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Structural Analysis of Titan's Tholins by Ultra-High Resolution Mass Spectrometry

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The structure, composition and formation processes of the aerosols constituting Titan's haze are largely unknown. In situ chemical analysis by the Huygens probe proved to be unsuccessful and remote optical data do not allow the retrieval of information about their molecular structure. As a consequence, analogs (called tholins) are produced in laboratories by depositing energy in a gas mixture of nitrogen and methane. Tholins have been extensively studied with various analytical methods (IR, UV and Raman spectroscopy, NMR, pyrolysis-GC/MS, etc.) and appear to be hydrogenated carbon nitrides with a very complex structure [1].
While the techniques mentioned above provide general information on the tholins, ultra-high resolution mass spectrometry is necessary to determine the atomic composition of each individual molecule making up the samples [2]. Moreover, tandem mass spectrometry (MS/MS) experiments can provide complementary information on the functional group inventory in tholins [3]. However, the MS/MS fragmentation spectra gathered so far not sufficient for determination of structural information. Based on the previous work, we propose here a systematic ultra high resolution mass spectrometry analysis (MS) in a Fourier Transform LTQ-Orbitrap mass spectrometer with an ElectroSpray Ionization (ESI) source. It is combined with an MS/MS study in order to provide a more coherent and complete characterization of the structure of the molecules making up the soluble fraction of the tholins.
Our tholins samples are synthesized in a reactor called PAMPRE by exposing N2-CH4 gas mixtures with various CH4 concentrations to a cold plasma discharge [4]. While tholins are usually synthesized on surfaces, in the PAMPRE reactor, tholins are produced in levitation in the plasma. This allows an excellent control over the growth conditions, and the tholins thus formed are very homogeneous.
Tandem mass spectrometry of standard molecules of general formula CxHyNz having structures (aliphatics, aromatics, heterocycles) and chemical functionalities (azines, nitriles, imines, amines, etc.) similar to those expected in the tholins are also performed. Analysis of the fragmentation patterns allows the retrieval of some generic rules for the fragmentation of specific functional groups. These rules will be used as a basis to interpret the results of the tholins MS/MS experiments and will lead us to possible structures for the tholins.
These results highlight the importance and necessity of ultra-high mass resolution, accurate mass measurements and tandem mass spectrometry (MS/MS) experiments for a more coherent and in-depth characterization of complex organic solids. In the context of a return to Titan, development of ultra-high resolution (m/m > 105) mass spectrometers for spaceflight capable of in situ sampling of the atmosphere is mandatory.

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