

SOLUBILITY AND DETECTABILITY OF ACETONITRILE IN TITAN LAKES. M. Leitner^{1, 2}, V. F. Chevrier¹, S. Singh¹ ¹Arkansas Center for Space and Planetary Sciences, University of Arkansas, Fayetteville, Arkansas 72701, ²Dept. of Physics and Astronomy, Humboldt State University, Arcata, California 9521, mal174@humboldt.edu.

Introduction: Titan is the only body aside from Earth on which stable bodies of liquid have been found [1]. Its lakes contribute to a methane-driven hydrological cycle making it a good analog to an early Earth. The exact composition of its lakes however is still a subject of study. They are thought to be composed predominantly of methane (CH₄) and ethane (C₂H₆) as well as a variety of other hydrocarbons and hydrocarbon ices [2, 3]. However current results lack precision and the solubility of these various molecules under Titan conditions is not very well studied. Acetonitrile (CH₃CN) in particular is of great interest due to its astrobiological implications and its role as a precursor in the formation of amino acids [4].

In order to study acetonitrile's solubility in CH₄ and C₂H₆ and whether it can be spectrally detected, bench-top experiments were performed in which spectra was taken of acetonitrile-saturated hexane (C₆H₁₄). To study CH₃CN under Titan conditions, it was mixed with CH₄ and C₂H₆ within a chamber which simulates Titan surface temperature, pressure and atmosphere [5].

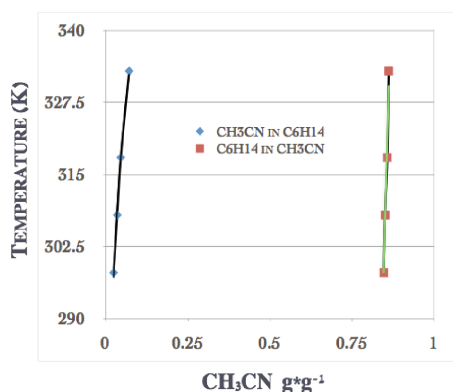


Figure 1. Phase diagram for C₆H₁₄ and CH₃CN. The left side of the graph represents the percent at which C₆H₁₄ is saturated with CH₃CN with varying temperature. Image credit [6].

Methods:

Bench-top experiment. The bench-top experiment was performed saturating C₆H₁₄ with liquid CH₃CN. C₆H₁₄ was chosen because it remains in liquid form at ambient temperatures and because of its spectral similarities to CH₄ and C₂H₆

C₆H₁₄ was saturated by gradually mixing in CH₃CN drop by drop. Mixing between drops was performed using a closed container. The solution was then transferred to an open container in which spectra was taken using FTIR so that comparisons could be made with increasing concentration. The saturation concentration was estimated using a phase diagram (Fig. 1).

Chamber experiments. Experiments under Titan conditions were performed using a Titan simulation chamber in which Titan temperatures and pressures are reached using liquid nitrogen [5].

N₂ gas was first bubbled through liquid CH₃CN allowing us to introduce CH₃CN to the chamber in gas form (Fig. 2). The gas mixture flowed into the condenser over a time-span of approximately 20 minutes, during which time the pressure valve was kept open to allow the CH₃CN-N₂ gas to flow as well as the bottom solenoid valve which allowed the N₂ gas to escape after the CH₃CN condensed onto the condenser's walls. Next, CH₄ or C₂H₆ was condensed over CH₃CN within the condenser. The liquid then passes through a filter and collects onto a petri dish exposed to the Titan-simulated atmosphere of approximately 94 K and 1.5 bar where spectra is then taken.



Figure 2. CH₃CN saturation apparatus. N₂ gas bubbles in from the top and the gas mixture flows out through the side to the chamber.

Results and Discussion:

Bench-top experiment. CH₃CN-saturated C₆H₁₄ spectra can be seen in Figure 2 with pure CH₃CN and C₆H₁₄ spectra present for comparison. No definite CH₃CN features could be confirmed in the saturated spectra, although potential features might be made clearer with further analysis. It is unclear as to why these features could not be detected. It is possible that with the amount of mixing required to dissolve the CH₃CN in the C₆H₁₄, evaporation prevented full saturation from being reached. Although the mixing was done in a closed container, the spectra were taken using an open container.

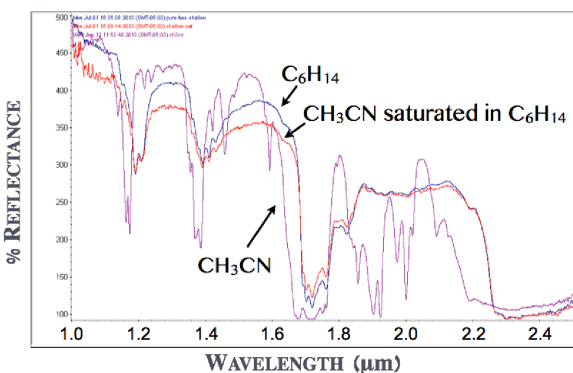


Figure 3. NIR spectra from bench-top experiment of CH_3CN -saturated C_6H_{14} with pure CH_3CN and C_6H_{14} spectra for comparison

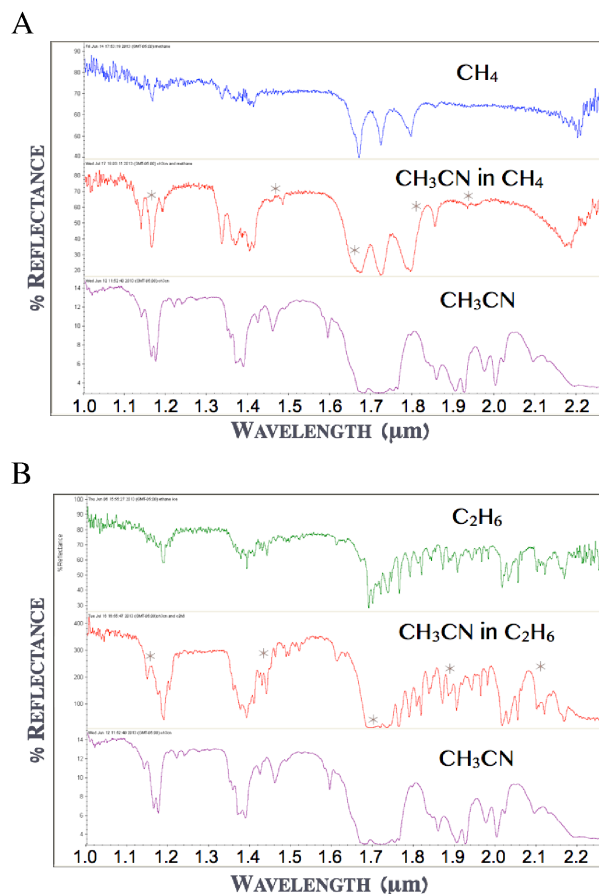


Figure 4. NIR spectra from chamber experiments of CH_3CN in CH_4 (A) and C_2H_6 (B). The starred locations indicate the presence of CH_3CN features

Chamber experiments. CH_3CN features are clearly defined in both CH_4 and C_2H_6 experiments as is seen in Fig. 4A and Fig. 4B. In CH_4 , features can be seen at wavelengths: 1.14, 1.46, 1.48 and 1.94 μm with distinct widening between 1.65-1.68 μm . The features at 1.46 and 1.48 μm correspond to CH_3CN CN stretch. In C_2H_6 , features can be seen at wavelengths: 1.14, 1.46 and 2.8 μm with clear evidence of saturation having been reached between 1.68-1.74 μm . Once again, evidence of the CN stretch is present in the 1.46 μm feature.

Applications to Titan: Solubility experiments of hydrocarbon ices within Titan lakes is not very well studied nor understood under Titan conditions. Knowledge of this can be very useful when studying the compositions of evaporites as lake levels decrease through evaporation. Using spectroscopy as a tool to determine these solubilities is even more valuable considering it's one of the few tools we have at our disposal directly on Titan (e.g. VIMS instrument on Cassini).

Spectrally studying CH_3CN in particular under Titan conditions is of value to the astrobiological studies being done as CH_3CN is one of the precursors in the formation of amino acids--one of the hypothesized first steps in the creation of life.

Conclusions and Future Studies: Solubility calculations still have not yet been made. Future studies will include attempting to use a spectra-unmixing program along with mass data obtained from chamber experiments to calculate values for the solubility of CH_3CN in C_2H_6 and in CH_4 . Future studies could also extend to other hydrocarbon ices such as benzene (C_6H_6), acetylene (C_2H_2) or butane (C_4H_{10}) and applying the same methods to calculate the solubilities of each compound. It might also be of interest to repeat these experiments to check for consistency, as well as to spectrally observe the effects of CH_4 as it evaporates, leaving CH_3CN evaporites behind.

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References: [1] E.R. Stofan, et al. (2007) *Nature*, 445:61. [2] D. Cordier, et al. (2011) *PSS*, 3101. [3] G. Mitri, et al. (2007) *Icarus* 186, 385-394. [4] F. Raulin (2008) *Space Sci. Reviews* 135, 37-48. [5] Wasiak, F. C., Luspay-Kuti, A., Welivitiya, W. D. D. P., Roe, L. A., Chevrier, V. F., Blackburn, D. G. and Cornet, T., 2012. A facility for simulating Titan's environment. *Adv. Space Res.* 51, 1213-1220. [6] V.A. Keskinov, A.K. Pyartman, N.A. Charykov, 2009, *Zhurnal Neorganicheskoi Khimii*, 54, 701-704.