Spectra as windows into exoplanet atmospheres

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Understanding a planet’s atmosphere is a necessary condition for understanding not only the planet itself, but also its formation, structure, evolution, and habitability. This requirement puts a premium on obtaining spectra and developing credible interpretative tools with which to retrieve vital planetary information. However, for exoplanets, these twin goals are far from being realized. In this paper, I provide a personal perspective on exoplanet theory and remote sensing via photometry and low-resolution spectroscopy. Although not a review in any sense, this paper highlights the limitations in our knowledge of compositions, thermal profiles, and the effects of stellar irradiation, focusing on, but not restricted to, transiting giant planets. I suggest that the true function of the recent past of exoplanet atmospheric research has been not to constrain planet properties for all time, but to train a new generation of scientists who, by rapid trial and error, are fast establishing a solid future foundation for a robust science of exoplanets.

The study of exoplanets has increased exponentially since 1995, a trend that in the short term shows no signs of abating. Astronomers have discovered and provisionally studied more than a hundred times more planets outside the solar system than in it. Statistical and orbital distributions of planets across their broad mass and radius continuum, including terrestrial planets/Earths, “super-Earths,” “Neptunes,” and giants, are emerging at a rapid pace.

However, understanding its atmosphere is a necessary condition for understanding not only the planet itself, but also its formation, evolution, and (where relevant) habitability, and this goal is far from being realized. Despite multiple ground- and space-based campaigns to characterize their thermal, compositional, and circulation patterns (mostly for transiting giant planets), the data gleaned to date have (with very few exceptions) been of marginal utility. The reason is that most of the data are low-resolution photometry at a few broad bands that retain major systematic uncertainties and large error bars. Moreover, the theory of their atmospheres has yet to converge to a robust and credible interpretive tool. The upshot of imperfect theory in support of imprecise data has been ambiguity and, at times, dubious retrievals. To be fair, (i) telescope assets are being used with great effort at (and, sometimes, beyond) the limits of their designs; and (ii) most planet/star contrast ratios are dauntingly small. As a consequence, the number of hard facts obtained over the last 10 y concerning exoplanet atmospheres is small and by no means commensurate with the effort expended.

An important aspect of exoplanets that makes their characterization an extraordinary challenge is that planets are not stars. They have character and greater complexity. A star’s major properties are determined once its mass and metallicity are known. Most stars have atmospheres of atoms and their ions. However, planets have molecular atmospheres with elemental compositions that bespeak their formation, accretional, and (where apt) geophysical histories. Anisotropic stellar irradiation, clouds, and rotation can break planetary symmetry severely, with the clouds themselves introducing multiple degrees of complexity, still unresolved even for our Earth. Molecules have much more complicated spectra than atoms, with a hundred to a thousand times more lines, and irradiated objects experience complicated photochemistry in their upper reaches. It took stellar atmospheres ~100 y to evolve as a discipline, and it still is challenged by uncertainties in oscillator strengths and issues with Boltzmann and thermal equilibrium. Furthermore, the spectroscopic databases for molecules (1), particularly at the high temperatures (500–3,500 K) experienced by close-in transiting planets, are much more incomplete than those for atoms, and the relevant collisional excitation rates are all but nonexistent. Therefore, it can reasonably be suggested that the necessary theory for detailed studies of exoplanets is in its early infancy.

One might have thought that the study of our solar system had prepared us for exoplanetology, and this expectation is in part true. The solar system has been a great, perhaps necessary, teacher. However, most solar-system spectra are angularly resolved with a long time baseline and high signal-to-noise. Exoplanets will be point sources for the foreseeable future, and signal-to-noise will remain an issue. Perhaps more importantly, much solar-system research is conducted by probes in situ or in close orbit, with an array of instruments for direct determination of, for example, composition, surface morphologies, B-fields, charged-particle environments, and gravitational moments. Masses and radii can be exquisitely measured. Orbits are known to standard-setting precision. Moreover, when comparing measured with theoretical spectra, the latter are often informed by direct compositional knowledge.

The exoplanet scientific landscape will be more challenging. Exoplanet science is an observational science that must rely on the astronomical tools of remote spectroscopic sensing to infer the physical properties of individual planets. Therefore, there is a premium on obtaining spectra and developing interpretative toolkits in the tradition of classical astronomy, without the luxury of direct, in situ probes. Therefore, although solar-system variety will continue to inform exoplanet thinking and motivate many calculations,

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the methodology of solar-system research is not the best model for conducting exoplanet research. Rather, we must determine the most robust and informative methods with which to interpret remote spectra and perform credible spectral retrievals of physical properties. Therefore, the science of exoplanet characterization is better viewed as a science of spectral diagnostics, and developing this art should be our future focus.

To date, planets that transit their stars due to the chance orientation of their orbit planes have provided some of the best constraints on hot exoplanet atmospheres. The variation of transit depth and, thus, apparent planet radius \((R_p)\), with wavelength \((\lambda)\) is an ersatz spectrum and can be used to infer the presence of chemical species with the corresponding cross-sections. Water, sodium, and potassium have been unambiguously detected by this means. Approximately 180° out of phase with the primary transit, when the same planet is eclipsed by its star, the difference between the summed light of planet and star and that of the star alone reveals the planet’s light. This is the secondary eclipse, and such measurements, when performed as a function of wavelength, render the planet’s emission spectrum; measurements taken between primary and secondary eclipse provide phase light curves. The secondary eclipse planet/star flux ratio is lower than the transit depth by \(\sim \left(\frac{R_p}{R_*}\right)^2\), where \(a\) is the orbital semimajor axis and \(R_*\) is the stellar radius. This ratio can be a factor of one tenth.

The transit and radial-velocity techniques with which most exoplanets have been found select for those in tight orbits. Tight orbits at the distances of stars in the solar neighborhood subtend very small angles (microarcseconds to 10s of milliarcseconds), and such angular proximity to a bright primary star mitigates against direct planet detection, imaging, or characterization. For wider separations of tens of milliarcseconds to arcseconds, the resulting contrast ratios for terrestrial and giant planets in the optical of \(10^{-10} – 10^{-6}\), and in the near- to mid-infrared of \(10^{-8} – 10^{-4}\), are quite challenging (2). However, such direct planet imaging is not only now conceivable, but has been accomplished. Four giant exoplanets around HR 8799 (3, 4) and one around \(\beta\) Pictoris (5), with masses of \(\sim 5-15\) Jupiter masses \((M_J)\) and angular separations between \(0.3\) and \(\sim 1.5\) arcseconds, have recently been found.

As direct imaging techniques mature, more and smaller directly imaged planets will be discovered. However, as articulated earlier, it is only with well-calibrated spectral measurements at useful resolutions that we can hope to characterize wide-separation exoplanet atmospheres robustly. Polarization measurements will also have an important diagnostic role, particularly for cloudy atmospheres, which at quadrature should be polarized in the optical to tens of percent.

Currently, due to their larger size, the photometric and spectroscopic techniques mentioned above have been applied mostly to giant exoplanets. Earths are ten times smaller in radius and one hundred times smaller in mass. Therefore, while astronomers and theorists hone their skills on the giant exoplanets, fascinating in their own right, these giants are also serving as stepping stones to the smaller planets, in anticipation of future routine campaigns to characterize them as well. Therefore, I concentrate in this article on the giant population, but all of the basic methodologies used in their study can be translated bodily to the investigation of smaller “exo-Neptunes,” terrestrial planets/Earth, and super-Earths.

A comprehensive review would necessitate more pages than this more synoptic and summary opinion piece can provide, but, for those readers interested in an expanded treatment, there are numerous archival papers from which to draw. They cover topics such as the general theory of giant exoplanets (6), giant planet atmospheres (7–9), analytic atmosphere theory (10, 11), opacities (1, 12, 13), thermochemistry and elemental abundances (14–17), the chemistry of hot Earth atmospheres (18), albedos (19–22), giant planet models at wide separations (2, 4, 23), phase functions (24, 25), irradiated atmospheres and inversions (10), basic transit theory (26, 27), transit spectra for Earths (28), emission spectra of Earth-like planets (29), transit spectra of Earth-like planets (30), habitable zones (31), theoretical exo-Neptune spectra (32), planet polarization (33), and clouds and hazes (34–36). In this paper, I refer preferentially to my own work but suggest that the general conclusions arrived at here have broad applicability.

**Compositions and Opacities**

The variety of compositions found in the gaseous atmospheres of solar-system planets suggests that the corresponding variety for exoplanet atmospheres must be at least as broad. Generally lower in temperature than stellar atmospheres, planetary atmospheres are dominated by molecules. Although fractionation and differentiation processes are no doubt involved in their formation, their elemental abundances should reflect the most abundant elements in the Universe. For giant exoplanets (like brown dwarfs\(^1\)), this fact means \(\mathrm{H}_2, \mathrm{He}, \mathrm{H}_2\mathrm{O}, \mathrm{CO}, \mathrm{CH}_4, \mathrm{NH}_3, \mathrm{PH}_3, \mathrm{H}_2\mathrm{S}, \mathrm{Na}, \mathrm{K}\) predominate, with most of the metals sequestered in refractories at depths not easily penetrated spectroscopically. However, titanium and vanadium oxides (\(\mathrm{TiO}\) and \(\mathrm{VO}\)), identified in cool-star and hot-brown-dwarf atmospheres, have been suggested to reside in quantity in the upper atmospheres of some hot Jupiters to heat them by absorption in the optical and create inversions (37). However, \(\mathrm{TiO}\) and \(\mathrm{VO}\) too are likely condensed out (38). Because such inversions require an optical absorber at altitude, what this absorber is, molecule or absorbing haze/cloud, remains a major mystery (39).

For terrestrial planets, the molecules \(\mathrm{N}_2, \mathrm{CO}_2, \mathrm{O}_2, \mathrm{O}_3, \mathrm{N}_2\mathrm{O}, \) and \(\mathrm{HNO}_3\) must be added to the list above, with \(\mathrm{O}_2\) (ozone), and \(\mathrm{N}_2\mathrm{O}\) considered biosignatures, along with the “chlorophyll red edge” (or its generalization). Many other compounds could be envisioned, and there is added complexity to terrestrial planet atmospheres due to atmosphere–surface interactions that are so important, for example, for our Earth. The major constituents of Neptune atmospheres are likely closer to those of giants, but the relative abundances in any exoplanet atmosphere must be considered as yet poorly constrained. Constraining these abundances is a goal, however, and one does so by identifying their unique signatures in measured atmospheric spectra and comparing the observed spectrum in its totality with spectral models. This extraction is “retrieval,” which at a minimum should also yield temperatures and temperature profiles. Because many parameters characterize exoplanet atmospheres (e.g., species, abundances, temperatures, spatial distributions, gravities, haze, and cloud layers), the low information content of few-band photometry is not adequate to avoid the pitfalls of parameter degeneracy. With too few data points in pursuit of too many

\(^1\)It is likely that the brown dwarf and giant planet mass functions overlap so that a tentative assignment is generally premature. A flexible and open-minded philosophy toward nomenclature is then best (8), which more data will progressively guide toward a more reasonable classification scheme. I do note, however, that much recent data for giant planets has been for the close-in transiting subset. For this subset, the fact that these planets are irradiated, whereas free-floating brown dwarfs are not, significantly alters the colors and atmospheric characteristics of the former, when they might otherwise have had spectra like isolated low-mass brown dwarfs (Fig. S1). One can speculate that, barring the irradiation difference, differences in atmospheric abundances, rotation rates, and orbital regimes might eventually distinguish brown dwarfs from giant planets (at least statistically).
expected to be important in giant exoplanet atmospheres (for which we currently have the most data) but are also likely important (to varying degrees) in terrestrial, super-Earth, and exo-Neptune atmospheres. In Fig. 1A, we focus on the 1.0- to 5.0-μm range and include the TiO, Na, and K opacities so prominent in the optical whereas the plot in Fig. 1B extends to 15 μm to reveal the behavior in the midinfrared and the signature nature of CO₂ at ~15 μm.

As indicated in Fig. 1, strong water features are ubiquitous and are found at (roughly) 0.94, 1.0, 1.2, 1.4, 1.9, 2.6, and 5–7 μm, defining between them the I, Z, J, H, K, and M bands through which much of ground-based near-infrared astronomy is conducted. Methane has important features at 0.89, 1.0, 1.17, 1.4, 1.7, 2.2, 3.3, and 7.8 μm. Carbon monoxide stands out at 2.3 and 4.5 μm whereas CO₂ has diagnostic features near 2.1, 4.3, and 15 μm. Ammonia has many features, but the one at 10.5 μm is most noteworthy. Molecular hydrogen (H₂) has no permanent dipole but one can be induced by collisions (“collision-induced absorption”) at high pressure, and the result is a family of undulations from ~2.2 to ~20 μm that has been seen in Jupiter, Saturn, and brown dwarfs. A central goal of transit, reflection, or emission spectroscopy of exoplanets is to identify these species (and perhaps infer their abundances) by these distinctive features.

**Clouds and Hazes**

Condensates can form and reside in exoplanet atmospheres as clouds or hazes (21, 35) and can have a disproportionate influence on spectra. This influence is because, assemblage in a grain, such aggregations can respond coherently to light (depending upon the particle size and wavelength). So, very little areal mass density can translate into a large optical depth, and a trace species can loom large. In addition, with a spectrum of particle sizes and enhanced line broadening in the grain, their absorption and scattering cross-sections can have a continuum character and veil a wide spectral range. The result can be partial (or complete) muting of the gas-phase spectral features, making understandable condensates and incorporating their effects into models as important as it is difficult. To properly handle the effects of clouds, we need to know the condensate species, grain size and shape distributions, the complex index of refraction, and the spatial distribution in the atmosphere. Such knowledge is generally in short supply.

The possibility of water clouds in terrestrial atmospheres is uncontroversial, the presence of ammonia clouds in the atmospheres of Jupiter and Saturn has been observed in detail, and the central role of silicate and iron clouds in brown dwarf L dwarfs is reasonably inferred by their very red infrared colors. These situations are in part informed by known thermochemistry. However, water clouds are expected in cold giant exoplanet and brown dwarf atmospheres (24, 41); Na₂S and KCl clouds are thought to reside in late T dwarf brown dwarfs; an extra absorber in the optical and at altitude has been invoked to explain the inversions and over-hot atmospheres inferred from the spectra of secondary eclipse of some transiting hot Jupiters (39); a thick haze envelopes the atmosphere of Saturn’s Titan; and there is a trace absorber in the blue that makes Jupiter and Saturn redder than Neptune or Uranus. None of the causative species in these situations is either known, or if known, well-modeled. The case of Jupiter’s color is a cautionary tale. The factor of two suppression in its reflected blue flux could be due to traces at the part in 10⁻¹⁰ level of either polycytylenes, sulfur or phosphorus compounds, tholins, or something else (19). Such leverage by a small (and unknown) “actor” in the interpretation of such a large effect should give one pause and emphasizes the potential complexity of the task of exoplanet characterization. Photolytic chemistry is likely a cause in Titan’s atmosphere, as in many other contexts, but this explanation is small comfort when designing a modeling effort aimed at anticipating all reasonable possibilities.

Scattering in general is important only in reflection and transit spectra, not in emission, and is most prominent for hazes and clouds. In fact, longward of the UV, clouds are necessary to give a planet any appreciable reflection albedo above ~1% (19). Also, in reflection, as a general rule, cloud or UV/blue Rayleigh scattering can yield highly polarized fluxes (20). The polarized fraction is higher when the absorption fraction is higher and the scattering albedo is low, but in this case the overall reflected flux is low. This reasoning suggests that polarization might in some circumstances be a useful ancillary diagnostic of exoplanet atmospheres. Unlike for gas species, for many realizations of likely hazes or clouds in exoplanet atmospheres, the scattering albedo can be either high or low, depending upon species and wavelength range, and is frequently high. This fact suggests that reflection spectra can be dominated by the effects of such layers and, moreover, that transit spectra can be affected by particulate scattering (as opposed to only...
absorption). Clearly, one must be aware of the possible presence of clouds and hazes when performing exoplanet spectral retrievals.

**Transit Spectra**

Transit spectra are direct probes of atmospheric scale heights and atmospheric abundances near the terminator(s). However, if the atmosphere is optically thick and overlays a rocky core, there is no obvious way to determine the core’s contribution to the measured radius. Therefore, it is standard practice to analyze transit spectra with respect to an arbitrarily determined reference radius, often taken to be the inferred discovery radius in the optical. When the solid surface of a terrestrial or super-Earth planet is not a priori known, or is inaccessible by measurement, then there will be ambiguity with respect to its contribution to the transit depth. Interpretation will not be ambiguous with an airless planet, and is moot for a gaseous planet, but is an issue to consider when falsifying theory.

The measured fractional diminution in the stellar light at a given wavelength is the transit depth (27, 42). The stellar beams pointed at the Earth probe the planet’s atmosphere transversely along a chord perpendicular to the impact radius. Therefore, the relevant optical depth, \( \tau \), is not the depth in the radial direction associated with emission, but much larger. The contribution of the annulus, or partial annulus in the case of the ingress or egress phases, to the blocking of stellar light is \( 1 - e^{-\tau} \) times the annular area. The sum of such terms over the entire atmosphere provides the integrated blocking fraction due to the atmosphere. That this \( \tau \) is larger than the radial \( \tau \) allows transit depth to be more sensitive to trace chemical species than emission or secondary eclipse spectra and amplifies their effect. This effect may be particularly relevant of atmospheric hazes that may be too thin in the radial direction to affect emission, but are thick along the chord (43), and may be why Pont et al. (44) see an almost featureless transit spectrum for HD 189733b and infer a veiling haze whereas the associated InfraRed Array Camera (IRAC) and Infrared Spectrometer (IRS) data at secondary eclipse clearly reveal water signatures (45). Another reason may be that, because transit spectra probe the terminator, the transition region between day and night, a condensate is more likely to form as the temperature transitions to lower values. Be that as it may, the terminator is a complicated region that introduces special challenges for the theory of transit spectra.

Despite this challenge, a simple analytic model (8, 43, 46) can be developed that captures the basic elements of general transit theory. Integrating along a chord at a given impact parameter and assuming an exponential atmosphere with a pressure scale height, \( H \), yields an approximate amplification factor for the chord optical depth (\( \tau_{chord} \)) over the radial optical depth of \( \sqrt{2 \pi R_p / H} \), which can be \( 5 - 10 \). This fact means that the \( \tau_{chord} = \tau_{solar} \) condition that approximately defines the apparent planet radius at a given wavelength is pushed to larger impact parameters (radii) and that the fractional transit depth is increased by a factor \( \propto 2H/R_p \). Moreover, it is straightforward to show that

\[
\frac{dR_p}{d\lambda} = H \frac{d\sigma}{d\lambda} \tag{1}
\]

where \( \sigma \) is the total species-weighted interaction cross-section (the sum of absorption and scattering). Note that, whereas emission spectra (ignoring reflection) depend upon only absorption, transit spectra depend upon both scattering and absorption processes. In fact, the haze inferred for HD 189733b could be purely scattering and, as such, would make no contribution to the emission at secondary eclipse. However, it is likely that any haze has a nonunity scattering fraction/albedo, introducing flexibility, but also further complexity, into the simultaneous interpretation of transit and emission spectra.

Eq. 1 suggests that significant wavelength variations in cross-section, as across an absorption band, translate into a change in the apparent radius of order \( H \). This fact is the essence of the use of transit measurements as a function of wavelength to determine compositions. Because \( R_p \) depends upon the logarithm of \( \sigma \), Eq. 1 also indicates that the dependence upon abundance is logarithmic and, thus, weak. Although it is “easy” to discern a molecular feature, it is not easy with transit spectra to determine its abundance. Note that, because \( H = kT/\mu g \), a low (high) temperature, high (low) gravity, or high (low) mean molecular weight atmosphere will yield weaker (stronger) indications of composition. Therefore, as long as spectroscopically interesting species reside in the atmosphere in reasonable abundances, a hot, \( H_2 \)-rich atmosphere (without a veiling haze/cloud) yields the largest, most diagnostic radius variations with wavelength.

If there are differences in the compositions and scale heights at the east and west limbs of a planet, such differences are in principle discernible as differences in ingress and egress transit spectra. Although difficult even for a giant exoplanet, such measurements might be doable in the future and could shed light on atmospheric dynamics and any pronounced zonal flow asymmetries.

In addition, narrow-band, very-high-resolution spectroscopy before and during transit has great potential to reveal planetary orbital, spin, and wind speeds, as well as compositions (compare the measurement of CO lines by ref. 47). Although giant exoplanets are the most studied population to date via multiband transit photometry and spectrophotometry [as opposed to wide-single-band observations à la Kepler (48)], such data around small M dwarfs for terrestrial planets and super-Earths (such as GJ 1214b) (see ref. 43 and references therein) have great promise to probe the atmospheres of these smaller, but likely more numerous, planets. Measuring the emission spectra of Earths around solar-like stars will be much more challenging.

Fig. 2 portrays the general character of representative theoretical exoplanet transit spectra from 0.4 to 5.0 \( \mu \)m. The models are for the giant WASP-19b and include isothermal atmospheres at \( T = 2500 \) K, with and without a uniform gray haze with an opacity of 0.01 cm\(^2\)g\(^{-1}\), a model that attempts to fit its IRAC data at secondary eclipse (49) with an unknown “extra absorber” at altitude of constant optical opacity 0.05 cm\(^2\)g\(^{-1}\) (from 0.4 to 1.0 \( \mu \)m), and a similar model using TIO as the extra absorber. For clarity, the latter two are shifted arbitrarily from the former two. We note that the transit depth is of order \( \sim 2\% \) and that the variation due to the presence of water bands is approximately one part in a thousand. The depths for other hot Jupiters could vary with wavelength by as little as a few parts in ten thousand.

One sees immediately that the extra optical absorber, whatever its nature, increases the ratio of the optical to infrared radii, that the TIO hypothesis can readily be falsified, that the spectral features of (here) water should be readily detected,** that the radius variations in the midinfrared can be of larger amplitude, and that even low-opacity hazes can mut
reprocessed stellar light (52, 53). Stellar irradiation and zonal atmospheric winds and dynamics break the simple spherical symmetry, so that 3D models would seem most appropriate. However, such models have yet to prove themselves, and simpler 1D hemisphere-averaged models have been used, however profitably, to compare with data. Issues with such a prescription include what average flux to use to derive a representative dayside temperature/pressure (T/P) profile, how to incorporate longitudinal and latitudinal surface flows into the energy budget, nonequilibrium chemistry (54), photochemistry, and day–night differences when interested in total phase curves (53, 55, 56). Nevertheless, such simple models are still commensurate with the information content of the extant observations.

The various quantities and topics that influence secondary eclipse spectra and have exercised the community include (i) the presence or absence of an extra absorber of currently unknown origin in the upper atmosphere that could heat those regions, at times producing thermal inversions over a restricted pressure range (39, 57); (ii) the temperatures and temperature profiles of the atmosphere; (iii) the phase shifts from the orbital ephemeris of the light curves at various wavelengths and spectral bands due to zonal winds that redistribute heat (58); (iv) the compositions and elemental abundances of the atmospheres; (v) the presence of hazes and clouds; (vi) the day/night flux contrast; (vii) Doppler signatures of atmospheric motions; (viii) reflection albedos (59); and (ix) the presence and role of evaporative planetary mass loss. I mention these challenges only to indicate the range of complex problems to be addressed but will focus in this paper on only the simplest of approaches taken to extract information from secondary-eclipse data.

A few conceptual points are worth noting in passing: (i) An atmosphere calculation with external incident flux will automatically generate a reflection albedo and is not extra physics. (ii) For a given elemental ratio set, the metallicity dependence of the emergent spectrum is quite weak. Most relevant species (such as water) have one bond to another so implied (60). Inferences of isothermality are not as content-neutral as is often implied (60).

One can derive an average temperature profile in a radiative-equilibrium exoplanet atmosphere under stellar irradiation by generalizing the classical Milne atmosphere (10, 11). One obtains:

$$T^4 = \frac{3}{4} T_{\text{eff}}^4 \frac{\kappa_f}{\kappa_B} \left[ \frac{\tau_B + 1}{\sqrt{3}} \right] + \frac{\kappa_f}{\kappa_B} W T^4, \quad [3]$$

where $W$ is the dilution factor $(R_* / a)^2$, $\tau_B$ is the Rosseland depth, $\kappa_f$ is the photon energy-density weighted opacity, $\kappa_B$ is the corresponding local black-body-weighted opacity, and we have used the Eddington approximation for the angular moments. For an isolated atmosphere, $\kappa_f$ is close to one, but, for an irradiated atmosphere, $\kappa_f$ and $\kappa_B$ can differ appreciably. The former at altitude is dominated

$$T_{\text{eq}} = T_* \left( \frac{R_*}{a} \right)^{1/2} (f(1-A_B))^{1/4}, \quad [2]$$

where $T_*$ is the stellar effective temperature, $f$ is the heat redistribution factor\(^\dagger\), and $A_B$ is the Bond albedo (8, 19). While providing a measure of the mean temperature achieved in a planet’s atmosphere, assuming this can be used as the inner boundary condition, $T_{\text{eq}}$ has introduced quite a lot of confusion. Very different T/P profiles can yield the same total flux but very different flux spectra. Fig. S1 shows two models with the same emergent flux, and, thus, $T_{\text{eq}}$. One consistently incorporates stellar irradiation whereas the other puts a flux with $T_{\text{eff}} = T_{\text{eq}}$ at the base of the atmosphere. Both are in radiative and chemical equilibrium. As Fig. S1 demonstrates, despite the fact that the emergent fluxes are the same, the corresponding T/P profiles are hugely different and the flux densities at a given wavelength can be off by factors of 2–4! Irradiated atmospheres are different from isolated atmospheres.

Lastly, (v) if an atmosphere is in fact isothermal, there must be an extra absorber in the optical at altitude. Even under irradiation, the temperature gradient must otherwise be negative from base to height, with characteristic temperature changes of ~500–1,500 K for close-in giant exoplanets. Therefore, inferences of isothermality are not as content-neutral as is often implied (60).

Secondary Eclipse

For a circular orbit, when 180° out of phase with the transit, the planet is occulted by the star and is in secondary eclipse. During the eclipse, the summed light of the planet and star being monitored shifts to that of the star alone and by the difference the planet’s emissions are determined. The Spitzer space telescope (51) has been particularly productive in this mode, providing near- and midinfrared photometric points for ~30 nearby transiting planets (mostly giants). For close-in planets, for which the transit probability is largest, the planet is emitting mostly

\(^\dagger\dagger$T\dagger_f = 1/4 for isotropic models.
Spitzer/IRAC data, in particular at 5.8 μm, extra heating of the upper atmosphere by an absorber in substellar fluxes at these given planets, as well as the IRAC data at secondary eclipse and demonstrate the span collection of transiting giant exoplanets. These models a wide wavelength range.

by the stellar spectrum whereas the latter reflects the local atmospheric black-body spectral distribution. If this difference is an interesting function of altitude, an inversion can result [10]. We note that $T_{\text{eff}}$ is generally small for close-in hot Jupiters. In this case, the temperatures at depth are determined by the second term, which yields something like Eq. 2. In reality, gas giants are convective at high optical depths (~100–1,000) and the T/P profile becomes an adiabat. Otherwise, it would be flat.

Representative theoretical average day-side temperature-pressure profiles for a subset of transiting gas giants are given in Fig. 3A.

These profiles are provided to communicate the range of atmospheric temperatures encountered for hot Jupiters and the matching to adiabats at depth above ~100 bars. The atmospheres of close-in giants can vary in temperature, depending upon $W$ and $T_{\ast}$, by ~1,000–2,000 K. Importantly, the difference in upper-atmosphere temperatures between “inverted” and noninverted situations can be ~1,000–1,500 K, a huge difference that can translate into flux spectrum differences of factors of ~2–4 for ostensibly the same object. This fact is depicted in Fig. 3B, which provides the corresponding planet/star flux ratios versus wavelength. Among this set of exoplanets, the theoretical flux ratios vary at a given wavelength by an order of magnitude. Moreover, as the comparison between (i) the model for WASP-12b with solar abundances, chemical equilibrium, and an extra upper atmosphere absorber in the optical (upper black) and (ii) the model for WASP-12b with enhanced CH$_4$ and CO, depleted H$_2$O, and no inversion (gray) attest, mid-infrared planetary spectra can vary significantly for the same stellar irradiation regime and gravity. Fig. 3B, together with Fig. 1, demonstrates the great diagnostic potential of multifrequency spectra to extract compositions. One can also determine the presence or absence of extra heating by enhanced absorption of stellar light that leads to inversions, but also hotter upper atmospheres and elevated fluxes of features formed in the heated zone. The pronounced bump at ~4.5–5.5 μm on the inverted spectrum for WASP-12b is due to water in emission and the fact that this band forms where the corresponding temperature profile has a positive (inverted) slope.

Although inversions have been inferred from enhanced Spitzer IRAC band fluxes (in particular at 5.8 μm), the nature of the absorber is still unknown. It is suggested that TiO could do it, but there are good reasons to believe this compound would be rained out to depth by various cold traps (38). There may be photochemical hazes with the right optical absorbing properties, but this possibility has not been demonstrated. Still, it is tantalizing to hypothesize that the haze inferred by Pont et al. (44) in the atmosphere of HD 189733B and that inferred by Deming et al. (50) in the atmosphere of HD 209458b might in some way be implicated, or at least be of similar composition. Although the interpretative and diagnostic promise of good spectra is suggested in Fig. 3B, the current reality is depicted in Fig. 4. Here, I plot representative measured planet/star flux ratios for 17 transiting giant exoplanets. Most of the data are Spitzer/IRAC photometry in four bands whereas some of the data are from the ground and the Hubble Space Telescope. For HD 189733b, we have Spitzer/IRS spectra from ~5–15 μm as well (45). To keep the plots from being any more cluttered, error bars for only a few measurements are shown. The quoted 1 − σ error bars generally range from ~10–30%. In an attempt to divide out universal expectations and to focus on what may distinguish one planet from another, I have normalized the planet/star flux ratio with the corresponding black-body value.

First, we see from Fig. 4 that the normalized ratio is rather flat over a broad range of wavelengths and close to one, perhaps a bit higher. However, the mean level could just reflect the crudeness of the $T_{\text{eff}}$ used for the comparison. We see undulations, but they have little information content, aside from the possible suggestion of enhanced or reduced flux in particular broad spectral regions. The IRS data near 6.2 μm for HD 189733b do imply the presence of water, but what is the feature near 12.5 μm? There is a systematic increase in the ratios to shorter wavelengths, and this increase is probably real. As Fig. S1 implies, fluxes from irradiated planets are expected to be mostly in the near infrared.

The comparison of Figs. 3B and 4 starkly emphasizes that we have a long way to go before comparative exoplanetology becomes a richly diagnostic science. At times, data such as are depicted in Fig. 4 have been used to find temperatures, compositions, albedos, inversions, carbon-to-oxygen ratios (91), metallicities, and day–night heat redistribution factors, etc. Clearly, these data, and the still primitive state of exoplanet atmosphere theory, do not justify attempts to constrain such quantities simultaneously, or perhaps at all. Until high-quality transit and emission spectra across a wide range of wavelengths are routinely available, only the most primitive and conservative conclusions will be justified. I reiterate that the data in Fig. 4 are for giant exoplanets. Smaller Neptunes, super-Earths, and terrestrial planets around similar stars will be much more difficult targets.
generally the space-based and ground-based observations have been problematic. Data for the same object at the same wavelength, but taken by different teams, have varied by up to factors of \( \sim 2 \), and such a factor can completely alter the conclusions drawn about abundances, C/O ratios, inversions, etc.

Given this list of limitations, one should be highly skeptical of extraordinary claims based on imperfect data with low intrinsic information content. Many published model fits have been highly underconstrained. This observation is all the more important given the gross imperfections in current exoplanet atmosphere theory. With a few photometric points, one cannot simultaneously determine with any confidence, or credibly incorporate into the fitting procedures, chemical and elemental abundances, wind dynamics, longitudinal heat redistribution, thermal profiles, albedos, the potential influence of hazes and clouds, nonequilibrium chemistry and photochemistry, and magnetic fields. Furthermore, the opacities for many chemical species are only imperfectly known, convection at depth is frequently handled with a mixing-length approach, and emissions over a planetary hemisphere are never calculated with correct, multidimensional radiative transfer. Moreover, most of the current generation of 3D general circulation models (GCMs) filter out sound waves but derive transonic flow speeds with Mach numbers at and above one, and new high-contrast coronagraphic imaging programs now coming on line [such as Gemini Planet Imager (96) and SPHERE (94), and perhaps dedicated Explorer, M-Class (e.g., EchO) (95), or Probe-Class space missions. The continued creative use of existing ground-based telescopes is assured, and new high-constraining geometric imaging programs can now address some of the above limitations. The continued creative use of existing ground-based telescopes is assured, and new high-contrast coronagraphic imaging programs now coming on line [such as Gemini Planet Imager (96) and SPHERE (97)] show great promise. Importantly, there is the exciting possibility of putting a coronagraph on Wide-Field Infrared Survey Telescope (WFIRST)/Astrophysics Focused Telescope Assets (AFTA) (98). In the farther future, once a cost-effective plan can be articulated, a major dedicated space mission of exoplanetary atmosphere characterization, such as was envisioned with the Terrestrial Planet Finder (TPF) and Darwin, should be possible. Currently, giant planets and Neptunes pose the most realistic targets, but terrestrial planets and the possibility of discerning signatures of life are major goals of many. Soon, the spectra of terrestrial 

Fig. 4. (A) Planet/star flux ratio data points at secondary eclipse for eight giant planets (WASP-19b, HD 149026b, HAT-P-7b, HAT-P-2b, CoRoT-2b, CoRoT-1b, HD 189733b, and HD 209458b), normalized to the corresponding ratio if both star and planet were black bodies at the corresponding measured stellar temperature, \( T_\text{eq} \approx T_\odot \sqrt{T_\text{intrinsic}/T_\text{host}} \), respectively. The lines connect points for the same object. Most of the data are Spitzer/IRAC points, but points at shorter wavelengths, where available, are also included. For HD 209458b and HD 189733b, points at 16 and/or 24 \( \mu \)m are also given, along with points (unconnected and for comparison) derived from other reductions. To avoid further clutter, quoted error bars are given only for the IRS spectrometer data for HD 189733b and the Spitzer data for HD 209458b. (B) The same as in A, but for XO-3b, XO-2b, XO-1b, WASP-18b, WASP-12b, TrES-4, TrES-3, TrES-2, and TrES-1. Error bars for only WASP-12b are given. The normalization provided helps to rationalize the interpretation potential of such photometric and low-resolution data and to facilitate planet-planet comparison. The data were taken from refs. 45, 49, 57, 60, and 61–90.

**Systematic Uncertainties in the Data and Theory**

Theorists and observers alike, anxious to extract all of the conclusions they can from this first generation of measurements of exoplanet atmospheres, have tended to overinterpret them. A comparison between Figs. 3B and 4 is a sober indication of the current limitations of the science. The telescopes being used were not designed with exoplanets in mind. For example, Spitzer was designed for photometry at the \( \sim 1\% \) level, yet it is being used (however heroically) to obtain numbers at the \( \sim 0.1–0.01\% \) level. Generally, the space-based and ground-based data have limited signal-to-noise, the systematic effects/errors are variously and imperfectly corrected for, there is no absolute calibration across disparate wavelength regions, stellar spots are difficult to account for, and corrections for the Earth’s atmosphere for ground-based observations have been problematic. Data for the same object at the same wavelength, but taken by different teams, have varied by up to factors of \( \sim 2 \), and such a factor can completely alter the conclusions drawn about abundances, C/O ratios, inversions, etc.

Given this list of limitations, one should be highly skeptical of extraordinary claims based on imperfect data with low intrinsic information content. Many published model fits have been highly underconstrained. This observation is all the more important given the gross imperfections in current exoplanet atmosphere theory. With a few photometric points, one cannot simultaneously determine with any confidence, or credibly incorporate into the fitting procedures, chemical and elemental abundances, wind dynamics, longitudinal heat redistribution, thermal profiles, albedos, the potential influence of hazes and clouds, nonequilibrium chemistry and photochemistry, and magnetic fields. Furthermore, the opacities for many chemical species are only imperfectly known, convection at depth is frequently handled with a mixing-length approach, and emissions over a planetary hemisphere are never calculated with correct, multidimensional radiative transfer. Moreover, most of the current generation of 3D general circulation models (GCMs) filter out sound waves but derive transonic flow speeds with Mach numbers at and above one without a means to handle shock waves. Many of these codes have also inherited from Earth GCM practice various ad hoc "Rayleigh drag" and hyperdiffusivity terms with arbitrary coefficients calibrated on the Earth that compromise the wind dynamics on strongly irradiated gas giants, even if magnetic torques are subdominant. Importantly, GCMs were configured to look at winds and pressures, not spectral emissions, highlighting the mismatch between the traditional goals of planetary and Earth scientists and exoplanet astronomers.

At times, basic atmosphere practice has been shunted aside in attempts to retrieve thermal and compositional information from a few (although precious) data points. Examples are (i) using unphysical, parametrized T/P profiles and arbitrary compositions, while not addressing local energy and chemical balance; (ii) using 1D averaged models for what is a 3D planet; (iii) using \( T_\text{eq} \) as if it were a real physical quantity of relevance to spectra; and (iv) defining and deriving a reflection albedo when the planet is mostly emitting thermally; or (v) fitting photometric points with \( T_\text{eq} \) and a Bond albedo. Such approaches might seem right-sized to the data at hand but are likely to generate an erroneous sense of confidence in the conclusions derived. For example, it is long been known that small errors in \( \Delta T \) can translate into large spectral flux errors, even if the total reprocessed emitted flux is ostensibly addressed.

**The Future**

Therefore, I suggest that once high-quality, well-calibrated, stable spectra across a broad range of wavelengths from the optical to the midinfrared are finally available, many conclusions reached recently about exoplanet atmospheres will be overturned. The current interpretations and theories are just not robust enough to survive intact into the future. However, despite the generally cautionary tone of much of this paper, I see an exciting future. The past \( \sim 20 \) y has been but a training period for a new generation of exoplanet scientists, forged by trial and error and educated in the new questions posed by exoplanets. Its growing membership is testing its tools—new technologies, concepts, theories, and techniques—that will serve to establish a solid foundation for a true science of planets not tethered to the solar system. Informed by the latter, but optimized to address its unique challenges as a remote-sensing science, comparative planetology’s youth is rapidly maturing.

The near- and midterm future of exoplanet atmosphere characterization will include the James Webb Space Telescope (JWST) (92, 93), ground-based Extremely-Large/Giant-Segmented-Mirror Telescopes (ELTs/GSMTs) (94), and perhaps dedicated Explorer, M-Class (e.g., EchO) (95), or Probe-Class space missions. The continued creative use of existing ground-based telescopes is assured, and new high-contrast coronagraphic imaging programs now coming on line [such as Gemini Planet Imager (96) and SPHERE (97)] show great promise. Importantly, there is the exciting possibility of putting a coronagraph on Wide-Field Infrared Survey Telescope (WFIRST)/Astrophysics Focused Telescope Assets (AFTA) (98). In the farther future, once a cost-effective plan can be articulated, a major dedicated space mission of exoplanetary atmosphere characterization, such as was envisioned with the Terrestrial Planet Finder (TPF) and Darwin, should be possible. Currently, giant planets and Neptunes pose the most realistic targets, but terrestrial planets and the possibility of discerning signatures of life are major goals of many. Soon, the spectra of terrestrial
planet atmospheres around small M-dwarf stars may be within reach. Given this landscape, it is clear that, for the field to remain vibrant and grow, it needs a heterogeneous and balanced program of ground-based and space-based facilities and programs. If anything has been demonstrated by the first ~20 y of exoplanet research, it is that some of the best techniques for studying them are unanticipated. The transit technique for close-in planets has been a game changer but was not envisioned in previous planning documents. High-context imaging, only now coming of age, was to inaugurate the era of atmospheric characterization. It is also clear that large, expensive missions are counterproductive until they are demanded by the science, in fact until the science indicates that further progress demands them. Precursor technologies for such missions should certainly be pursued and allowed to compete. However, overlarge and expensive missions without the requisite credibility and technological heritage in place can fatally squeeze the smaller programs that have proven so fruitful. Implied is an international roadmap crafted for exoplanet’s next ~20 y. This roadmap’s guiding principle should be a balanced approach of small, medium, and large initiatives that encourages flexibility and scientific return and does not presume (or proscribe) a specific future. The clear goal is to understand in rich detail the planets that we now know exist in profusion in the galaxy and universe. One is only left to ask: Are we ready to assume the challenge?

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Burrows


Fig. S1. (A) Shown are the temperature–pressure profiles for two models of HD 209458b. The black curve was generated including the stellar irradiation flux at the orbital distance of the planet and a token effective temperature (T_{eff}) of 200 K at the base. Note that T_{eff} for such a model reflects the net flux, not the emergent flux. The red curve is for an isolated model with roughly the same total emergent flux at an effective temperature T_{eff} of 1,700 K. Despite having the same emergent flux, these temperature–pressure profiles are profoundly different. (B) The corresponding normalized spectra, F_\nu, versus wavelength (in \mu m). These spectra are vastly different, although the total emergent fluxes are the same, and demonstrate that one cannot assume that an equal emergent flux constraint will translate into useful spectra or colors. They also demonstrate that one must be careful when quoting an effective temperature, and not confute T_{eff} with an “equilibrium temperature,” T_{eq}.