Identification of Complex Organic Molecules in PAMPRE Tholins.

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The destruction of N_2 and CH_4 and subsequent complex chemical processes lead to the formation of organic aerosols in Titan's atmosphere. The CAPS (CAssini Plasma Spectrometer) detection of large negative ions (up to 10,000 u/q) in the upper atmosphere (approximately 950 km) [1] suggests that production of aerosols begins in the upper atmosphere [2]. Although CAPS is able to detect these very large molecules and a few of the molecules have been identified [3], it does not have the mass resolution necessary to infer their chemical composition. The ability to create large organic molecules in the upper atmosphere of Titan, or any planet, is of significant astrobiological interest.

To further our understanding of the formation and composition of these aerosols, laboratory experiments have been designed to produce aerosols under Titan atmospheric conditions. We have characterized Titan aerosol analogues or Titan tholins generated by the PAMPRE (Production d'Aérosols en Microgravité par Plasma REactif) experiment. The PAMPRE experiment uses capacitively coupled RF plasma discharge to initiate the chemistry between N_2 and CH_4 that leads to the production of micron size solid particles [4]. The tholins form and grow while levitated in the plasma, which minimizes any possible wall effects. Tholins were generated using N_2/CH4 gas mixtures that range from 2-10% CH_4.

Due to the extreme complexity of the samples, ultrahigh resolution mass spectrometry is necessary to determine the chemical composition of the tholins. The samples were characterized using an LTQ-Orbitrap XL mass spectrometer, which has a resolving power of better than 10^5 up to 400 u and accuracy in exact mass determination of ± 2 ppm. Both the large number of molecules and the very similar mass defects of C, N, and H make manual molecule identification impossible. Accordingly, custom computer software has been written to quickly and accurately determine the identity of the measured peaks. Thousands of molecular formulae have been identified ranging in mass from 50 to 800 u. The spectra exhibit groups of peaks with a mass periodicity of 13.5, which results from the large amount of nitrogen incorporated into the tholins and provides insight into the chemical processes involved in tholin synthesis.

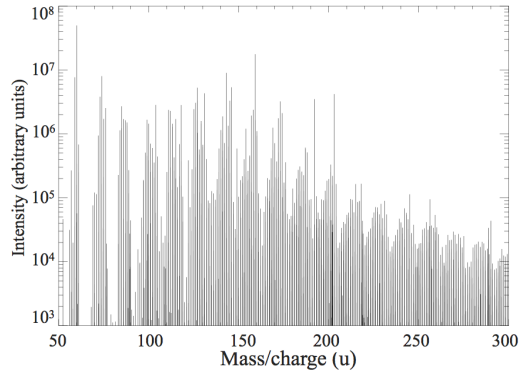

Figure 1: This figure shows a typical Orbitrap tholin positive ion mass spectrum. The sample shown was produced using 98% N_2 and 2% CH_4. It was dissolved in CH_3OH before injection into the Orbitrap. The groups of peaks have a mass periodicity of 13.5.

References

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