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Exploring strange new worlds with high-dispersion spectroscopy

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Chapter 1

Introduction

The contemplation of planets beyond Earth and the Solar System is recorded to stretch back millennia, though perhaps not always phrased in such precise terms. For instance, the Greek philosopher Epicurus (c. 341–271 BCE) mused that there exist "an infinite number of worlds, some like this world, others unlike it" (Laertius & Hicks 2015). Such openness to worlds unlike our own is rather prescient, and foreshadows the themes of investigating unfamiliar, often extreme, objects and pushing observational and theoretical capabilities that are recurrent in the more recent scientific study of exoplanets — those worlds beyond our Solar System. Over the past three decades, many such unfamiliar worlds have been discovered and explored in the pursuit of answers to the key questions of exoplanetary science, such as *What kinds of planets exist beyond the Solar System? Of what are these planets made? How did they form?* and *Is there life beyond Earth?*

Indeed, the first exoplanet discovered orbiting a main-sequence star proved to be one of these extreme objects. By measuring periodic Doppler shifts in the radial velocity of the solar-type star 51 Pegasi, Mayor & Queloz (1995) inferred the presence of the orbiting planet 51 Peg b (see Figure 1.1). This radial velocity method of exoplanet detection provides both the minimum mass of the perturbing planet and the orbital period. While the derived mass of about half that of Jupiter for 51 Peg b was not surprising, the same could not be said of the roughly four-day orbital period. For comparison, the closest orbit in the Solar System — the only other main-sequence planetary system known at the time — is that of Mercury lasting 88 days.

This extreme discovery, with no analogue in our own planetary system, immediately challenged and subsequently advanced the contemporaneous understanding of planet formation. Astonishment is readily evident in the discovery paper, in which Mayor & Queloz (1995) tried to reconcile the rather hot 0.05-AU orbit of 51 Peg b with the expectation that gas giant planets form in icy regions of protoplanetary disks, beyond several AU. Confronted with this new class of so-called hot Jupiters, planet formation theory developed further, and it is now accepted that planet migration is capable of decaying a gaseous planet's orbit from several AU to a few hundredths of an AU (e.g., Lin et al. 1996; Armitage et al. 2002). The extreme radiation environment of such planets also spurred studies into the nature of their atmospheres. Particular interest has been paid to how strong stellar irradiation impacts the chemistry, structure, and dynamics of hot Jupiters (e.g., Showman & Guillot 2002; Fortney et al. 2008; Showman et al. 2009, 2013) — a topic that will recur frequently throughout this dissertation.

Observationally, the discovery of 51 Peg b and similar hot Jupiters gave way to a series of survey programs to discover more exoplanets. The afore-

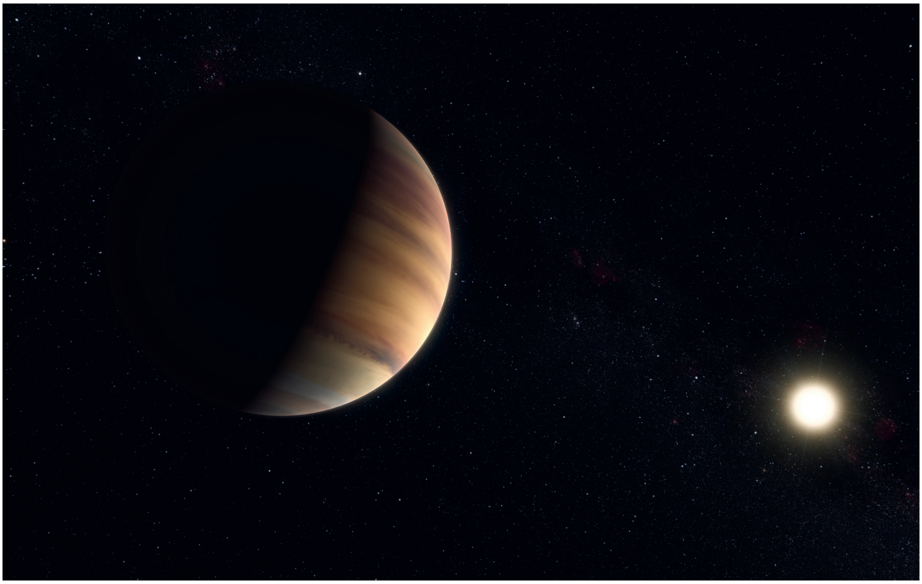

Figure 1.1. Artist's depiction of the archetypal hot Jupiter 51 Peg b. In addition to being the first exoplanet discovered orbiting a main-sequence star, 51 Peg b represents an extreme class of planet with no analogue in the Solar System. Image credit: ESO/M. Kornmesser/Nick Risinger (skysurvey.org).

mentioned radial velocity method, in which an orbiting planet is inferred by its gravitational perturbations of the host star's radial velocity, has been successfully employed using several ground-based spectrographs (e.g., HARPS/La Silla, HIRES/Keck), leading to the discovery of more than 900 planets. The success of this technique was later surpassed by transit surveys, in which fortuitously-aligned planets are detected from periodic decreases in stellar light as they orbit in front of their host stars. Following the successful application of this technique by Charbonneau et al. (2000) to the known hot Jupiter HD 209458 b, various ground-based (e.g., TrES, HATNet, WASP) and space-based (e.g., CoRoT, Kepler, TESS) surveys set out to detect planets from their transits. To date, in excess of 4900 planets have confirmed detections[1], with over 75% discovered using the transit method. In combination, the radial velocity and transit methods have provided 95% of all exoplanet discoveries.

[1]NASA Exoplanet Archive (https://exoplanetarchive.ipac.caltech.edu)

In addition to detecting exoplanets, radial velocity and broadband transit studies allow basic analysis of planetary bulk properties. Being a gravitational effect, radial velocity analyses provide a lower limit on the planet mass $M_\mathrm{p} \sin i$, dependent on the inclination angle i between the orbital plane and the sky plane. On the other hand, the transit technique constrains the radius ratio of the planet and star $R_\mathrm{p}/R_\star$ and the inclination. In those cases where both radial velocity and transit observations are performed, and the stellar properties (e.g., stellar radius) are well known, the average planetary density may be derived. This can provide a basic characterization of the planet, for instance, as a gaseous or rocky body. Such basic information is valuable for understanding the diversity of planet types. However, to more fully understand the characteristics of exoplanets, spectroscopic studies specifically probing their atmospheres are required.

1.1 Methods for probing exoplanet atmospheres

Studies to detect and characterize the atmospheres of exoplanets developed nearly contemporaneously with the first discoveries of these objects. Soon after the first broadband transit detection, Charbonneau et al. (2002) used a similar method to detect the first exoplanet atmosphere. By comparing the amount of light blocked by the hot Jupiter HD 209458 b during transit in different visible wavelength bands, they found excess absorption by the planet in the wavelength range containing the sodium D-lines at 5893 Å. Charbonneau et al. (2002) were thus able to infer the presence of sodium in the atmosphere of HD 209458 b.

Since then, the spectroscopic study of exoplanet atmospheres has advanced and expanded to observations across various wavelength ranges, spectral resolutions, and orbital phases, as well as planets spatially resolved from their host star. These various methods contribute complementary information about planets and their atmospheres.

1.1.1 Transit spectroscopy

Transit spectroscopy involves observing a planet at different wavelengths as it passes in front of its host star and attenuates a fraction of the stellar light. In addition to the broadband attenuation due to, for instance, the rocky core of a terrestrial planet or optically-thick atmospheric layers of gaseous planets, the optically-thin limb of the planetary atmosphere imprints a wavelength-dependent extinction due to its constituent spectroscopically-active species. As

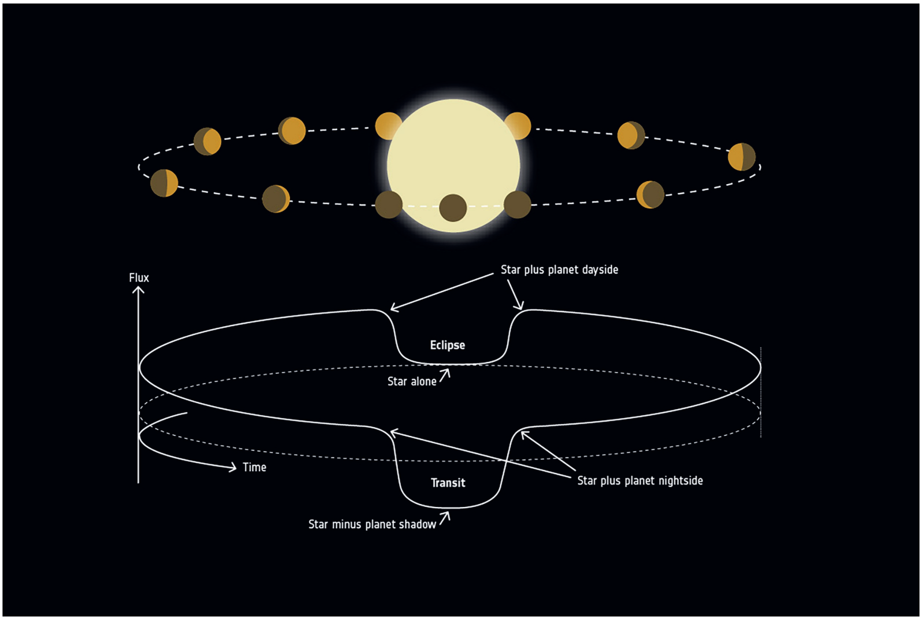

Figure 1.2. Flux variations in a transiting planetary system over the course of an orbit. The upper diagram shows how a greater fraction of the hotter planetary dayside is visible at orbital phases adjacent to secondary eclipse. The lower diagram plots the corresponding flux modulations. Image credit: ESA.

a result, the amount of light blocked — and thus the effective radius of a planet — will exceed the broadband radius for wavelengths corresponding to spectroscopic transitions. It is therefore possible to infer the presence of specific chemical species based on a transit spectrum.

Since transit spectroscopy probes the extinction of stellar light, rather than the emergent spectrum of the exoplanet, such observations are less sensitive to the vertical thermal structure of the planetary atmosphere than emission spectroscopy (see Section 1.1.2). Instead, by virtue of the observation geometry, transit spectra are most useful for probing the composition of the limb regions between the day- and nightside of the planet, as well as the atmospheric dynamics at these regions.

1.1.2 Emission spectroscopy

In contrast, emission spectroscopy measures the emergent flux of exoplanetary atmospheres. For hot Jupiters, such measurements probe the dayside atmosphere since these planets are expected to be in synchronous rotation and, as a result, the same side of the planet continuously faces the host star. This sets up a relatively strong temperature contrast between the dayside and nightside. As shown in Figure 1.2, as the planet orbits, various fractions of the hotter, brighter planet dayside are visible from Earth. Taking spectroscopic observations during the out-of-transit phases of the orbit allows the dayside planetary emission spectrum to be derived.

Since emission spectroscopy measures the flux from the planetary atmosphere itself, in addition to revealing the atmospheric composition, it provides constraints on the vertical temperature structure. Depending on the opacity, the spectrum will probe a different atmospheric layer at each wavelength, and thus a different point in the atmospheric temperature–pressure (T–P) profile. Fitting observed emission spectra with models that link T–P profiles to emergent spectra enable a characterization of the vertical temperature structure (e.g., Stevenson et al. 2014).

1.1.3 Imaging spectroscopy

Emergent spectra can also be measured for planets that are spatially resolved from their host stars. These directly-imaged planets are usually first detected with photometric and low-dispersion spectral observations in the near-infrared using some combination of physical obstruction (e.g., coronagraphs) and processing procedures to suppress the stellar flux (e.g., Marois et al. 2008; Lagrange et al. 2010; Chauvin et al. 2017). Planets manifest as temporally-persistent flux sources. Follow-up observations conducted over wider spectral ranges and at higher spectral resolutions enable more detailed analyses of planetary spectra (e.g., Konopacky et al. 2013; Barman et al. 2015; Petit dit de la Roche et al. 2018; Hoeijmakers et al. 2018b; Petrus et al. 2021).

Due to current observational limitations, this technique is most sensitive to widely orbiting ($\gtrsim$10 AU) planets, and in particular, young or still-forming planets. This is because planets are expected to cool on timescales of billions of years after their formation (e.g., Phillips et al. 2020), leading to a higher planet-to-star flux contrast for younger objects. For directly-imaged planets, it is not practical to derive mass and radius information from transit or radial velocity studies due to their relatively long orbital periods of tens of years. Therefore, bulk properties such as mass, radius, and temperature must be derived using other techniques, for instance, analysis of the planet's luminosity and spectral energy distribution (e.g., Marois et al. 2008), or astrometric analysis of planet-induced perturbations of the proper motion of the host star (e.g., Snellen & Brown 2018).

1.1.4 Spectral resolution

The spectroscopic methods of observing exoplanet atmospheres presented and discussed in the preceding sections can be conducted at various dispersions. This is often quantified by the resolving power $\mathcal{R} = \lambda/\Delta\lambda$, where λ is the wavelength of observation and $\Delta\lambda$ is the spectral resolution. Higher values of $\mathcal{R}$ indicate a finer resolvability along the spectral axis, allowing greater differentiation of spectral features and velocity shifts. Spectra are generally referred to as low resolution for $\mathcal{R} < 10^3$, medium resolution for $\mathcal{R} \sim 10^3$, and high resolution for $\mathcal{R} \gtrsim 10^4$.

The main motivation for using medium- and high-resolution spectroscopy is the ability to resolve individual spectral lines, for instance, in molecular bands. Using model-matching techniques such as cross-correlation (e.g., Snellen et al. 2010) and atmospheric retrievals (e.g., Brogi & Line 2019), the signals of the unique set of individual lines of a chemical species, or blend of species, in high-dispersion data can be combined. For this reason, chemical detections based on high-resolution spectroscopic analysis are often considered more unambiguous than those using low-resolution spectroscopy, though quantifying the robustness of high-dispersion detections is still a matter of discussion (Cabot et al. 2019).

A corresponding critical advantage of high-dispersion spectroscopy is the increase in velocity resolution. Current high-resolution spectrographs typically have $\mathcal{R} \sim 10^5$, corresponding to velocity resolutions of $\sim$1 km s^{-1}. This allows the changing radial velocity of the exoplanet to be resolved as it orbits, which assists in differentiating the planetary atmospheric signal from that of the host star and Earth's atmosphere. This contributes to the greater unambiguity of high-resolution detections. As will be discussed in subsequent sections, this more precise velocity resolution enables the study of dynamics within planet atmospheres.

1.2 Studies of exoplanet atmospheres

Over the past several decades, studies of exoplanet atmospheres have consistently pushed observational and theoretical capabilities in an effort to better understand various aspects of these objects, including chemical makeup, structure and dynamics, young and forming planets, and habitability and the search for extraterrestrial life. Thoroughly investigating each of these avenues, often for extreme cases, has promoted a better understanding of the nature of planets and their atmospheres in the round. The following sections highlight some of the significant advances in the field of exoplanet atmospheres, with a focus on results from high-dispersion studies and topics that have particular relevance to subsequent chapters.

1.2.1 Chemical composition

One of the earliest characteristics to be probed in the study of exoplanet atmospheres was chemical composition. As previously mentioned, the first detection of a planetary atmosphere outside the Solar System was conducted by finding sodium absorption in the transmission spectrum of a hot Jupiter (Charbonneau et al. 2002). This discovery was but the first in a continuing effort to tally the inventory of chemical species present in exoplanets. Due to current sensitivity limitations, this inventorying has rather exclusively been done for gas giant exoplanets, and in particular, hot Jupiters and young super Jupiters.

Through a combination of high- and low-dispersion transit, emission, and imaging spectroscopy from ground- and space-based observatories, dozens of different chemicals have been detected in the atmospheres of exoplanets. These include neutral atoms and ions across several grouping in the periodic table, including alkali metals (e.g., Li I, Na I, K I), alkaline Earth metals (e.g., Mg I, Ca I, Ca II, Sr II), transition metals (e.g., Sc II, Ti I, Ti II, V I, Cr I, Cr II, Mn I, Fe I, Fe II, Ni I, Y II), and nonmetals and metalloids (e.g., H I, He I, Si I). Additionally, various molecules have been detected, including CO, H_2O, CH_4, and HCN. High-dispersion studies have been particularly useful in detecting the presence of molecules (e.g., Snellen et al. 2010; Birkby et al. 2013) and transition metals (e.g., Hoeijmakers et al. 2018a, 2019), given the relatively high number of narrow, resolved spectral lines for these species that may be co-added.

Expanding this inventory to more chemical species across a wide range of exoplanets is important to understanding the various processes at work in exoplanet atmospheres. For instance, comparing observed chemical inventories to expectations from atmospheric chemical models enables the validation and refinement of these models. Consider the case of the transition-metal molecule titanium (mon)oxide (TiO), which has strong visible-wavelength opacities and is prominent in the spectra of cool stars and hot brown dwarfs, in which gaseous TiO is expected to be most abundant for atmospheric temperatures ∼2000–3000 K (Lodders 2002). The dayside temperatures of ultra-hot Jupiters ($T_{\rm day} \gtrsim 2200$ K; Parmentier et al. 2018) have similar values. Despite predictions of the presence of gaseous TiO in these hottest of exoplanets (Hubeny et al. 2003; Fortney et al. 2008), unambiguous detections have proven scarce. Various effects have been invoked to explain this discrepancy between observation and theory, such as gravitational settling of TiO and its condensates to lower, less-observationally-accessible altitudes (Spiegel et al. 2009), transport of TiO to the planet's nightside by winds and subsequent condensation (Parmentier et al. 2013), and thermal dissociation in the cases of highest stellar irradiation (Lothringer et al. 2018). Pushing atmospheric models to extreme cases and attempting to validate them using observed chemical inventories has thus enabled advances in our understanding of potential non-equilibrium processes in exoplanet atmospheres.

Assembling complete chemical inventories of exoplanet atmospheres also enables a better understanding of how planets and their atmospheres form and evolve. The protoplanetary disks in which planets form are complex, with physical and chemical properties that vary with time (Eistrup et al. 2018). In general, though, it is expected that bulk chemical properties like elemental abundance ratios vary with temperature, and thus radial distance, from the host star. As a result, different planet formation models predict different trends of bulk chemical properties for exoplanet atmospheres depending on the orbital distance of formation, relative importance of gas and solid accretion to the atmospheric envelop, and accretion during any orbital migration (Madhusudhan 2019, and the references therein). Determining the abundances of these inventoried species by modeling and fitting exoplanet spectra can enable the empirical determination of elemental abundances and metallicity. Comparison with the associated trends predicted by planet formation scenarios can constrain the formation process for individual objects. For instance, Line et al. (2021) recently performed the first robust determination of the C/O value and metallicity of a hot-Jupiter atmosphere using high-dispersion dayside emission spectroscopy. The solar C/O value and subsolar metallicity they found in the hot Jupiter WASP-77Ab is inconsistent with general predictions made by various planet formation models, leading Line et al. (2021) to propose constraints on, for instance, the orbital distance at which atmospheric accretion occurred and the degree of planetesimal bombardment.

Another recent development that is pushing the boundaries of current chemical inventorying capabilities is the differentiation and analysis of isotopes in exoplanet atmospheres. Isotopes, and their molecular counterparts isotopologues, of a given species behave slightly differently in radiative, chemical, nuclear, and dynamical processes. As a result, variations in relative isotope abundances trace these processes, and in a complementary fashion to elemental abundance ratios and metallicities, can constrain the formation and evolution of exoplanets. Recently, an isotopologue abundance ratio was robustly measured for the first time in a young, widely-orbiting super Jupiter. Zhang et al. (2021a) concluded that the enhanced $^{13}CO/^{12}CO$ value relative to that of the interstellar medium that they measured in the planet TYC 8998-760-1 b may indicate accretion of ices enriched in ^{13}CO during its formation. After performing a similar measurement for a brown dwarf and finding a $^{13}CO/^{12}CO$ value consistent with that of the interstellar medium, Zhang et al. (2021b) suggested that the difference in isotopologue abundance ratio could be indicative of different formation mechanisms for these two objects. As a result, isotope and isotopologue studies have begun to serve as a complementary tool to trace planet formation through chemical inventorying.

1.2.2 Structure and dynamics

In addition to itemizing the chemical inventories of exoplanet atmospheres, efforts have been made to characterize and understand exoplanets as three-dimensional objects. As alluded to in the discussion of TiO in the previous section, atmospheric analyses are pushing beyond simply determining whether chemical species are present in planet atmospheres, to trying to understand how these species are distributed and the associated impact on atmospheric structure. In turn, these studies drive a better general understanding of the structure and dynamics in exoplanet atmospheres.

Determining T–P profiles for exoplanets probes the vertical structure of their atmospheres and has been a major contribution of emission spectroscopy at both low and high spectral resolution. The variation of temperature with altitude is heavily influenced by the strength of the incident stellar radiation, as well as the chemistry of the atmosphere, which determines the opacities available for heating and cooling at each pressure layer. Unlike cooler hot Jupiters ($T \lesssim 2000$ K), most extremely-irradiated ultra-hot Jupiters exhibit T–P profiles that are isothermal or inverted, in which case the temperature increases with altitude over a certain range of pressures (Madhusudhan 2019; Baxter et al. 2020). Understanding the mechanisms that produce these inversions is of particular interest, as it involves the interplay between stellar irradiation, atmospheric chemistry, and atmospheric opacities in these extreme objects. Originally, it was proposed that inversions are driven by strong optical absorption of stellar radiation by gaseous TiO and/or VO (Hubeny et al. 2003; Fortney et al. 2008). However, given the scarcity of unambiguous detections of either molecule in exoplanets known to have inverted T–P profiles, further theoretical developments have suggested that various atoms (e.g., Fe I, alkali metals), ions (e.g., H^-, Fe II), and molecules (e.g., metal oxides, metal hydrides) besides TiO and VO have sufficiently strong optical opacities to drive temperature inversions (Mollière et al. 2015; Parmentier et al. 2018; Lothringer et al. 2018; Lothringer & Barman 2019; Gandhi & Madhusudhan 2019). Indeed, recent high-dispersion studies have found clear evidence for Fe I emission lines in several ultra-hot Jupiters (e.g., Pino et al. 2020; Yan et al. 2020; Nugroho et al. 2020a). Analysis of these extreme objects has thereby advanced the understanding of the impact of stellar radiation fields and atmospheric chemistry on the vertical structure of exoplanet atmospheres.

Observations have also started to reveal the structure and dynamics at work across the surfaces of hot Jupiters, often confirming the predictions of three-dimensional global circulation models of these tidally-locked planets (e.g., Showman et al. 2009, 2013). For instance, high-resolution transit spectroscopy has revealed net velocity offsets between atmospheric species and the orbital rest frames of exoplanets (e.g., Snellen et al. 2010; Brogi et al. 2016, 2018; Alonso-Floriano et al. 2019; Casasayas-Barris et al. 2019; Nugroho et al. 2020b), as well as asymmetries in these offsets when determined separately for the start and end of transit (e.g., Louden & Wheatley 2015; Ehrenreich et al. 2020). These findings reflect the impact of various dynamical factors, such as day-to-nightside winds, zonal jets, and planetary rotation. Additionally, these velocity asymmetries between the leading and trailing limbs have been shown to vary for different species in the ultra-hot Jupiter WASP-76b, which may trace different wind patterns at different altitudes in this planet (Kesseli et al. 2021).

Chemical gradients have also recently been inferred based on signal strength asymmetries in high-dispersion transit spectra. For instance, in the same study analyzing transit velocity asymmetries in the ultra-hot Jupiter WASP-76b, Ehrenreich et al. (2020) also found stronger Fe I absorption at the end of transit, when only the trailing (evening) limb was probed. This was interpreted as evidence for the condensation of Fe I on the night side and morning limb. These regions are expected to be cooler than the dayside and the evening limb due to the day-to-nightside temperature contrast of synchronously-rotating hot Jupiters and the shift in the dayside hot spot from the substellar point towards the evening limb due to zonal jets. Asymmetries in transit signal strength have also been found in other chemical species, with transition metal atoms similarly presenting stronger signals in the hotter, inflated evening limb of WASP-76b, while more readily-ionized alkali atoms produce stronger signals at the cooler morning limb of this hot Jupiter (Kesseli et al. 2021). Such advances in understanding the dynamics and structure of exoplanets have thereby enabled the probing of their weather patterns.

1.2.3 Young planets

Characterizing planets at various ages allows for the study of their atmospheres at different stages of evolution and, for the youngest planets and protoplanets, during formation. Such observations uniquely complement studies that infer constraints on planetary histories based on current atmospheric properties such as elemental abundance ratios, metallicities, and isotope and isotopologue abundance ratios (see Section 1.2.1). Finding and characterizing planets early in their development also facilitates a better understanding of their impact on their formation environment. Rings, gaps, and spiral arm patterns have been observed in various disks around young stars, and it is expected that young planets may drive these substructures (ALMA Partnership et al. 2015; Andrews et al. 2016; Andrews 2020). Studying still-forming exoplanets, like those in the PDS 70 system (see Figure 1.3), allows these objects to be directly linked to observed disk structures (Bae et al. 2019; Toci et al. 2020), which may in turn influence the formation and evolution of their atmospheres.

As mentioned in Section 1.1.3, studies of young planets and their atmospheres are largely the province of direct imaging studies, which probe the emergent spectrum of these objects. Like high-dispersion transmission and spatially-unresolved emission spectroscopy, medium-resolution imaging spectroscopy has allowed unambiguous molecular detections. In particular, the molecule mapping technique developed by Hoeijmakers et al. (2018b), in which the spectra of the spatial pixels containing planet signal are probed for chemical signatures using cross-correlation with model atmosphere templates, has revealed the presence of CO and H_2O in several young planets (Hoeijmakers et al. 2018b; Petit dit de la Roche et al. 2018; Petrus et al. 2021), as well as provided constraints on planet parameters such as temperature and surface gravity. This method has also been applied to data of embedded, accreting protoplanets (Cugno et al. 2021) and protoplanet candidates (see Chapter 4), but produced ambiguous results.

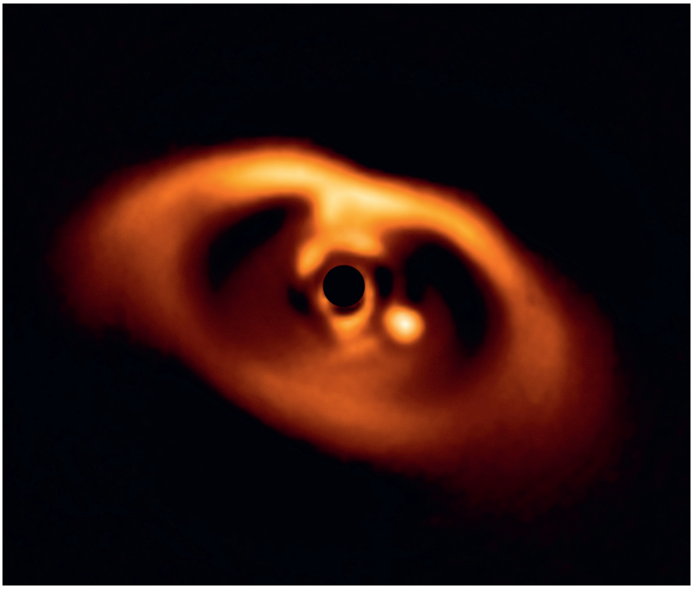

Figure 1.3. VLT/SPHERE near-infrared image of the young PDS 70 system. To the right of the central mask, the accreting protoplanet PDS 70 b is readily visible as an isolated emission source. Image credit: ESO/A. Müller et al.

1.2.4 Habitability and extraterrestrial life

The previous sections on the characterization of exoplanet atmospheres have exclusively focused on gas-giant planets, with a particular emphasis on hot Jupiters. Despite the significant advances made in understanding planetary atmospheres through studies of these extreme objects, hot Jupiters are relatively rare compared to terrestrial planets (Fressin et al. 2013). With the recent launch and deployment of the James Webb Space Telescope, upcoming ground-based extremely large telescopes (ELT, TMT, GMT), and planned future space-based observatories such as LUVOIR and HabEx, observational capabilities will improve and enable routine and robust measurements of atmospheres for progressively smaller, and eventually terrestrial, exoplanets. Studying terrestrial planet atmospheres is not only important for understanding planetary characteristics across various classes of planets, but also offers the opportunity to search for extraterrestrial life.

Many factors impact whether a terrestrial planet is capable of sustaining life as we know it (Kaltenegger 2017). Perhaps one of the most relevant from a planet detection standpoint is whether a given planet orbits within the habitable zone — the range of orbital distances where the equilibrium temperature of the planet can sustain liquid water. Several dozen such planets has been discovered,[2] but due to current observational constraints, have largely been out of reach of robust atmospheric analysis. Such analysis will be critical to determining whether life is indeed present on planets we believe to be habitable.

In particular, searching for atmospheric biosignatures — chemical species we associate with life on Earth — is seen as the most promising method for probing life on exoplanets. It has long been advocated that detecting multiple biosignatures in thermodynamic disequilibrium will be necessary to serve as robust evidence of extraterrestrial life (Lovelock 1965). Canonically, the specific combination of molecular oxygen and methane in the atmosphere of terrestrial planets has been proposed, since these two molecules should react rapidly and would therefore require substantial and ongoing replenishment to maintain their individual abundances (Lovelock 1975; Lippincott et al. 1967; Sagan et al. 1993). On the present-day Earth there are no such processes known to produce appreciable quantities of O_2, absent life (Meadows et al. 2018, and the references therein). However, for other planets the situation may not be as straightforward. For instance, it has been theorized that the vaporization and subsequent photodissociation of large bodies of water could be a substantial abiotic source of molecular oxygen in terrestrial planets (Luger & Barnes 2015). Recent studies have therefore advocated a more holistic approach to determining whether life is present, involving as complete a characterization of a planet and its atmosphere as possible to investigate the possibilities for such false positive scenarios (Meadows 2017; Meadows et al. 2018). In such an endeavor, the insights gained by studying the atmospheres of various classes of planet, including the most extreme hot Jupiters, will be invaluable.

[2]Habitable Exoplanets Catalog, The Planetary Habitability Laboratory, UPR Arecibo

1.3 This dissertation

The subsequent chapters in this dissertation present several works studying exoplanet atmospheres at medium- and high-spectral resolution, spanning a diverse set of topics in the field. In Chapter 2, the atmosphere of one of the hottest ultra-hot Jupiters WASP-33b is probed, in an attempt to verify a previous high-dispersion detection of gaseous TiO in its dayside emission spectrum. Despite expecting to retrieve a stronger signal using an improved spectral template for TiO, the signal detected in this reanalysis was weaker and found at inconsistent orbital velocities. An analysis of these results is presented and discussed in the context of the fidelity of high-resolution spectral observations.

For exoplanets in which TiO is unambiguously detected, Chapter 3 demonstrates how high-resolution emergent spectra can be used to determine the absolute and relative abundances of the isotopologues of TiO, and by extension, the relative abundances of Ti isotopes. As previously discussed, such isotope ratios can constrain processes at work during the formation and evolution of planet atmospheres. In this study, the impact of commonly-used high-dispersion processing techniques on measured abundances and abundance ratios is shown to be minimal, and the observing time required to perform such Ti isotope measurements is determined for upcoming observational facilities.

Chapter 4 investigates candidate protoplanets in a young protoplanetary disk system. A search for planetary atmospheric signatures in medium-resolution integral field spectroscopic data is conducted using molecule mapping, but does not reveal any compelling signals at the locations of the candidates. A sensitivity analysis indicates that the data is too noisy to probe the most promising candidate. Detectability requirements for upcoming, improved integral field spectrographs are estimated, and the impact of possible obscuring disk material is discussed.

This dissertation concludes in Chapter 5 with a forward-looking investigation into the feasibility of using the next generation of large ground-based telescopes to detect O_2 in the atmospheres of habitable-zone terrestrial planets. Previous studies have focused on determining the observing time necessary to detect this biosignature in high-resolution transmission spectra of temperate planets orbiting M-dwarf stars — a favorable planetary system set-up for such an endeavor due to the comparatively high planet-to-star flux contrast and relatively frequent transit occurrence. Chapter 5 improves upon previous works by incorporating real data with similar uncorrelated and correlated noise levels expected for future observations targeting O_2 in such terrestrial planets using the upcoming 39-meter Extremely Large Telescope.