Astro2010 Science White Paper: Exoplanet Molecular Spectroscopy

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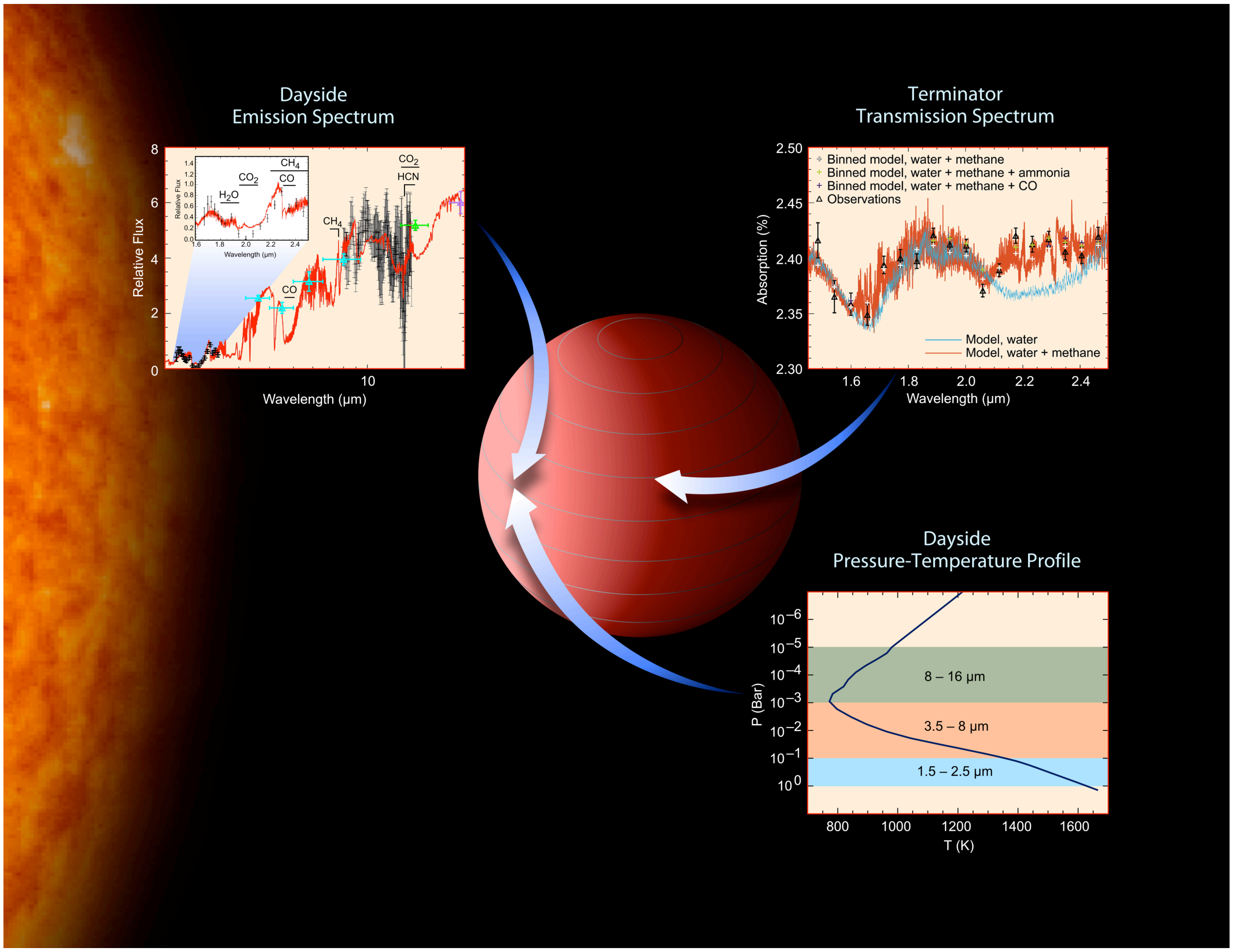

Understanding composition, chemistry and dynamics in exoplanet atmospheres.

Abstract

Detection of molecules in an exoplanet atmosphere, a long-term scientific and technology program goal, has recently been demonstrated with the Hubble and Spitzer Space Telescopes for a transiting hot-Jupiter exoplanet. Because molecules serve as probes of an exoplanet atmosphere and allow us to answer fundamental questions about the temperature, composition, and chemistry, molecular spectroscopy is emerging as the most powerful tool available for characterizing exoplanet atmospheres. To date, water (H_2O), methane (CH_4), carbon dioxide (CO_2), and carbon monoxide (CO) have been detected via infrared spectroscopy; several of these molecules have potential prebiotic or biological significance, and thus their detection in a hot-Jupiter atmosphere is an important step towards the eventual characterization of habitable-zone planets, including searching for biomarkers. The detection of molecules in both primary and secondary eclipses (which probe the terminator region and the dayside, respectively) has allowed some degree of longitudinal localization of knowledge about the atmospheric conditions, while the detection of CO_2 has raised the possibility that non-equilibrium chemistry may play a significant role in establishing the atmospheric radiation balance. By recovering the pressure-temperature profile and determining whether the atmospheres are in radiative equilibrium, we can estimate the radiative-forcing of the atmospheric dynamics and the redistribution of heat. The emergence of detectable spectroscopic variability presents both an opportunity and a challenge that has important ramifications for any future exoplanet characterization mission. ***Perhaps the most surprising aspect of the recent results is the realization that today, with existing instruments, we can begin to answer the detailed questions about exoplanets that are only possible with molecular spectroscopy.*** The recent results prove beyond doubt that (1) molecular spectroscopy is an essential tool for characterizing the composition, structure, and dynamics of exoplanets and (2) that there are near-term, modest investments that would dramatically expand our understanding of exoplanets while producing high-impact science results.

Introduction

Molecules have recently been detected via infrared spectroscopy in an exoplanet atmosphere; this was accomplished using the “combined light” method in which temporal changes (e.g. during a primary or secondary eclipse) are used to infer properties of the exoplanet atmosphere. With the benefit of hindsight, we now understand that exoplanet molecular spectroscopy has been feasible with both Spitzer and Hubble for several years. However, the calibration requirements for a “molecular abundance grade” spectrum of an exoplanet are substantial, and it has taken the leading groups some time to develop adequate calibration methods. To give an approximate sense of the difficulty of the problem, for molecular spectroscopy in a hot-Jupiter type planet, one needs to obtain a dynamic range of ~1000 in the Spitzer bands and a dynamic range ~10,000 in the near-infrared bands over an observational time span of several hours. Given the bright host stars of many transiting planets, the desired dynamic range limits (set by photon, detector, and background noise contributions) are frequently higher, but the measurement dynamic range is limited by systematic errors (e.g. telescope pointing). Current calibration methods identify and remove instrument systematic errors; this has been highly successful, and these techniques now permit measurements that are very close to the photon-noise limit. Development of these calibration methods is an ongoing process, and it is likely that both a nightside spectrum and a spectrum of a non-transiting planet will be demonstrated in the near future.

Exoplanet molecular spectroscopy can answer fundamental questions concerning the nature of a planet's atmosphere and, by allowing the determination of elemental abundances, it can constrain the formation/evolution history. In the case of transiting planets, the primary eclipse sequence is used to obtain a transmission spectrum, while the secondary eclipse is used to obtain a dayside emission spectrum (Fig. 1); the light-curve can be used to obtain the emission spectra for disk-averaged views around the planet. The emission spectrum is sometimes termed an "emergent" spectrum because molecular signatures can appear either in absorption, emission, or both, depending on the shape of the pressure-temperature profile and the molecular vertical mixing ratio. This complexity, together with the potential for overlapping molecular bands, means that the spectra can be understood only through comparing them to detailed atmospheric models. These models depend on accurate molecular opacity data, and existing exoplanet spectra are reaching the limitations of our current knowledge of opacities. Spectral retrieval methods and forward models are used to infer the presence and abundance of specific molecules and, in the case of an emission spectrum, the pressure-temperature profile; this can lead to a natural ambiguity (in the case of an emission spectrum) between composition and temperature. Once the composition and temperature structure has been determined, knowledge of the atmospheric chemistry is inferred from the abundance estimates and vertical mixing ratios of individual molecules; for example, if the mixing ratio of CO_2 is higher than would be expected from purely equilibrium chemistry, a non-equilibrium chemistry mechanism (such as photochemistry) may be needed to explain the additional CO_2.

Science

Exoplanet molecular spectroscopy has exceptional breadth and depth in terms of the questions that can be addressed. In the case of transiting planets, the spectra of different regions of the atmosphere can be obtained (via primary and secondary eclipse today – see Fig. 1); this allows the composition of the terminator region to be compared to the hotter dayside region. Where Hubble and Spitzer have both observed the same exoplanet, one can construct a composite spectrum with broad spectral coverage (see Fig 2.); this type of spectrum probes the atmosphere over a wide range of pressures, provides powerful constraints for models, and allows some molecules to be detected in multiple bands. Extending these kinds of measurement to non-transiting planets should be possible given stable, well-calibrated, space-based instruments; light-curve photometry of a non-transiting planet has already been demonstrated with Spitzer (Harrington et al. 2006). While extending these techniques to non-transiting planets provides a significant increase in the number of possible targets, transiting planets provide special opportunities for characterization. For example, the secondary eclipse ingress/egress portions of a transiting light curve can be used to search for spatial structure (e.g. detecting a spectral difference due to the presence of the hot-spot displaced by zonal winds). Temporal variability has been detected (see Fig. 2); whether this is due primarily to changes in temperature or changes in composition is unknown. However, the emergence of significant variability raises questions about the validity of the "composite spectrum". As we look forward to characterizing exoplanets via molecular spectroscopy in the 2010-2020 decade, we identify the following **key questions:**

- What is the atmospheric composition and temperature structure?
- Does non-equilibrium chemistry play a significant role in determining atmospheric composition?
- What significant dynamical processes are present, and do they influence atmospheric composition and chemistry through mechanisms such as quenching or vertical transport?
- What is the extent and origin of temporal and spatial variability?
- What are the elemental abundances, and how do they constrain the formation and evolution histories?
- What are the conditions on habitable-zone “super-Earths,” and is there potential for generating and sustaining life?
- What do exoplanets reveal about the origin, evolution, and destiny of the planets in our solar system?

These key questions can be answered during the next decade using existing technology and methods. Answering the questions broadly for a large sample of exoplanets will require a dedicated mission; a dedicated mission could characterize non-transiting exoplanets, including those orbiting M dwarfs. Significant scientific progress with Hubble and James Webb is possible, but reliance on these observatories will limit exoplanet characterization for two reasons. First, both are general-purpose observatories and are not designed for high-stability measurements; this will almost certainly limit these instruments primarily to transit events and make observations of non-transiting planets a rare event because large amounts of calibration time will be required. Second, neither Hubble nor James Webb will be able to obtain broad spectral coverage as simultaneous measurements (e.g. covering just the mid-IR with James Webb requires four different observing configurations). If variability can significantly influence our understanding of the atmospheric conditions for a large number of exoplanets, only simultaneous measurements over a wide spectral band will provide a representative picture of the atmosphere.

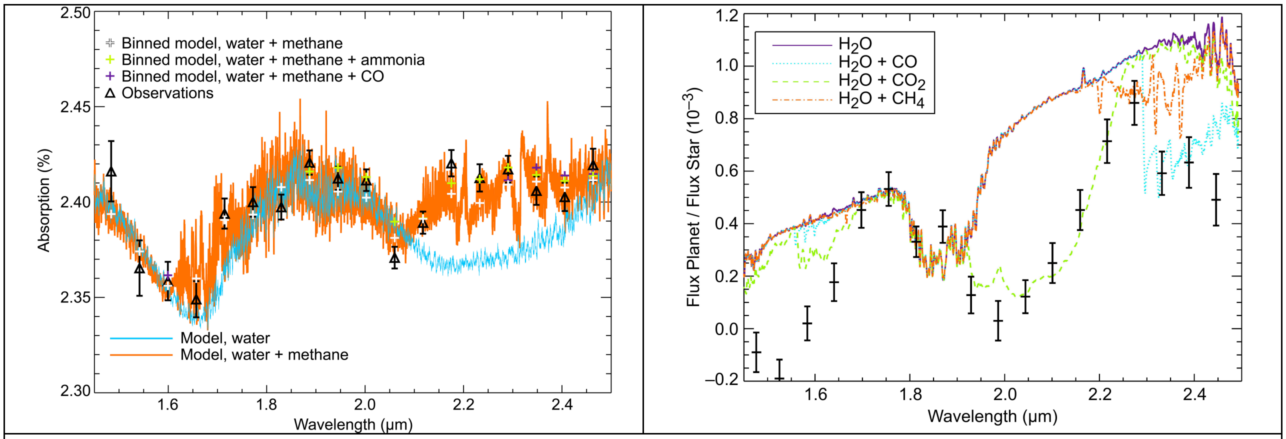

Fig. 1 **left:** A transmission spectrum (primary eclipse) of the terminator region of HD 189733b, showing the presence of water and methane (Swain et al. 2008). **right:** An emission spectrum (secondary eclipse) of the dayside region of HD 189733b, showing the presence of water, carbon dioxide, and carbon monoxide (Swain et al. 2009). Taken together, these spectra probe how the atmosphere changes from the hotter dayside to the cooler terminator regions. These results show the maturity of exoplanet molecular spectroscopy. There are observations for at least four additional exoplanets in the Hubble archive where we expect to detect molecules via infrared spectroscopy.

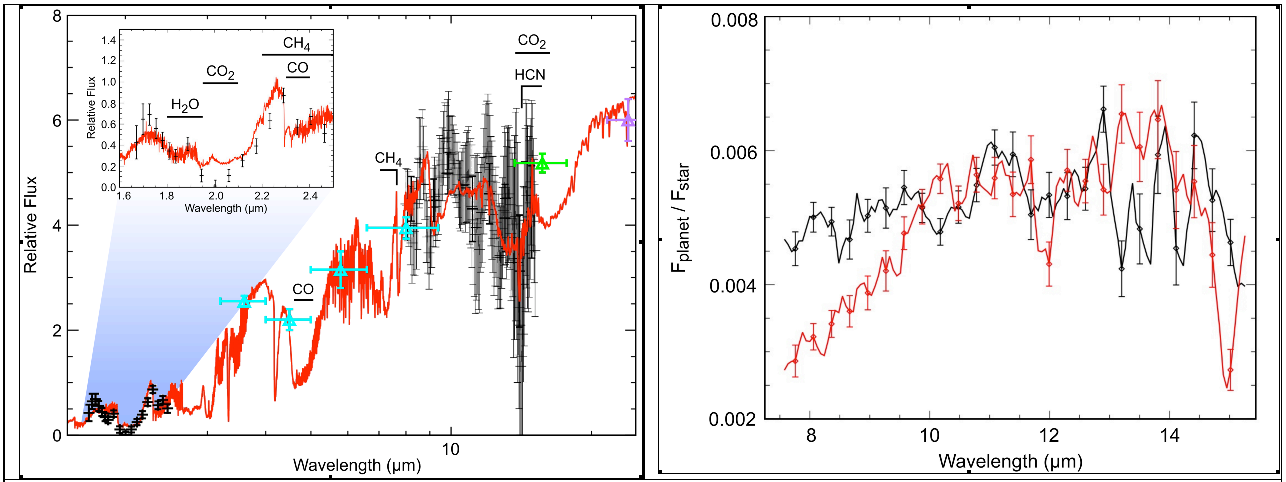

Fig. 2 **left:** A composite Hubble/Spitzer dayside spectrum for the hot-Jupiter HD 189733b, together with Spitzer photometry data and a model by Tinetti. The broad spectral coverage shown here probes the atmosphere from about 1 bar to about 10^{-6} bar and provides powerful constraints on the dayside pressure-temperature profile and atmospheric composition. The near-IR spectrum is from HST (Swain et al. 2009), the mid-infrared spectrum is based on data obtained by Grillmair et al. (2007); the light blue, green, and purple photometry points are from Charbonneau et al. (2008), and Deming et al. (2006) respectively. **right**: an analysis of data obtained by Grillmair et al. (2008) showing two spectra, taken 4.4 days apart, with significant differences around 8 μm; this raises significant questions about the validity of composite spectra.

Needed Data and Mission Requirements

The data needed to answer the detailed questions of exoplanet characterization are relatively simple to obtain. We need:

1. **Broad, instantaneous spectral coverage** from approximately the visible to the mid-infrared where the data are obtained simultaneously. This enables resolving the temperature/composition ambiguity in an emission spectrum.
2. **Excellent intrinsic stability**. This enables measurements of non-transiting planets and atmospheric variability.

The spectral resolution need not be high – a spectral resolution of a few hundred is adequate. The measurements should be photon noise limited (or background noise at the longest wavelengths); this implies stable, purpose-built instruments operating from space. If the combined-light method is used for obtaining the spectra, a ~1.5 m telescope enables dramatic scientific progress and is capable of probing super-Earth-type planets (both transiting and non-transiting) in the habitable zone around nearby M dwarfs. Regular calibrator measurements (as was done with the IRS instrument on Spitzer) make it possible to extend the photon-noise-limited calibration period beyond a single source; this is crucial for spectroscopy of non-transiting planets or for understanding long-term variability. To amplify the previous points, we are including a few "lessons learned" based on the recent results:

- **Small telescopes "advantage":** Small telescopes (~ 1m) have a large discovery space for exoplanet spectroscopy using the combined-light technique because the observable scales as the square root of the number of photons in the photon-noise limit. Thus, everything else being constant, larger telescopes have a sensitivity advantage that scales as diameter, not area. To illustrate the potential for small telescopes, the Hubble detection CH_4 required a low duty cycle, which effectively reduced the Hubble telescope aperture to ~ 70 cm.
- **New technology not required**: Exoplanet molecular spectroscopy does not require new technology. The "combined-light" method is capable of providing molecular-abundance-grade spectroscopy of habitable-zone super-Earths' and non-transiting planets.
- **Stability is crucial:** Achieving photon-noise-limited calibrated stability requires removing instrument systematics. Although decorrelation methods have been used with great success with Hubble (where a spectro-photometric dynamic range of 20,000:1 has been demonstrated), a spectrometer *with no moving parts* (like Spitzer's Infrared Spectrograph) would dramatically enhance instrument stability and would make routine spectroscopy of non-transiting planets possible.
- **Broad spectral coverage essential:** The interpretation of an exoplanet emission spectrum, which is the only kind of spectrum that can be obtained from a non-transiting planet, benefits enormously from spectral coverage from near visible to mid-infrared wavelengths. This is because there is a natural ambiguity between the shape of the vertical temperature profile and atmospheric composition. For an emission spectrum, the shape of the temperature profile is crucial; an approximately isothermal temperature profile hides the presence of molecules, a decreasing T-profile shows absorption features, while an increasing T-profile shows emission features. Different wavelengths probe the atmosphere at different levels, and thus broad spectral coverage provides the only observational method for resolving the temperature-composition ambiguity.
- **Simultaneous measurements:** The detection of significant variability has profound implications for exoplanet spectroscopy. Currently, it is common practice to "assemble" a composite exoplanet spectrum (or SED in the case of photometry) using all available measurements. As these observations cannot be obtained at the same time (either using current instrumentation or with JWST) the assembled spectrum is only representative if approximate time-stationarity can be assumed over the period of the observations.

The calibration technology for the "combined-light" method, the approach of determining the planet emission/absorption by taking temporal differences of spatially unresolved measurements, is still in a rapid development phase. Although ground-based measurements will never match space-based measurements in terms of wavelength coverage or absolute calibrated stability, it is possible that calibration methods will be developed for ground-based telescopes, permitting molecular spectroscopy of exoplanet atmospheres. This is especially likely for the detection of narrow molecular features where it may be possible, in some atmospheric bands, to achieve results comparable to James Webb.

Recommendations

Spectroscopy of molecules in exoplanet atmospheres is poised to make a major impact on the field of exoplanet characterization over the next few years. Given the rapid rate of current progress and exceptional scientific potential, we urge the committee to consider the following recommendations.

- Recognize that exoplanet molecular spectroscopy will have a central role for characterizing exoplanets, especially in determining the conditions, composition, chemistry, and likely formation histories. Although general-purpose observatories such as Hubble and James Webb may make important discoveries, they cannot match the breadth and depth of exoplanet characterization science possible with a purpose-built mission.

- Recommend that a purpose-built, modest cost (~300 to 500 M) mission for exoplanet spectroscopy be considered for the 2010-2020 timeframe. Instead of focusing on a technique, this mission should be science driven in terms of the number/kind of exoplanets observable together with a strong emphasis on broad and simultaneous wavelength coverage to provide the strongest possible science return.

- Advocate that the NASA sub-orbital program aggressively undertake the modest (~ 2 – 3 M) technology development effort for ~ 1 arcsec telescope pointing that would allow exoplanet molecular spectroscopy from a balloon-borne platform. There is enormous scientific potential for sub-orbital exoplanet spectroscopy in the 0.5 – 5 µm range.

- Encourage ground-based telescopes to continue to make high-risk/high-return time awards to continue the development of high-dynamic-range spectroscopy observing techniques. It is possible, perhaps even likely, that calibration methods will be developed allowing ground-based telescopes to have a significant scientific impact in the area of exoplanet molecular spectroscopy.

- Insist that priority be given to obtaining better molecular line lists via laboratory spectroscopy and theoretical calculations. Our ability to interpret exoplanet spectra is completely dependent on quality models that depend critically on accurate opacity data.

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