New Statistical Measures of Atmospheric Disequilibria and Implications for Detecting Life and Technology

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Abstract

Exoplanets exhibit properties suggestive of a diversity of worlds far exceeding that observed within our own solar system. This diversity, combined with limited data, poses challenges for future exoplanet characterization, especially regarding life detection: not only is the diversity planets unprecedented, but the low resolution and s/n data available to current and near-future technology demand we improve our ability to infer properties of planetary atmospheres, surfaces and potential signs of life from very little data. For this reason, recent consensus recommendations from both within the exoplanet science community, and without, are directing the field to move from searching from specific products of life to developing probabilistic frameworks for inferring the presence of life that encompass entire planetary systems. Here, we demonstrate a new framework based on statistical characterization of planetary atmospheric chemistries with the goal to provide the quantitative tools required by this approach. We validate these tools against current observational constraints available for Jovian worlds by constructing chemical reaction networks (CRNs) from the atmospheres of hot jupiters simulated over a wide range of temperatures and metallicities using VULCAN. For each model, we calculated measures of the CRN topology and more traditional measures of disequilbrium. To model the uncertainty in observations, these properties were then used as the basis for an interpolation function, which was then fed a series of 10,000 point Gaussian distributions of possible initial conditions to simulate the likelihood distribution of possible atmospheric models centered around a specific observable such as T or metallicity. We present results demonstrating how our multivariate, statistical approach permits quantifying distance from disequilibrium in Jovian atmospheres. We discuss implications for inferring the presence of life as a driver of atmospheric disequilibrium on terrestrial worlds, and how technologically produced molecules could influence CRN topology.

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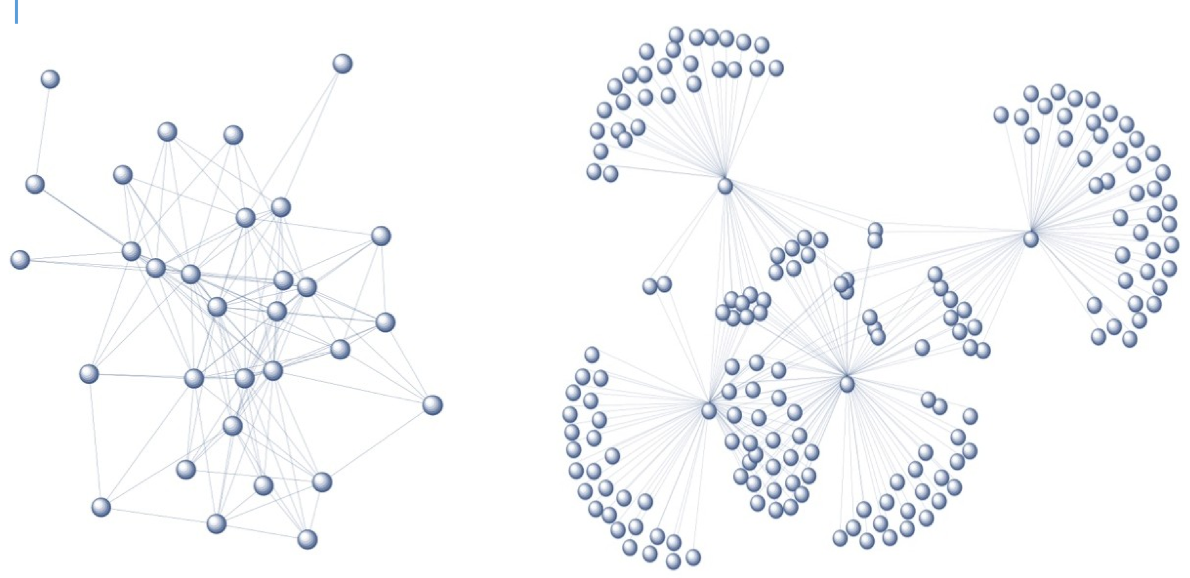
Introduction

As spectral analysis of the atmospheres of Earth-like exoplanets becomes technologically possible, the need for more reliable biosignature detection grows—especially in light of the vast diversity of worlds, risk of false positives[1] and the possibility of exotic biochemistry[2]. One possible solution is network theory: chemical reaction networks—where molecules are represented by nodes, and reactants and products of reactions are connected by edge—have noticeably different topology when arising from biology[3], and this appears to carry over to atmospheres, as well[4]



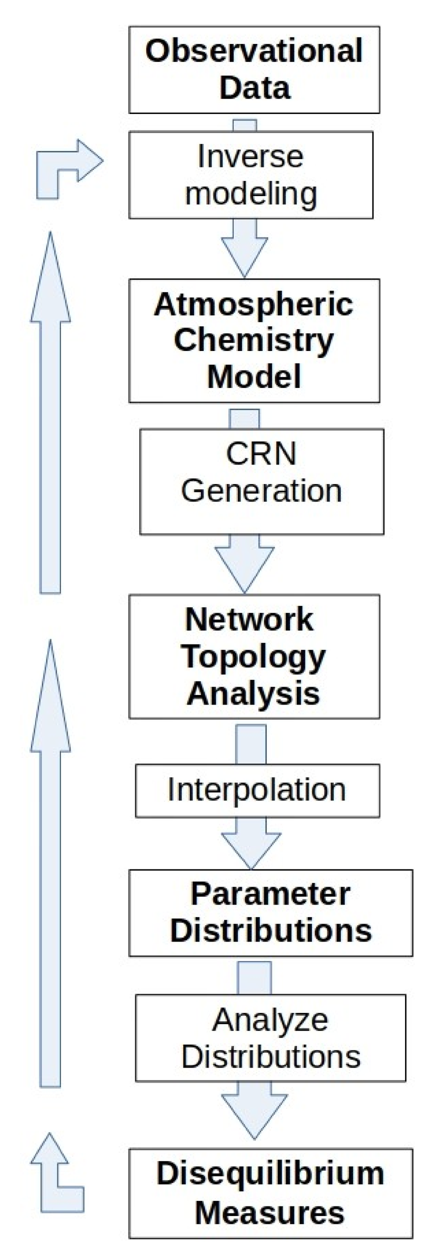
CRNs for Mars and Earth, after[5]

Methodology

Hot jupiters used since they're simpler and well characterized, both in terms of observational data and chemical kinetics. Simulated hot jupiter atmospheres were constructed using VULCAN over wide range of initial conditions[5]. The reaction list and kinetics were then extracted from these model results, and used to construct the chemical reaction networks.

The parameters of these networks--such as mean degree, average shortest path length, and average clustering coefficient--were measured, and used as the basis for an interpolation function. This function can be fed a 10,000 point Gaussian distribution of initial conditions (in terms of temperature, pressure, and metallicity), and will return the corresponding network measurements. To understand how the network measurements changed as function of distance from chemical equilibrium, vertical mixing coefficient (Kzz) was used as a proxy for level of disequilibrium, with Kzz = 0 being at equilibrium. The resulting distributions of network measurements were then compared statistically using the Kolmogorov-Smirnoff test.

Additionally, the sensitivity to the network analysis was tested by feeding in distributions that incorporated a range of uncertainties in the initial temperature value,ranging from +/- 50K all the way up to +/- 1000K.



.Schematic of the analysis pipeline used for the network topology approach.

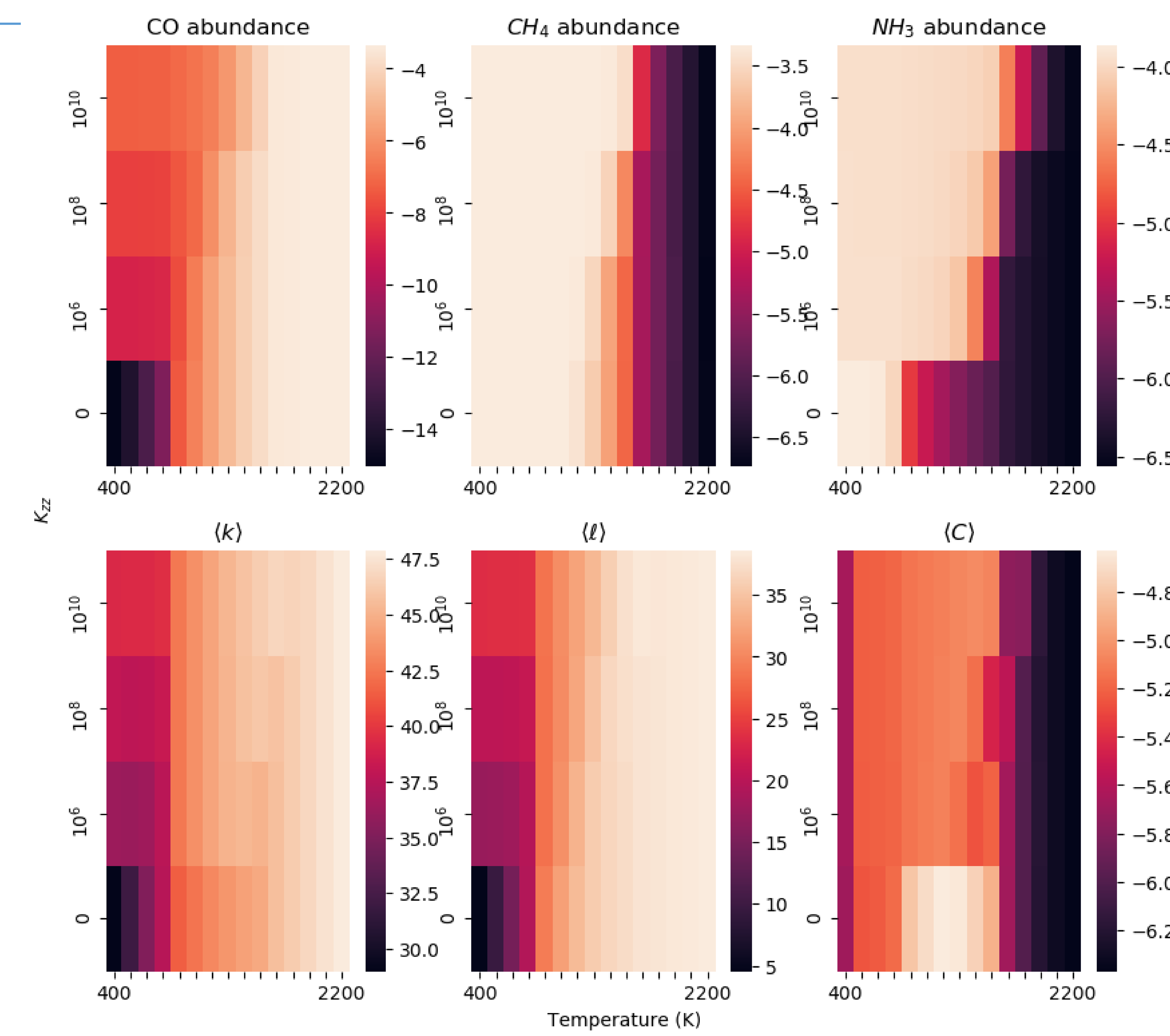
Results

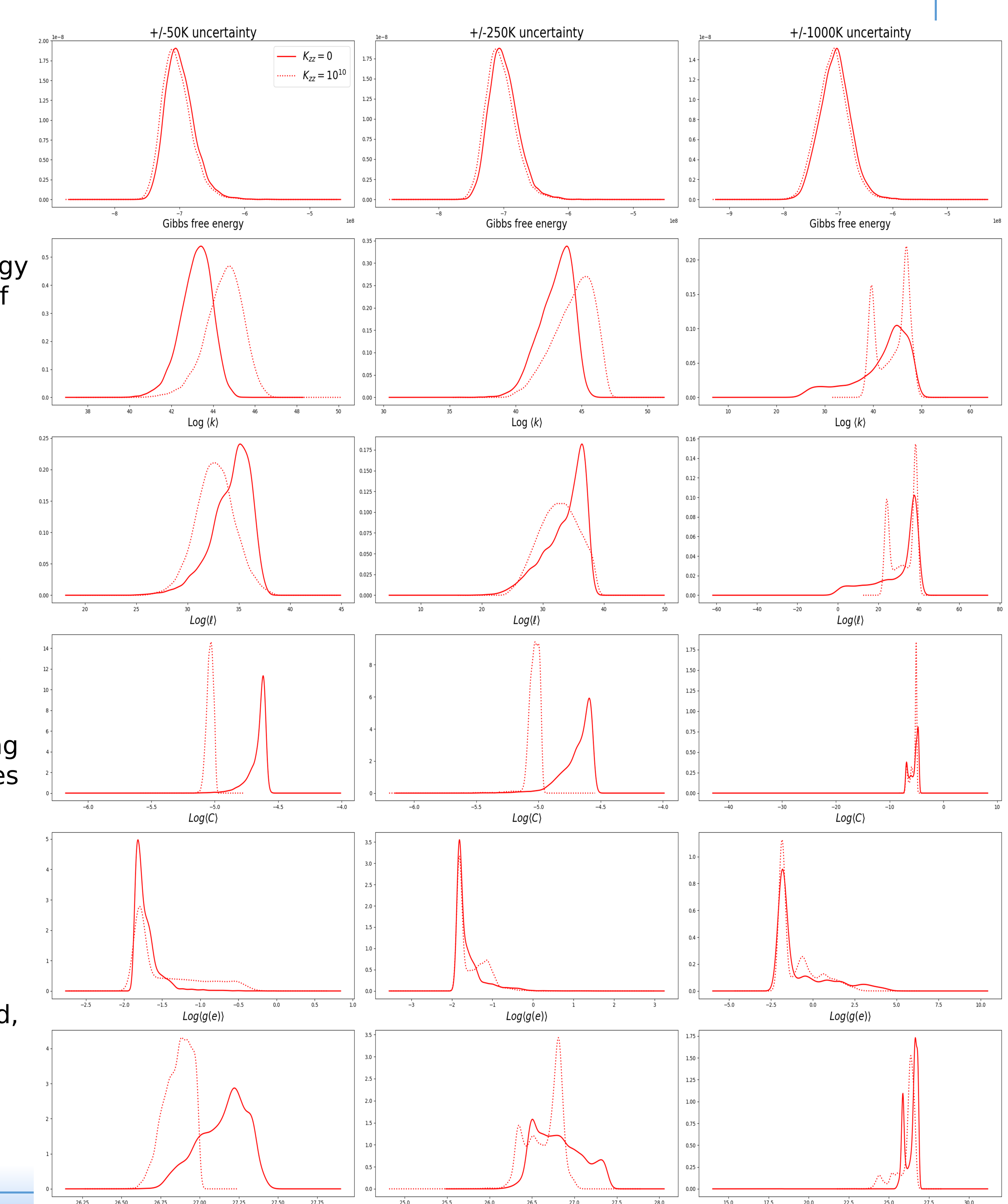
The resulting distributions of network parameters appear to be statistically distinguishable based on the distance from equilibrium. In particular, mean degree and average shortest path length can indicate the distance from equilibrium, while average clustering coefficient lacks that sensitivity, it has high utility at determining if a network is at equilibrium or disequilibrium. Furthermore, preliminary results suggest that it may be possible to infer network parameters from observable trace gases, with CO appearing to correlate with mean degree and average shortest path length.

The ability to determine the level of disequilibrium also appears to be resilient in the face of uncertainty in initial conditions. The distributions were still distinguishable at temperature uncertainties of +/- 250K and above.

Above, right: Heat maps of network parameters and species abundance as a function of temperature and vertical mixing coefficent.

Right:Distributions of network parameters and molecular abundances, interpolated from a 10,000 point normal distribution of initial conditions centered on a temperature of 1200K, at vertical mixing coefficients of 0 and 1010, and uncertainties in temperature of 50K, 250K, and 1000K.





Discussion

If network measures can be inferred from observable abundances of species such as CO, then our methodology represents a new and useful technique in the tool box of exoplanet science. From network measures, other properties, such as level of disequilibrium can then potentially be inferred, expanding our understanding of the system-level behavior of planetary atmospheres.

While our results demonstrate that the level of disequilibrium in an atmosphere is measurable using topological measurements of atmospheric chemical reaction networks, it remains to be seen if these measurements can also inform us of the type of disequilibrium, in terms of the major physical processes driving the atmosphere away from equilbrium. If this proves to be the case, then, as hoped, network measurements could provide invaluable in differentiating biologically-driven disequilibria in planetary atmospheres from abiotic disequilibria. As such, our next goal is to apply these methods to terrestrial planets with and without biospheres.

Furthermore, it is possible the that the presence of industrial compounds may alter the topology of atmospheric CRNs, While further investigation is needed, this

Conclusion

IOur results show that the topology of atmospheric chemical reaction networks can successfully distinguish between disequilibria in the atmosphere of hot jupiters. This new technique offers exciting have opportunities to expand our ability to more fully understand the atmospheres of exoplanets, and potentially better detect the presence of life on terrestrial exoplanets.

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