

Some inconvenient truths about biosignatures involving two chemical species on Earth-like exoplanets

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The detection of strong thermochemical disequilibrium in the atmosphere of an extrasolar planet is thought to be a potential biosignature. In this article we present a previously unidentified kind of false positive that can mimic a disequilibrium or any other biosignature that involves two chemical species. We consider a scenario where the exoplanet hosts a moon that has its own atmosphere and neither of the atmospheres is in chemical disequilibrium. Our results show that the integrated spectrum of the planet and the moon closely resembles that of a single object in strong chemical disequilibrium. We derive a firm limit on the maximum spectral resolution that can be obtained for both directly imaged and transiting planets. The spectral resolution of even idealized space-based spectrographs that might be achievable in the next several decades is in general insufficient to break the degeneracy. Both chemical species can only be definitively confirmed in the same object if absorption features of both chemicals can be unambiguously identified and their combined depth exceeds 100%.

astrobiology | detection of life | biomarker | exomoon | habitability

With almost a thousand confirmed exoplanets [Open Exoplanet Catalogue (1)], the prospects of detecting signs of a biosphere on a body outside our own solar system are more promising than ever before. However, there are still huge technological and theoretical challenges to overcome before one can hope to make a clear detection of life on an exoplanet. In this article, we discuss one of these complications, the possibility of false positives due to the presence of an exomoon orbiting the exoplanet.

There are many ways that life on an exoplanet might affect the planet's appearance, ranging from deliberate signals from intelligent civilizations (2) to subtler signs of simple life. To characterize an extrasolar world as fully as possible, we ideally would measure its spectrum as a function of time in both the optical and the infrared parts of the spectrum (e.g., refs. 3–6). For example, spectral evidence of water could suggest that a planet might be habitable. It has also been suggested that an intriguing indication of life might be an increase in the planet's albedo toward the infrared part of the spectrum, which on Earth can be associated with vegetation (7). However, these features alone would not be smoking-gun proof of the presence of life. The terms “biomarker” and “biosignature” generally refer to chemicals or combinations of chemicals that could be produced by life and that could not be (or are unlikely to be) produced abiotically; hereafter, we use these terms interchangeably. If biosignature gases are detected in the spectrum of an exoplanet, the probability that they actually indicate life depends both on the prior probability of life (8) and on the probability that the observed spectroscopic feature could be produced abiotically. The latter possibility is the subject of this paper.

Byproducts of metabolism are often thought of as the most promising biomarker (9–15). More specifically, an extreme thermodynamic disequilibrium of two molecules in the atmosphere is considered a biosignature (16–18). An example of two such species is the simultaneous presence of O₂ and a reduced gas such as CH₄. It is important to point out that a disequilibrium in

a planet's atmosphere should not be considered as clear evidence for life. [Also note that the Earth might have never had a phase of strong, observable O₂/CH₄ disequilibrium (19).] There is a long list of abiotic sources that could also create a disequilibrium such as impacts (20), photochemistry (21), and geochemistry (14).

In this article, we describe a previously unidentified scenario for a possible false positive biosignature. If the exoplanet hosts a moon that has an atmosphere itself, the simultaneous observation of the planet and moon modifies the observed spectrum (see also refs. 22 and 23) and can produce a signal that looks like a disequilibrium in one atmosphere but is in fact created by two atmospheres blended together. It might be extremely difficult to discern that an exoplanet even has a moon, let alone that one component of a two-chemical biosignature comes from the moon instead of the planet.

The outline of this article is as follows. We first describe our model atmospheres and present simulated spectra. Using those synthetic spectra, we show that the combined spectrum from an oxygen-rich atmosphere such as that of the Earth and a methane-rich atmosphere such as that of Titan indeed looks like it could have come from a single atmosphere with a strong disequilibrium. We then calculate a strong upper limit on the spectral resolution of such a system as observed from Earth under ideal conditions with a plausibly sized space telescope. Our estimate shows that the spectral resolution $R \equiv \lambda/d\lambda$ for such a system is unlikely to exceed $\sim 1,600$ with foreseeable technology. Given this maximum possible resolution, discriminating between a single planet and a planet-moon system is in general unlikely to be possible.[†] Nevertheless, we

Significance

The search for life on planets outside our own solar system is among the most compelling quests that humanity has ever undertaken. An often suggested method of searching for signs of life on such planets involves looking for spectral signatures of strong chemical disequilibrium. This article introduces an important potential source of confusion associated with this method. Any exoplanet can host a moon that contaminates the planetary spectrum. In general, we will be unable to exclude the existence of a moon. By calculating the most optimistic spectral resolution in principle obtainable for Earth-like planets, we show that inferring a biosphere on an exoplanet might be beyond our reach in the foreseeable future.

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[†]If an exomoon transits its planet, its secondary eclipse (when it dips behind the planet) offers a way to break the degeneracy because it presents an opportunity to obtain the spectrum of the planet alone. Transits, however, are unlikely. For instance, Earth's moon transits Earth for only $\sim 2\%$ of randomly oriented observers.

Table 1. Basic assumptions for planet and moon

Description	Symbol	Planet	Moon
Radius	r	r_{\oplus}	$0.4r_{\oplus}$
Surface gravity	g	9.8 m/s^2	1.35 m/s^2
Surface temperature	T_0	300 K	300 K
Surface pressure	P_0	1,013 mbar	1,500 mbar
Surface albedo	a	0.3	0.3
Mean molecular weight	μ	28.8	27.0
Heat capacity	c_p	1.0	1.0
Dry adiabatic lapse rate	Γ	9.8 K/km	1.35 K/km
Cloud or haze	—	No	No

conclude with a summary and a positive outlook with two possibilities that can provide genuine biosignatures. The first possibility is to find a single chemical species that is sufficient to indicate life. The second one requires the unambiguous identification of both species' absorption features and the combined depth of the features needs to exceed 100%.

Models

To demonstrate how a planetary spectrum with two biosignature molecules could be spoofed by an unseen moon, we compare two simulated spectra: case 1, that of a planet that has both O₂ and CH₄ in its atmosphere, and case 2, that of a (spatially unresolved) planet + moon system where each body contains either O₂ or CH₄ but not both. We calculate 1D line-by-line radiative transfer based on Discrete Ordinates Radiative Transfer Program for a Multi-Layered Plane-Parallel Medium (24) and the high-resolution transmission molecular absorption database (25).

Although absorption by other chemical species is naturally expected for habitable planet candidates, we exclude all species besides O₂ and CH₄ from our model because doing this clarifies our argument. Nevertheless, water, for instance, has strong absorption features that overlap with some oxygen and methane bands. This can further complicate inferring the presence of any biosignatures in a spectrum (we address this in [Supporting Information](#)).

The geometric configuration is fixed at $\theta_0 = \theta_1 = 45^\circ$ and $\phi = 0^\circ$, where θ_0 , θ_1 , and ϕ are the zenith angle of the incident light, that of the observation, and the relative azimuthal angle ($\phi = 0^\circ$ represents the forward scattering), respectively, as a representative geometry for a planet at quadrature. We assume that the model atmospheres are characterized by the ideal gas equation of state, hydrostatic equilibrium, and (dry) adiabatic temperature profiles from the 300-K surface up to 150 K:

$$P = \frac{\rho}{\mu} \mathcal{R} T, \quad \frac{dP}{dz} = -\rho g, \quad \frac{dT}{dz} = -\Gamma = -\frac{g}{c_p}, \quad [1]$$

where \mathcal{R} is the ideal gas constant; ρ and z have their usual meanings; and the other symbols are described in Table 1.

Real planetary atmospheres do not follow an adiabat above the tropopause and therefore do not continue to get arbitrarily colder with altitude. Stratospheric temperature profiles can be complicated, but for illustrative purposes we simply take the model atmosphere to be isothermal above the altitude at which the adiabat reaches $T = 150 \text{ K}$. Furthermore, for the sake of simplicity, we neglect the effects of clouds or hazes. The physical parameters to specify the atmospheric profiles are as listed in Tables 1 and 2, where the planet mimics a (cloudless) Earth, whereas the moon has Titan-like properties. We can neglect the Doppler shift of the spectral lines as the relative Doppler shift of the Earth-moon system in an edge-on orbit is only $\Delta\lambda/\lambda \sim 3 \times 10^{-6}$.

Fig. 1 compares the spectrum of a planet with 15% O₂ and 30 ppm CH₄ (case 1) to that of a planet with 20% O₂ plus a moon

with 50 ppm CH₄ (case 2). For case 2, we independently calculated the spectra for the planet and for the moon, found the sum of the two, and normalized by the total area of the planetary and moon disks $r_{\oplus}^2 + (0.4r_{\oplus})^2 = 1.16r_{\oplus}^2$, where r_{\oplus} is the radius of the Earth.

At very high resolution ($R = 1,000,000$; Fig. 1, *Top*) where lines are well resolved, the difference between cases 1 and 2 is clear. In the spectrum of a planet alone, many of the line cores of both O₂ and CH₄ hit zero, whereas in the spectrum of a planet plus a moon, the lines are peculiarly cut well above 0. In the latter case, many of the O₂ and CH₄ lines are actually saturated in the spectrum of the planet and that of the moon, respectively. After adding the two, the scattered light from the other body contributes as an offset.

At lower resolutions, however, the two spectra are almost indistinguishable. The saturated line cores are smoothed off, resulting in very similar shallow absorption bands. The direct comparison is shown in Fig. 2 with the uncertainty bars corresponding to signal-to-noise ratio (SNR) of ~ 10 . Although subtle differences exist in the shapes of the band and the slope of the continuum, it would be impossible to discern such differences from moderate-resolution ($R = 100$) observations without a priori knowledge of the detailed chemistry and physical properties of the target bodies. We therefore conclude that the presence of an unseen moon may be responsible for the apparent coexistence of two species in disequilibrium.

There is one other possibility to confirm the presence of two species in the same object. Unfortunately, this requires one to be able to unambiguously identify absorption bands, which is hard or even impossible in a low-resolution spectrum without any a priori knowledge of the atmosphere's composition. Let us ignore these difficulties for now and assume that we have measured the depth of two uniquely identified absorption features A and B as q_A and q_B with values between 0% and 100%. If the combined depth $q_A + q_B$ is larger than 100%, then this implies that at least the larger of the two bodies (the planet) must have both chemical species in its atmosphere.

In reality, planetary spectra are far more complicated than demonstrated here, for example, due to the presence of condensates in the atmosphere (clouds and haze) and spectroscopic features of other molecules. Even in the event that the summed absorption depths of two species exceeds 100%, the proportion of the planetary light and moon light can significantly change within the observed wavelength interval, for instance, because of broad absorption by other atmospheric species. In that case it would still be possible that one absorption trough comes from the planet and the other from a moon. A definitive conclusion would require detailed modeling of the atmospheric properties of the planet and a possible moon.

Several techniques have been proposed that might reveal the existence of an exomoon for both transiting (e.g., refs. 26 and 27) and directly imaged systems (22, 28, 29). Such techniques could provide some constraints on the interpretation of the spectra, although in most cases the detailed atmospheric properties would remain unknown.

Estimate of Spectral Resolution

To estimate the spectral resolution we might expect in an observation, let us consider an Earth twin around a Sun-like star at

Table 2. Models to compare

Description	Case 1	Case 2	
Target	Planet	Planet	Moon
Composition	15% O ₂ + 30 ppm CH ₄	20% O ₂	50 ppm CH ₄
Normalization	r_{\oplus}^2	$1.16r_{\oplus}^2$	

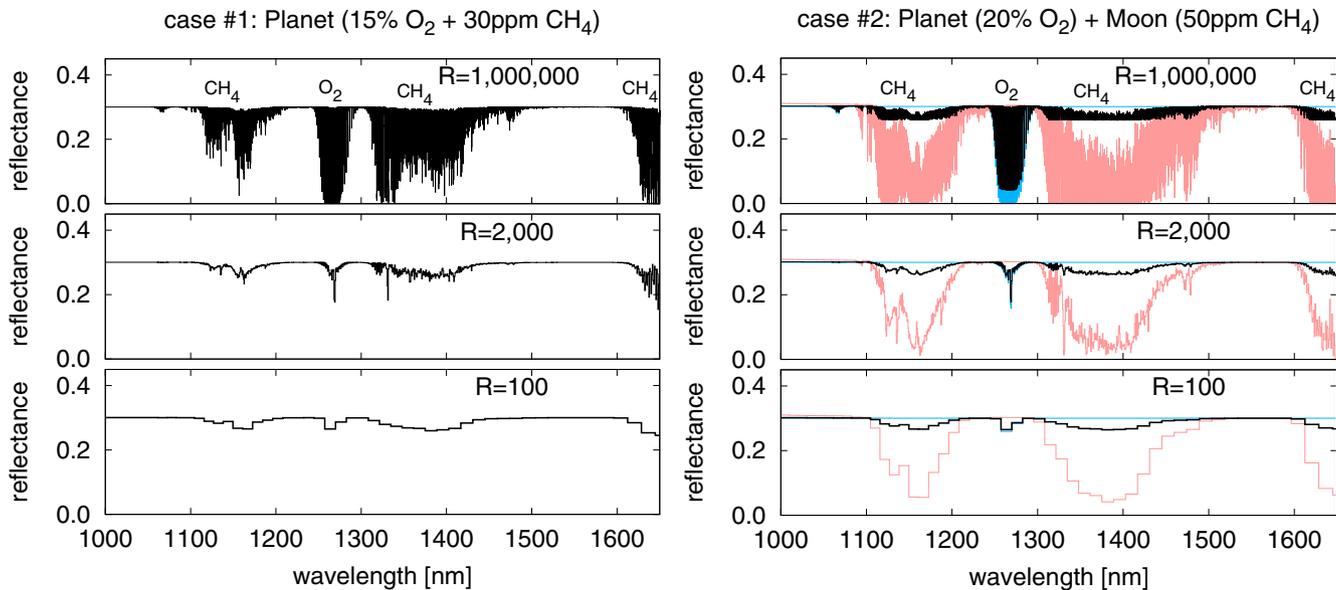


Fig. 1. Model spectra for cases 1 and 2 with varying resolution. (*Left*) Model spectra of a planet with 15% O₂ and 30 ppm CH₄. (*Right*) Black lines show combined spectra of a planet with 20% O₂ and a moon with 50 ppm CH₄. Blue lines show model spectra of a planet with 20% O₂. Red lines show model spectra of a moon with 50 ppm CH₄.

a distance $d = 10$ parsec away from the solar system. The flux of the star as seen from Earth is $F_* = L_*/(4\pi d^2)$, where L_* is the star's luminosity. In the following discussion we will assume a solar-type star with solar luminosity, $L_* = 3.8 \cdot 10^{33}$ erg/s, and temperature, $T_* = 5780$ K.

Rate of Photons. We are interested in a specific wavelength λ and can use Planck's law to estimate that portion of a given stellar or reflected planetary flux F that is emitted in a small wavelength band $d\lambda$ around λ :

$$f[\lambda, d\lambda] \approx F \frac{\pi B_\lambda [T_*]}{\sigma T_*^4} d\lambda, \text{ where} \quad [2]$$

$$B_\lambda [T_*] = \frac{2hc^2}{\lambda^5} \frac{1}{\exp[hc/(\lambda k_B T_*)] - 1}.$$

The Planck function $B_\lambda [T_*]$ is referred to as the spectral radiance, σ is the Stefan–Boltzmann constant, and T_* is the effective temperature of the star. We can convert $f[\lambda, d\lambda]$ to a photon flux f_γ (number of photons per area per time interval) using the relation $f_\gamma \equiv f/E = f\lambda/(hc)$, where $E = hc/\lambda$ is the energy of a photon of wavelength λ . The rate of photons captured with an idealized telescope of diameter D and 100% photon efficiency is then given by

$$\dot{N} = f_\gamma \pi \left(\frac{D}{2}\right)^2 = F \frac{\pi^2}{4\sigma hc} \frac{\lambda B_\lambda [T_*]}{T_*^4} D^2 d\lambda. \quad [3]$$

Spatially Resolved Planet. The flux of reflected light from a spatially resolved exoplanet is a fraction of the incident stellar flux. Let us consider a planet at a distance a from the star. If we ignore thermal radiation, the total luminosity of the planet is $L_{\text{reflected}} = L_* A r_p^2 / (4a^2)$, where A is the Bond albedo. The planet is most easily observed at quadrature when its projected distance from the host star is maximized. At quadrature the planet appears as a half circle. The reflected light flux is usually obtained by approximating the planet's reflection properties with, for

example, a Lambertian bidirectional reflectance distribution function (see, e.g., ref. 30). Here we use an even simpler argument which is nevertheless correct to within 10% compared with a Lambert sphere. We assume that the night side of the planet does not radiate and the star-facing side of the planet shines uniformly in each direction. From the perspective of Earth, we see a semicircle of the dayside and a semicircle of the nightside. Then, by conservation of energy, the flux of the planet as seen from Earth is simply

$$F_{\text{reflected}} = \frac{L_{\text{reflected}}}{4\pi d^2} = \frac{L_* A r_p^2}{16\pi a^2 d^2}. \quad [4]$$

Note that for an Earth-like planet with a Bond albedo of $A = 0.3$ and a separation of $a = 1$ AU the contrast of the planet with respect to the star is $F_p/F_* \sim 1.3 \cdot 10^{-10}$ (consistent with the results of ref. 30). We can now use Eq. 3 to calculate the rate of photons $\dot{N}_{\text{reflected}}$ captured with our telescope. If we want a signal to noise ratio of $\text{SNR} = 10$ per spectral bin in integration time Δt , we need at least $\text{SNR}^2 = 100$ photons in the wavelength band $d\lambda$ in

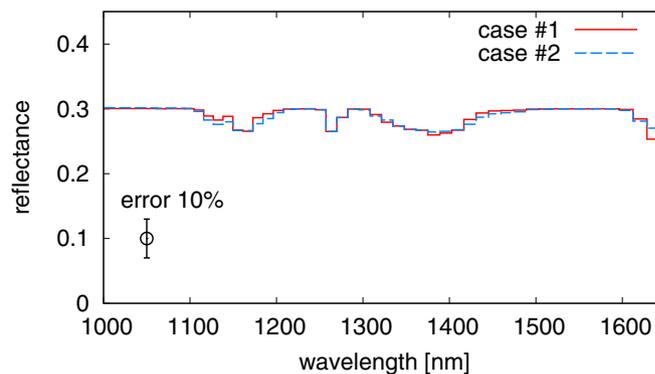


Fig. 2. Comparison between the low-resolution spectra ($R=100$) of cases 1 and 2. An uncertainty bar corresponding to $\text{SNR} = 10$, simply estimated as 10% of the average signal, is also shown at the bottom left.

the Poisson noise limit, considering only noise from the planet's photons. This condition gives us a maximum spectral resolution of

$$\begin{aligned}
 R_{\text{reflected}}^{\text{max}} &= \frac{\lambda}{d\lambda} = \frac{\lambda}{d\lambda} \frac{\dot{N}_{\text{reflected}} \Delta t}{\text{SNR}^2} \\
 &= \frac{\pi}{64\sigma hc} \underbrace{\frac{A r_p^2}{a^2}}_{\text{constants planet}} \underbrace{\frac{L_* \lambda^2 B_\lambda [T_*]}{T_*^4}}_{\text{star/band}} \underbrace{\Delta t \frac{D^2}{d^2}}_{\text{telescope}} \text{SNR}^{-2} \quad [5] \\
 &= 1683 \left(\frac{d}{10\text{pc}}\right)^{-2} \left(\frac{D}{6.5\text{m}}\right)^2 \left(\frac{\Delta t}{12\text{hrs}}\right) \left(\frac{\text{SNR}}{10}\right)^{-2}.
 \end{aligned}$$

In essence, this value tells how much we can possibly learn about the planet in the most idealized observation: not enough to distinguish the two spectra presented above.

It is important to point out that this calculation is likely to vastly overestimate the spectral resolution for several reasons. For example, we set the photon efficiency of the telescope and the spectrograph to 100%, which is clearly not realistic. Any sort of coronagraph will reduce the throughput dramatically. We further ignore all sources of noise except the photon noise from the planet. In a real observation, other sources of photon noise such as those from the host star and from exozodiacal light might dominate over the photon count from the planet. Astrophysical systematics (such as star spots) and instrumental systematics might dominate over all purely statistical noise sources. Nevertheless, the above result gives a firm upper limit on the spectral resolution we can achieve in the best case scenario for an Earth twin.

Indeed, future space observatories such as NASA's proposed Terrestrial Planet Finder (TPF) and the European Darwin mission (31) are expected to give spectral resolutions of only $\lambda/d\lambda \sim 50$ (32) in the most ideal scenario.[‡] Missions such as these will probably happen decades in the future. Even then, it seems highly unlikely that Earth-twin exoplanetary spectra will be achievable with significantly better SNR or spectral resolution than indicated in Fig. 2 in the foreseeable future.

Transiting Planet. If we are lucky enough to find a transiting Earth twin, would a transit spectrum allow a better opportunity to characterize the atmosphere than we can achieve in a high-contrast-imaging direct observation? The technical hurdles that must be cleared to obtain a transit spectrum are much lower because there is no need for a coronagraph to block the light from the star. As it turns out, however, the maximum achievable spectral resolution is worse, not better, in the case of a transit spectrum. Here we show why.

We will consider the same Earth twin as before. Let us further assume that the atmosphere has a scale height of $H = 7.6$ km and that $n_H = 5$ such layers will contribute to the spectrum, resulting in an effective scale height of $n_H H = 6.0 \cdot 10^{-3} r_p$. [At the resolutions that are possible, $n_H \lesssim 5$ is a reasonable assumption that applies to both jovian (33, 34) and Earth-like (35) planets, although Eq. 8 shows how the spectral resolution scales with n_H if the reader would like to explore other values.] The flux directed toward Earth during a transit and passing through the planet's atmosphere is then

$$F_{\text{transit}} = \frac{(r_p + n_H H)^2 - r_p^2}{r_*^2} F_* \approx 2n_H \left(\frac{r_p}{r_*}\right)^2 \left(\frac{H}{r_p}\right) F_*, \quad [6]$$

where r_* is the radius of the star. Using Eq. 3, this corresponds to a photon rate that is much larger than in the nontransiting case,

$$\dot{N}_{\text{transit}} = \frac{8n_H H a^2}{A r_p r_*^2} \dot{N}_{\text{reflected}} \sim 7.3 \cdot 10^3 \dot{N}_{\text{reflected}}. \quad [7]$$

Initially, this looks promising for the transiting case because the signal is now given by the rate of photons passing through the atmosphere, \dot{N}_{transit} . However, the signal-to-noise ratio is what matters, and the noise comes from the stellar flux, \dot{N}_* , which dominates over the flux through the planet's atmosphere by a factor of a million ($\dot{N}_* \sim 10^6 \dot{N}_{\text{transit}}$). Requiring the same signal to noise ratio as above gives us the condition $\text{SNR}^2 = 100 = (\dot{N}_{\text{transit}} \Delta t)^2 / (\dot{N}_* \Delta t)$ or, equivalently, the spectral resolution of

$$\begin{aligned}
 R_{\text{transit}}^{\text{max}} &= \frac{\lambda}{d\lambda} = \frac{\lambda}{d\lambda} \frac{\dot{N}_{\text{transit}}^2 / \dot{N}_*}{\text{SNR}^2} \Delta t \\
 &= \frac{\pi}{4\sigma hc} \underbrace{r_p^2 n_H^2 H^2}_{\text{constants planet}} \underbrace{\frac{L_* \lambda^2 B_\lambda [T_*]}{r_*^4 T_*^4}}_{\text{star/band}} \underbrace{\Delta t \frac{D^2}{d^2}}_{\text{telescope}} \text{SNR}^{-2} \quad [8] \\
 &= 12.2 \left(\frac{d}{10\text{pc}}\right)^{-2} \left(\frac{D}{6.5\text{m}}\right)^2 \left(\frac{\Delta t}{12\text{hrs}}\right) \left(\frac{\text{SNR}}{10}\right)^{-2}.
 \end{aligned}$$

Thus, we have shown that the expected spectral resolution of a transiting Earth twin is extremely small. We might not even be able to take a spectrum of the atmosphere at all.

In particular, this result shows that taking a spectrum of a transiting Earth-like planet will be worse than that of a directly imaged analog (putting the issue of building a coronagraph aside). Note that taking a secondary-transit spectrum will be extremely challenging as well because the noise is similarly inextricably dominated by the stellar photon flux.

Another factor adding to the limitations is that an Earth twin transits only once per year and for just 13 h, setting a firm upper limit on the maximum integration time. Also note that the transit probability for an Earth twin is $r_*/a \sim 1/200$. Thus, the closest transiting Earth twin is likely to be about $200^{1/3} \sim 6$ times farther away than the closest nontransiting Earth twin because 200 times the volume needs to be surveyed to find a transiting Earth twin. Because the distance enters the equation for the spectral resolution as d^{-2} , this further hurts our ability to probe the atmospheres of transiting Earth twins via their primary- or secondary-transit spectra.

Conclusions

In this article, we studied a false-positive scenario that could spoof biosignatures in spectroscopic observations of exoplanets. We showed that a detection of two chemical species in a spectrum could be caused by light originating from two different bodies. This is particularly important because it has been suggested that a chemical disequilibrium (which involves two or more species) could be a biomarker. However, an observation of two species does not show that they are in fact in the atmosphere of a single object (the planet). An almost identical spectrum would be measured if the two species are in the atmospheres of two different bodies, one of them being on the planet and the other on the planet's moon. Because it is impossible to resolve the moon-planet system (most likely we would not even know of its existence), the two spectra will be blended together, creating a spectrum with absorption bands of both species.

To test this scenario, we calculated synthetic spectra of an exoplanet and an exomoon, both with an atmosphere. Using molecular oxygen and methane as the chemical species of interest, we showed that with the spectral resolution that will be achievable with foreseeable technology, it will be impossible to tell the difference between the true-biosphere case where both

[‡]More information about TPF and Darwin can be found at <http://sci.esa.int/jump.cfm?oid=40843> and <http://exep.jpl.nasa.gov/TPF-I/astrophysics.cfm>.

species are in the same atmosphere and the false-positive case where one chemical is on the planet and the other is on the moon. Although our specific false-positive example involves oxygen and methane, the effect is the same for any two gases that are considered a biosignature when observed together. Our results show clearly that it is in general not possible to break the degeneracy between the two cases in a low-to-moderate resolution Earth-twin spectrum. The only case where we can safely conclude the coexistence of two species in one planet is the case in which the smooth continuum level is well determined and the sum of the absorption depths of two species exceeds 100%.

We considered a large, idealized space telescope and show that even using the most optimistic assumptions possible, the spectral resolution is unlikely to be higher than $R \sim 1,600$ for an Earth twin around a solar-type star. This is a fundamental physical limit just based on the photon noise. Unless we find a planet very close to us ($d \ll 10$ pc) or develop space telescopes significantly larger than considered in this article, the only way to tweak the maximum spectral resolution is by relaxing the assumption of an Earth twin around a solar-type star. For example, planets that are orbiting low-mass stars and/or are somewhat larger than Earth (so-called super-Earths) have larger planet-star size ratios and could allow improved spectral resolution (Eq. 8).

Another way to avoid the exomoon false-positive scenario altogether is to reconsider single-molecule biomarkers, which

do not suffer from the degeneracy presented here. Molecular oxygen (O_2) and ozone (O_3) have been suggested as potential single-species biosignatures. However, either or both of them might show up in the spectrum of an abiotic planet (36), so they do not definitively indicate life. Nevertheless, progress has been made in recent years on more rigorous constraints on the abiological nature of these gases (13).

From the perspective of the human race exploring space and searching for life on other worlds, the results of this paper are inconvenient, yet unavoidable: we will only learn the most fundamental properties of Earth twins unless we find one right in our solar neighborhood. It will be possible to obtain suggestive clues indicative of possible inhabitation, but ruling out alternative explanations of these clues will probably be impossible for the foreseeable future. Because our results are based on fundamental physical laws, they are unlikely to change, even as technology advances. The logical step forward is to widen our search for life in the universe and include objects, in the solar system and beyond, that are less similar to Earth but more easily observable.

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