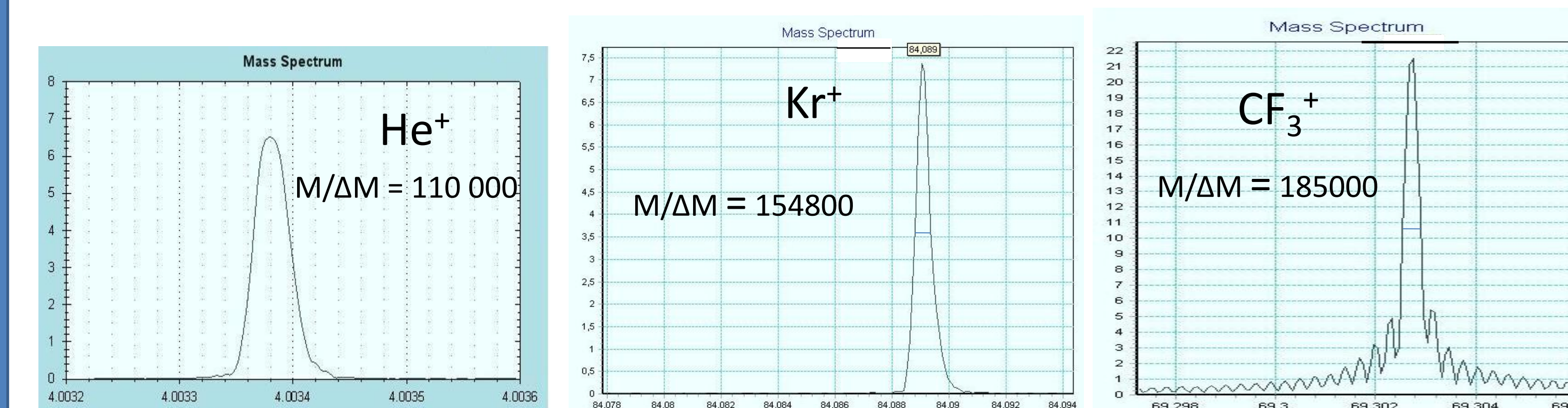


CF_3^+ can be used for ionization of alkanes or chlorofluorocarbons which are not ionized with H_3O^+ or OH^+ .

As an example the kinetic of the reaction of CF_3^+ with CHF_2Cl (R22) is shown here.

Resolution as a function of mass

Resolution is limited by the homogeneity of the magnetic field, deviation of the electrostatic potential from a quadrupolar potential, and ion-ion interactions. The resolution obtained for different ions vary inversely proportional to mass, except at very small masses where the measured resolutions are smaller than expected from a $1/m$ law, as shown below for He^+



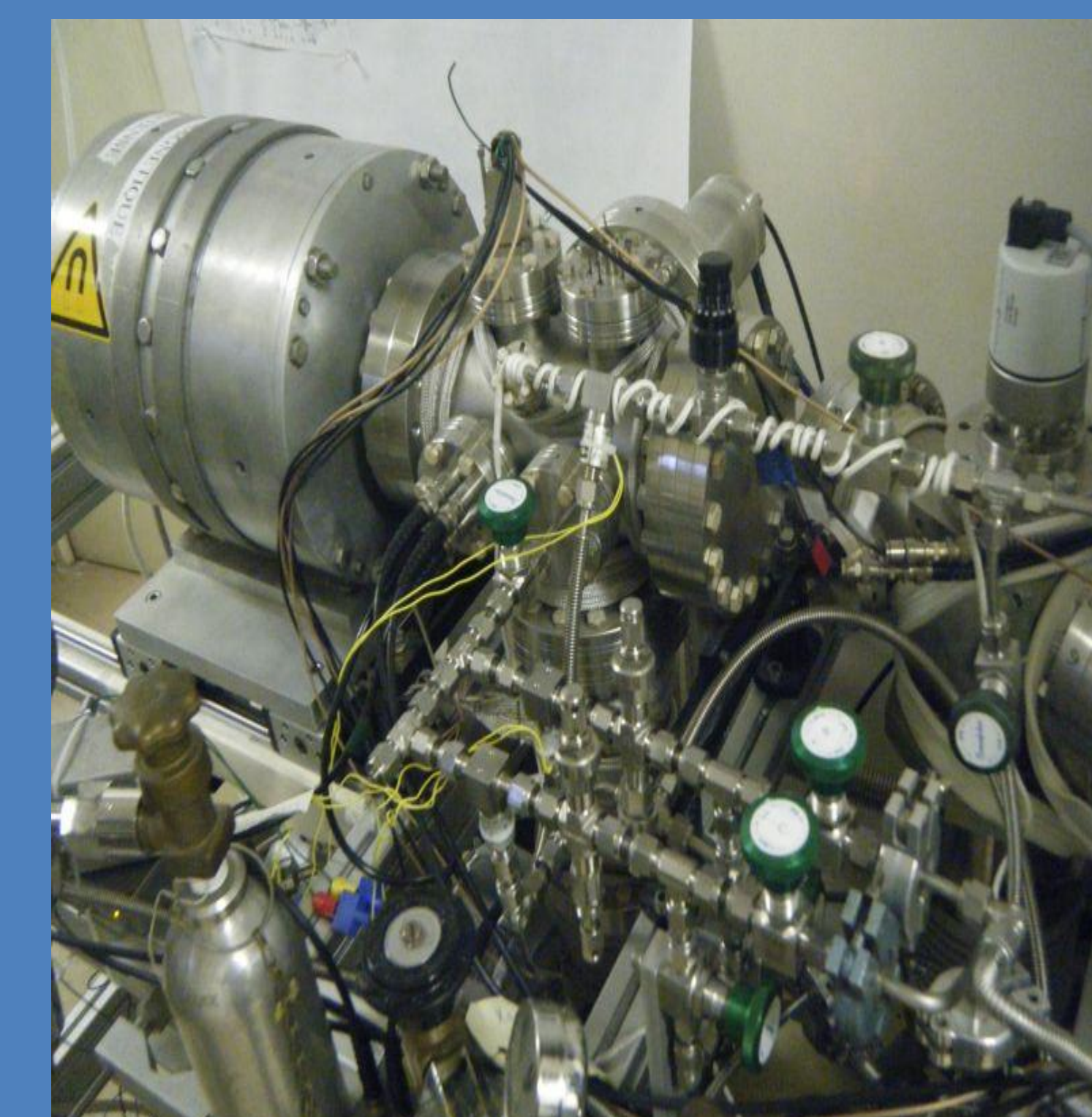
Conclusions.

Permanent magnet based FTICRs allow measurement of volatile compounds in air in a wide range of mass and concentrations.

The limit of detection is of the order of 1ppm for direct introduction and in the ppb range with membrane inlet. High concentrations, up to several %, can also be measured.

Use of different precursors such as H_3O^+ , OH^+ , CF_3^+ allows the detection of a wide range of compounds.

Measurements are quantitative since the chemical ionization is realized with well controlled pressures and reaction times.



Acknowledgement.

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