Analysis and Characterization of Titan Aerosol Simulants by Mass Spectrometry

Thesis by

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Saturn's large moon of Titan is unique as the only solid body in the outer solar system to possess a dense atmosphere, which is comprised of mostly nitrogen and methane. Atmospheric chemistry on this moon creates aerosols comprised of carbon, hydrogen, and nitrogen. Laboratory based synthesis of simulated Titan aerosols, also called tholins, led to molecules with rich chemical diversity, functionalities, and molecular weights. While this diversity has intriguing implications for Titan, it complicates the analysis and characterization of these simulants. This thesis discusses three different mass spectrometry methodologies, prioritizing a combination of mission applicability, broad spectrum characterization, and specific functional group identification. Chapters 2 and 3 utilize a home-built Direct Analysis in Real Time (DART) ionization source, termed EZ-DART, to test its suitability for the analysis of these simulants and the source's mission applicability. Chapter 2 focuses on the development and characterization of the EZ-DART source. Chapter 3 presents the analysis of Titan aerosol simulants, produced in a new and unique way, by EZ-DART, allowing for the identification of various compounds of astrobiological significance. Solid phase microextraction gas chromatography mass spectrometry (SPME-GC-MS) is utilized in Chapter 4 with different Titan aerosol simulants, identifying multiple compounds of significance to Titan and astrobiology. The versatility allowed by SPME increases the applicability of GC for future lander missions. While not mission applicable, Chapter 5 shows the breadth of primary amines in Titan aerosol simulants through the use of supramolecular complexation to 18-crown-6 ether. This technique not only enabled the unambiguous identification of primary amines, but also allowed for the structural characterization of some components. The range of methods and identified compounds

discussed within this thesis demonstrates not only the rich chemistry of these Titan aerosol
simulants, but also introduces intriguing possibilities for Titan's atmospheric chemistry and presents potential significance to astrobiology.

Chapter 2 is reproduced in part from:

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K.T.U. was the lead researcher on this project and main author of the manuscript

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NOMENCLATURE

DART. Direct Analysis in Real Time

MS. Mass Spectrometry

Tholin. Same as Simulated Titan Aerosol

PDN. Pulsed Discharge Nozzle

COSmIC. NASA Ames cosmic simulation chamber

RADI. Reagent Assisted Desorption Ionization

CID. Collision Induced Dissociation

ESI. Electrospray Ionization

DC. Direct Current

PPG. Poly(propylene glycol)

SPME. Solid Phase Microextraction

GC. Gas Chromatography

TIC Total Ion Chromatogram

EIC Extracted Ion Chromatogram

EI Electron Impact