



Aromatic Structures in Simulated Titan Aerosol

M. G. Trainer, M. J. Loeffler, C. M. Anderson, R. L. Hudson, R. E. Samuelson, and M. A. Moore

Solar System Exploration Division, Goddard Space Flight Center, Greenbelt, MD, USA
(melissa.trainer@nasa.gov / Fax: +1-301-614-6406)

Abstract

Observations of Titan by the Cassini Composite Infrared Spectrometer (CIRS) between 560 and 20 cm^{-1} (~ 18 to 500 μm) have been used to infer the vertical variations of Titan's stratospheric ice abundances, as well as those of the aerosol from the surface to an altitude of 300 km [1]. The aerosol has a broad emission feature centered approximately at 140 cm^{-1} (71 μm). As seen in Figure 1, this feature cannot be reproduced using currently available optical constants from laboratory-generated Titan aerosol analogs [2].

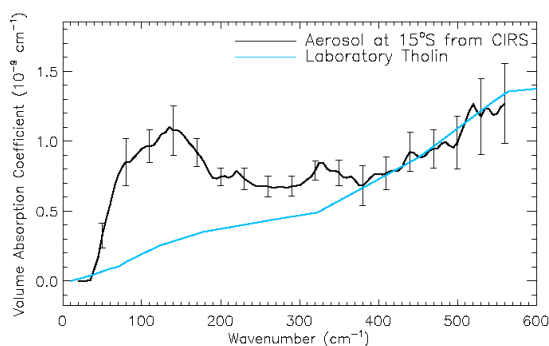


Figure 1: Derived spectral variations of absorption coefficients of aerosol (black) at an altitude of 77.5 km. 1σ uncertainties are also shown. The blue curve is derived from the Khare et al. [2] laboratory measurements of simulated Titan aerosol (tholin) in the small particle limit. Figure is adapted from Anderson and Samuelson [1].

The far-IR is uniquely qualified for investigating low-energy vibrational motions within the lattice structures of complex aerosol. The feature observed by CIRS is broad, and does not likely arise from individual molecules, but rather is representative of the skeletal movements of macromolecules. Since

Cassini's arrival at Titan, benzene (C_6H_6) has been detected in the atmosphere at ppm levels as well as large positive ions that may be polycyclic aromatic hydrocarbons (PAHs) [3]. We speculate that the feature may be a blended composite that can be identified with low-energy vibrations of two-dimensional lattice structures of large molecules, such as PAHs or nitrogenated aromatics. Such structures do not dominate the composition of analog materials generated from CH_4 and N_2 irradiation.

We are performing studies forming aerosol analog via UV irradiation of aromatic precursors – specifically C_6H_6 – to understand how the unique chemical architecture of the products will influence the observable aerosol characteristics. The optical and chemical properties of the aromatic analog will be compared to those formed from CH_4/N_2 mixtures, with a focus on the as-yet unidentified far-IR absorbance feature. Preliminary results indicate that the photochemically-formed aromatic aerosol has distinct chemical composition, and may incorporate nitrogen either into the ring structure or adjoined chemical groups. These compositional differences are demonstrated in the aerosol mass spectra shown in Figure 2.

The aromatic aerosol also demonstrates strong chemical reactivity when exposed to laboratory air, indicating substantial stored chemical potential. Oxidation and solubility studies will be presented and implications for prebiotic chemistry on Titan will be discussed.

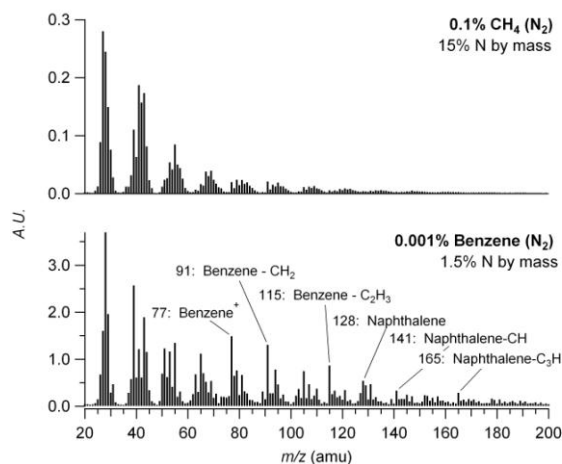


Figure 2: Mass spectra of aerosol analogs produced from the photolysis of 0.1% CH₄ in N₂ (top) and 10 ppm benzene in N₂ (bottom). The aerosol spectrum is produced using procedures outlined in previous work [4]. The photolyzed benzene sample shows that the aerosol is composed of a large variety of PAHs and aromatic rings with hydrocarbon chains attached, and that several percent of nitrogen has been incorporated.

haze on Titan and the early Earth, PNAS, Vol. 103, Pp. 18035 – 18042, 2006.

Acknowledgements

The authors thank the Planetary Atmospheres and Cassini Data Analysis Programs at NASA for funding.

References

- [1] Anderson, C. M. and Samuelson, R. E.: Titan's aerosol and stratospheric ice opacities between 18 and 500 μm : Vertical and spectral characteristics from Cassini CIRS, *Icarus*, Vol. 212, pp. 762-778, 2011.
- [2] Khare, B. N., Sagan, C., Arakawa, E. T., Suits, F., Callcott, T. A., and Williams, M. W.: Optical constants of organic Tholins produced in a simulated Titanian Atmosphere: From soft X-ray to Microwave Frequencies. *Icarus*, Vol. 60, pp. 127-137, 1984.
- [3] Waite, J. H., Young, D. T., Cravens, T. E., Coates, A. J., Crary, F. J., Magee, B., and Westlake, J.: The process of tholin formation in Titan's upper atmosphere, *Science*, Vol. 316, pp. 870-875, 2007.
- [4] Trainer, M. G., Pavlov, A. A., DeWitt, H. L., Jimenez, J. L., McKay, C. P., Toon, O. B., and Tolbert, M. A.: Organic