



Titan's Organic Aerosols : Molecular Composition And Structure Inferred From Systematic Pyrolysis Gas Chromatography Mass Spectrometry Analysis of Analogues

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In spite of numerous studies carried out to characterize the chemical composition of laboratory analogues of Titan aerosols (tholins), their molecular composition as well as their structuration are still little known. If Pyrolysis gas chromatography mass spectrometry (Pyr-GCMS) has been used for years to give clues about this composition, the highly disparate results obtained show that they can be attributed to the analytical conditions used, to differences in the nature of the analogues studied, or both. In order to have a better description of Titan's tholins molecular composition, we led a systematic analysis of these materials by pyr-GCMS, exploring the analytical parameters to estimate the biases this technique can induce.

With this aim, we used the PAMPRE experiment, a capacitively coupled RF cold plasma reactor (Szopa et al. 2006), to synthesize tholins with 2%, 5% and 10% of CH₄ in N₂. The three samples were systematically pyrolyzed in the temperature range 200-600°C with a 100°C step. The evolved gases were then injected into a GC-MS device for molecular identification. This systematic pyr-GC-MS analysis had two major objectives: (i) optimizing all the analytical parameters for the detection of a wide range of compounds and thus a characterization of the tholins composition as comprehensive as possible, and (ii) highlighting the role of the CH₄ ratio on the tholins molecular structure.

About a hundred of molecules have been identified in the pyrolysis products. Although an identical major pattern of nitriles and ethylene appears clearly for the three samples, some discriminant signatures were highlighted. The samples mainly differ by the number of released compounds. The results show especially an increase in the hydrocarbonaceous chains when the CH₄ ratio increases. At the opposite, the formation of poly-nitrogenous compounds seems to be easier for lower CH₄ ratios. We also performed a semi-quantitative study on the best represented chemical family in our chromatograms – namely nitriles: the existence of a relation between the quantity of a released compound and its molecular mass is consistent with the quantification of nitriles in the PAMPRE gas phase done by Gautier et al., 2011. Moreover, numerous species are present both in tholins and in the gas phase. That allowed us to make out potential precursors of the solid organic particles.

From all these results, we conclude that the optimal pyrolysis temperature for a GC-MS analysis of our tholins is 600°C. This temperature choice results from the best compromise between the number of released compounds, the quality of the signal and the appearance of pyrolysis artefacts.

Lastly, thanks to a review of pyr-GCMS studies carried out on Titan tholins since the first work of Khare et al. (1981), we compared all the previous analyses between them and with our own results in order to better understand the differences.

References

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