**A Database for the Material Properties of Titan's Organic Liquids, Ices, and Hazes.** Xinting Yu[1], Yue Yu[1], Jialin Li[2], Julia Garver[2], Xi Zhang[1], [1]Department of Earth and Planetary Sciences, University of California Santa Cruz, 1156 High Street, Santa Cruz, CA 95064 (xintingyu@ucsc.edu). [2]Department of Physics, University of California Santa Cruz, 1156 High Street, Santa Cruz, CA 95064.

**Introduction:** Titan's thick methane ($CH_4$) and nitrogen ($N_2$) have enabled rich photochemistry to occur in its upper atmosphere. The photochemistry leads to the creation of numerous organic molecules in Titan's atmosphere, such as ethane ($C_2H_6$), acetylene ($C_2H_2$), benzene ($C_6H_6$), hydrogen cyanide (HCN), etc. [1]. Most of the simple organic molecules are in the gas phase when produced in the upper atmosphere (for a complete list of the observed gaseous molecules, see Table 1). Titan's unique temperature profile allows these simple gaseous organic molecules to condense into liquids or solids in its stratosphere, forming liquid or ice clouds [2]. Various types of organic clouds have been detected in Titan's atmosphere through both ground-based and spacecraft observations by Voyager 1 and Cassini (see references in [3]). The simple organic molecules in Titan's atmosphere can further coagulate and react to form complex refractory organic particles that constitute Titan's thick haze layers [4].

After the clouds and hazes are formed, they would eventually fall onto the surface of Titan. If they land on dried surfaces on Titan, species that are able to remain in the solid form will become surface sediments. For example, Titan's sand dunes are likely derived partially from the organic hazes [5]. Solid acetylene has also been detected on Titan's surface [6]. While species that remain in liquid form or transform into liquids can modify and wet Titan's surface by rainfalls and storms (e.g., [7]). For those clouds and hazes that land on the surfaces of lakes and seas, they could either dissolve in the methane-ethane-nitrogen-dominated lakes, float on the lake surfaces, or sink and form lakebed sediments [8]. After the lake dries, the dissolved organics could precipitate as solids and form evaporites on Titan's surface. Organic evaporites have been discovered in the polar regions [9] and the equatorial regions [10] at the bottom of presumably dried lakebeds and sea-beds.

Thus, it is crucial to have a database summarizing various material properties of the hazes and the organic condensates, made of organic liquids or ices, to prepare for future in-situ Titan explorations such as the Dragonfly mission, due to arrive at Titan in 2034. In this work, we summarize and calculate a range of material properties of organic liquids, ices, and hazes that can be used for future modeling, data analysis, and comparison to observations. These properties include thermodynamic properties (saturation vapor pressure and latent heat for vaporization and sublimation), optical property (refractive indices at the visible wavelength), electric property (dielectric constant), physical property (density), and surface properties (liquid surface tensions and solid surface energies).

**Methods:** We include the material properties of 18 organic species (summarized in Table 1), all of which have been observed as gas-phase compounds in Titan's atmosphere. We also include the material properties for Titan haze analogs, the so-called "tholins" made in different laboratories.

| *Compound name* | *Mixing ratio range* |
|---|---|
| Methane ($CH_4$) | 5e-3 – 2.2e-2 |
| Acetylene ($C_2H_2$) | 2e-6 – 1e-5 |
| Ethane ($C_2H_6$) | 7e-6 – 3e-5 |
| Ethylene ($C_2H_4$) | 7e-8 – 6e-6 |
| Diacetylene ($C_4H_2$) | 9e-10 – 1e-7 |
| Benzene ($C_6H_6$) | 6e-11 – 2e-7 |
| Propadiene ($C_3H_4$-a) | (6.9 ± 0.8) e-10 |
| Propyne ($C_3H_4$-p) | 5e-9 – 1e-7 |
| Propene ($C_3H_6$) | 2e-7 – 3e-6 |
| Propane ($C_3H_8$) | 1e-9 – 6e-9 |
| Hydrogen cyanide (HCN) | 4e-8 – 3e-4 |
| Cyanoacetylene ($HC_3N$) | 6e-11 – 9e-7 |
| Carbon dioxide ($CO_2$) | 1e-8 – 3e-8 |
| Acetonitrile ($CH_3CN$) | 4e-10 – 1e-8 |
| Propionitrile ($C_2H_5CN$) | 8e-10 – 3e-9 |
| Acrylonitrile ($C_2H_5CN$) | 2e-10 – 8e-10 |
| Cyanogen ($C_2N_2$) | 5e-11 – 7e-9 |
| Dicyanoacetylene ($C_4N_2$) | < 5e-10 |

We collect from literature the sublimation and vaporization saturation vapor pressures as functions of temperature, $P_{sat}(T)$ for the 18 species. The latent heat of sublimation and vaporization can then be estimated using the Clausius-Clapeyron equation:

$$L_{vap/sub}=RT^2/P_{sat}(T)dP_{sat}(T)/dT.$$

We collect from the literature the measured densities ($\rho_{l/s}$) for the organic liquids and ices at different temperatures and fit the experimental data as polynomial functions. We also collected the measured refractive indices in the visible wavelengths ($n_{vis}$) and the static dielectric constants ($\varepsilon_0$) of the organic ices and liquids on Titan. We collect from the literature the surface tensions of the organic liquids. We also use $\rho_l$, $n_{vis}$, $\varepsilon_0$ to compute the missing surface tensions of the organic liquids using the MacLeod-Sugden method [11, 12]. We calculate the surface energies of the organic ices using the surface tension of the liquids, their $L_{vap}$ and $L_{sub}$, and $\rho_s$, following two empirical methods described in [13].

**Results:** Using the collected $P_{sat}(T)$ and the mixing ratio of each species, we find that all these observed 18 species in the gas phase could condense. Most of them condense from the gas phase to the liquid phase, and only propane ($C_3H_8$) condenses into a liquid.

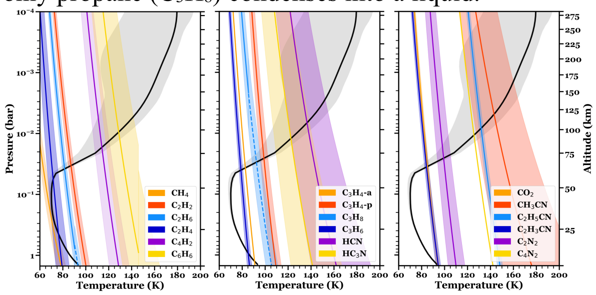


**Figure 1**: Condensation curves for observed gaseous organic species in Titan's atmosphere. The black line in each panel represents Titan's mean temperature profile, and the shaded grey area represents the range of retrieved temperature profiles using Cassini/CIRS data throughout the Cassini mission [14]. The solid condensation curves are plotted with the average mixing ratio, and the shaded regions are plotted using the observed upper and lower bond mixing ratios listed in Table 1. Solid condensation curves represent gas-solid transitions, and dash lines represent gas-liquid transitions.

We also summarized all the properties as a function of temperature for the organic liquids and ices. For tholins, we complied all measured material properties for tholins produced at different laboratories and specified their production conditions. and tholins as data tables. For example, in Table 1, we show the complied and fitted liquid densities of the 18 organic species as functions of temperature.

| Species | $\rho_l$ (kg/m$^3$) | Temp (K) | Ref |
|---|---|---|---|
| $CH_4$ | $756.75 - 6.2806T + 4.4541 \times 10^{-2}T^2 - 1.3583 \times 10^{-4}T^3$ | $T_{tri}$–180 | [a] |
| $C_2H_2$ | $1048.7 - 2.2548T$ | 194–298 | [a] |
| $C_2H_6$ | $800.67 - 2.2197T + 8.1971 \times 10^{-3}T^2 - 1.9941 \times 10^{-5}T^3$ | $T_{tri}$–300 | [a] |
| $C_2H_4$ | $876.67 - 3.1890T + 1.3578 \times 10^{-2}T^2 - 3.2485 \times 10^{-5}T^3$ | $T_{tri}$–280 | [a] |
| $C_4H_2$ | $2165.6 - 5.2315T$ | 237–278 | [a] |
| $C_6H_6$ | $1457.9 - 3.5779T + 7.8879 \times 10^{-3}T^2 - 8.2593 \times 10^{-6}T^3$ | $T_{tri}$–520 | [a] |
| $C_3H_4$-(a) | $922.05 - 0.88621T - 8.1467 \times 10^{-4}T^2$ | 156–298 | [a] |
| $C_3H_4$-(p) | $977.69 - 1.2267T$ | 185–298 | [a] |
| $C_3H_8$ | $843.37 - 1.5313T + 3.5869 \times 10^{-3}T^2 - 8.0831 \times 10^{-6}T^3$ | $T_{tri}$–320 | [a] |
| $C_3H_6$ | $900.91 - 1.8447T + 4.7704 \times 10^{-3}T^2 - 1.0179 \times 10^{-5}T^3$ | $T_{tri}$–320 | [a] |
| HCN | $1111.4 - 1.4473T$ | $T_{tri}$–298 | [a] |
| $HC_3N$ | $1189.6 - 1.2850T$ | $T_{tri}$–315 | [b] |
| $CO_2$ | $6295.8 - 60.676T + 0.25108T^2 - 3.6941 \times 10^{-4}T^3$ | $T_{tri}$–290 | [a] |
| $CH_3CN$ | $1133.1 - 1.1958T$ | 278–373 | [a] |
| $C_2H_5CN$ | $1031.9 - 0.68308T - 5.8010 \times 10^{-4}T^2$ | 208–533 | [a] |
| $C_2H_3CN$ | $1131.3 - 1.1103T$ | 213–443 | [a] |
| $C_2N_2$ | $1423.6 - 1.8839T$ | $T_{tri}$–293 | [a] |
| $C_4N_2$ | 970.8 | 298 | [c] |

**Table 1**: Densities of Titan-relevant organic liquids along the saturation line. [a] this work; [b] [15]; [c] [16].

The calculated surface tensions of the organic liquids and surface energies of the organic solids are essential for understanding cloud formation and cloud-lake interactions on Titan, methods as detailed in [17]. The results will be published in a forthcoming paper [18].

**Conclusion**: We started a preliminary database summarizing measured and calculated material properties of organic liquids, ices, and hazes on Titan. The database can not be used as inputs for models and theoretical studies on understanding various atmospheric and surface processes on Titan. It can direct future laboratory work to study species with few measured material properties, such as diacetylene ($C_4H_2$) and dicyanoacetylene ($C_4N_2$).

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