THE SEARCH FOR N-BUTANE IN TITAN'S ATMOSPHERE USING IRTF/TEXES DATA.

B. L. Steffens[1] (BrendanSteffens@gmail.com), C. A. Nixon[2], N. A. Lombardo[3], T. K. Greathouse[4], J. H. Lacy[5], H. G. Roe[6], K. Sung[7] and P. G. J. Irwin[8]. [1]Florida Institute of Technology, [2]NASA Goddard Space Flight Center, [3]Yale University, [4]Southwest Research Institute, [5]University of Texas, [6]Gemini Observatory/NSF's NOIRLab, [7]Jet Propulsion Laboratory, California Institute of Technology [8]University of Oxford.

Introduction: In this work, we summarize the latest results from our search for *n*-butane (n-C_4H_{10}) in Titan's atmosphere. The atmosphere of Titan has a rich organic chemistry which is initiated through photolysis and photodissociation of CH_4 and N_2. The dissociated, intermediate species undergo a chain of reactions as they propagate downward toward the surface, forming a variety of hydrocarbons and nitriles in the process. Though it has yet to be detected there, butane (a fourth order hydrocarbon) is predicted by many photochemical models to be present at Titan in similar abundance to other hydrocarbons such as propane (C_3H_8), for example, which has already been detected.[1-3] Butane has two (spectroscopically unique) isomers: *n*-butane (n-C_4H_{10}) and isobutane (i-C_4H_{10}), which are schematically depicted in Figure 1. We have focused our search on the *n*-butane isomer, primarily due to the availability of recently derived, high resolution laboratory spectra and cross sections specific to *n*-butane, obtained at NASA JPL.[4] We note that isobutane, on the other hand, has also previously been studied in the laboratory and rough upper limits for its abundance on Titan have been derived.[5]

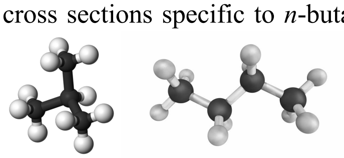

Figure 1: Two isomers of butane, i-C_4H_{10} (left) and n-C_4H_{10} (right).

Motivation: Explicit detection of *n*-butane, or at least the further constraining of its maximum abundance at Titan, will help to continue the development of numerical photochemical models, the use of which will improve our understanding of atmospheric processes on Titan and in other planetary atmospheres as well. Constraining the butane abundance at Titan may also provide insight as to the rise of even more complex molecules, haze, and other molecular structures of interest in Titan's atmosphere. Lastly, there is evidence to suggest that Titan's current atmosphere may resemble that of the prebiotic Earth. Therefore, study of Titan's current atmosphere may provide crucial insight into the early Earth environment and even the origin of life.[6]

Methodology: We searched for *n*-butane signals in high resolution ground-based observations undertaken by NASA's Infrared Telescope Facility (IRTF), via the TEXES (Texas Echelon Cross Echelle Spectrograph) instrument, on Mauna Kea, Hawaii.[7] The data include observations collected in June of 2010, centered on wavenumbers 956 cm^{-1} and 962 cm^{-1}, as well as separate observations collected earlier in May of 2009 centered on wavenumbers 1222 cm^{-1} and 1226 cm^{-1}, with the TEXES instrument operating in "High-Medium" mode (resolving power R≈80,000) in both cases.

We modeled the IRTF/TEXES observations using the NEMESIS (Non-linear optimal Estimator for MultivariatE Spectral analySIS) planetary atmosphere and retrieval tool.[8] NEMESIS consists of both a forward model calculation as well as an inversion or retrieval calculation, allowing for the retrieval of temperature, aerosol, and gas profiles, as well as retrieval of optimum scaling factors for the gas profiles implemented in the model atmosphere. This, and all other NEMESIS calculations discussed in this work, were performed in "Line-by-line" (LBL) mode, rather than making use of the correlated-k approximation. We used NEMESIS to model the methane lines in the 2009 data (1219–1229 cm^{-1}) in order to retrieve a temperature profile for Titan (Figure 2), as the stratospheric abundance of methane is well constrained. This was assumed to be an effective approximation to the Titan temperature profile during

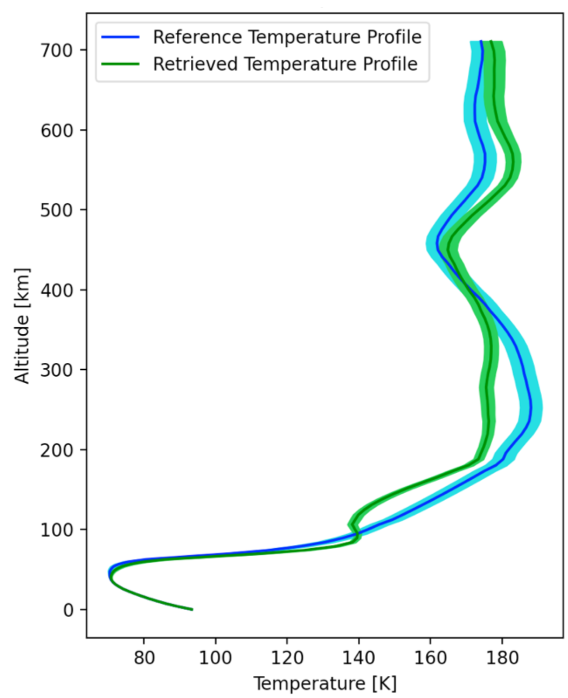

Figure 2: Reference and retrieved temperature profiles, and associated uncertainty envelopes.

the collection of the later data in 2010. We implemented the retrieved temperature profile in our modeling of the 2010 data, for which we retrieved an abundance of ethylene (C_2H_4) the most spectrally active of Titan's gases in this region.

The primary spectral region studied (953-966 cm^{-1}, see Figure 3) contains the ν_{35} (trans conformer, 965.8 cm^{-1}) and ν_{33} (gauche conformer, 957.0 cm^{-1}) bands of *n*-butane.[4] We calculated the difference between our model and the observations and searched in the residuals for signs of these *n*-butane bands. This approach was taken as we were unable to explicitly include *n*-butane in our model due to the lack of a sufficiently high resolution line list.

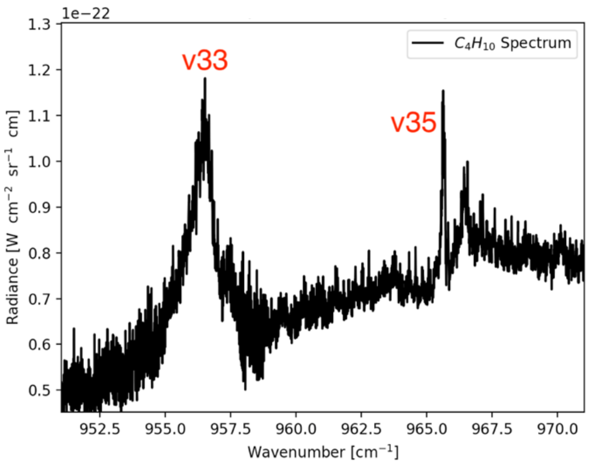

Figure 3: High resolution *n*-butane spectrum (collected at NASA JPL) containing the ν_{33} and ν_{35} bands of *n*-butane.[4]

Results: Presently, this search is still considered to be a work in progress. We anticipate being able to derive an updated upper bound on the *n*-butane abundance at Titan, should an explicit detection prove to be unattainable. A sample model fit to the 956 cm^{-1} data from 2010 is included as Figure 4. Current fits to this and the other data sets are achieving χ^2 of approximately 1.7 in the ν_{35} and ν_{33} regions for *n*-butane. In our poster, we will also discuss steps taken to improve the model's fit to the observations, as well as future work concerning the search for *n*-butane on Titan.

Acknowledgments: We wish to thank the NASA Solar System Observations (SSO) program, as well as the NASA Astrobiology Institute (NAI) for funding this research. Part of the research carried out at the Jet Propulsion Laboratory was funded through contracts and co-operative agreements from the National Aeronautics and Space Administration.

References:

[1] Yung, Y. L., M. Allen, and J. P. Pinto. *The Astrophysical Journal Supplement Series* 55 (1984): 465. [2] Willacy, K., M. Allen, and Y. Yung. *The Astrophysical Journal* 829, no. 2 (2016): 79. [3] Vuitton, V., R.V. Yelle, S.J. Klippenstein, S.M. Hörst, and P. Lavvas. *Icarus* 324 (May 2019): 120–97. [4] Sung et al. *Journal of Quantitative Spectroscopy and Radiative Transfer* (2020) 107011.[5] Hewett et al. *Icarus* 344 (2020): 113460. [6] Clarke et al. *Planetary and Interstellar Processes Relevant to the Origins of Life*, 225–48. (1997). [7] Lacy et al. *Publications of the Astronomical Society of the Pacific* 114, no. 792 (2002): 153–68. [8] Irwin et al. *Journal of Quantitative Spectroscopy and Radiative Transfer* 109, no. 6 (2008): 1136–50.

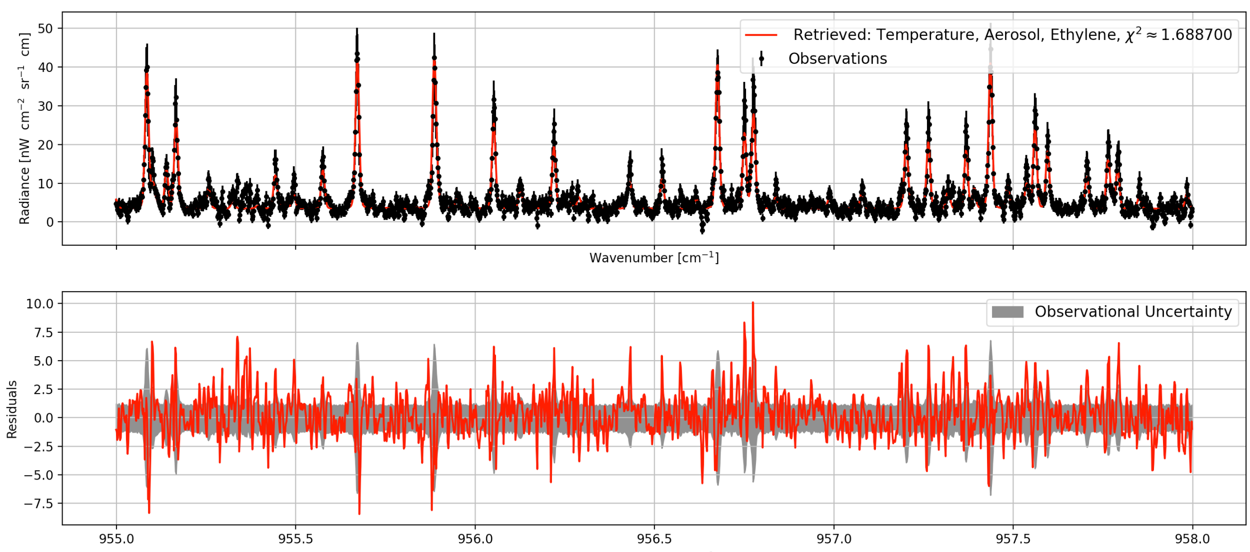

Figure 4: High quality image of model fit (red curve in top plot) to IRTF observations (black points in top plot), achieving χ^2 of approximately 1.7. Residuals (data minus model) are displayed in red in bottom plot, with associated uncertainty estimates in gray. Please zoom in PDF reader for more detail.