A Material Property Database of Organic Liquids, Ices, and Hazes on Titan and A Cross-Laboratory Comparison Study of Titan Haze Analogs. Xinting Yu[1], Jialin Li[2], Yue Yu[3], Julia Garver[2], Abigale Hawthorn[2,3], Erik White[3], Ella Sciamma-O'Brien[4], Chao He[5], Joshua Sebree[6], Farid Salama[4], Sarah Horst[5], Xi Zhang[3], Erika Barth[7], [1]Department of Physics and Astronomy, the University of Texas at San Antonio, One UTSA Circle, San Antonio, TX 78249 (xinting.yu@utsa.edu). [2]Department of Physics, University of California Santa Cruz, 1156 High Street, Santa Cruz, CA 95064. [3]Department of Earth and Planetary Sciences, University of California Santa Cruz, 1156 High Street, Santa Cruz, CA 95064. [4]NASA Ames Research Center, Space Science & Astrobiology Division, Astrophysics Branch, Moffett Field, CA 94035. [5]Department of Earth and Planetary Sciences, Johns Hopkins University, 3400 N. Charles Street, Baltimore, MD 21218. [6]Department of Chemistry and Biochemistry, University of Northern Iowa, 1227 W. 27th Street, Cedar Falls, IA 50614. [7]Southwest Research Institute, 1050 Walnut St Suite 300, Boulder, CO 80302.

Introduction: The methane (CH_4) and nitrogen (N_2) in Titan's upper atmosphere enable rich photochemistry, creating numerous organic molecules in Titan's atmosphere. At least 18 organic species have been detected with space- and ground-based observations in Titan's atmosphere (see the list of species in Table 1). Most of the simple organic molecules are in the gas phase when produced in the upper atmosphere. During their descent through the atmosphere, Titan's unique temperature profile allows these gaseous organic molecules to condense into liquids or solids in its stratosphere, forming liquid or ice clouds [1]. It is expected the organics in Titan's atmosphere will eventually fall toward the surface of Titan. If they land on dry surfaces on Titan, species that are able to remain in the solid form will become surface sediments [2]. While species that remain in liquid form or transform into liquids can modify and wet Titan's surface with rainfalls and storms (e.g., [3]). In a nutshell, because of the diverse range of temperature and pressure regimes that can exist on Titan, from its atmosphere to the base of its lakes and seas, it is anticipated that many simple organic species are present in multiple phases (gas, liquid, and solid phases).

These simple organic molecules in Titan's atmosphere can further react, polymerize, and coagulate to form the complex refractory organic particles that constitute Titan's thick haze layers. These complex organics are also expected to fall towards Titan's surface and form surface sediments, forming sedimentary features such as the dunes seen in the equatorial regions of Titan [4].

***Table 1**: The 18 detected simple organic compounds included in this work [8].*

Compound name	
Methane (CH_4)	Ethane (C_2H_6)
Ethylene (C_2H_4)	Acetylene (C_2H_2)
Diacetylene (C_4H_2)	Benzene (C_6H_6)
Propane (C_3H_8)	Propene (C_3H_6)
Propadiene (C_3H_4-a)	Propyne (C_3H_4-p)
Hydrogen cyanide (HCN)	Cyanoacetylene (HC_3N)
Carbon dioxide (CO_2)	Acetonitrile (CH_3CN)
Propionitrile (C_2H_5CN)	Acrylonitrile (C_2H_5CN)
Cyanogen (C_2N_2)	Dicyanoacetylene (C_4N_2)

All the above organics (simple and complex) actively participate in various processes such as cloud formation, lake interaction, sediment transport, and abrasion on Titan. The unique material properties of each species/material are found to play an important role in shaping these different processes (e.g., [5-7]) and therefore represent critical input parameters to model these processes and prepare for the future in-situ explorations of Titan (i.e., the Dragonfly mission). Thus, a comprehensive database to archive the material properties for all possible material candidates is timely and necessary to better model these processes and support future missions. In this work, we present the first comprehensive database that is dedicated to summarizing the material properties of organics on Titan [8]. The database has also helped us identify some gaps between existing material property measurements. This leads us to conduct some new laboratory material characterization on the analogs of Titan's complex organics through a cross-laboratory comparative study [9, 10]. 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.

Methods: For the material properties of the simple organics, we review and compute several important material properties of organic liquids and ices for the 18 species detected on Titan. Here is a list of properties we fitted using existing laboratory data or computed in this work [8]: 1) sublimation saturation vapor pressures as a function of temperature of C_3H_8, C_3H_6, C_3H_4-p, HC_3N, CH_3CN, C_2H_5CN, C_2H_3CN; 2) vaporization saturation vapor pressures as a function of temperature of HCN and C_4N_2; 3) latent heat of all species in Table 1 at their triple point; 4) organic liquid densities as a function of temperature of CH_4, C_2H_6, C_2H_4, C_4H_2, C_6H_6, C_3H_8, C_3H_6, C_3H_4-p, and CO_2; 5) organic ice densities as a function of temperature of C_2H_6, C_2H_4, C_2H_2, C_4H_2, C_6H_6, C_3H_8, HCN, CO_2, CH_3CN, C_2H_5CN, and C_2N_2; 6) liquid surface tensions of HC_3N and C_4N_2 at their triple points, 7) solid surface energies of all species in Table 1 at their triple point.

For the material properties of the complex organics on Titan, since no sample returned from Titan is available, the data on their properties rely upon the laboratory-made organic aerosol analogs ("tholins"). Many laboratory facilities have been synthesizing tholins since the 1970s. However, modern research studies often adopt the properties of tholins from one particular laboratory. It is an open question whether/which tholins are representative of the actual complex organics on Titan. To approach this question, we think the best way to proceed would be to compare material properties of tholins produced in different laboratory facilities to existing/future data on the complex organics on Titan. To minimize the effect of measuring techniques/conditions on the measured sample properties, we used a standardized approach and measured tholin samples produced by three independent facilities (the Planetary Haze Research (PHAZER) chamber at Johns Hopkins University, the Cosmic Simulation Chamber (COSmIC) at NASA Ames Research Center, and the photochemical aerosol chamber at the University of Northern Iowa). All samples are made with a gas mixture of 95% N_2 and 5% CH_4. After all the samples are made and deposited on the same substrate provided to each facility, they are shipped in custom-built vacuum vessels to avoid sample contamination/oxidation and then measured in an inert atmosphere. We conducted a pilot study characterizing the solid surface energies of seven samples from three facilities (without the standardized transportation under vacuum) [9]. We also recently conducted the full standardization sample characterization on four freshly-made samples and measured the surface energy, elastic modulus, and hardness of these samples.

Results and Discussion: In the Titan material database [8], we presented the following material properties: thermodynamic properties (phase change points, sublimation and vaporization saturation vapor pressure, and latent heat of the simple organics), physical property (density of the simple organic liquids and ices, and tholins made in various laboratories), optical property (refractive indices at the visible wavelength of the simple organic liquids and ices), electric property (dielectric constant of the simple organic liquids and ices), and surface properties (liquid surface tensions of the simple organic liquids and solid surface energies of the simple organic ices and tholins made in various laboratories). All data are presented in easy-to-use tables that allow users to compute property quickly at certain temperatures. As an example, we show the simple organic liquid density table we compiled in Table 2.

Table 2*: Density expressions of Titan-relevant organic liquids along the saturation line. [a] this work; [b] Daubert & Danner, 1989; [c] Kroenlein et al. 2011; [d] Dannahauser & Flueckinger, 1963; [e] Rumble, 2020.*

Species	Liquid density, $\rho_l(T)$ (kg/m^3)	Temp (K)	Ref
CH_4	$162.70 + 291.23(1-T/T_{cri})^{0.35} + 142.42(1-T/T_{cri}) - 121.96(1-T/T_{cri})^2 + 107.38(1-T/T_{cri})^3$	T_{tri}-T_{cri}	[a]
C_2H_6	$206.20 + 390.80(1-T/T_{cri})^{0.35} + 161.80(1-T/T_{cri}) - 90.702(1-T/T_{cri})^2 + 88.144(1-T/T_{cri})^3$	T_{tri}-T_{cri}	[a]
C_2H_4	$214.20 + 402.42(1-T/T_{cri})^{0.35} + 177.02(1-T/T_{cri}) - 99.181(1-T/T_{cri})^2 + 101.65(1-T/T_{cri})^3$	T_{tri}-T_{cri}	[a]
C_2H_2	$63.816/0.27448^{1+(1-T/T_{cri})^{0.28752}}$	T_{tri}-T_{cri}	[b]
C_4H_2	$2165.6 - 5.2315T$	T_{tri}–278–[T_{cri}]	[a]
C_6H_6	$304.70 + 596.41(1-T/T_{cri})^{0.35} + 292.04(1-T/T_{cri}) - 296.31(1-T/T_{cri})^2 + 378.24(1-T/T_{cri})^3$	T_{tri}-T_{cri}	[a]
C_3H_8	$220.50 + 429.60(1-T/T_{cri})^{0.35} + 167.26(1-T/T_{cri}) - 87.547(1-T/T_{cri})^2 + 96.621(1-T/T_{cri})^3$	T_{tri}-T_{cri}	[a]
C_3H_6	$229.60 + 447.91(1-T/T_{cri})^{0.35} + 181.53(1-T/T_{cri}) - 102.10(1-T/T_{cri})^2 + 121.01(1-T/T_{cri})^3$	T_{tri}-T_{cri}	[a]
C_3H_4-a	$243.20 + 508.18(1-T/T_{cri})^{0.35} + 66.874(1-T/T_{cri}) + 232.07(1-T/T_{cri})^2 - 159.04(1-T/T_{cri})^3$	T_{tri}-T_{cri}	[c]
C_3H_4-p	$244.90 + 469.73(1-T/T_{cri})^{0.35} + 409.34(1-T/T_{cri}) - 658.50(1-T/T_{cri})^2 + 600.71(1-T/T_{cri})^3$	T_{tri}-T_{cri}	[a]
HCN	$195.00 + 451.55(1-T/T_{cri})^{0.35} + 1249.0(1-T/T_{cri}) - 3452.1(1-T/T_{cri})^2 + 3809.9(1-T/T_{cri})^3$	T_{tri}-T_{cri}	[c]
HC_3N	$1189.6 - 1.2850T$	T_{tri}–315.2–[T_{cri}]	[d]
CO_2	$467.60 + 925.62(1-T/T_{cri})^{0.35} + 465.51(1-T/T_{cri}) - 412.21(1-T/T_{cri})^2 + 509.61(1-T/T_{cri})^3$	T_{tri}-T_{cri}	[a]
CH_3CN	$247.37 + 556.17(1-T/T_{cri})^{0.35} + 214.71(1-T/T_{cri}) + 34.189(1-T/T_{cri})^2 + 34.820(1-T/T_{cri})^3$	T_{tri}-T_{cri}	[c]
C_2H_5CN	$244.85 + 447.66(1-T/T_{cri})^{0.35} + 601.25(1-T/T_{cri}) - 658.21(1-T/T_{cri})^2 + 497.05(1-T/T_{cri})^3$	T_{tri}-T_{cri}	[c]
C_2H_3CN	$252.09 + 757.67(1-T/T_{cri})^{0.35} - 448.60(1-T/T_{cri}) + 1307.2(1-T/T_{cri})^2 - 944.27(1-T/T_{cri})^3$	T_{tri}-T_{cri}	[c]
C_2N_2	$352.99 + 734.98(1-T/T_{cri})^{0.35} + 191.04(1-T/T_{cri}) + 216.84(1-T/T_{cri})^2 - 248.71(1-T/T_{cri})^3$	T_{tri}-T_{cri}	[c]
C_4N_2	970.8	298.15	[e]

To accommodate this rapidly evolving field where more laboratory experiments are being conducted on the material properties of simple organics, we also created a publicly available database website to serve as a repository for all the data presented in this work: https://titanmaterials.sites.ucsc.edu/.

Through the comparison study between the material properties of tholins, we find that the properties of tholins produced from different laboratories with varying setups/experimental conditions have varying properties. We also find that sample preservation and the measuring condition play a significant role in the accuracy of the material property characterization. The samples that are preserved during transportation and measured in an inert atmosphere have different properties than our pilot study without sample preservation [9] and a previous study conducted in the ambient atmosphere [7]. Overall, the total surface energies of all tholin samples span from 45-75 mJ/m^2. The elastic moduli of the tholin samples span from 10-30 GPa, and the hardness of the tholin samples spans from 0.5-3 GPa.

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