National Aeronautics and Space Administration

Exploring Titan's Organic Mineralogy

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Program: FY21 R&TD Topics **Strategic Focus Area: Planetary Atmospheres and Geology**

Objectives

Understanding the material properties of Titan's cryogenic organics is critical for future surface missions to Titan. Our proposed efforts will deliver a new, comprehensive understanding of the physicochemical properties of the most common Titan surface organics.

The overall objective of this work is to measure the physical and mechanical properties, morphology, heat capacity, and microstructure of the most probable major organic mineral constituents within Titan's surface (i.e. benzene, naphthalene, acrylonitrile), and to use this information to (1) provide the basic scientific foundation for constraining the extent of surface geological processes and (2) determine technological requirements for in-situ surface sampling instruments. These physical parameters will be used to make specific predictions of geochemical processes that should occur on Titan's surface and subsurface, and estimates of their extent and surface expression and tie them to Cassini's observations of features on Titan's surface. The design of solid sampling systems requires information about material strength, deformability, resistance to fracture, and stiffness, all of which will be uncovered in the course of this study. The proposed basic scientific and technological research tasks are highly interdisciplinary; they combine chemistry, geology, and astrobiology.

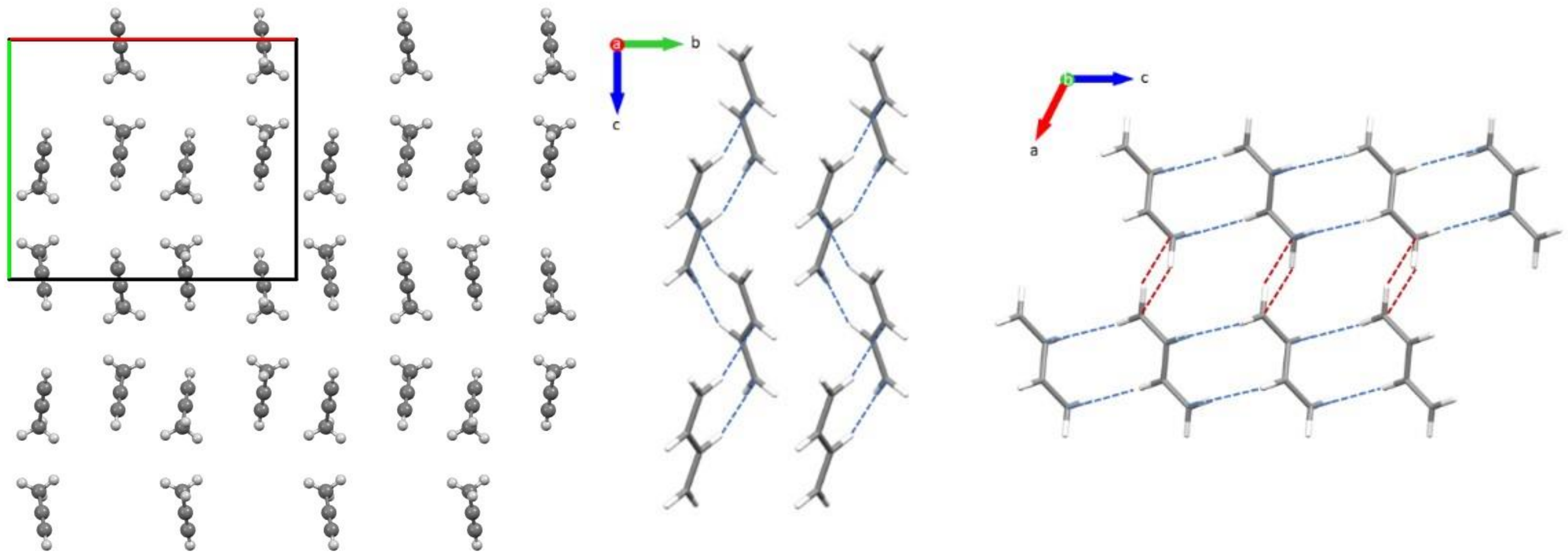
Background

The Cassini-Huygens mission has revealed a wide variety of Earth-like landforms on Titan's surface: plains, mountains, dunes, lakes, seas and rivers. Titan's surface appears to be constructed from organic molecules, rather than rocks and minerals that make up Earth's surface. At a surface temperature of ~92 K, the non-covalent interactions are sufficiently strong to enable stable interactions among these organic molecules, which form an entirely new class of cryogenic organic "minerals," or naturally occurring compounds with a specific composition. **The physical properties of these organic minerals have rarely, and in most cases never, been investigated.**

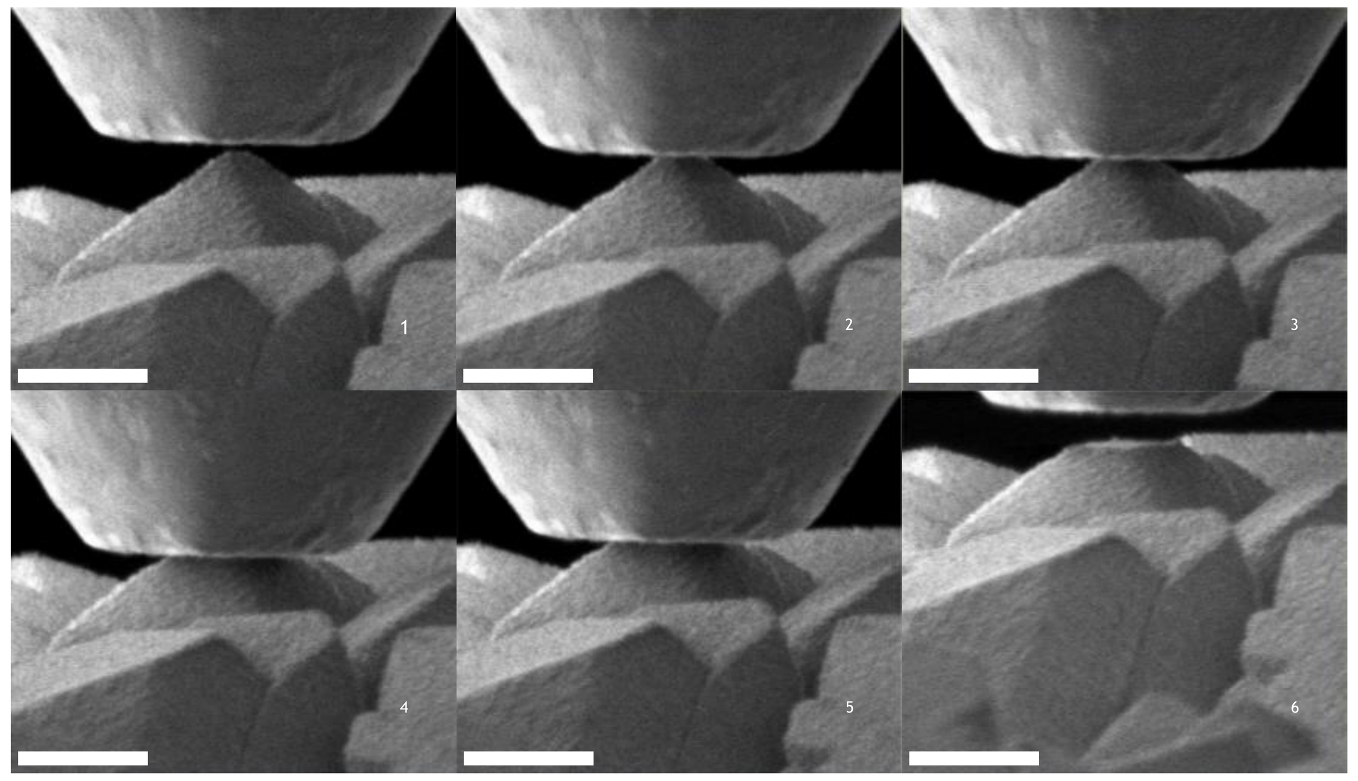
Table 1. Expected abundant molecular species on Titan's surface

Molecule	Surface Flux (molecules cm^{-2} s^{-1})	Known Structures
acetylene (C_2H_2)	3.22×10^8	orthorhombic (Acam) → cubic (Pa3) at 130 K
hydrogen cyanide (HCN)	1.54×10^8	orthorhombic (Imm) → tetragonal (I4mm) at 170.4 K
butadiene (C_4H_6)	1.71×10^7	Crystal structure determined in FY20 by this group: monoclinic (Pc)
acrylonitrile (C_3H_3N)	1.62×10^7	crystalline phase 1 → crystalline phase 2 at ~94 K. Crystal structure not available.
acetonitrile (CH_3CN)	1.27×10^7	β (orthorhombic - Cmc2_1) → α (monoclinic - P2_1/c) at 216.9 K Possible γ form on rapid quenching from liquid
benzene (C_6H_6)	1.08×10^6	orthorhombic Pbca
Propyne (C_3H_4)	2.60×10^6	Crystal structure determined in 2021 by this group

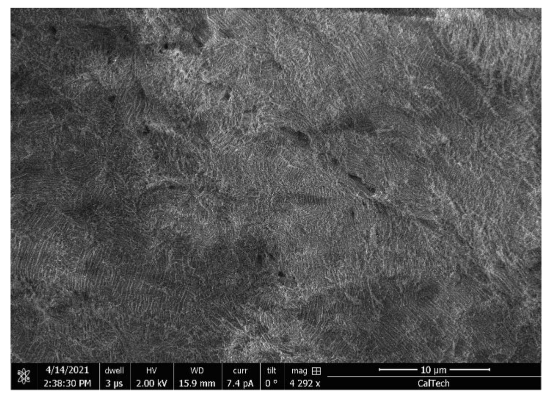
Approach and Results



Crystal structures of propyne (left) and butadiene (right) determined for the first time by this project.



Compression tests on single crystals of benzene at cryogenic temperatures (125 K) have allowed us to measure the yield stress, ~2 GPa. We have performed analogous tests on a acetonitrile. Greer lab, Caltech



Solid crystalline acetonitrile at 143 K, exhibiting crystal steps of ~ 200 nm.

Significance/Benefits to JPL and NASA

Our highly interdisciplinary work represents the first comprehensive investigation of the physical and chemical properties of the solid phase of the organic minerals that make up Titan's surface. Over the past decade, our labs at JPL have developed extensive, state-of-the-art capabilities for the study of organic materials at cryogenic temperatures. We are currently the world leaders in the study of Titan organic minerals. Our collaboration with Prof. Greer at Caltech has added novel cryogenic nanomechanical testing instrumentation to our capabilities, and this collboration is continuing through JROC funding. No other laboratories have these combinations of instrumentation and expertise.

This work has helped retain and advance JPL's leadership in Titan surface chemistry, is complementary to the ongoing Titan NAI (PI Rosaly Lopes), and would likely help capture Dragonfly Participating Scientist positions, and enable JPL to be significantly involved in the science of Dragonfly.

Publications

Cable, M. L.; Vu, T. H.; Malaska, M. J.; Maynard-Casely, H. E.; Choukroun, M.; Hodyss, R., *A Co-Crystal between Acetylene and Butane: A Potentially Ubiquitous Molecular Mineral on Titan*. ACS Earth Space Chem 2019, 3 (12), 2808-2815

Courtney Ennis, Morgan L. Cable, Robert Hodyss, and Helen E. Maynard-Casely *Mixed Hydrocarbon and Cyanide Ice Compositions for Titan's Atmospheric Aerosols: A Ternary-phase Co-crystal Predicted by Density Functional Theory.* Acs Earth Space Chem 2020, 4 (7), 1195-1200

Morgan L. Cable, Tuan H. Vu, Michael J. Malaska, Helen E. Maynard-Casely, Mathieu Choukroun and Robert Hodyss. *Properties and behavior of the acetonitrile-acetylene co-crystal under Titan surface conditions.* Acs Earth Space Chem 2020, 4 (8), 1375-1385.

Tuan H. Vu, Helen E. Maynard-Casely, Morgan L. Cable, Robert Hodyss, Mathieu Choukroun and Michael J. Malaska. *Anisotropic Thermal Expansion of the Acetylene-Ammonia Co-crystal under Titan's Conditions.* J. Appl. Cryst. (2020). 53, 1524-1530

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