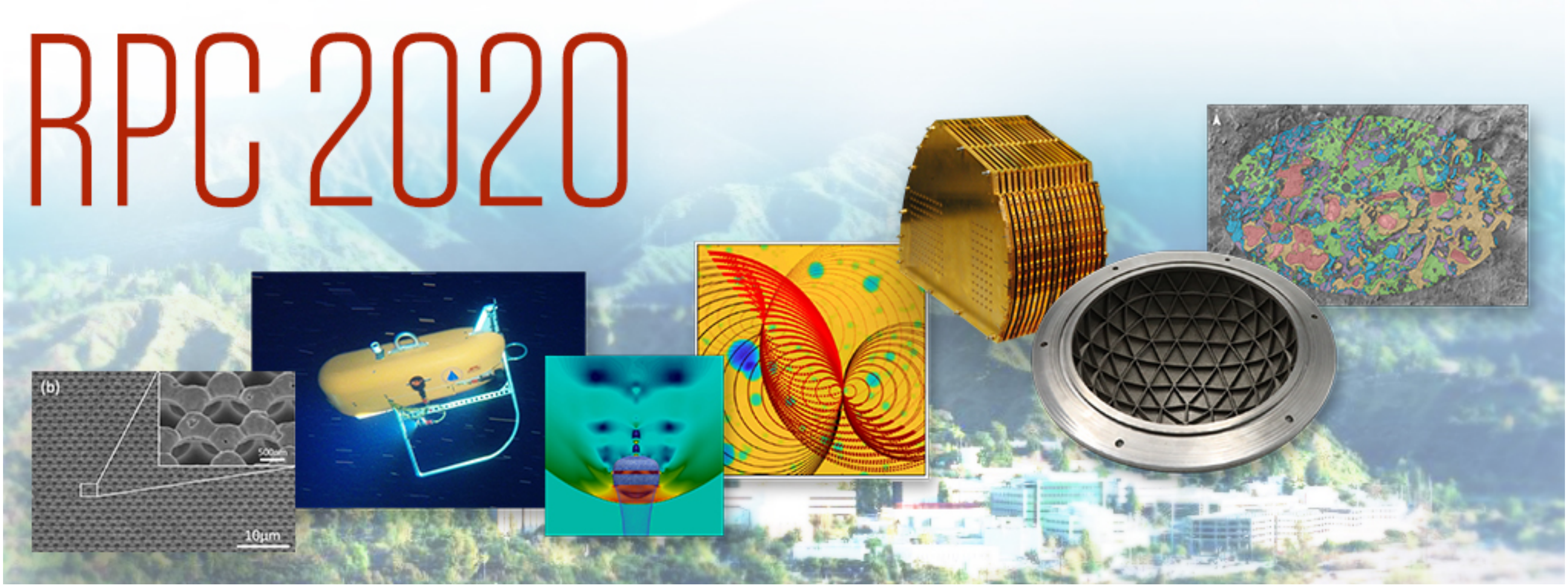

Virtual Research Presentation Conference

Laboratory Spectral Simulations of Habitable Exoplanet Atmospheres

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Tutorial Introduction

Abstract

Our goal is to understand the composition of Earth-like and Jupiter-like atmospheres around other stars in our galaxy. In order to do this, we need to simulate much hotter conditions in the laboratory, because most of those extra solar planets (exoplanets) so far observed are very hot, as much as 3000 K, compared to Earth (~300 K). Those stars also emit a lot of ultraviolet (UV) light, just like our Sun. For this reason, those exoplanets are very hot and at the same time drenched with UV-light.

So, we built an instrument named as CAAPSE (Cell for Atmospheric and Aerosol Photochemistry Simulations of Exoplanets) to reproduce those exoplanet conditions in our laboratory at JPL. Our research results took us by surprise.

For example, we found that a hydrogen-dominated (H_2) atmosphere with a small amount of carbon monoxide (CO) produces CH_4, CO_2, H_2O, and organic aerosols at these high temperatures under UV-light. So, two fundamental molecules in our Universe are sufficient to start producing several other important molecules.

Our data will be used by fellow scientists who do astronomical observations of exoplanet spectroscopy as well as those who develop and use models to interpret those observations.

Some 40 light-years from Earth, a planet called TRAPPIST-1e offers a heart-stopping view: brilliant objects in a red sky, looming like larger and smaller versions of our own moon. But these are no moons. They are other Earth-sized planets in a spectacular planetary system outside our own. These seven rocky worlds huddle around their small, dim, red star, like a family around a campfire. Any of them could harbor liquid water, but the planet shown here, fourth from the TRAPPIST-1 star, is in the habitable zone, the area around the star where liquid water is most likely to be detected. This system was revealed by the TRAnsiting Planets and PlanetesImals Small Telescope (TRAPPIST) and NASA's Spitzer Space Telescope. The planets also are excellent targets for NASA's James Webb Space Telescope. Take a planet-hopping excursion through the TRAPPIST-1 system.

www.nasa.gov

NASA's Exoplanet Exploration Program, Jet Propulsion Laboratory, Pasadena CA.
exoplanets.nasa.gov

Source: https://exoplanets.nasa.gov/resources/2159/planet-hop-from-trappist-1e/

Problem Description

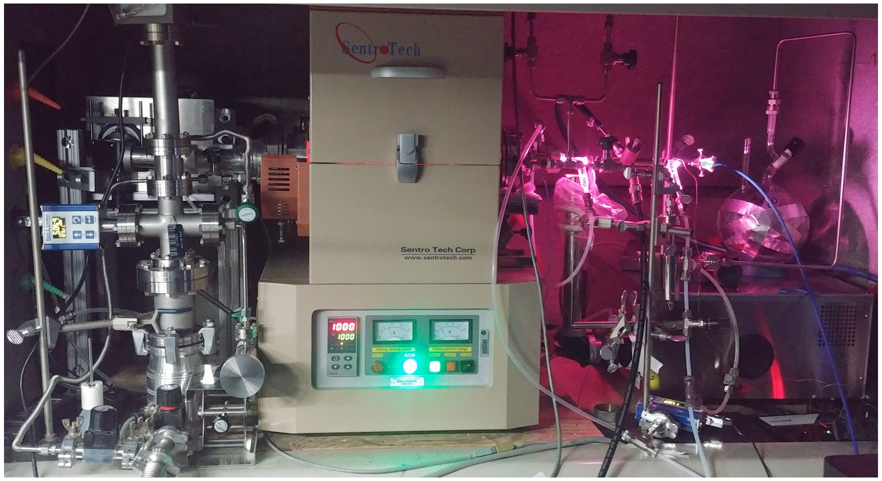
Hot Jupiter type exoplanets are much closer to their parent stars and experience high temperatures and UV radiation, which are conditions that represent a new and mostly unexplored frontier in atmospheric photochemistry and aerosol formation. There is mounting evidence of aerosol/haze in the atmospheres of exoplanets ranging from these hot Jupiter to cooler super Earth like exoplanets.

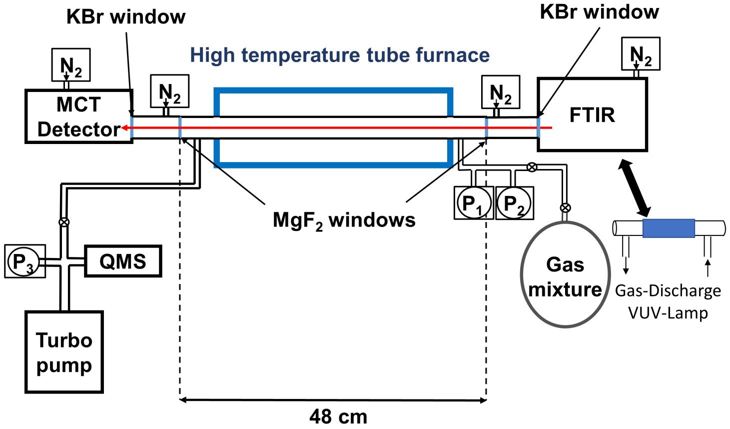
Laboratory data are lacking under these conditions, making general understanding and modeling of these hot Jupiter atmospheres difficult. Our laboratory research is aimed at providing the data needed and insight into the chemical processes occurring in these environments.

In our laboratory we have successfully simulated for the first time simultaneous UV-light exposure of atmospheric gases at relatively high temperatures these hot Jupiter exoplanets experience. Our laboratory work addresses a variety of atmospheric compositions that evolve with temperature, pressure, and ultraviolet (UV) irradiation, which are crucial for these efforts.

Our work provides equilibrium mixing ratios of exoplanet atmospheric gases as well as organic aerosol formation efficiencies. This data will help the exoplanet community for interpreting hot planet atmospheric transmission spectra (with their wealth of observations – 20 planets with HST transmission spectra). Our data for lower-temperature Earth-like or Neptune-like exoplanets will help simulate atmospheres of cooler planets that will be found by the K2 and TESS missions and which will be extensively studied by JWST and ARIEL/CASE.

Methodology





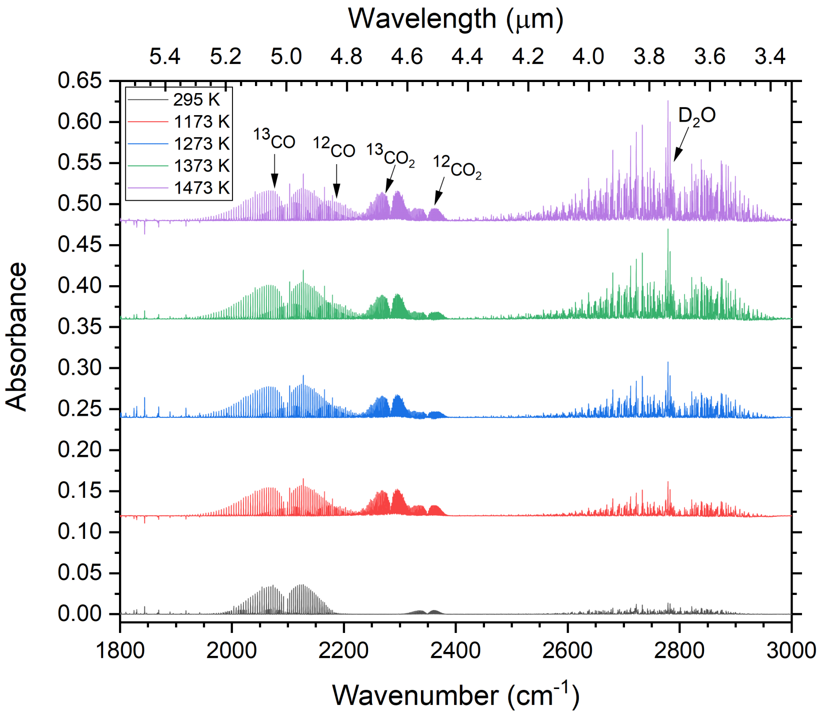
- The CAAPSE (Cell for Atmospheric and Aerosol Photochemistry Simulations of Exoplanets) experimental setup (left) is a unique facility to study simultaneous thermochemistry (<1800 K) and photochemistry (Lyman-alpha at 121.6 nm and above) in exoplanet atmospheres of up to a few tens of millibar (limited for safety reasons).

- In the present study, to simulate different stellar H:C:N:O ratio, the cell is filled with 15 mbar of gas mixture: D_2:^{13}CO:D_2O (99.26%:0.26%:0.48%), H_2:CO:N_2 (96.4%:1.7%:1.9%) and H_2:CH_4 (690:1).

- The gases are heated at temperatures up to 1473 K for several hours to study equilibrium thermochemistry.

- While heating, the gaseous mixture is irradiated at Lyman-α (121.6 nm) + a broad emission band (140–170 nm), mimicking the VUV stellar flux received by the hot Jupiter like exoplanet atmospheres.

Results: C/O Ratio and Mixing Ratios of Exoplanet Atmospheres



Transmission-Absorption IR spectra of the gaseous mixtures at the equilibrium thermochemistry at different temperatures. Isotopically labelled carbon monoxide (^{13}CO) and water (D_2O) were used for these experiments.

- **Thermochemistry:**

  In atmospheres with C/O = 0.35 (oxygen is ~3 times more abundant than carbon), thermochemistry alone resulted in a significant formation of carbon dioxide ($^{13}CO_2$) and water (D_2O) at each studied temperature.

  In contrast, in our previous studies, when C/O = 1, thermochemical formation of CO_2 was less efficient, but a small amounts of CH_4 was observed.

- **Thermochemistry Augmented by Photochemistry:**

  In atmospheres with C/O = 0.35, a small additional increase of the CO_2 mixing ratio by a factor of 2–3 is observed.

  In contrast, in our previous studies, when C/O = 1, a significant increase of CO_2 mixing ratio by a factor of 10 was observed under UV-irradiation, increasing with temperature.

- **Conclusions:**

  Thermochemical reactions are primarily responsible for the formation of CO_2 in solar-like low C/O ratio (0.35) atmospheres, while photochemistry is the major process responsible in carbon-rich high C/O ratio (C/O = 1.0) atmospheres.

Results: C/O Ratio and Aerosol Formation in Exoplanet Atmospheres

- **High C/O ratio promotes more organic aerosol formation:**
  Photochemical formation of organic aerosols was not observed in the low C/O ratio (0.35) gas mixture contrary to the one with a high C/O ratio of 1 (Fleury et al., ApJ 871:158, 2019).

- **Low C/O ratio promotes oxidation of organics:**
  For atmospheres with a C/O ratio << 1, water and its dissociation products (OH and O) likely inhibit the growth of organic molecules and the formation of aerosols, suggesting that photochemical organic aerosols are likely to be observed in planets presenting a carbon enrichment compared to their host stars.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Sample 1


Sample 2

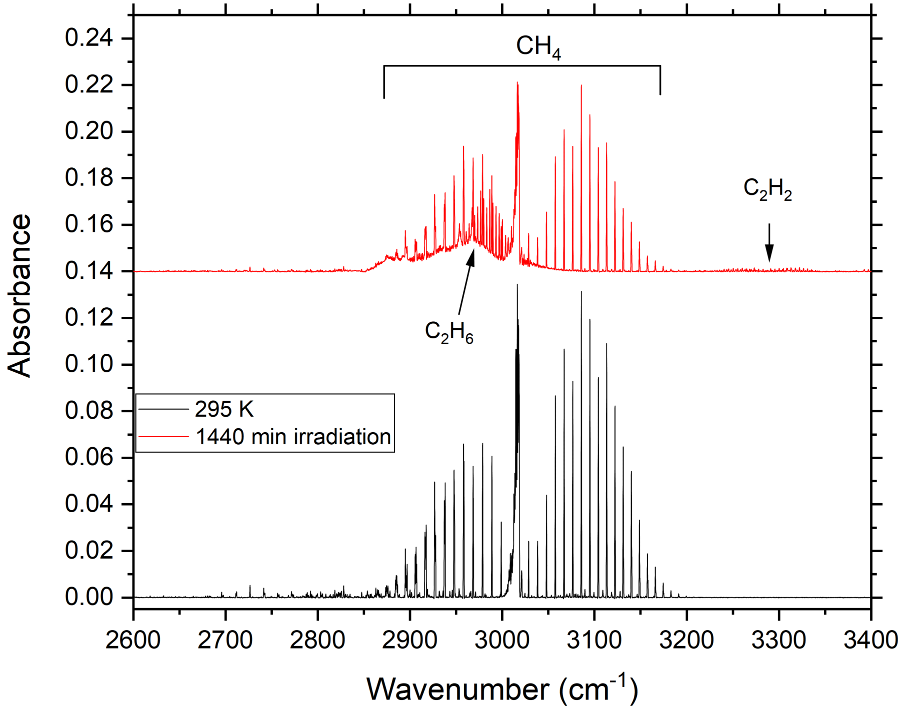
High C/O ratio (C/O = 1.0) UV-irradiation augmented thermochemistry produced organic aerosols. There was no such non-volatile residue formation when C/O ratio was lowered to 0.35.

Results: Nitrogen Chemistry in hot Jupiter Atmospheres

N_2 does not undergo chemistry at low pressures (15 mbar) and UV > 121.6 nm

- Analysis of the gas mixture composition did not reveal the presence of any new chemical species (containing N) compared to what we observed previously for gas mixture without N_2.
- Nitrogen is not directly reactive at the wavelength (MgF_2 window cut-on of 115 nm) used in our experiments because its absorption in the vacuum ultraviolet (VUV) starts at $\lambda < 100$ nm.
- N_2-chemistry will not takes place in H_2 dominated exoplanet atmospheres at altitudes where photons < 100 nm do not penetrate. It is likely that direct N_2-chemistry can only be activated in the highest atmospheric layers (i.e. mesosphere and thermosphere) where photons with sufficient energy are present to directly dissociate or ionize N_2.

Results: Equilibrium Mixing in Warm CH_4-rich H_2-dominated Exoplanet Atmospheres



H_2/CH_4 (690:1) warm-exoplanet atmosphere simulations. Bottom: equilibrated at 295 K; Top: UV-irradiation with Ly-alpha (121.6 nm) at 295 K that results in the formation of C_2H_2 and C_2H_6 as well as other molecules (to be studied in detail)

- **Goal:** We conducted preliminary experiments to explore chemistry and aerosol formation in warm (300-900 K) H_2 dominated exoplanet atmospheres with CH_4 as the main carbon carrier
- **Results:** Photochemistry led to a consumption of CH_4 and a significant formation of simple hydrocarbons: acetylene (C_2H_2) and ethane (C_2H_6). These products were not formed with the rmochemistry only.
- **Conclusion:** Photochemistry is very efficient in CH_4-rich exoplanet atmospheres that may lead to the formation of complex organic molecules, including aerosol. Work is ongoing to extend these experiments to higher temperature: 473 K, 673 K, and 873 K.

Publications

A. Fleury, et al., (2020), “Influence of C/O Ratio on Chemistry in Hot Jupiter Exoplanet Atmospheres”, The Astrophysical Journal, 899:147, (10pp.)

B. Fleury, et al., (2019), “Photochemistry in Hot H_2-dominated Exoplanet Atmospheres”, The Astrophysical Journal, 871:158, (14pp.)