OBSERVATIONS OF TERRESTRIAL EXOPLANET ATMOSPHERES FOR BIOSIGNATURES: STATE OF SCIENCE

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ABSTRACT

Exoplanetary science remains at the forefront of astronomical research, with the atmospheres of terrestrial planets remaining an elusive – yet integral – component in the search for life. This paper highlights the historical strides and current state of the atmospheric spectroscopy of terrestrial atmospheres – the science of which consists of a great deal of unknowns. Since the discovery of the first exoplanet atmosphere in 2002, water and basic organic compounds have been located within the infrared spectra of many "hot Jupiter" exoplanets and a few "super-Earth" candidates. And only three years ago, water vapor was first found in the atmosphere of a terrestrial Earth-analog exoplanet (Tsiaras et al. 2019). Many astronomers favor studying "Earth as an exoplanet" given its atmosphere's obviously ideal composition and ability to host life – analysis of the "Earthshine" infrared spectrum can reveal key features indicative of life that can be compared to other, less-resolved exoplanet spectra. The future of the field will contain even more certain and fruitful discoveries than its past, with the science to be bolstered by the ongoing discovery of new exoplanets and the analysis of their spectra with powerful new observatories.

INTRODUCTION

Since the discovery of the first exoplanet orbiting a main-sequence star in 1995 (Mayor & Queloz 1995), astronomers and astrobiologists have gazed beyond our solar system in search of other worlds – worlds that could host extraterrestrial life. A key ingredient to the persistence of life (or life as we know it) is the presence of a thick atmosphere with an appropriate composition for life. We have yet to work out the entire dynamics of our *own* atmosphere or trace the evolution of its chemical composition fully enough to determine how life evolved on Earth, but astrobiologists apply the prevailing theories of the *overall* requirements for life to our study of other terrestrial planets. Our theory on the "origin of life" involves the exchange of a thin atmosphere, consisting of residual hydrogen and helium gas from its proto-stellar progenitor, for a thick atmosphere consisting of nitrogen and carbon compounds via its delivery by meteorites. Small anaerobic, single-cellular life would accelerate the production of complex molecules, and the eventual development of plants is thought to be responsible for the ubiquity of oxygen on our planet, required for animal life.

Naturally, there are *many* more pieces to the puzzle of evolution that humans must work out, but astronomers can observe other planets' atmospheres for their chemical composition to determine if it contains the overall ingredients or hallmarks of life – hallmarks which are a subclass of *biosignatures*. Exoplanetary atmospheric science is done entirely with spectroscopy, where a small fraction of scattered infrared light that has passed through a thin sliver of an exoplanet's atmosphere reaches observers along with the planet's spectrum. Upon resolving this spectrum, certain biosignatures can be searched for based on the emission patterns of their associated chemical components.

On Detections

Exoplanets are detected by a variety of methods, each of which yields different information about the target planet. Detection by *transit*, for example, occurs when the incoming flux from a star dims as a result of a planet passing along our line of sight of the star (Figure 1). The fraction by which the light is reduced is directly proportional to the planet's radius, and the length of the transit is related to the planet's distance to the star and mass (which can be easily proven using Kepler's third law). As a result, this method of detection usually favors very large planets orbiting extremely close to their host stars (usually M-dwarfs), a subclass known as "hot Jupiters." These planets are, via their high temperature and gaseous composition, inherently inhospitable to life as we know it. The first exoplanet discovered to have an atmosphere, HD 209458b, was one such hot Jupiter; additional dimming in its photometric measurements were attributed to the presence of sodium in the planetary atmosphere (Charbonneau et al. 2002).

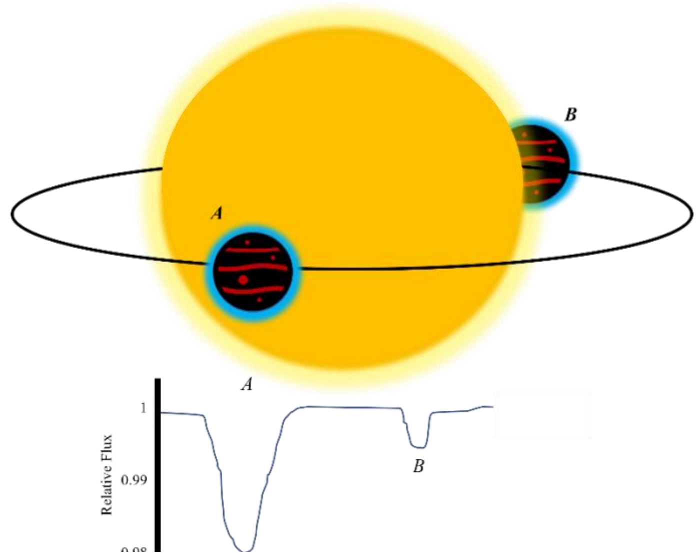

***Figure 1** | Detection via Transit.* Primary eclipse "A" occurs as the planet transits across the star, creating a dim in the flux as measured by an observer located far away and aligned with the planet's orbit. Some starlight passes through the planet's atmosphere, picking up its spectral features. During secondary eclipse "B", the planet passes behind the star, reducing the total incoming flux but revealing the total spectrum of the star alone.

A sizable number of detected exoplanets fall into two categories that may be able to host life: Neptune-sized "Ocean Worlds" and short-period "super-Earths" that have a radius near or above that of Earth. Most detected exoplanets that are potentially habitable are close to their stars and have a large planet-to-star radius ratio, which allows for easy detection via transit, radial velocity (which attributes the "wobble" of a star to an orbiting planet), or other means. Finding more Earth-analog planets, as well as other small terrestrial worlds, remains a frontier in exoplanet science.

This review paper will focus on the general advances in exoplanet atmospheric spectroscopy over the past three decades, biosignatures that astronomers have obtained from our small sample of terrestrial Earth-analogs via atmospheric spectroscopy, and the consideration of "Earth as an exoplanet" as a means of exploring this scientific frontier.

Discussion

Exoplanet Atmospheres: A Brief History

In 2010, Drs. Sara Seager and Drake Deming published a review paper in the Annual Review of Astronomy and Astrophysics (ARA&A) explaining the state of science in the study of exoplanet atmospheres (Seager & Deming 2010). In their paper, the study of planetary atmospheres is discussed at length, while *this* paper summarizes the key advances highlighted by this paper that are relevant to the study of terrestrial Earth-analogs. However, it is useful to recount a generalized scientific history of exoplanet atmospheric science to provide context for our discussion.

Hot Jupiters have comprised the majority of atmospheric detections due to their high temperatures (and high infrared intensity) and close proximity to their host stars (Seager & Sasselov 1998) (e.g., Figure 2). After the detection of first exoplanet atmosphere in HD 209458b (Charbonneau et al. 2002), many theory papers were published that attempted to model the atmosphere of these planets, and the *Spitzer* Space Telescope was used extensively in the detection and infrared atmospheric observation of the hot Jupiters.

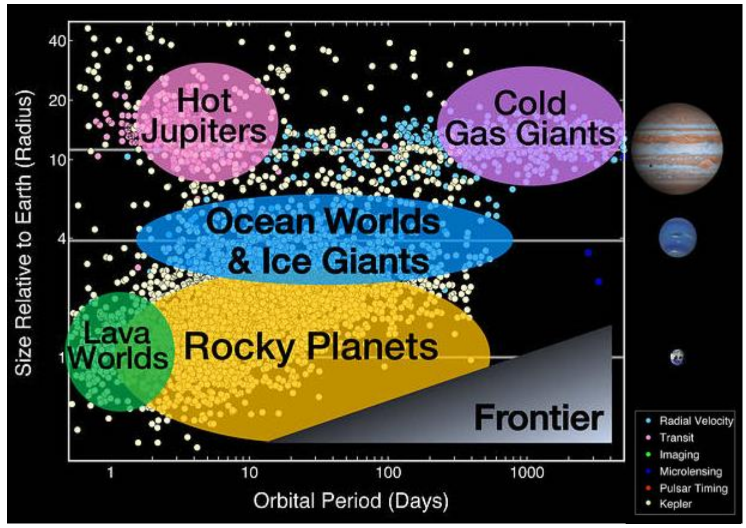

***Figure 2** | Distribution of detected exoplanets and their categories*. Most detections by transit favor Hot Jupiters due to their close proximity to their host stars and large size. Other methods are used to discover planets of varying mass and types, though long-period low-mass planets remain elusive on all frontiers. *Adapted from Chen 2017*.

While direct imaging is one obvious route in detecting exoplanets, it turns out that the transit method has proven a far more successful method of finding and categorizing exoplanets and their atmospheres. When a planet passes in front of its star, some starlight passes through the planet's atmosphere, and the incoming flux will contain the spectral features of its planet's atmosphere. The planet's spectrum alone can be obtained, then, by subtracting the spectrum of the star alone (obtained outside of transit or, for planets with circular orbits, during "secondary eclipse" when the planet passes behind its host star) from that of the planet-star system (obtained during transit) (Seager & Deming 2010). Utilizing chemical models and based on the radiative transfer equation (the solution of which is influenced by clouds), the composition of the atmosphere can be obtained.

A major stride toward the identification of molecules within exoplanet atmospheres came when water was identified within the transmission spectrum of HD 189733, a hot Jupiter (Swain et al. 2008). Atomic sodium, methane, carbon monoxide, and carbon dioxide are also staples in hot Jupiter atmospheres (Seager & Deming 2010); the detections of these models are considered largely model-independent because they agree with *Hubble Space Telescope* and *Spitzer* data and rely only on molecular absorption information. However, the relative abundances of these molecules are poorly constrained (e.g. Madhusudhan & Seager 2009), limited by the number of observations of hot Jupiters available (relative to the amount of model parameters required in spectroscopy). Hot Jupiters have also been shown to display atmospheric haze, likely have a strong day-night temperature gradient due to tidal locking, and experience atmospheric hydrogen escape (Seager & Deming 2010).

Instrumental difficulties have been a challenge within the field. *Spitzer* and *Hubble* both contain systematic errors (and *Hubble* is located in low-Earth orbit) that influences the thermal readings of these exoplanets; future improved space telescopes like *James Webb* are likely to remedy/mitigate these errors. Additionally, the turbulence of Earth's atmosphere in ground-based observations and various disagreements within scientific literature in the field has made progress in the characterization of exoplanet atmospheres somewhat stifled, despite increasingly high interest in these worlds.

Since Seager & Deming's 2010 publication, several more great strides have been made in the analysis of the atmospheric composition of exoplanets. In 2013, several more exoplanets were discovered to contain water in their atmospheres (e.g., Demory *et al.* 2013, Northon 2013), and in 2014, water vapor was found in the atmosphere of the Neptune-sized exoplanet HAT-P-11b; the first time these molecules have been found in a relatively small exoplanet (JPL 2014). In 2014, studies were also undertaken to resolve the thermal structure of an exoplanet's atmosphere, and little heat redistribution was found in the hot Jupiter WASP-43b (Stevenson *et al.* 2014). A 2015 study examined the abiotic methods of production of atmospheric oxygen on planets in the habitable zones of M-class stars; the results of their study found that water loss as a result of high ultraviolet flux and runaway greenhouse effects can make these “super-Earths” uninhabitable, ruling oxygen out as a biosignature alone (Luger & Barnes 2015). And in 2015, it was found that the exoplanet WASP-33b (the hottest exoplanet discovered (Shiga 2011)) has a stratosphere – atmospheric layering that was caused by differential heating due to different chemical compounds in the hot Jupiter’s atmosphere (Haynes *et al.* 2015).

Exoplanets alone comprise a *vast* category of science, from modeling and analyzing their atmospheres to understanding how their orbital dynamics contribute to their overall habitability. Perhaps the most intriguing exoplanets to study, though, are the Earth-analogs and super-Earths (or mini-Neptunes); the subclasses of exoplanets imagined to contain vast oceans and teeming with the possibility of containing life. In recent years, great progress in observing these planets’ atmospheres have been made, and this will be the focus of the next section’s discussion.

Super-Earth Atmospheres: What We Know

The short answer is not very much. Terrestrial exoplanets and their associated astrobiology remain one of the most elusive fields of astronomy because of the scarcity of observational samples which can be studied. The first successful analysis of a super-Earth’s atmosphere came in 2016, when an atmosphere composed of hydrogen and helium was discovered around 55 Cancri e (Tsiaras et al. 2016) (ESA/Hubble Information Centre 2016). The team of astronomers, led by Angelos Tsiaras from the University College London, used observations from *Hubble* and a specialized pipeline to observe the atmosphere; they also detected a significant amount of hydrogen cyanide in the planet’s atmosphere, indicating that it has a particularly high carbon-to-oxygen ratio. Such an atmospheric composition makes this planet a very exotic place, though certainly not the kind that could host life. The planet orbits very close to its star, and likely has surface temperatures upwards of 2000 K; 55 Cancri e is more aptly dubbed with the popular nickname “lava world” than it is a “super-Earth.” Nonetheless, the discovery of its atmosphere marks a major stride in the atmospheric analysis of terrestrial atmospheres.

In 2019, the next great feat of terrestrial exoplanet atmospheric science was reported in *Nature Astronomy*: the discovery of water vapor in the atmosphere of K2-18b, an eight-Earth-mass planet orbiting in the habitable zone of its host star (Tsiaras *et al.* 2019). Prior to the 2019 study, no spectroscopic signatures of water had been detected in terrestrial exoplanets (even, as a side-note, for the TRAPPIST family of exoplanets a system of several exoplanets located in their stars habitable zone that are relatively close to Earth). This is due to their small size and cold temperature (and low infrared emission). The observations were likewise recorded using the *Hubble* Space Telescope’s Wide Field Camera 3 and were completed by a team led by A. Tsiarias, who called the planet the “best candidate for habitability that we know right now” (Greshko 2019). The same results were also obtained in an independent study lead by Björn Benneke (Benneke *et al.* 2019), who also predicted the presence of water vapor and clouds in the planet’s mid-atmosphere, supplementing their results with *Spitzer* and *K2* (an extension of the original *Kepler* mission). Though habitability around M-dwarfs indeed remains a subject of debate among astrobiologists (due to the possibility of tidal locking in close orbit and a large degree of solar activity), the discovery marks a milestone in the atmospheric science of these planets.

We are still very much at the frontier of this vein of research; considering it was only three years ago that the first signature of water was discovered on an Earth-like planet (and the COVID-19 pandemic has hindered progress in this field of astronomical science). Because the observational sample is low, and observations of these planets are clearly hard to obtain, much of exoplanet science relies on the construction of computer models that seek to explain the origin and composition of these types of planets. While this work is largely outside the scope of this review (which focuses on the state of science of *observed* atmospheric biosignatures), some recent papers are worth mentioning. A paper published in 2021 takes a novel approach to analyzing the formation of primary exoplanet atmospheres via outgassing: by testing it on meteorites, which are representative of the building blocks of terrestrial planets. By heating the carbonaceous chondrites to almost 1500 K and analyzing the samples with a mass spectrometer, a water-rich atmosphere with substantial carbon compounds (CO and CO_2) and some hydrogen compounds (H_2 and H_2S), the study provides some context and insight into what the initial atmospheres of forming Earth-analog planets (including ours!) might have looked like (Thompson *et al.* 2021). The formation of Earth-like planets has been an especially hot topic among astronomers who wish to examine the "Origins of Life" subfield of astrobiology, which is concerned with the methods via which Earth and other terrestrial planets developed life (and as a means of finding it). For example, a 2020 study led by Mariah G. MacDonald focuses on simulating systems of super-Earths "in situ," examining which orbital parameter of these systems best leads to habitability. Atmospheric considerations are also of key importance to these results; not only does the formation of atmospheres depend on the rocky composition of the planets, but collisions between them can result in stripping of the planets' atmospheres in ways that reduce their detectability (MacDonald *et al.* 2020).

Biosignatures: The Frontier

Finding and classifying additional "biosignatures" – the hallmarks of life – in a planet's atmosphere remains at the forefront of extraterrestrial atmospheric science. Instrumentational development is currently underway to better analyze these Earth-like exoplanets; projects such as the Habitable Exoplanet Observatory (HabEx) and the Large UV/Optical/IR Surveyor (LUVOIR) will directly image these super-Earths in ways that minimizes scattering to obtain clear atmospheric data (Science & Technology). The *James Webb Space Telescope*, which is now in its calibration phase, will detect spectroscopic biosignatures from various atmospheric compounds. For the meantime, much of this field has been dedicated to studying the atmospheres of planets and moons within our own solar system. These objects, which are closer and easier to analyze with telescopes or via probes, may serve as a laboratory for what the atmospheres of "potentially habitable" exoplanets may look like and will help astronomers better interpret the signals received from extrasolar planets. Take the atmospheric modeling of Venus as an example; although Venus is the classic example of the "runaway greenhouse," it is an Earth-analog planet in every other way; it is feasible that other exoplanets that orbit in their star's habitable zone (but are too hot to support life) could have developed in the way of Venus (or have done so like Mars, the "icehouse"). It also teaches scientists to be wary of false alarms of biological life. When phosphine was found on Venus in 2020, many became excited at the strange prospect of life on the planet; it was later found out to be a trace gas, and most likely attributed to volcanic activity (Friedlander 2021).

The best laboratory for studying terrestrial exoplanets, however, doesn't even require another planet. According to many astronomers, it's Earth; and when trying to analyze planets that could host extraterrestrial life, the a key candidate for study is the one on which we live.

Earth as an Exoplanet

It goes without saying that Earth's atmosphere contains the perfect chemical balance and thermal structure to support life. Oxygen and ozone, which together compose of about 21% of the gases in Earth's atmosphere, are robust biosignatures (e.g., Leger et al. 1993), and although there is some debate surrounding oxygen's utility as a biosignature alone, its concentration in Earth's atmosphere is far higher than anything producible by abiotic processes. Like on Earth, a terrestrial exoplanet with a large and replenishing supply of O_2 is likely to host plant or bacterial life. Other spectral features, like CO_2 and CH_4, reveal information about a planet's atmosphere and biotic processes, respectively.

Taking the spectrum of our own planet requires inventive methods. These include sending probes millions of miles away to take a spectrum of our planet, as was done by the Mars Global Surveyor (Pearl & Christenson 1997) or with NASA's *EPOXI* spacecraft (Ballard *et al.* 2009). However, we can obtain this information even without these probes using a form of light called "Earthshine" – the reflection of the sunlight-illuminated Earth's light from the night side of the Moon. While most Earth-orbiting infrared satellites only see a small patch of Earth's surface at a time, the spectrum obtained from the "Earthshine" data is representational of Earth as viewed as an exoplanet (Turnbull et al. 2006). Hemispherical flux integration can be done over the spatially unresolved data to obtain a spectrum representative of our planet's reflection.

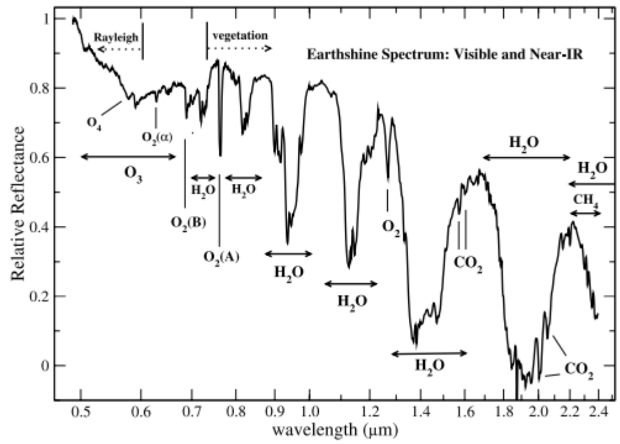

Figure 3 *| Earthshine Spectrum. Adapted from Figure 7, Turnbull et al. 2006.*

The reflectance spectrum (Figure 3), adapted from the image presented in Turnbull et al. 2006, is a composite of the authors' 0.8-2.4 µm data and 0.5-0.8 µm data from Earthshine measurements taken by Woolf *et al.* 2002. Many salient features present themselves upon analysis of the spectrum; not only do water, carbon dioxide, methane, oxygen and ozone have significant absorption features, but several structures particular to our planet emerge. Rayleigh scattering from the particles in our atmosphere marks the lower-wavelength range of the spectrum, and – most pertinently a biosignature – "vegetation" is marked with an order-of-magnitude rise in albedo at around 750 nm. Vegetation has a strong spectroscopic reflection feature known as the "red edge", a cooling mechanism in leaves to prevent overheating (Seager *et al.* 2005). The spectral feature, which would be strongest on planets with low cloud cover and large continents, is clearly indicative of life, but will have to be interpreted with caution. Several mineral reflectance edges have a similar strength and slope as the red edge. Additionally, any direct image or transit observations of Earth-analog exoplanets will not be able to spatially resolve the planet's surface to identify continents or clouds; several observations will be needed to distinguish surface vegetation biosignatures from atmospheric biosignatures. Thus, as the planet rotates, the spectral signal associated with the red edge should change accordingly (Seager & Deming 2010).

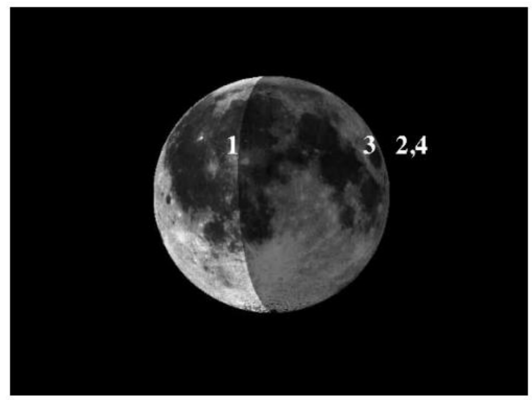

Figure 4 *| The Moon on 11/18/2003 when the earthshine reflectance spectrum was taken.* A CG-rendition. Points 2 and 4 include the night sky taken as a background for the spectra, Point 1 as the light/sun-reflecting side of the moon, and Point 3 as the dark/Earth-reflecting side of the moon. *Adapted from Figure 1, Turnbull et al. 2006.*

In the analysis of biosignatures, astrobiologists do not worry about *how* life produces atmospheric gases; an assumption of the field is that it *does* by metabolic processes, and that the byproducts of metabolism can be used to detect them. Earth's spectrum has a prominent oxygen absorption feature at 0.76 µm, and contains far more oxygen than would be present via abiotic thermodynamic processes. According to Seager, a key element in studying biosignature gases involves those produced in reduction-oxidation (redox) reactions. Oxygen, an oxidized element, and methane, a reduced species, are both abundant in Earth's atmosphere; however, the latter is far less concentrated and weaker spectroscopically. Conversely, an early Earth from billions of years ago would have seen vastly abundant CH_4 (produced by bacteria) but only trace amounts of abiotic oxygen; exoplanet spectra that contain pairs of species severely out of redox equilibrium would present a potential biosignature (Seager & Deming 2010).

In fact, methane has recently fallen under even greater consideration as a key biosignature of interest. One of the few terrestrial biosignature gases that JWST will be able to detect, methane was also a prominent molecule in the atmosphere of the Archean Earth, so its detection in terrestrial atmospheres makes those planets candidates for potentially habitable planets (Thompson et al. 2022). According to Thompson *et al.,* who published an article in 2022 supporting the further consideration of methane as a biosignature, although CH_4 is often considered an "ambiguous" indicator of life due to its ability to be produced abiotically, methane has a short photochemical lifetime (under one million years) on rocky planets in their habitable zones. Especially in the presence of other oxidizing chemicals (which can also be biosignatures), methane is quickly depleted in the atmosphere and thus requires steady production – a flux that is most easily produced biogenically on Earth. Furthermore, abiotic methane-generating processes often produce other molecules or atmospheric signatures that can be used to rule biota out. The authors present criteria for CH_4 as a biosignature, the investigation of which JWST will greatly aid (Thompson et al. 2022):

1. The planet's bulk density is largely terrestrial
2. Atmosphere has a high molecular weight and is oxygen-poor,
3. Its host star is comparatively old.
4. Atmospheric CH_4 abundance is high (replenishment exceeds abiotic processes)
5. Atmospheric methane is accompanied by high CO_2 but little CO.

As must remain abundantly clear, however, one must take the *entirety* of atmospheric data into account before jumping to conclusions regarding biosignatures. Additionally, it is becoming more and more apparent to astronomers that Earth's atmosphere does not have the only composition that could foster life. Research into other organic compounds that are less abundant on Earth but that are rapidly produced by bacteria and other lifeforms as a potential environment-determined biosignature is underway (Seager & Deming 2010). Finally, life may not need be restricted to only forming in water and via carbon; the presence of a liquid solvent and molecules that can support many covalent bonds – even at high temperatures – could open up entirely new avenues and planets in which life can persist (Baross et al. 2007).

CONCLUSION

The infancy of exoplanetary science as a field – especially on its astrobiological front – is simultaneously daunting and encouraging to twenty-first century astronomers. The scientific progress on uncovering extraterrestrial biosignatures from exoplanets described in this paper isn't just a snapshot of the *current* state of science, but a representation of the field in its three-decade entirety. Only *three years* ago did Angelo Tsiaras and his team report the first discovery of water vapor in the atmosphere of a terrestrial exoplanet via spectroscopic methods (2019); however, the presence of liquid water on exoplanets via their *density* (as a mere function of mass and radius, which can be found by transit observations) has long been inferred during their prospective classification. But life as we know it depends on far more than liquid water alone, but likely a precise arrangement of planetary air pressure and composition requirements that are satisfied by a sufficiently thick atmosphere.

The first exoplanetary atmosphere to be discovered belonged to a hot Jupiter (Charbonneau et al. 2002), the subclass of exoplanets that tends to dominate detections due to selection effects. Since then, water and other biologically-friendly molecules have been discovered in the transmission spectra of these planets' atmospheres; the detections of these compounds are significant but the relative abundances of them are very poorly constrained (Madhusudhan & Seager 2009). It is up to future research to reduce the uncertainties of these compound detections and develop more reliable models for the infrared spectra of exoplanets; the most significant contributor towards these goals will likely be the rapidly increasing rate of exoplanet detection and the identification of planets that can be studied closely. New missions such as the *James Webb Space Telescope* will enable great strides in the in-depth study of terrestrial planets and their atmospheres (JWST).

Since the major review of exoplanet atmospheric science conducted by Seager & Deming (2010), several more exoplanets have been discovered to have water in their atmospheres. Starting in 2016, the realm of super-Earth atmospheres was entered with the analysis of 55 Cancri e by Tsiaras et al. (2016), and water was discovered by the same team on the terrestrial exoplanet K2-18b in 2016. One consensus among many astrobiologists is the utility of studying Earth as the "ideal" terrestrial exoplanet candidate; given its clear ability to support life, focusing on the mechanisms by which Earth supports life and studying our atmosphere's own infrared spectrum provides a laundry list of features that astronomers can search for in other planets.

The future of astrobiology and exoplanetary science is as uncertain as their guiding question regarding the existence of life in the universe. Repeated observations of terrestrial exoplanets to obtain highly-resolved infrared spectra, which can reveal the molecular composition of their atmospheres and the presence of biosignatures, should be a key science goal for astronomers. Because it is unlikely that humans will send a probe or spacecraft of any kind to any extrasolar planet in the next century for direct atmospheric analysis (rather, intrasolar objects will remain the focus of human space exploration), the construction of a larger range of multiwavelength telescopes/spectrometers and the focus on imaging and categorizing a broader diversity of exoplanets should be a main area of investment. If anything is made apparent by this paper, it is that this field is limited only by the technology and detections available to its researchers; the desire to learn about extraterrestrial atmospheres and to engage with the search for life is strong, and more and more young astronomers continue to enter the field. A defining characteristic of terrestrial exoplanetary atmospheres, then, is how much we *don't* know given the novelty of the field. With time and discovery, though, the field may soon have far more definite examples of viable models *and* observed samples of atmospheres, teaching us more about the strange new worlds beneath them.

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