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Introduction of ion mobility for the structural elucidation of soluble organic matter: Application to Titan's Haze

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Abstract

Titan's photochemical haze is one important example of primitive organic matter in the solar system. The simulation in the laboratory of analogs of this fog has proved itself to be a useful tool to improve our knowledge of the aerosols formation on Titan. However, the global structure of molecules composing this complex organic matter remains so far unknown. In this work, ion mobility coupled with mass spectrometry was used, for the first time, to gain information on the preferential shape of molecules present in Titan's haze analogs.

1. Introduction

Thanks to the Cassini-Huygens space mission, lots of information were recovered on Titan's haze [1]. Because of large mass-to-charge measurements of ions detected by *in situ* mass spectrometry and infrared spectral signatures of the haze, a Poly-Aromatic Hydrocarbon (PAH) based structure of molecules composing the haze has been suggested.

On Earth, we propose to investigate this hypothesis thanks to ion mobility by comparing analogs of the haze with standard compounds such as PAH. The goal of the present work is to give a hypothesis of a possible structure according to the obtained results.

2. Sample preparation

Tholins were produced using the PAMPRE experiment and following the procedure detailed in previous publications [2]. In order to separate soluble and insoluble fractions, 4 mg of tholins were dissolved in 1 mL of methanol in a vial under ambient atmosphere. The vial was vigorously stirred for 3 minutes to dissolve the maximum amount of species. The brown mixture was then filtered using a 0.2 μm polytetrafluoroethylene (PTFE) membrane filter on a filter holder. The soluble fraction was transferred in a glass vial. Half dilution with a 50/50 water/methanol mixture was performed just before analysis in mass spectrometry.

3. Results: analysis by ion mobility-mass spectrometry

The ion mobility coupled with mass spectrometry allows the recovering of the Collision cross section (CCS) and the m/z ratio for each detected species. The CCS represents an intrinsic property of the molecules characteristic of its size and charge. For a same m/z value, the higher is the CCS, the more deployed (/spread out) is the molecule.

Two instrumental setups were used in the present work, with increasing mass resolution.

First a Synapt G2 hybrid Q-TOF (Waters, Manchester) was used. Comparison between sample and reference compound was made as well as computational prediction of possible molecular structure (Figure 1). This study excluded poly-HCN scenarios and highlighted a possible chemical structure intermediate between PAH and ramified amines (Maillard et al, Submitted to GCA).

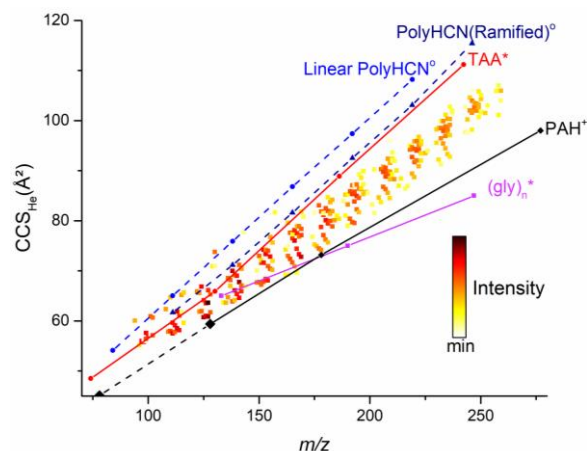


Figure 1: Collision cross section *versus* mass to charge ratio of the tholins sample recorded with the Synapt G2. TAA: Tetraalkyammonium, (Gly): Glycin polymer.

Secondly a 12-Tesla FTICR coupled with a TIMS cell was used in order to resolve more species at higher masses. The gain of resolution will be discussed in this work as well as the possible predictable structures.

4. Summary and Conclusions

In summary, this work introduces ion mobility spectrometry coupled with mass spectrometry analysis for the structural study of soluble organic matter by presenting a case study on analogues of the Titan's haze. This new analysis allows an isomeric separation of the sample and additional structural information are recovered.

As a conclusion, several hypotheses will be given concerning Titan haze regarding the obtained ion-mobility results.

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