

## High resolution mass spectrometry for Titan's aerosol analysis

N. Carrasco (1), C. Szopa (1), A. Bouabdellah (1), P. Pernot (2), R. Thissen (3), P. Puget (3), B. Arezki (3), C. Briois (4), A. Boukrara (4), L. Thirkell (4), H. Cottin (5), N. Grand (5), and A. Makarov (6)  
(1) LATMOS, Guyancourt, France, (2) LCP, Orsay, France, (3) LAOG, Grenoble, France, (4) LPC2E, Orléans, France, (5) LISA, Créteil, France, (6) Thermo Fisher Scientific, Bremen, Germany  
(nathalie.carrasco@latmos.ipsl.fr)

### Abstract

We present recent high resolution mass spectrometry analysis performed in laboratory on Titan's aerosols analogs (tholins) by orbitrap measurements. New representative diagrams are developed for this nitrogen-rich organic matter based on modified Van Krevelen-type diagrams. The high resolution provided by the orbitrap technology reveals the polymeric structure of Titan's tholin and provides new horizons for future missions towards Titan's atmosphere.

### 1. Complexity of the organic composition of Titan's aerosols: orbitrap analyses of Titan's lab analogs

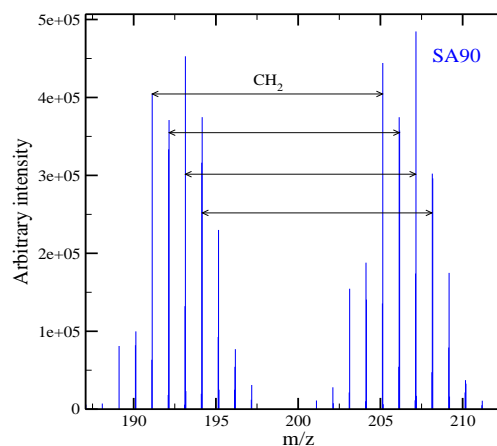
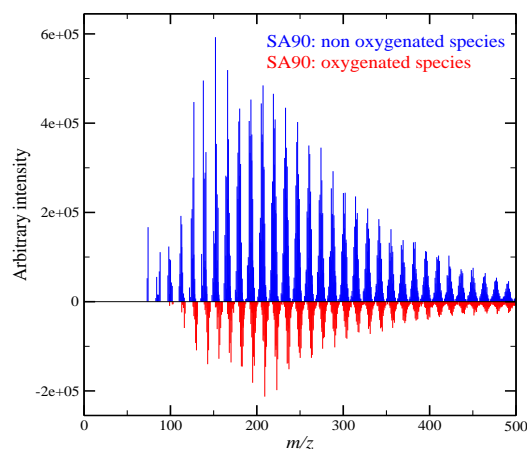


Figure 1: (upper panel) ESI/orbitrap mass spectrum of tholin sample. Oxygenated/<sup>13</sup>C species are shown with negative intensities; (lower panel) detail of the same mass spectrum for m/z 185-215.

Tholins are produced by the radio-frequency plasma setup PAMPRE, in suspension in a gaseous nitrogen-methane mixture [1]. The polymeric composition of Titan's tholins is elucidated using high-resolution mass spectrometry with a hybrid linear trap/orbitrap mass-spectrometer (see Figure 1) [2].

The highly structured mass spectra are treated with tools developed for petroleomics (Kendrick and van Krevelen diagrams), with original adaptations for nitrogen-rich compounds (see Figure 2).

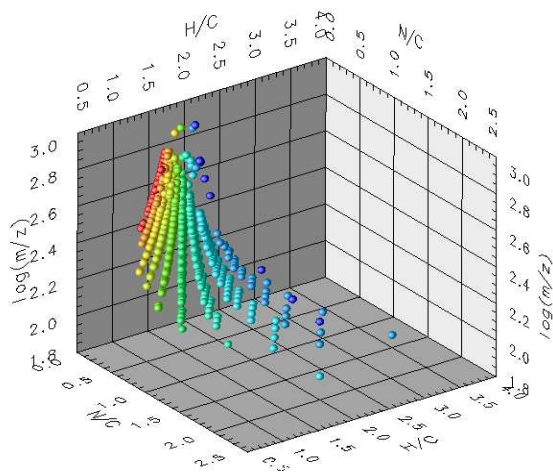


Figure 2: Tholins mass spectrum projected on a 3-dimensional plot:  $m/z$  and Van Krevelen  $N/C$ ,  $H/C$  axis.

This allows us to identify polymeric families in the complex tholins mass spectrum, which can be assigned to a small number of regularly distributed  $X-(CH_2)_m(HCN)_n$  families. We also identify the smallest species of a subset of families as linear and cyclic amino nitrile compounds of great astrobiological interest: biguanide, guanidin, acetamidine, aminoacetonitrile, and methylimidazole.

## 2. Space orbitrap project

The high complexity of Titan's analogs composition clearly demonstrates the necessity for high resolution mass spectrometry for a future in situ mission towards Titan's atmosphere. The best mass resolution ( $M/\Delta M$ ) currently achieved by mass spectrometers in space is about 3000 at mass 28 u (ROSINA on board ESA's comet chaser Rosetta), insufficient for Titan's aerosols study. Yet, purely electrostatic orbital traps in laboratory are showing mass resolution above 100 000 for  $m/z \leq 400$  [3,4]. This is the reason why our French consortium of laboratories, in collaboration with Thermoelectron which commercializes the orbitrap used in laboratory analyses, intends to suit this type of mass spectrometer to the space instrumentation requirements. We will thus present this innovative concept of high resolution mass spectrometry for space, based on the orbitrap capabilities.

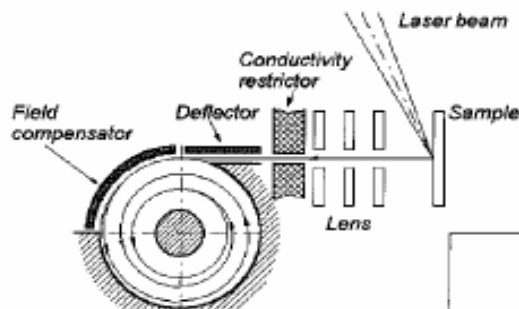


Figure 3: Conceptual picture of instrument that leads our prototype development [3]

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## References

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