

Above the Clouds:

Probing the atmospheres of ultra-hot Jupiters at high-resolution

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Cathal Maguire, B.A. (Mod.)

School of Physics, Trinity College Dublin

Supervisor:

Prof. Neale P. Gibson



Trinity College Dublin

Coláiste na Tríonóide, Baile Átha Cliath

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Summary

One of the most surprising discoveries of the numerous exoplanet surveys conducted over the past two decades is the existence of close-in giant planets orbiting their host stars at orbital separations smaller than that of Mercury’s orbit. Although their large numbers are partly due to observational biases, these planets—namely hot Jupiters and ultra-hot Jupiters—offer astronomers a unique opportunity to study atmospheric physics and chemistry in extreme environments, for which there are no Solar System analogues.

The recent significant advancements in ultra-stable, ground-based, high-resolution spectrographs have enabled the detection and characterisation of these objects in unprecedented detail, using techniques that complement similar studies conducted with space-based observatories. This thesis aims to investigate these worlds during transit using high-resolution observations. From these observations, advanced statistical and atmospheric modelling frameworks are employed to infer the physical, chemical, and dynamical properties of their atmospheres

The key results of this thesis are primarily based on data from the Echelle SPectrograph for Rocky Exoplanets and Stable Spectroscopic Observations (ESPRESSO) installed at the Very Large Telescope (VLT) at Paranal Observatory, Chile. Firstly, ESPRESSO was used to observe three transits of the ultra-hot Jupiter WASP-121b. The chemical and dynamical properties of the atmosphere of WASP-121b, such as the vertical temperature structure, chemical abundances, and wind velocity, were monitored using observations taken months/years apart.

Similarly, in the second study, three transits of the ultra-hot Jupiter WASP-76b were observed, separated by months/years. A novel rotational broadening kernel was developed to analyse these observations. This kernel allows the contributions from the morning (leading) and evening (trailing) limbs of the planet to be separated in velocity, enabling the extraction of atmospheric properties across the planet’s hemispheres. Thus, these properties were monitored with respect to both time and longitude.

Finally, two of the most common methods for removing contamination of ground-based spectra from the Earth’s atmosphere were compared on simulated exoplanetary signals injected into real ESPRESSO data. These signals were injected on varying orbital architectures, and subsequently reduced using the different telluric removal methods, before recovering them via an atmospheric retrieval. The methods’ efficacy, as well as any biases they might impose on the inferred atmospheric parameters, were compared.

The key findings are summarised before highlighting future avenues of research which may be extended from the research presented in this thesis to advance the knowledge of the complex, multidimensional nature of these alien worlds.

*“Ever tried. Ever failed. No matter.
Try again. Fail again. Fail better.”*

– Samuel Beckett, *Worstward Ho*

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Publications

1. **Cathal Maguire**, Elyar Sedaghati, Neale P. Gibson, Alain Smette, and Lorenzo Pino.
“Assessing methods for telluric removal on atmospheric retrievals of high-resolution optical exoplanetary transmission spectra”,
Astronomy & Astrophysics, 692, A8, December 2024.
2. **Cathal Maguire**, Neale P. Gibson, Stevanus K. Nugroho, Mark Fortune, Swaetha Ramkumar, Siddharth Gandhi, and Ernst de Mooij.
“High resolution atmospheric retrievals of WASP-76b transmission spectroscopy with ESPRESSO: Monitoring limb asymmetries across multiple transits”,
Astronomy & Astrophysics, 687, A49, June 2024.
3. Mark Fortune, Neale P. Gibson, Daniel Foreman-Mackey, Thomas M. Evans-Soma, **Cathal Maguire**, and Swaetha Ramkumar.
“How do wavelength correlations affect transmission spectra? Application of a new fast and flexible 2D Gaussian process framework to transiting exoplanet spectroscopy”,
Astronomy & Astrophysics, 686, A89, June 2024.
4. Swaetha Ramkumar, Neale P. Gibson, Stevanus K. Nugroho, **Cathal Maguire**, and Mark Fortune.
“High-resolution emission spectroscopy retrievals of MASCARA-1b with CRIRES+: strong detections of CO, H₂ O, and Fe emission lines and a C/O consistent with solar”,
Monthly Notices of the Royal Astronomical Society, 525, 2, 2985, October 2023.
5. Siddharth Gandhi, Aurora Kesseli, Yapeng Zhang, Amy Louca, Ignas Snellen, Matteo Brogi, Yamila Miguel, Núria Casasayas-Barris, Stefan Pelletier, Rico Landman, **Cathal Maguire**, and Neale P. Gibson.
“Retrieval Survey of Metals in Six Ultrahot Jupiters: Trends in Chemistry, Rain-out, Ionization, and Atmospheric Dynamics”,
The Astronomical Journal, 165, 6, 242, May 2023.
6. **Cathal Maguire**, Neale P. Gibson, Stevanus K. Nugroho, Swaetha Ramkumar, Mark Fortune, Stephanie R. Merritt, and Ernst de Mooij.
“High-resolution atmospheric retrievals of WASP-121b transmission spectroscopy with ESPRESSO: Consistent relative abundance constraints across multiple epochs and instruments”,
Monthly Notices of the Royal Astronomical Society, 519, 1, 1030, February 2023.

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7. Neale P. Gibson, Stevanus K. Nugroho, Joshua Lothringer, **Cathal Maguire**, and David K. Sing.
“Relative abundance constraints from high-resolution optical transmission spectroscopy of WASP-121b, and a fast model-filtering technique for accelerating retrievals”,
Monthly Notices of the Royal Astronomical Society, 512, 3, 4618, May 2022.

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Introduction

For millennia, humanity has postulated the existence of worlds such as our own beyond our Solar System, so-called extrasolar planets, or *exoplanets*. As far back as Ancient Greece, in the 5th century BCE, Atomist philosophers deduced that if the Universe consisted of an infinite number of unchangeable, indivisible components, then these components may be rearranged to form an infinite number of worlds. Democritus (460 BCE – 370 BCE) stated: “*In some worlds there is no sun and moon, in others they are larger than in our world, and in others more numerous.*” This belief was held by the Democritean scholar Epicurus (341 BCE – 270 BCE) who theorised: “*There are infinite worlds both like and unlike this world of ours.*” However, for the following two millennia, the Aristotelian (384 BCE – 322 BCE) view that “*there cannot be more worlds than one*” was upheld.

That was until the year 1584 when the Italian monk Giordano Bruno published *On the Infinite Universe and Worlds* in which he postulated the existence of worlds orbiting stars other than our Sun, and that “*those worlds have no less virtue nor a nature different from that of our Earth.*” It was for these cosmological beliefs, alongside his religious views and support of Nicolaus Copernicus’ heliocentric worldview, that Bruno was burned alive at the stake by the Roman Inquisition of 1600. Fortunately, his modern successors are not subjected to the same fate.

1.1 Exoplanet Detection

1.1.1 The Age of Exoplanet Discovery

In recent years, the study of exoplanets and their atmospheres has undergone a rapid development. Just over thirty years ago, in the early 1990s, the first extrasolar planetary system was discovered orbiting the millisecond pulsar PSR B1525-12 (Wolszczan

& Frail, 1992). This was soon followed by the first detection of an exoplanet orbiting a Sun-like star (Mayor & Queloz, 1995), 51 Pegasi b, a Jupiter-sized companion with an orbital period of approximately 4.2 days—a discovery for which the authors were awarded the Nobel Prize in Physics in 2019. These groundbreaking discoveries were soon followed by the first detection of an exoplanetary atmosphere, with the detection of sodium in the atmosphere of HD 209458b, after four transits of the HD 209458 system were observed using the Hubble Space Telescope (HST; Charbonneau et al. 2002). In the years that followed, a diverse range of exoplanets were discovered, in both their orbital properties and composition, forcing astronomers to rethink their hypotheses regarding planetary system formation, extrapolated from the architecture of our own Solar System.

1.1.2 Exoplanet Demographics

In the subsequent decades, numerous exoplanet surveys have been successfully conducted to quantify the frequency and distribution of these objects over a broad range of physical parameters, with particular reference to both the planetary and host star properties. At the time of writing, there have been over 5,700¹ confirmed exoplanet detections. This large sample now enables well-constrained statistical analyses, whose physical trends can then be used to infer the formation and evolution processes of planetary systems. The most successful exoplanet survey to date, the Kepler mission (Borucki et al., 2010), with over 2700 confirmed detections, resulted in one of the more surprising conclusions of such analyses—the “Neptunian Desert”, a deficiency of Neptune-sized planets with short orbital periods (see Fig. 1.1). Although some observed trends have been the result of the observational biases of exoplanet detection methods, the Neptunian Desert might indicate different mechanisms of formation and evolution between *hot Jupiters* and short-period *super-Earths* (Mazeh et al., 2016).

For a planetary system comparable to the Solar System, direct observation of an exo-

¹<https://exoplanetarchive.ipac.caltech.edu/>, 2/9/2024.

planet via reflected starlight is extraordinarily challenging. For instance, Jupiter—at the same orbital distance—would achieve a planet-star brightness contrast of approximately 10^{-9} . Thus, astronomers have employed a suite of creative detection methods, relying on both direct and indirect observations of exoplanets to yield their detection and characterisation.

1.1.3 Exoplanet Detection Methods

An understanding of the various detection methods used in exoplanet surveys is important when interpreting the trends observed in their subsequent analyses. Each of the following techniques provides astronomers with a unique insight, allowing for both the detection and characterisation of these worlds. The transit method, and consequently *transmission spectroscopy*, will be discussed in detail as the primary technique used in this study to probe exoplanetary atmospheres, and has been described as the “royal road” of exoplanetary science (Winn, 2011).

1.1.3.1 Radial Velocity

When one visualises a planet such as the Earth in orbit around its host star, one would be excused for assuming the host star is stationary. However, in reality, both bodies orbit a common centre of mass or barycentre. As the star ‘wobbles’ about the star-planet barycentre, its light is periodically redshifted and blueshifted relative to the observer, inducing a periodic radial velocity signal. As this effect is due to the gravitational effect of the orbiting planet, one can estimate its *minimum mass* using the radial velocity method by measuring its host star’s radial velocity semi-amplitude, K_* . In reality, $M_p \sin i$ is estimated, where M_p and i are the planetary mass and orbital inclination, respectively. This method introduces an inherent bias toward more massive planets with short orbital periods and close proximity to their hosts, as these planets produce more readily detectable radial velocity signals.

With $K_\oplus \simeq 0.09 \text{ m s}^{-1}$ and $K_J \simeq 12.5 \text{ km s}^{-1}$ the radial velocity semi-amplitudes

induced by the Earth and Jupiter on our Sun over a period of 1 and 11.86 years, respectively, as indicative goals, the detection and characterisation of similar planets around Sun-like stars would require radial velocity accuracies of $\approx 10 \text{ cm s}^{-1}$ maintained over many months or years (e.g., Perryman, 2011). High-resolution spectrographs ($\lambda/\Delta\lambda \gtrsim 10^5$), such as the Echelle SPectrograph for Rocky Exoplanet and Stable Spectroscopic Observations (ESPRESSO) at the Very Large Telescope (VLT), are capable of achieving such precision (Pepe et al., 2021)—owing to the thousands of individual stellar absorption lines in their given wavelength range, as well as their high instrumental stability.

1.1.3.2 Direct Imaging

This method aims to directly image exoplanets on the plane of the sky, via their intrinsic thermal emission. This is a tremendously complex problem, as one must separate the light from the exoplanet from that of its host star, a contrast that typically ranges from $10^{-6} - 10^{-8}$, depending on the observed wavelength range (e.g., Heng, 2017). However, for young giant planets still possessing their remnant heat of formation ($>1000 \text{ K}$), at large orbital distances, the planet-star flux contrast approaches 10^{-4} , making these planets detectable with current facilities (e.g., Madhusudhan, 2019). Direct imaging also allows for atmospheric characterisation via spectroscopy, once the exoplanet’s emission has been isolated.

1.1.3.3 Microlensing

Gravitational microlensing, or microlensing, is a relativistic effect that occurs when a background star and a foreground object (such as another star) are both located along the line of sight of the observer. As the foreground star, or gravitational lens, passes in front of the background star, the background starlight is warped due to the mass of the lens, creating a smooth rising and falling light curve. However, if the foreground star hosts an exoplanet, the orbiting planet will distort this light curve, in such a manner that the planet/star mass ratio and orbital distance may be estimated (Gaudi,

2012). However, despite being a useful method for detecting planets, particularly ‘rogue’ planets or planetary systems at large distances, the detections are unrepeatable and typically do not allow for the characterisation of planetary atmospheres.

1.1.3.4 Transit

Transit photometry is the most effective method for both detecting and characterising exoplanets, with roughly 4200 detections to date, facilitating the study of their atmospheres via transmission spectroscopy. Both methods utilise the fact that for a population of planet-hosting stars, some fraction will host planets whose orbit will be edge-on (i.e., an orbital inclination $\approx 90^\circ$) relative to the observer. Light from the host star is then periodically obstructed by the transit of a planet across its disk. This dip in starlight relative to the flux of the star (i.e., the transit depth) can be measured as a function of the planet’s orbital phase, resulting in what is known as a *transit light curve* (see Fig. 1.3). The measured transit depth is proportional to the ratio of the area of the planetary disk to the area of the stellar disk, $R_p^2/R_\star^2$. This effect is often a small fraction of the stellar flux, making it a formidable challenge, such that a planet of radius $1 R_\oplus$ transiting a star of radius $1 R_\odot$ at 1 AU would produce a differential flux ($\Delta F/F$) $\simeq 8.4 \times 10^{-5}$. Since the early 2000s, the number of exoplanets identified using this technique has increased dramatically, with just 3 detected in total by 2003 (Sasselov, 2003). This dramatic increase is due to the success of a number of ground- and space-based transit photometric surveys, such as Kepler, the Transiting Exoplanet Survey Satellite (TESS; Ricker et al. 2015), and the Wide Angle Search for Planets (WASP; Pollacco et al. 2006), among others.

Due to the dependence of the transit depth on the planet/star radius ratio, the transit method is inherently biased towards larger planets with highly inflated radii or planets in orbit around smaller stars, such as M dwarfs (Beatty & Gaudi, 2008). There is also an inherent detection bias towards short-period planets, which is present in the majority of exoplanet surveys (see Fig. 1.1).

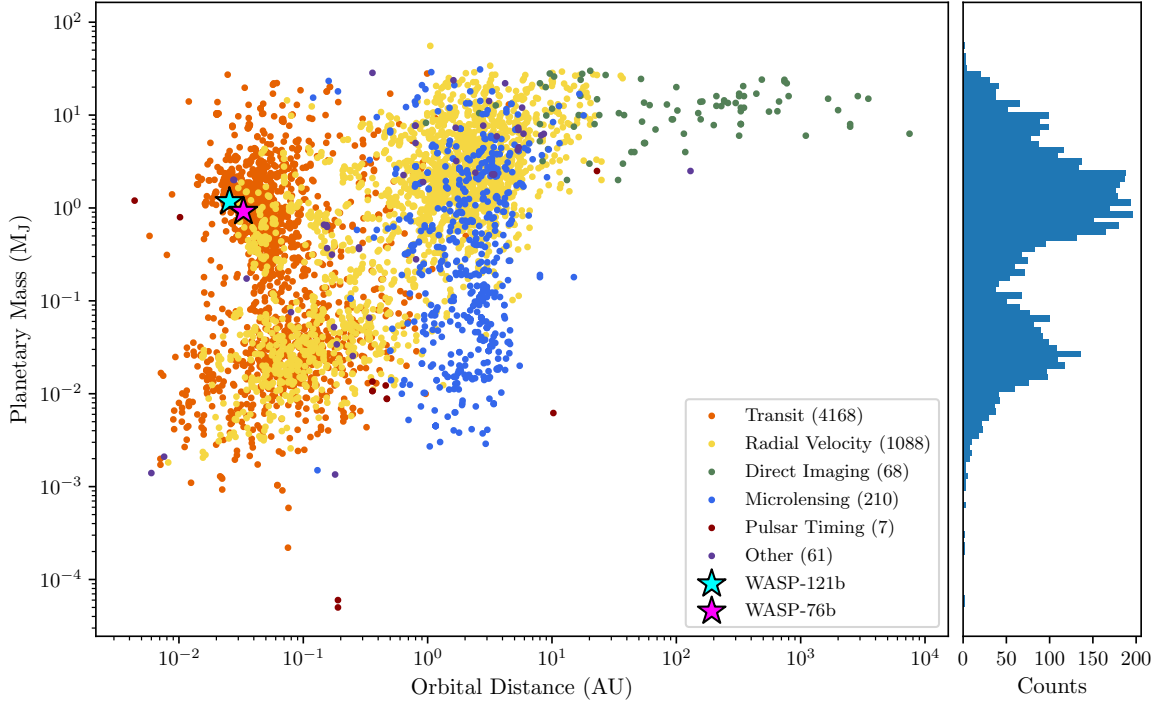


Figure 1.1: The confirmed exoplanet detections to date, displayed as a planetary mass vs orbital distance diagram (retrieved 2/9/2024). The method used for their detection is also indicated. The primary subjects of this study, WASP-121b and WASP-76b, are highlighted with a cyan and magenta star, respectively. The bimodality of this distribution as a function of planetary mass is shown on the right, clearly displaying the aforementioned “Neptunian Desert”.

Whilst transit photometry has now eclipsed the radial velocity method as the most successful detection method in current use, both methods can be used in conjunction to provide a more comprehensive description of both the planets’ physical and orbital parameters. As previously mentioned, the transit depth gives the planet/star radius ratio, and one may estimate the minimum mass of a transiting planet using the radial velocity method. A transiting planet also allows for the measurement of i , thus, the $M_p \sin i$ degeneracy is broken. Assuming a stellar radius value from stellar-evolutionary models, and knowing the total transit duration, one can obtain values for R_p , M_p , ρ_p , g , i , and b . These quantities represent the planetary radius, mass, bulk density, surface gravity, orbital inclination, and impact parameter, respectively (Winn, 2011). However, to fully characterise the planet’s atmosphere via its chemical composition, temperature-pressure (T - P) structure, and global weather patterns, one must utilise the complementary technique of transmission spectroscopy.

1.2 Exoplanetary Atmospheres

The study of planetary atmospheres unsurprisingly began in our own Solar System. The atmospheres of Solar System planets have been studied since the 18th century (Lomonosov, 1761; Herschel, 1784; Challis, 1863), where astronomers noted the varying refraction of the Sun’s rays during transits of Venus. The discovery of this phenomenon caused by the Venusian atmosphere is attributed to the Russian polymath Mikhail Lomonosov, who, whilst observing the 1761 transit of Venus, wrote:

Afterwards, I watched with keen attention for the ingress of the trailing limb of Venus, which, it seemed, had not yet taken place, for there seemed to be a small segment not yet entered upon the Sun. However, there suddenly appeared between the trailing limb of Venus and the following [solar] limb a hair-thin luminous sliver. The time that separated the two appearances was not more than a second. ... From these observations, I concluded that the planet Venus is surrounded by an extensive atmosphere of air, similar to (if not even greater than) that which surrounds our own globe.

The English translation of the original Russian text (Lomonosov, 1761) provided above was taken from Pasachoff (2012). Thus, remarkably, the study of planetary atmo-

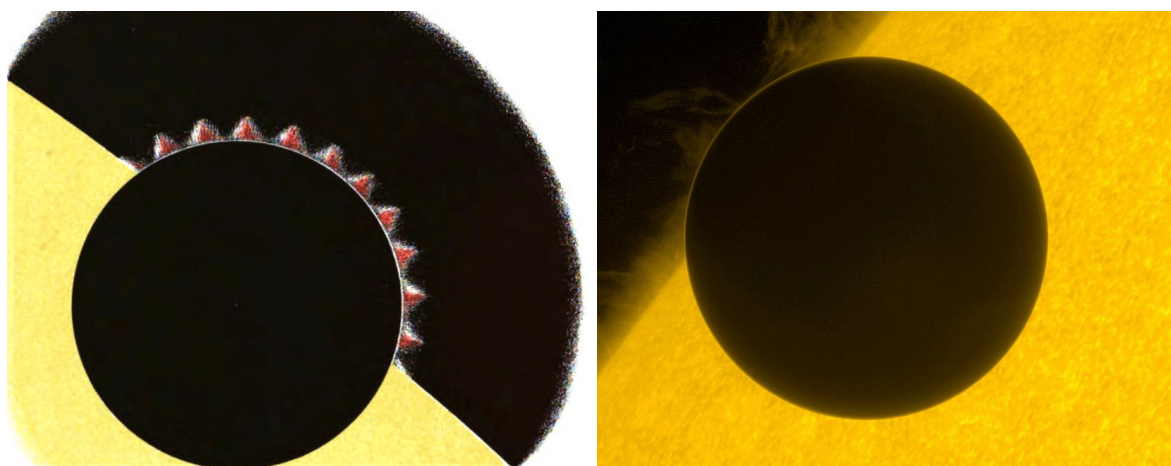


Figure 1.2: (left) An illustration of the 1874 transit of Venus by Mr. A Fairfax, published in Russell (1892), showing the Venusian “ring of light” (i.e., atmosphere). (right) The 2012 transit of Venus observed with HINODE, showing this “hair-thin luminous sliver” of an atmosphere. Image Credit: NAOJ/JAXA/NASA.

spheres in transmission is over 250 years old and continues to be used today to study the atmospheres of exoplanets.

1.2.1 Hot Jupiters and Ultra-hot Jupiters

If one were to extrapolate planet formation mechanisms solely from the architecture of our Solar System, the formation of close-in giant planets within the orbit of Mercury wouldn't seem feasible. However, over the last 25 years, exoplanet surveys have discovered an abundance of close-in giant planets. Although these discoveries are enhanced by observational biases, once corrected for, it is estimated that roughly 1% of Sun-like stars host a HJ (Wright et al., 2012). The diverse and often perplexing nature of these newfound planetary systems has posed new questions for astronomers, such as: How do they form? How do they evolve over time? And what are they composed of?

1.2.1.1 Formation and Evolution

The formation of giant planets is thought to occur via two primary mechanisms: core accretion (Perri & Cameron, 1974) and gravitational instability (Boss, 1997). Core accretion occurs when a solid, rocky core or planetesimal reaches a critical mass within the protoplanetary disk, allowing for runaway accretion of gas to form a massive gaseous envelope. Such a formation scenario is difficult to obtain close to the host star at the current orbital architecture of a close-in giant planet, known as *in situ* formation, where building a sufficiently large core ($\sim 10 M_{\oplus}$) is challenging. However, it has been shown that HJs can form via *in situ* core accretion, a mechanism which can also account for their semi-major axis-mass distributions shown in Fig. 1.1 (Batygin et al., 2016; Bailey & Batygin, 2018). Alternatively, giant planets may form via core accretion in the outer regions of the protoplanetary disk beyond the snow line—such as in the Solar System. These planets then migrate through the disk to their current orbits via a number of various mechanisms, discussed below. In contrast, gravitational instability can cause the rapid formation of giant planets as small, dense regions of the protoplanetary disk become gravitationally unstable, collapsing directly to form large planetary

bodies. This mechanism is favoured in the outer regions of the protoplanetary disk, where the gas conditions are more favourable as these ‘clumps’ can cool and coalesce more efficiently. Furthermore, a disk-star mass ratio greater than $\approx 10^{-2}$ is typically required for disks to become subjected to self-gravity effects. (Kratter & Lodato, 2016).

There are numerous viable mechanisms through which these giant planets, formed in the outer regions of the protoplanetary disk, could migrate and evolve to their current orbital configurations. Disk migration via planet-disk interaction occurs when a giant planet is formed and migrates inwards through torques from the gaseous disk (Lin et al., 1996). Alternative inward migration mechanisms begin when the planet is perturbed into a highly elliptical orbit (Fortney et al., 2021). The migrating planet’s orbit is then stabilised and circularised via tidal interactions with the star. It is not known for certain what triggers this perturbation, and many mechanisms have been theorised, such as: planet-planet scattering (Rasio & Ford, 1996; Weidenschilling & Marzari, 1996), Kozai-Lidov cycles (Kozai, 1962; Lidov, 1962), and secular chaos (Wu & Lithwick, 2011), among others. Planet-planet scattering occurs when two or more giant planets form and gravitationally interact, exchanging angular momentum and becoming dynamically unstable. This instability causes their orbital architectures to change drastically. These interactions typically lead to the orbits becoming highly eccentric and/or misaligned with the initial orbital plane. A possible outcome of such an interaction, particularly for unequal-mass planets, is that one planet is ejected from the system, while the remaining planet is left in a smaller, eccentric orbit that gradually becomes circularised through tidal interactions with the star (Davies et al., 2014). Kozai-Lidov cycles occur when a distant third body perturbs a system, such as a star-planet pair. This perturbation causes the smaller body (i.e., the planet) to undergo oscillations in both the eccentricity and inclination of its orbit. As the highly eccentric orbit brings the planet close to the host star at periastron, tidal interactions can occur, which shrink and circularise the planet’s orbit over time. Finally, secular chaos is analogous to planet-planet scattering, where planetary bodies within the protoplanetary

disk interact *gradually* over time, in contrast to the short-term interactions involved in planet-planet scattering. The long-term evolution of the inner Solar System, for example, is predominantly secular in nature (Laskar, 1989). The cumulative gravitational interactions of planets perturb and alter their orbits. Under certain circumstances, secular interactions can gradually increase the eccentricity of the inner planet to near unity (Wu & Lithwick, 2011). The current orbital architectures of HJs can provide insights into the formation channels through which they formed. Out to ~ 3 day orbital periods, HJs orbits have become circularised, and therefore their origin channel is difficult to ascertain. However, between 3 – 10 days, a broad range of moderate eccentricities are observed ($0.2 < e < 0.6$), which cannot be explained by in situ formation or disk migration, and thus must have formed via the various high eccentricity migration mechanisms (Dawson & Johnson, 2018). In order to determine where in the protoplanetary disk these objects formed, such observations must be coupled with observations of the planet’s composition.

1.2.1.2 Internal Structures

As mentioned in Sect. 1.1.3, the measurement of a planet’s orbital inclination via the transit method breaks the $M_p \sin i$ degeneracy, assuming $M_p \sin i$ has been measured via radial velocity. Thus, knowing the planet’s mass and radius, one may estimate the planet’s bulk density. This, to first order, allows for the determination of the planet’s bulk composition. As one cannot probe the opaque interior of an exoplanet via transmission spectroscopy, the bulk densities are typically coupled with planetary interior models. From this, a bulk planet metallicity or composition is determined (e.g., Thorngren et al., 2016). However, there are numerous degeneracies one encounters when one assumes a planet’s bulk composition from its mass and radius alone. This is highlighted in Rogers & Seager (2010), where three different gas accretion mechanisms could account for the gas layer required for the low density super-Earth GJ 1214b. This inherent degeneracy in the mass-radius diagram can be broken by measuring the atmospheric metal mass fraction in the envelope, which together with the mass

and radius enables the constraint of the individual mass fractions of the rocky/icy core, H/He dominated envelope, and volatile metals in the envelope (Benneke et al., 2024). Thus, measurement of a planet’s atmosphere, and its interior by extension, is required. However, this is not always trivial. As a planet evolves, the composition of its atmosphere can change dramatically relative to that of its interior, via various processes such as: volcanic activity (Gaillard & Scaillet, 2014), outgassing (Kite & Barnett, 2020), and atmospheric escape (Murray-Clay et al., 2009). These processes can alter the atmospheric composition over time, making it challenging to accurately infer the planet’s internal composition and evolutionary history based solely on atmospheric measurements.

1.2.1.3 Atmospheres

High-mass planets typically have larger radii and thus lower densities than expected from theoretical models, known as the *radius anomaly* (Thorngren & Fortney, 2018). These early theoretical models, derived from models of Solar System gas giants, did not account for effects such as the intense stellar irradiation received by close-in gas giants, which increases their radii (Guillot & Showman, 2002). These objects are thus assumed to contain H/He dominated envelopes to explain this discrepancy (Madhusudhan et al., 2016), which also comes from the assumption that they formed in a similar manner as Saturn and Jupiter—such that they accrete a high mass fraction of gaseous H/He from the protoplanetary disk (Pollack et al., 1996). Their close proximity to their host star means that HJ/UHJs undergo immense stellar irradiation, inflating their radii and enabling atmospheric characterisation via transmission/emission spectroscopy. The high temperatures of HJs mean that atomic metals such as Na and K are vapourised and thus are present in their atmospheres, primarily in the optical regime of their spectra (Brown, 2001). Additional sources of opacity in HJs include molecular absorption by species such as H₂, H₂O, CH₄, CO, CO₂, N₂, NH₃, TiO, and VO (Fortney et al., 2021); cloud and hazes composed of Si-O, Al-O, Fe-O, and Ti-O bearing condensates (see Wakeford & Sing (2015) for a theoretical description of HJ cloud condensates); and

various scattering and absorption processes, including collisionally induced absorption (CIA), Rayleigh scattering, H^- absorption, and Mie scattering, among others (Parmentier et al., 2018).

Although they are a rare outcome of planet formation (Wright et al., 2012), UHJs are the most amenable to atmospheric characterisation due to their extreme irradiation and highly inflated radii. These objects are the primary focus of the analyses presented in this work. At such extreme temperatures, atomic metals that are typically condensed deep in the atmosphere now become vapourised and absorb incoming stellar radiation. Atomic species detected in the atmospheres of UHJs thus far via high-resolution spectroscopy include: H, Li, O, Mg, Si, Ca, Sc, Ti, V, Cr, Mn, Fe, Ni, Rb, Sr, and Sm (Hoeijmakers et al., 2018, 2019, 2020; Yan & Henning, 2018; Casasayas-Barris et al., 2018; Cauley et al., 2019; Borsa et al., 2021; Tabernero et al., 2021; Cont et al., 2022; Prinoth et al., 2023; Jiang et al., 2023). Similarly, at these high temperatures, these gaseous atomic species are more readily ionised. A number of ionised species have also been detected with both low- and high-resolution spectroscopy, such as: Mg II, Ca II, Sc II, Ti II, V II, Cr II, Fe II, Ni II, Sr II, Y II, Ba II, and Tb II (Fossati et al., 2010; Hoeijmakers et al., 2019; Azevedo Silva et al., 2022; Borsato et al., 2023, 2024). To the best of my knowledge, this is a complete list of confident detections of neutral and ionised species in the atmospheres of HJ/UHJs, at the time of writing¹. At high-resolution (see Sect. 1.2.2.2), the accurate positions and shapes of these atomic/ionic lines can also be measured. This allows astronomers to infer atmospheric dynamics such as global wind patterns, including day-to-night flows, equatorial jets, and radially outflowing escape (Seidel et al., 2020).

As these planets are assumed to be tidally locked due to the tidal interactions with their host with which they evolved, they have a permanently irradiated dayside and a cooler

¹A special mention to the ExoAtmospheres database maintained by the IAC (<https://research.iac.es/proyecto/exoatmospheres/table.php>), without which the compilation of these lists would have been very difficult!

nightside. The temperature gradient between both day and nightside is thought to be ~ 1000 K (Parmentier et al., 2018). As a result, a wide variety of condensable species that are stable in the gas phase on the dayside may condense on the nightside, leading to the formation of particles there. If the atmosphere does not have sufficient vertical mixing, these condensed particles can gravitationally settle and become permanently ‘locked out’ of the observable atmosphere in a process known as “cold trapping” (Parmentier et al., 2013). These “cold traps”—atmospheric layers which are colder than the layers above them—are caused by thermal inversions, where the temperature of the atmosphere increases with altitude. The Earth’s atmosphere also possesses a cold trap between the troposphere and stratosphere, which prevents water vapour from rising to the stratosphere, thus regulating the moisture balance essential for life on Earth (Pierrehumbert, 2010). Thermal inversions have been theorised and detected in several HJ/UHJs through both low- and high-resolution spectroscopy (Fortney et al., 2008; Knutson et al., 2008; Nugroho et al., 2020a). At the extreme temperature regime, these inversion layers are thought to be driven by high-altitude optical absorbers, such as VO and TiO in the atmosphere of WASP-33b (Haynes et al., 2015), which heat the upper atmosphere. TiO was detected by Nugroho et al. (2017) in the atmosphere of WASP-33b via high-resolution emission spectroscopy. These high-altitude optical absorbers have also been used to explain the inverted dayside T - P profile of the UHJ WASP-121b (Evans et al., 2016). VO was first detected in the atmosphere of WASP-76b by Pelletier et al. (2023). Such a cold trap mechanism can also explain the absence of Ti, Al, and Sc, as these species have higher condensation temperatures relative to other refractory elements detected in WASP-76b.

By detecting atmospheric species across the hemispheres of these objects, and placing constraints on their dynamics and chemistry (i.e., abundance, temperature, etc.), astronomers not only learn how these objects are, but also how they came to be. Developing robust techniques to constrain relative elemental abundances—such as metallicity (Fe/H), the carbon-to-oxygen (C/O) ratio, the refractory-to-volatile ratio, the relative

abundances between species (χ_1/χ_2), and isotope ratios—from spectroscopic observations enables us to infer the formation and evolution mechanisms of these objects (Öberg et al., 2011; Madhusudhan et al., 2014; Mordasini et al., 2016; Lothringer et al., 2021). The relative abundances of a various species in a planetary atmosphere can be used as a tracer to determine where in the protoplanetary disk the planet formed. This has been a long-standing goal of exoplanet science. However, simply inferring planet formation processes from relative atmospheric abundances is a challenging task, due to the numerous complex processes which govern a planet’s formation history (Van der Marel et al., 2021; Mollière et al., 2022).

1.2.2 Transmission Spectroscopy

In transit photometry, it is implicitly assumed that the transiting planet is a solid, opaque disk, periodically eclipsing its host star. In reality, during the transit of an exoplanet, a small portion of the host starlight will filter through the planet’s atmosphere. The planet’s radius, and therefore the projected area of its silhouette, changes as a function of the wavelength of the filtered light. This wavelength dependence arises from the scattering/absorption properties of the atoms and molecules in the planet’s atmosphere. At wavelengths of strong atomic or molecular absorption, the atmosphere is more opaque, and the planet’s effective area relative to its host star is larger. Therefore, by measuring the planet’s effective radius or *transit radius*, by means of the transit depth, as a function of wavelength, one can gain an understanding of the chemical composition and physical structure of the planet’s atmosphere.

This technique was first modelled for extrasolar planets by Seager & Sasselov (2000) and successfully applied by Charbonneau et al. (2002), which led to the detection of neutral sodium in the atmosphere of HD 209458b using HST, marking the beginning of a new era in the study of transiting exoplanets. Since this pioneering discovery, a plethora of exoplanetary atmospheres have been identified, and their atmospheric properties studied, using transmission spectroscopy, with both ground- and space-based observatories.

Transmission spectroscopy observations of exoplanetary atmospheres can typically be classified into two distinct categories, low- ($R = \lambda/\Delta\lambda \sim 10^2 - 10^3$) and high-resolution ($R = \lambda/\Delta\lambda \gtrsim 10^5$) transmission spectroscopy.

1.2.2.1 Low-resolution Transmission Spectroscopy

In the past, low-resolution spectrographs have traditionally dominated the field of exoplanet atmospheric characterisation. The first spectroscopic measurements of exoplanetary atmospheres were made using space-based instruments (Sing et al., 2008; Sing et al., 2011), however, these techniques require extremely stable time-series measurements, with instrumental systematics having limited the measurement of transit depths to a precision of $\approx 10^{-3}$ (Gibson et al., 2019). In contrast to high-resolution transmission spectroscopy, ‘low-resolution’ directly measures the transit light curve as a function of wavelength, known as *spectroscopic light curves*. Ground-based observations at low-resolution have also shown some success, with the use of multi-object spectrographs increasing the stability of time-series observations (Bean et al., 2010; Nikolov et al., 2016; Gibson et al., 2017). Despite many efforts to develop statistical frameworks to account for these instrumental systematics and extract transmission spectra, there has been a history of ambiguous and often contradictory results (Sing et al., 2009; Gibson et al., 2011; Sedaghati et al., 2017; Espinoza et al., 2018).

However, with the launch of the James Webb Space Telescope (JWST) in December 2021, the stability and precision of low-resolution observations have improved dramatically (see Fig. 1.3). During the first 5 months of JWST science operations, the Transiting Exoplanet Community Early Release Science (ERS) Program (ERS Program 1366, PIs: Batalha, Bean, and Stevenson) observed 4 transits of WASP-39b using the NIRISS/SOSS, NIRCам/F322W2, NIRSpec/G395H, and NIRSpec/PRISM instruments, respectively (Feinstein et al., 2023; Ahrer et al., 2023; Alderson et al., 2023; Rustamkulov et al., 2023). With JWST’s enhanced sensitivity and wavelength coverage, these observations were able to recover the transmission spectrum of WASP-

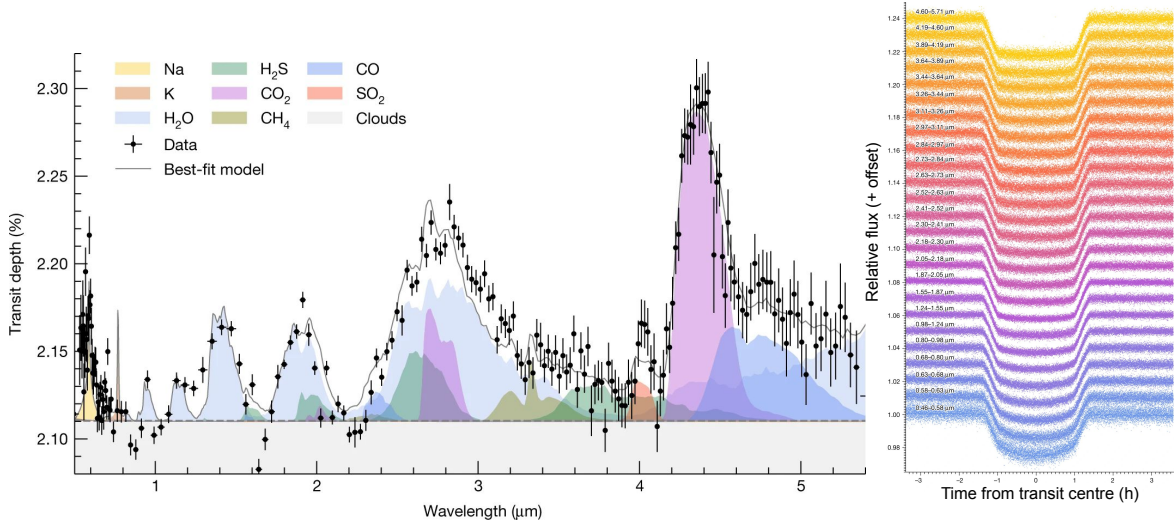


Figure 1.3: The NIRSpec/PRISM transmission spectrum of WASP-39b from Rustamkulov et al. (2023). The transit light curves are also shown on the right, highlighting the stability of JWST, with negligible time- and wavelength-dependent systematic effects present.

39b from $0.5 - 5.5 \mu\text{m}$ in unprecedented detail (see Fig. 1.3). These spectra include a notable SO_2 feature at $\approx 4\mu\text{m}$, thought to be the first unambiguous detection of a byproduct of photochemistry in an exoplanetary atmosphere (Tsai et al., 2023). Recent follow-up analysis of the NIRSPEC/PRISM observations analysed the inhomogeneous terminator of WASP-39b, by splitting the transmission spectrum into its morning (leading) and evening (trailing) limb contributions (Espinoza et al., 2024), finding a temperature difference of roughly 200 K between the two hemispheres. These observations, among others, have highlighted the power of JWST and of low-resolution transmission spectroscopy in enhancing our understanding of the atmospheres of these worlds.

Observations at low-resolution are typically sensitive to atmospheric layers deep within the atmosphere, from the troposphere ($P \sim 10 \text{ bar} - 10^{-4} \text{ bar}$), where clouds and molecular bands are formed, to the edge of the thermosphere ($P \gtrsim 10^{-6} \text{ bar}$) (Pino et al., 2018). At higher altitudes, the atmospheres of close-in giant planets such as hot Jupiters (HJs; $T_{\text{eq}} \gtrsim 1000 \text{ K}$) and ultra-hot Jupiters (UHJs; $T_{\text{eq}} \gtrsim 2200 \text{ K}$) experience thermal dissociation of their molecular species and thermal ionisation of their atoms (Parmentier et al., 2018). The cores of these atoms' absorption/emission lines can be

resolved via high-resolution spectroscopy, thus allowing astronomers to simultaneously probe these lower pressure/higher altitude regimes.

1.2.2.2 High-resolution Transmission Spectroscopy

Ground-based high-resolution spectrographs have recently emerged as an additional tool in characterising exoplanetary atmospheres. Ground-based low-resolution observations using multi-object spectrographs simultaneously observe a reference star, to compensate for instrumental systematics affecting the target star (Bean et al., 2010). Alternatively, high-resolution observations do not observe a reference star, and rely on out-of-transit observations of the target stellar spectrum to correct for systematics. These instruments are capable of resolving the individual spectral lines of atomic/molecular species in a transiting exoplanetary atmosphere, resulting in their unambiguous detection/non-detection through a variety of techniques.

There are several related and complementary methods that one might use to study these objects at high resolution in transmission. Firstly, one can measure the excess absorption in the cores of strong atmospheric transition lines by comparing the differential flux of in-transit and out-of-transit spectra (Wyttenbach et al., 2015; Casasayas-Barris et al., 2019; Seidel et al., 2021), a technique known as narrowband transmission spectroscopy. This technique involves analysing individual resolved absorption lines in a given wavelength range directly (see Fig. 1.4) and therefore is typically reserved for the strongest absorbing species (Borsa et al., 2020). The shapes of these absorption lines are governed by the dynamics of the atmosphere at the altitudes probed for a given species (Seidel et al., 2020, 2021; Hoeijmakers et al., 2020). However, this technique typically requires combining the signal over the entire transit to increase the S/N, thus losing information on the orbital velocity one might extract using alternative techniques.

Chromatic Rossiter-McLaughlin (CRM) can also probe the atmosphere of a transiting

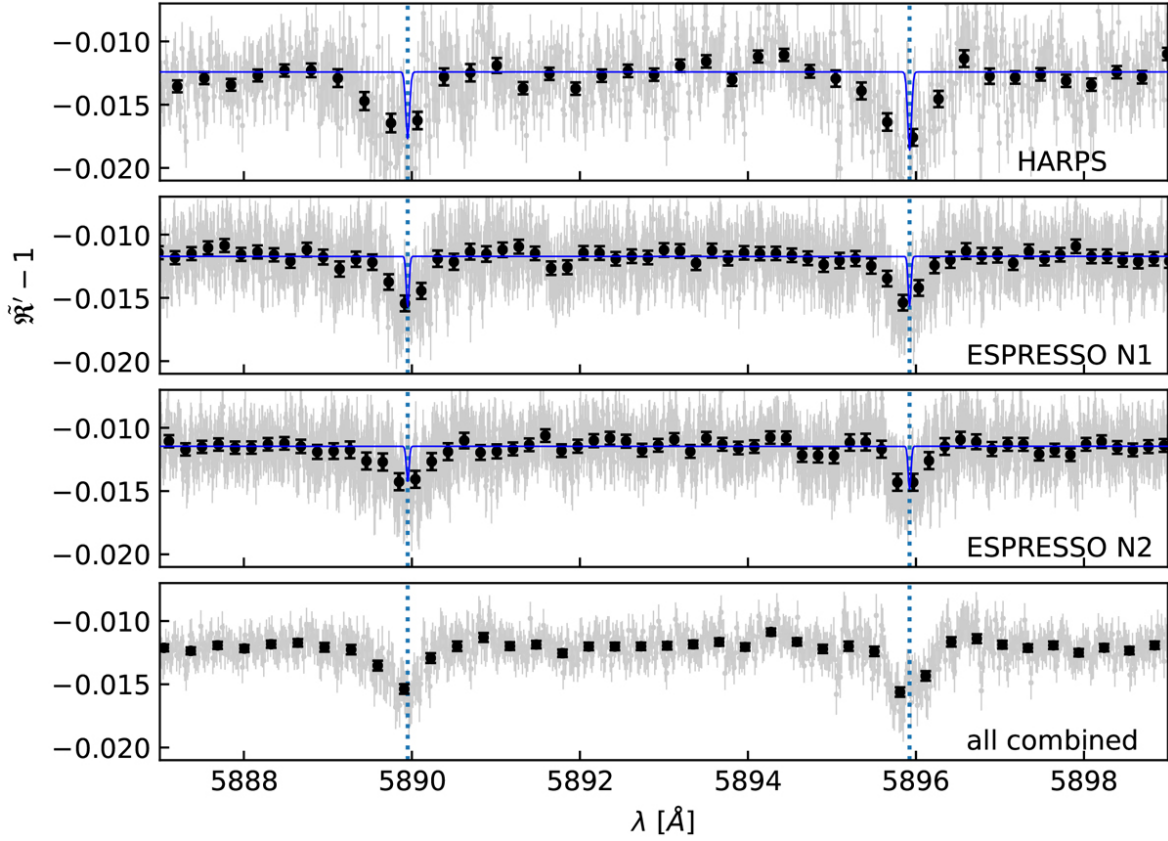


Figure 1.4: The sodium doublet, located at 5890 Å and 5896 Å, of WASP-76b observed via narrowband transmission spectroscopy with the High Accuracy Radial velocity Planet Searcher (HARPS) and ESPRESSO (Seidel et al., 2021). The individual transmission lines are typically shifted to the planet’s rest frame before combining, boosting the signal.

planet, by measuring the planetary radius as a function of wavelength, similar to the technique outlined in low-resolution studies (Snellen, 2004; Di Gloria et al., 2015; Borsa et al., 2020). The Rossiter-McLaughlin (RM) effect, discussed further in Sect. 2.2.3, refers to the apparent distortion of stellar spectral lines observed during a planetary transit. As the planet crosses the stellar disk, it successively obscures portions of the blueshifted and redshifted hemispheres caused by stellar rotation (assuming a synchronous orbit), creating a temporary anomaly in the star’s absorption line shapes and thus observed radial velocity (RV) signature. The amplitude and shape of this RV anomaly contains information regarding the planet-star radius ratio. As this changes as a function of wavelength, one can use the RM effect anomalies to measure the planet radius variations as a function of the wavelength, i.e., the transmission spectrum of the planet (Cristo et al., 2022).

A powerful technique which has emerged in recent years, high-resolution cross-correlation spectroscopy (HRCCS) or Doppler-resolved spectroscopy, can phase-resolve absorption/emission lines from transiting and non-transiting planets through the use of cross-correlation analysis (Snellen et al., 2010; Brogi et al., 2014). This approach utilises the large Doppler shift of atmospheric transition lines relative to its host star, with a significant shift between subsequent exposures. The quasi-stationary stellar and telluric lines (i.e., spectral lines due to absorption in the Earth’s atmosphere) can be removed from the observed data, and the planetary signal can then be detected through cross-correlation with an atmospheric model, shifted over a range of velocities, effectively summing up over many spectral lines in the observed wavelength range. This technique is discussed in detail in Sect. 2.4.1. HRCCS has not only proven proficient at unambiguously identifying chemical species in the atmospheres of transiting exoplanets, but it also has been developed upon to retrieve atmospheric abundances and T - P profiles in a Bayesian framework (Brogi & Line, 2019; Gibson et al., 2020). This is outlined in detail in Sect. 2.4.2. Furthermore, it has also been used to map day-to-night wind velocities, as well as variations in the wind measurements and abundance profiles of species between morning and evening hemispheres of HJ/UHJs (Louden & Wheatley, 2015; Ehrenreich et al., 2020; Seidel et al., 2020, 2021; Gandhi et al., 2022; Boucher et al., 2023; Maguire et al., 2024).

The higher pressure of deeper atmospheric layers can increase the opacity of atomic and molecular species in the optical, thus making their spectral signatures more readily accessible with high-resolution observations. However, in contrast to low-resolution observations, high-resolution observations are also sensitive to the fine cores of alkali atoms, as well as the spectral signatures of ionised/doubly-ionised atomic species, generated at higher altitudes in the lower thermosphere ($P \sim 10^{-4}$ bar) to the exosphere ($P \gtrsim 10^{-11}$ bar) (Pino et al., 2018; Hoeijmakers et al., 2019). This makes such observations complementary to near and far-UV transit observations, which probe the

transition between the upper thermosphere and the exosphere (Vidal-Madjar et al., 2013; Sing et al., 2019). Going forward, we will need to combine multiple complementary measurements and techniques from both the ground and space to further understand the nature and origin of these complex worlds.

Methodology

The following chapter outlines the various instrumentation and methods used for the reduction and analysis of the high-resolution, time-series, spectroscopic data presented in this work.

2.1 Instrumentation

2.1.1 ESPRESSO

The majority of the analysis and results presented in this work rely primarily on observations obtained with ESPRESSO installed at the incoherent combined Coudé focus (ICCF) of the VLT, Paranal Observatory, Chile. ESPRESSO is a fibre-fed, cross-dispersed, high-resolution echelle spectrograph.

2.1.1.1 The Echelle Spectrograph

An echelle spectrograph (from French *échelle*, meaning ladder) is a spectrograph in which the incident light is dispersed using an echelle grating. An echelle grating is a diffraction grating which is characterised by a relatively low groove density and a large angle of diffraction, facilitating the diffraction of higher orders (Chaffee & Schroeder, 1976). This property is evident in the diffraction equation:

$$n\lambda = a(\sin \theta_i + \sin \theta_m) \quad (2.1)$$

where n is the diffraction order, λ is the wavelength of the incident light, a is the groove spacing (which is relatively large for an echelle grating), θ_i is the incident angle, and θ_m is the diffraction angle for the m^{th} order, such that a large a and large θ_m ensures the diffraction of higher orders. From Eq. 2.1, for constant θ_i , it follows that:

$$d\theta_m/d\lambda = \frac{n}{a \cos \theta_m} \quad (2.2)$$

thus for higher orders, n , the angular dispersion increases. This also results in a higher resolution, $R = \lambda/d\lambda = nN$, where N is the total number of grooves in the diffraction grating. A consequence of operating at higher diffraction orders, and thus higher resolution, is the decrease in angular separation of adjacent orders produced from an echelle grating, resulting in order overlap. The wavelength difference between two wavelengths in successive orders at the same diffraction angle, θ_m , is given by $\Delta\lambda = \lambda/n$, which monotonically decreases for higher diffraction orders (Schroeder, 1970). In order to overcome overlapping orders on the detector, an additional optical element known as a cross-disperser—which is typically an additional diffraction grating or prism—is added to the light path to “cross-disperse” the light. This results in a two-dimensional image on the detector, known as an echellogram, with the spectral axis showing high-resolution dispersion of spectra within each order, and each separate order dispersed along the spatial axis (see Fig. 2.1c). In the case of ESPRESSO, the cross-dispersing elements are volume-phase holographic (VPH) gratings (Arns, 2016).

2.1.1.2 The ESPRESSO Project

The ESPRESSO spectrograph was designed initially with two main science objectives:

- the detection of Earth-mass planets in the habitable zone around GKM stars;
- the measurement of potential variations in the fundamental constants of the Universe

With these objectives in mind, it is essential that ESPRESSO reaches the required spectral resolution to impose an RV precision of 10 cm s^{-1} and a metrological stability which ensures its maintained precision over a timescale of several years (Pepe et al., 2021). For the first objective, this RV precision is akin to the RV semi-amplitude of an Earth-like planet orbiting within the habitable zone of a Sun-like star. Similarly, the metal transition lines of distant quasars are sensitive to the fine structure constant, α , whereas the molecular transitions which cause the Lyman-alpha forest from hydrogen clouds in the interstellar medium (ISM) are sensitive to the proton-to-electron

mass ratio, μ (Bahcall & Schmidt, 1967; Thompson, 1975). Therefore, by monitoring these quantities over several years via ultra-stable, high-resolution spectroscopic observations, one can search for potential non-trivial variations of these fundamental constants. These observations would also need to be monitored over a number of orbits/years, requiring extreme thermo-mechanical and illumination stability as well as a stable wavelength calibration source.

The target RV precision of 10 cm s^{-1} corresponds to a physical shift of the spectrum in the focal plane of the spectrograph by merely a few nanometres. Thus, the optical system of ESPRESSO (see Fig. 2.1) is mounted inside a vacuum vessel in which a 10^{-5} mbar class vacuum is permanently maintained. The temperature of the optical system is also stabilised at the mK level by enclosing the spectrograph in a multishell thermal enclosure system, to avoid variations in the optical refractive index. Furthermore, any thermal “breathing” or instrumental drift of the detector due to the warming-up and cooling-down of readout electronics, for example, must also be monitored and accounted for. To do so, the instrument applies the ‘simultaneous-reference’ technique (Pepe et al., 2002; Mayor et al., 2003), successfully utilised on the predecessor to ESPRESSO: the High-Accuracy Radial velocity Planetary Searcher (HARPS). This technique requires two optical fibres running parallel, such that their light paths—and thus the optical aberrations and distortions they experience—are near-identical. Fibre A is the target fibre, which is placed on the scientific target. Fibre B is the reference fibre, which is placed on a simultaneous spectral reference, in this case a combination of a Thorium-Argon (ThAr) lamp and Fabry-Pérot etalon, which has a number of sharp and stable lines across the wavelength range of ESPRESSO. By monitoring the distortions of spectral lines on the reference spectrum from instrumental drift, one can maintain the precision and stability of the target spectrum. This reference spectrum also ensures an accurate wavelength calibration source for the detectors of ESPRESSO—two E2V CCDs of $9\text{k} \times 9\text{k}$ $10 \mu\text{m}$ -square pixels for the red and blue arms, respectively.

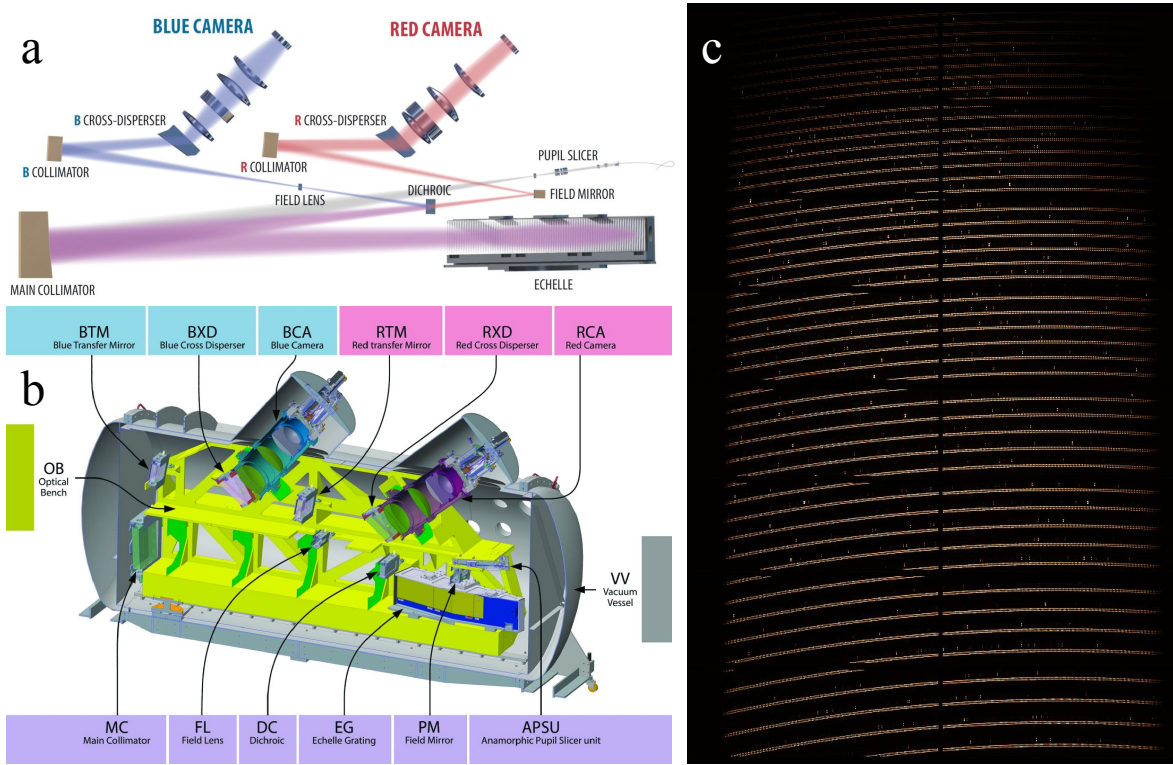


Figure 2.1: The ESPRESSO instrument configuration. (a) Layout of the ESPRESSO spectrograph and its various optical elements. (b) Optical system of the ESPRESSO spectrograph within the vacuum vessel. (c) Example of a raw frame, or echellogram, taken by the red CCD of ESPRESSO illuminated with the ThAr lamp. The horizontal axis is the spectral axis, and the vertical axis is the spatial axis. Each curved horizontal trace is an individual echelle order. The continuous dots are caused by Fabry P rot calibration source illuminating fibre B, whereas the intermittent dots above are caused by illumination of fibre A with the ThAr lamp.

2.2 Data Reduction

2.2.1 Error Estimation

Given the significant variation in flux with respect to both wavelength and time, it is important that realistic estimates of the uncertainties in the flux values are obtained, in order to optimally extract the information content of the spectra. The data were reduced using the ESPRESSO Data Reduction Software (DRS) v2.3.3, and the two-dimensional non-blaze-corrected S2D spectra were extracted. The DRS includes standard reduction procedures for echelle time-series spectra, such as bias and dark subtraction, flat-field and contaminated pixel correction, as well as wavelength calibration and barycentric velocity correction. Following the procedure outlined in Gibson et al. (2020), the uncertainties are estimated assuming Poisson-noise. Firstly, the out-

liers are removed from each ESPRESSO spectral order by subtracting a simple model of the data, constructed via the outer product of the median spectrum (i.e., median as a function of time) and median light curve (i.e., median as a function of wavelength), weighted by the mean of the median spectrum (to correct the scaling). A 10th order polynomial is then fitted to each spectrum of the residual orders, and any 5 σ outliers are replaced by their respective polynomial value, before adding the cleaned residual array back to the subtracted model. It is from this ‘cleaned’ array that the uncertainty values are estimated. For each spectral order, an initial Poisson uncertainty estimate of the form $\sigma_i = \sqrt{aF_i + b}$ is assumed for each pixel, where F_i is the respective pixel flux value, and a and b are the uncertainty scale factor and gain, respectively. A 5th order Principal Component Analysis (PCA) decomposition of the order is then constructed and subtracted, removing the stellar spectrum, resulting in a new residual array, R . Values for a and b , and thus σ_i , are then found via the optimisation of a Gaussian log-likelihood of the form:

$$\ln \mathcal{L}(a, b) = -0.5 \sum_i \left(\frac{R_i}{\sigma_i} \right)^2 - \sum_i \ln \sigma_i$$

The uncertainties are constructed from the best-fit values for a and b , before finally fitting this estimate with another 5th order PCA model, in order to remove biases in the Poisson uncertainty estimate. This model is the final estimate of the uncertainties. This uncertainty estimation routine was used for the analysis presented in Chaps. 3 – 5. Poisson uncertainty estimates from count rates and read-noise can bias fits to the residuals after removing the stellar spectra—which is fundamental to the high-resolution technique—by imposing that negative values of the residuals (i.e., lower count rates) will always have lower uncertainties than positive values. Therefore, the final step of fitting the uncertainty estimate with a 5th order PCA is included in order to mitigate these biases by removing any ‘noise’ at the pixel level in the uncertainty estimate.

2.2.2 Blaze Correction

After outlier removal and uncertainty estimation, the variation of the throughput of the spectrograph as a function of wavelength—which is characterised by the *blaze function*—must also be removed. The individual spectral orders are blaze-corrected following Merritt et al. (2020). Firstly, each order is divided by its mean spectrum. The resultant residual array is then smoothed with a median filter to remove outliers, followed by a Gaussian filter. The width and standard deviations of these filters vary depending on the analysis presented in Chaps. 3 – 5. The original orders and their respective uncertainties are then divided by these resultant smoothed residuals. This does not remove the blaze function, but instead places each spectrum on a common blaze function in time. This allows the blaze function to be readily removed after division through by the median spectrum of each order. After cleaning and blaze correction, the spectra are then Doppler shifted to the stellar rest frame via the stellar radial velocity:

$$v_{\star} = K_{\star} \cdot \sin(2\pi\phi) + \gamma \quad (2.3)$$

where $K_{\star}$, ϕ , and γ are the stellar radial velocity semi-amplitude, orbital phase, and systemic velocity, respectively. It is worth noting that the efficacy of this procedure relies heavily on a precise estimate of the stellar parameters. The result of each of these data reduction steps on a single spectral order of ESPRESSO observations of WASP-121b is shown in Fig. 2.2.

2.2.3 Removal of CLVs and the RM Effect

In addition to contamination, or spectral distortion such as the blaze, imprinted on the spectra, there are also spectral imprints due to the spatial and dynamical variation of the stellar spectrum across the stellar disk, whilst a planet is in transit, such as Centre-to-Limb variations (CLVs) and the Rossiter-McLaughlin (RM) effect. As has

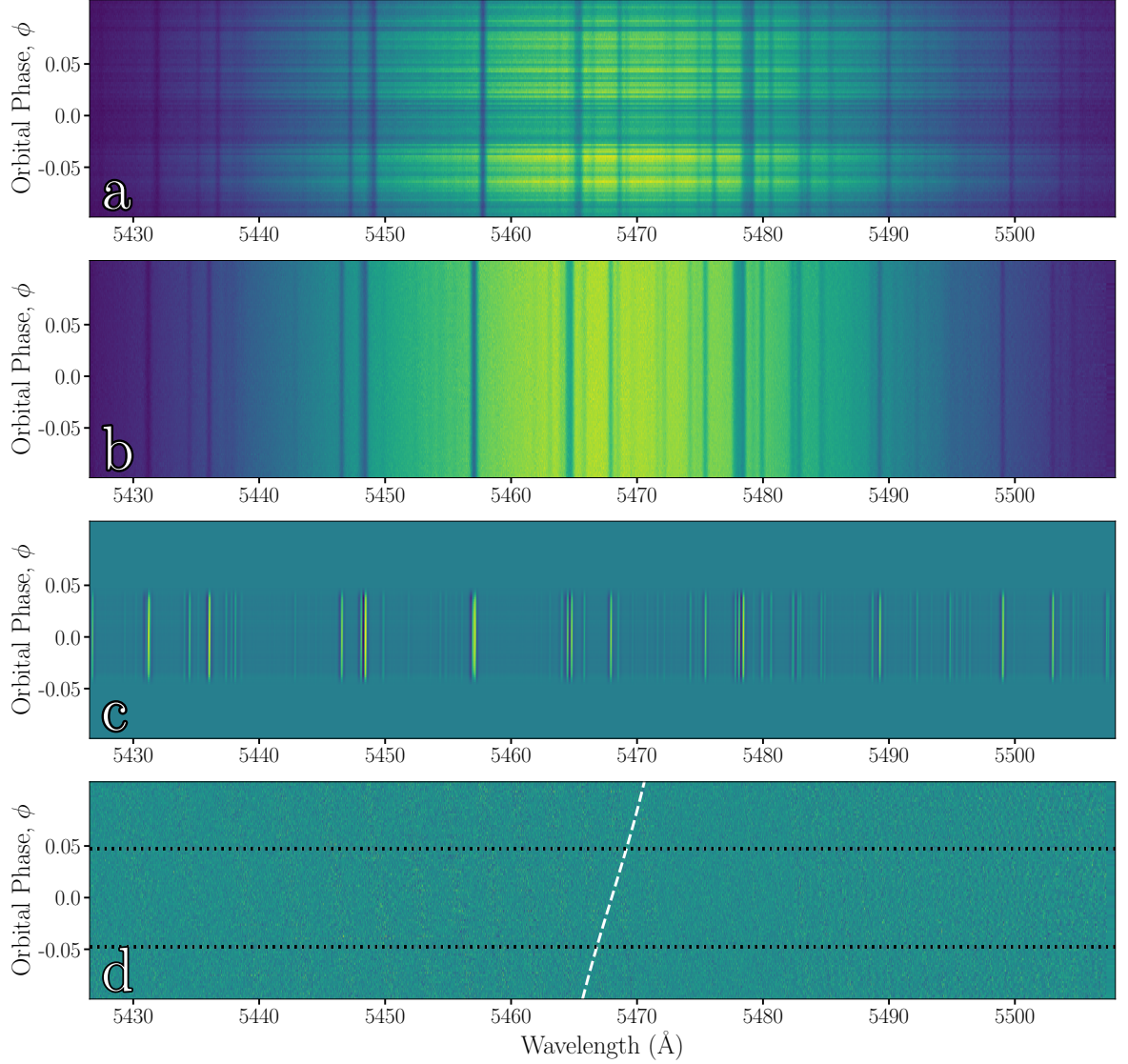


Figure 2.2: The data reduction steps applied to a single ESPRESSO order of T2 (see Chap. 3 for further details). **(a)** Cleaning and outlier removal. **(b)** Blaze correction and Doppler shift to the stellar rest frame. **(c)** The modelled CLV and RM distortions on the in-transit spectra. **(d)** After CLV and RM removal, and removal of stellar and telluric features with SYSREM. The black dotted horizontal lines show the orbital phases of ingress and egress, whereas the white dashed curve shows the approximate velocity shift of WASP-121b.

become common practice in the reduction of high-resolution transmission spectroscopy observations (Yan et al., 2017; Casasayas-Barris et al., 2017, 2018; Yan et al., 2019; Turner et al., 2020; Nugroho et al., 2020b), these distortions of the stellar spectral lines, caused by both CLVs and the RM effect, are modelled and removed from the data. Following Nugroho et al. (2020b), synthetic stellar spectra are generated at 21 different limb darkening coefficients, $\mu = \cos \theta$, where θ is the limb darkening angle, using SPECTROSCOPY MADE EASY (SME, Piskunov & Valenti 2017), with line lists obtained from the VALD3¹ database (Ryabchikova et al., 2015) using MARCS stellar models (Gustafsson et al., 2008). A μ value is then calculated for each pixel on a two-dimensional stellar grid ranging from $-1 R_\star$ to $+1 R_\star$ in steps of $0.01 R_\star$ in both the x and y dimensions, onto which the μ -dependent synthetic spectra are linearly interpolated. A projected equatorial rotational velocity, $v_{\text{eq}} \cdot \sin i_\star$, value is also calculated for each pixel, with the corresponding spectrum then Doppler shifted, assuming solid body rotation and ignoring gravity darkening. For each exposure of the observations, as the planet transits the stellar disk, the occulted pixels are masked using a binary mask, and the remaining spectra are integrated over the entire disk. This assumes the planet is an opaque disk of radius R_p across the entire wavelength range. A schematic diagram of these stellar grids, as well as the transiting planetary disk, is shown in Fig. 2.3. Thus, a model stellar spectrum is generated for each exposure, which includes the distortions from both CLVs and the RM effect in-transit. The stellar model spectra are then divided by the out-of-transit spectrum, ensuring only distortions caused by CLVs and the RM effect remain. The data is then divided by this final model, which is shown in Fig. 2.2c. Without this step, an anomalous ‘Doppler shadow’ is apparent in the cross-correlation maps ($\Delta v_{\text{sys}} \simeq 0 \text{ km s}^{-1}$) of species present in the stellar atmosphere (see Fig. 3.1a).

¹<http://vald.astro.uu.se>

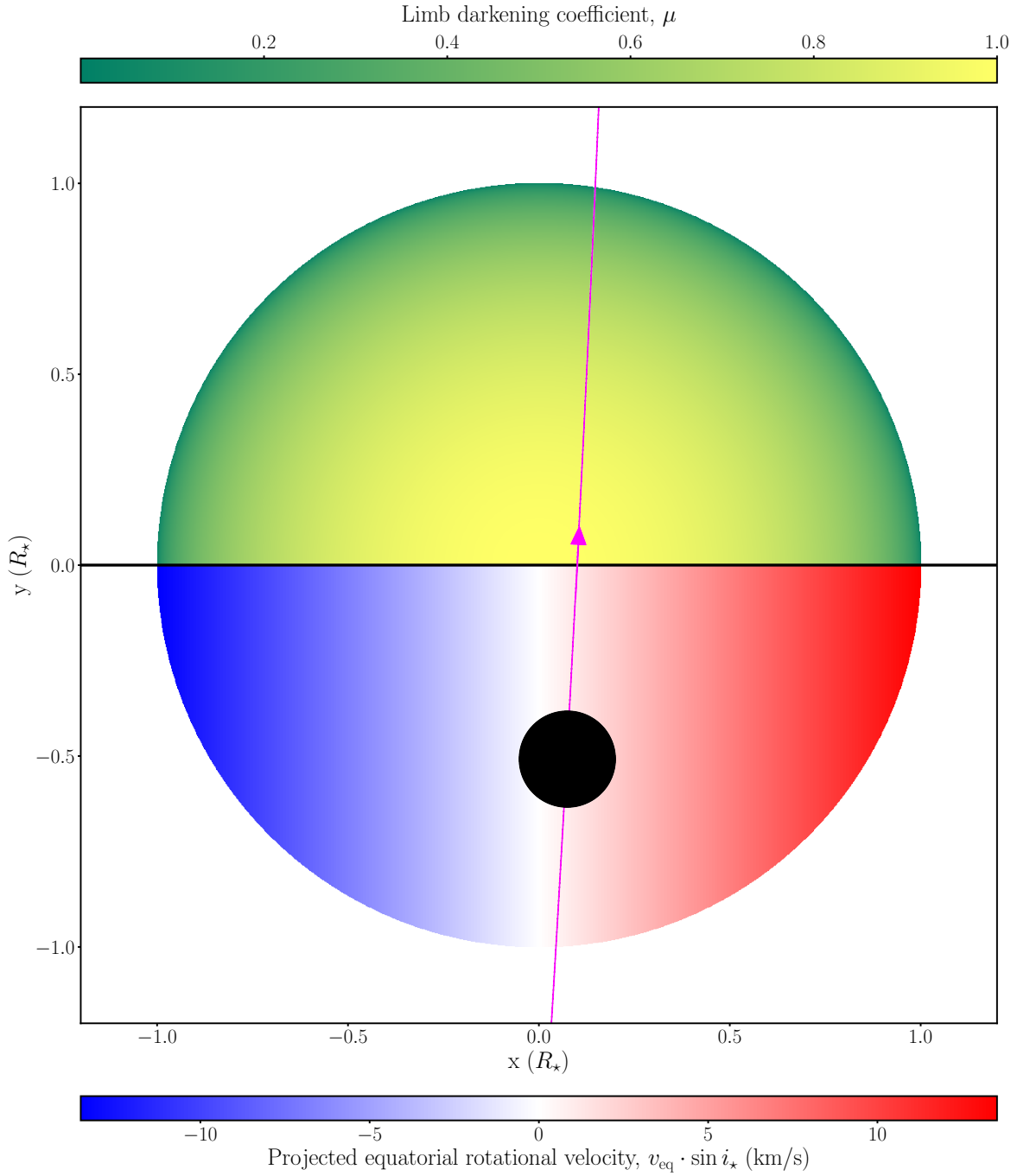


Figure 2.3: The stellar model used to compute the distortions caused by CLVs and the RM effect, outlined in Sect. 2.2.3. The upper half shows the variation of the limb darkening coefficient, μ , across the stellar disk. The lower half shows the projected equatorial rotational velocity of the star across the stellar disk. The stellar model in the above figure is WASP-121, which hosts an ultra-hot Jupiter WASP-121b, shown as a black disk to scale. The orbital trajectory of WASP-121b is also shown in pink.

2.2.4 Removal of Stellar and Telluric Lines

Observing a planet’s host star from the ground poses significant challenges, not least the removal of contamination by numerous stellar and telluric absorption and emission

lines caused by the host star and the Earth’s atmosphere, respectively. The extent of this telluric contamination in the optical and near-infrared is shown in Fig. 2.4. In the past, a telluric standard star would be observed alongside the target star, in order to correct for telluric contamination. This method, however, is costly, as it would require valuable telescope time to observe the telluric star, which would otherwise be used for other scientific observations (Smette et al., 2015). This method of telluric correction is also not perfect, as temporal variation of the Earth’s atmosphere over the course of an observation causes differences in the contamination of the reference and target spectra, particularly if both are not subsequently observed within a short time period and/or at small angular separations on the sky. Furthermore, normalising a telluric standard’s continuum, as well as its broad absorption lines, is never without imprecisions.

In more recent years, it has become common practice to model the telluric spectra directly, with tools such as MOLECFIT (Smette et al., 2015; Kausch et al., 2015) and TELFIT (Gullikson et al., 2014), which combine line-by-line radiative transfer calculations with on-site meteorological data to estimate the transmission spectrum of the Earth’s atmosphere across the wavelength range of the observations. MOLECFIT is further detailed below in Sect. 2.2.4.2. This method also accounts for the temporal variation of airmass above the telescope over the course of an observation, and has been successfully implemented in removing telluric contamination of high-resolution exoplanetary spectra (Sedaghati et al., 2021). This telluric removal method has also been shown to be more effective in removing the contamination on high-resolution X-Shooter spectra when compared to correcting with a telluric reference star (Kausch et al., 2015). It has also been shown to be more effective in removing the contamination on exoplanetary spectra when compared to obtaining a telluric reference spectrum directly from the data, assuming telluric line strength varies linearly with airmass (Langeveld et al., 2021). This telluric removal method is typically paired with division of a master out-of-transit spectrum, which represents the stellar spectrum free from additional planetary absorption/emission.

After the data has been shifted to the stellar rest frame via Eq. 2.3, the stellar and telluric features are (quasi-)static in time, meaning they undergo no significant Doppler shift across adjacent wavelength channels over the course of the observations. Another common method of removing time invariant features is constructing a model of the observed spectra directly using PCA-like algorithms and removing this model from the observations. However, these algorithms can often be overly aggressive in their removal, as there exists no obvious halting criterion, and thus run the risk of inadvertently distorting the underlying exoplanet signal (Birkby et al., 2017).

2.2.4.1 SYSREM

Many PCA-like algorithms have been successfully implemented to treat high-resolution spectroscopy observation of exoplanetary atmospheres, such as singular value decomposition (de Kok et al., 2013), eigenvalue decomposition (Damiano et al., 2019), and SYSREM (Tamuz et al., 2005, 2006; Birkby et al., 2013). SYSREM can be seen as a generalisation of PCA, which accounts for time- and wavelength-based uncertainties. The modelling and removal of telluric contamination from high-resolution exoplanetary spectra using SYSREM was first implemented by Birkby et al. (2013), and has since become common practice for both transmission and emission observations (e.g., Gibson et al., 2020; Nugroho et al., 2021). These methods model the stellar and telluric lines which are (quasi-)stationary in wavelength, as a function of time, which can then be subsequently removed from the observations. Birkby et al. (2013) developed upon the initial use of SYSREM by Tamuz et al. (2005) in which the algorithm was used to detrend light curves in photometric transit surveys. In its application to high-resolution spectroscopy, each wavelength channel may be treated as an individual light curve (see Fig. 2.2). SYSREM targets common modes or principal components, such as the variation in airmass between the 9111 wavelength channels in an ESPRESSO order (Birkby et al., 2017).

SYSREM is an iterative algorithm which aims to fit the (quasi-)static features in each column of a 2D array. As stated above, for high-resolution spectroscopy this amounts to fitting time invariant features across each column (i.e., wavelength channel). For each iteration of SYSREM, the input is the mean-subtracted data array, $\mathbf{R}$, and the inverse variance, $1/\sigma^2$, where σ is the data uncertainties. The mean-subtracted data $\mathbf{R}$ is decomposed into two column vectors, $\mathbf{u}$ and $\mathbf{w}$, where the SYSREM model for each iteration, p , is given by their outer product $\mathbf{u}_p \mathbf{w}_p^\top$. SYSREM removes the product $\mathbf{u}_p \mathbf{w}_p^\top$ from the residuals $\mathbf{R}$. However, $\mathbf{u}$ and $\mathbf{w}$ must first be calculated for each pass of SYSREM. In practice, the best-fit w_i is calculated which minimises the expression:

$$S_i^2 = \sum_j \frac{(R_{ij} - w_i u_j)^2}{\sigma_{ij}^2} \quad (2.4)$$

where i and j are the data columns and rows, respectively. Assuming u_j is known, the above expression is differentiated and equated to zero to estimate w_i :

$$w_i = \frac{\sum_j \frac{R_{ij} u_j}{\sigma_{ij}^2}}{\sum_j \frac{u_j^2}{\sigma_{ij}^2}} \quad (2.5)$$

With the updated w_i , the process is repeated for u_j by minimising:

$$S_j^2 = \sum_i \frac{(R_{ij} - w_i u_j)^2}{\sigma_{ij}^2} \quad (2.6)$$

whilst estimating u_j via:

$$u_j = \frac{\sum_i \frac{R_{ij} w_i}{\sigma_{ij}^2}}{\sum_i \frac{w_i^2}{\sigma_{ij}^2}} \quad (2.7)$$

This value of u_j is then used to recalculate the best-fitting w_i via Eq. 2.5, and the process continues iteratively. Thus, SYSREM is an iterative process which searches for the two sets— $\{w_i\}$ and $\{u_j\}$ —that best fit the common modes in the underlying data. Tamuz et al. (2005) performed many simulations that showed that this iterative

process converged to the same $\{u_j\}$ and $\{w_i\}$, no matter which initial values are used.

The model, $\mathbf{u}_p \mathbf{w}_p^\top$, is then subtracted from the input, to get the processed data, $\mathbf{R}_N$, after N iterations, such that:

$$\begin{aligned}\mathbf{R}_N &= \mathbf{R} - \sum_{p=1}^N \mathbf{u}_p \mathbf{w}_p^\top \\ \mathbf{R}_N &= \mathbf{R} - \mathbf{U} \mathbf{W}^\top\end{aligned}\tag{2.8}$$

where $\mathbf{U}$ and $\mathbf{W}$ are matrices containing each column vector $\mathbf{u}_p$ and $\mathbf{w}_p$. $\mathbf{U}$ is a $j \times N$ matrix where j is the number of rows (i.e., exposures) and N is the number of SYSREM passes. Similarly, $\mathbf{W}$ is an $i \times N$ matrix, where i is the number of columns (i.e., wavelength channels). An example of a single order of the final reduced array after running SYSREM, weighted on its uncertainties, is shown in Fig. 2.2d.

2.2.4.2 MOLECFIT

As mentioned above, it is also common practice to model the transmission spectrum of the Earth's atmosphere above the observatory over the course of the observations, and remove this model from your data. One of the most common telluric modelling tools is MOLECFIT. MOLECFIT has the advantage of being more physically motivated than PCA-like algorithms, as codes such as SYSREM have no prior information regarding observing conditions. The Earth's atmosphere consists of about 78% of N_2 , 21% of O_2 , 1% of Ar, and several trace gases and aerosols. Each of these molecules interact with incoming stellar irradiation via absorption and scattering, and the goal of telluric modelling/removal codes is to remove this contamination such that the spectrum (or photometry) of the target is recovered as it would appear as if the instrument was located above the Earth's atmosphere.

In order to model telluric absorption, MOLECFIT requires and computes the following:

- (1) Vertical atmospheric profiles are calculated by combining three input sources.

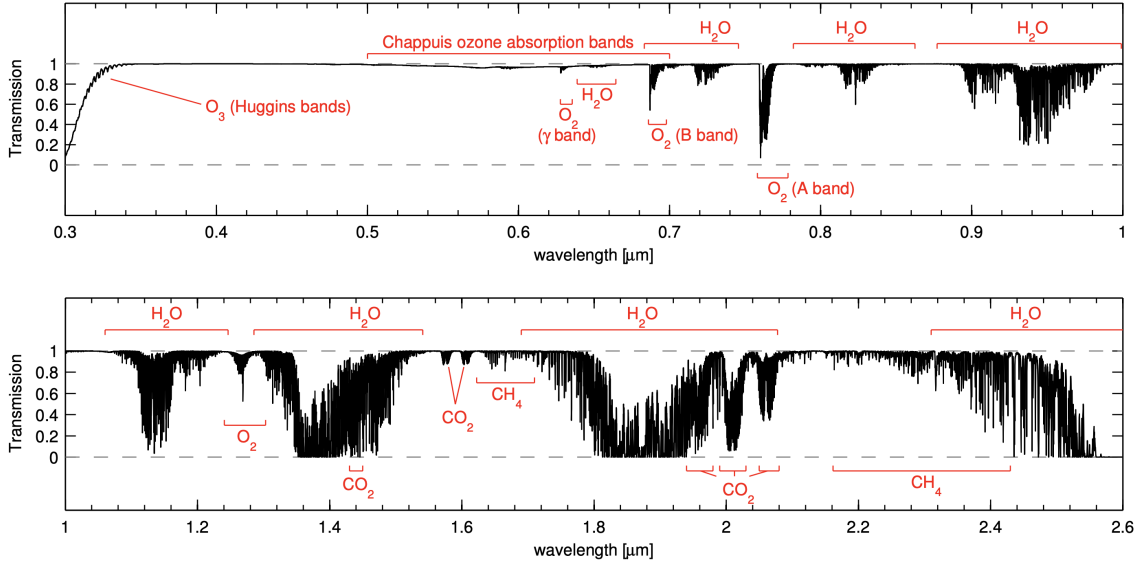


Figure 2.4: Synthetic absorption spectrum of the sky between 0.3 and 2.6 μm . The ESPRESSO wavelength coverage ranges from approximately 0.38 to 0.79 μm . Figure adapted from Smette et al. (2015).

These sources contain information regarding temperature, pressure, relative humidity, wind speed and direction, and abundances of several species as a function of altitude. The default reference profile is the equatorial profile derived from Michelson Interferometer for Passive Atmospheric Sounding (MIPAS¹) measurements onboard the Environmental Satellite (ENVISAT). This profile contains abundances of several molecular species up to an altitude of 120 km, which can either be fit for or adjusted manually. The reference atmosphere is then merged with the modelled Global Data Assimilation System (GDAS²) 3D data provided by the National Oceanic and Atmospheric Administration (NOAA). This model contains time-dependent information on the temperature, pressure, relative humidity, and wind speed/direction up to an altitude of ~ 26 km on a 3 h basis. In the case of ESPRESSO observations, the GDAS model is created by interpolating from four grid points closest to Paranal Observatory. Finally, the ESO Meteo Monitor (EMM) provides local meteorological information for both the La Silla and Paranal observatories. The EMM profiles more accurately represent the geographical position and altitude of the observing site

¹<https://eodg.atm.ox.ac.uk/RFM/atm/>

²<https://www.ready.noaa.gov/gdas1.php>

relative to the MIPAS and GDAS profiles.

- (2) The resultant atmospheric profiles are then used as input to the radiative transfer code LNFL/LBLRTM¹ (Clough et al., 2005). This radiative transfer code utilises line lists from the High-resolution TRANsmision (HITRAN) molecular absorption database (Rothman et al., 2009). Only molecules for which there is an atmospheric abundance available in the standard atmospheric profile (MIPAS) are used by default.
- (3) The model telluric transmission spectrum outlined thus far is then fit to the input science spectrum via the C version of the least-squares fitting library MPFIT. MPFIT is a χ^2 minimisation routine which uses the Levenberg-Marquardt algorithm (Moré, 1978). This fitting procedure requires the careful selection of ‘inclusion regions’, with sufficient continuum and telluric absorption to allow MOLECFIT to accurately determine the telluric column density and line spread function. These ‘inclusion regions’ must be free from intrinsic features from the science object and instrument, as these intrinsic features can disrupt the fitting procedure. The reader is referred to Smette et al. (2015) for further details regarding the radiative transfer calculation and fitting procedure.

MOLECFIT finally outputs a synthetic transmission spectrum and the division of the input spectrum by the transmission spectrum over the full spectral range of the input spectrum. This procedure is repeated for each exposure, or input spectrum, of the observations. The application of MOLECFIT to ESPRESSO data is explored further in Sect. 5.1.4 and shown in Fig. 5.1.

2.3 Atmospheric Modelling

In order to learn anything from the reduced data, these observations must be compared to *forward models*. These models are a theoretical description of the observations at hand. In this case, a spectrum of an exoplanetary atmosphere observed as it transits its

¹http://rtweb.aer.com/lblrtm_frame.html

host star—a *transmission spectrum*—discussed extensively in Sect. 1.2.2. The approach used to compute the atmospheric model presented henceforth was first developed and introduced by Gibson et al. (2022), however is similar to typical atmospheric radiative transfer procedures.

2.3.1 One-dimensional Model Transmission Spectrum

Firstly, the vertical layers of the atmosphere are defined across a range of pressures, which are uniform in log-space. The atmosphere ranges from 10^2 to 10^{-12} bar unless otherwise stated, where the lower pressure regime signifies a higher altitude. A vertical temperature-pressure (T - P) profile is then computed across the atmospheric layers. Many different parameterisations exist in the literature for defining T - P profiles (e.g., Madhusudhan & Seager, 2009; Guillot, 2010), with some more attuned to possessing thermal inversions, which is expected to occur in the upper atmospheres of UHJs. The T - P profile chosen for this study is outlined in Guillot (2010), which defines the temperature as function of pressure (i.e., altitude) as:

$$T(P) = \frac{3T_{\text{int}}^4}{4} \left[\frac{2}{3} + \tau \right] + \frac{3T_{\text{irr}}^4}{4} \mu_{\star} \left[\frac{2}{3} + \frac{\mu_{\star}}{\gamma} + \left(\frac{\gamma}{3\mu_{\star}} - \frac{\mu_{\star}}{\gamma} \right) e^{\frac{-\gamma\tau}{\mu_{\star}}} \right] \quad (2.9)$$

where T_{irr} , T_{int} , and γ are free parameters, representing the irradiation temperature, internal temperature, and the ratio of visible-to-infrared opacity, respectively. $\tau = \kappa_{\text{IR}}P/g$, where κ_{IR} is the remaining free parameter—the mean infrared opacity and P is the pressures at each layer of the atmosphere, respectively. $\mu_{\star} \equiv \cos \theta \equiv \sqrt{K_{\nu}/J_{\nu}}$, where θ is the angle between the incoming beam of radiation and a line extending from the centre of the planet to the point at which the beam reaches the planet’s surface, assuming plane-parallel radiation (see Fig. 2.5). K_{ν} and J_{ν} are defined as moments of the specific intensity of stellar radiation, such that J_{ν} is equivalent to the energy of the beam and $4\pi/cK_{\nu}$ the radiation pressure. In the case of isotropic stellar irradiation, which is assumed in this case, $\mu_{\star} = \sqrt{1/3}$. The vertical T - P structure is then used to compute the vertical extent, or physical height, of the atmosphere assuming hydro-

static equilibrium. This occurs when the internal outward pressure of the atmosphere balances the inward self gravitational force. This assumption is likely valid in the lower regions of the atmospheres of UHJs, but for highly irradiated planets on close-in orbits, their upper atmosphere is thought to be undergoing atmospheric escape, where this assumption breaks down. In order to compute the physical extent of the atmosphere, a reference pressure (P_0), radius (R_0), and surface gravity (g) are assumed for the atmospheric model, and the equations of hydrostatic equilibrium are solved, accounting for the varying gravity and temperature with altitude/pressure. This assumption leads to a well-known degeneracy in transmission spectroscopy studies, as these assumed values alter the location of the base of the atmosphere being observed (Heng & Kitzmann, 2017). Consequently, an incorrect reference pressure or radius could result in inaccurate estimates of the atmospheric species' abundance. This process effectively converts the vertical temperature-pressure structure into a temperature-radius structure (Mollière et al., 2019). Using the ideal gas law, $n = P/k_B T$, where n and k_B are the number density and Boltzmann's constant, respectively, the number density for each layer in the atmosphere is computed. This one-dimensional structure is assumed to represent the vertical structure of the atmosphere across all longitudes and latitudes of the atmospheric terminator probed during the transit. With the vertical structure of the atmosphere defined, the opacity at each layer of the atmosphere is computed. Following similar transmission spectroscopy models (e.g., Mollière et al., 2019), predefined absorption cross-sections across a pressure-temperature grid are used. From this grid, the cross-sections, σ_{species} , are linearly interpolated for each atmospheric species in the model, to the temperature and pressure at each layer of the atmosphere. The cross-sections are then weighted by the species' respective volume mixing ratios (VMRs), χ_{species} , and the number density to give the attenuation coefficient, $\alpha = n\chi_{\text{species}}\sigma_{\text{species}}$, at each atmospheric layer. From this, the grazing geometry of incoming stellar radiation through the different layers of the atmosphere can be computed (see Fig. 2.5).

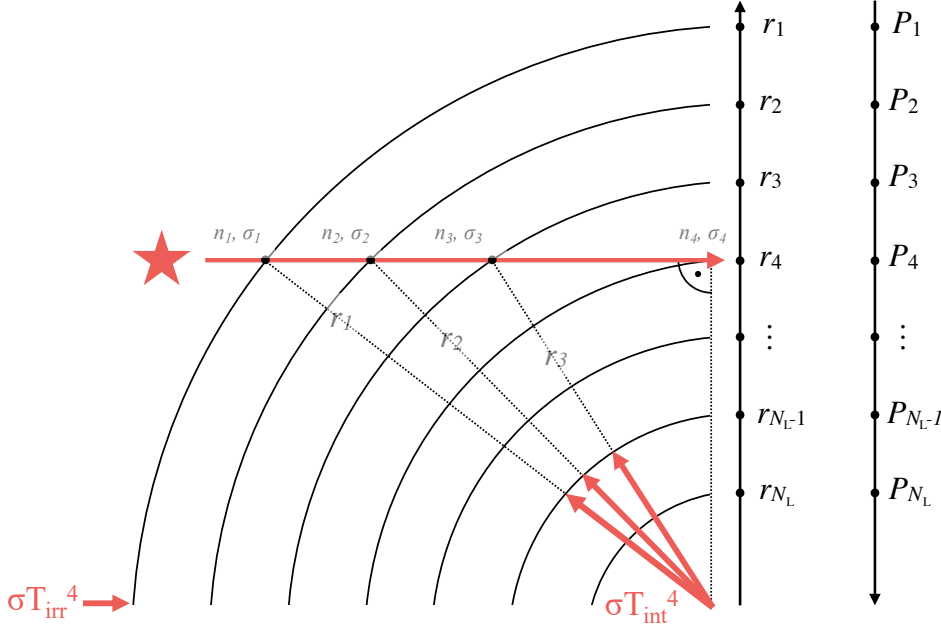


Figure 2.5: A diagram of the vertical structure of the atmospheric model. Incoming stellar flux at the substellar point is equated by the Stefan-Boltzmann law $F = \sigma T_{\text{irr}}^4$, where σ is the Stefan-Boltzmann constant. Similarly, the planet emits an intrinsic heat flux of σT_{int}^4 . Figure adapted from Guillot (2010) and Mollière et al. (2019).

The optical depth is defined as:

$$\tau = \int \alpha ds \quad (2.10)$$

$$= \int n \chi_{\text{species}} \sigma_{\text{species}} ds \quad (2.11)$$

where s is the path length travelled by the stellar photons. For stellar irradiation grazing the atmosphere at an altitude r_i above the planetary centre, this integral along the photon's optical path can be approximated using the Trapezoidal Rule:

$$\tau_i = \frac{1}{2} \sum_{j=1}^{i-1} (\alpha_j + \alpha_{j+1}) \left(\sqrt{r_j^2 - r_i^2} - \sqrt{r_{j+1}^2 - r_i^2} \right) \quad (2.12)$$

where the chord length between subsequent layers comes directly from the Pythagorean theorem. However, since the rays' incoming and outgoing paths are symmetrical around

the closest approach to the planet's centre, the factor of $1/2$ can be omitted, such that:

$$\tau_i = \sum_{j=1}^{i-1} (\alpha_j + \alpha_{j+1}) \left(\sqrt{r_j^2 - r_i^2} - \sqrt{r_{j+1}^2 - r_i^2} \right) \quad (2.13)$$

where α_j is the attenuation coefficient at an altitude r_j . The transmittance T of the planetary atmosphere along an incident ray's path, given by the Beer-Lambert law, is the fraction of incoming flux that is absorbed by the atmosphere:

$$T = e^{-\tau} \quad (2.14)$$

The effective area of the atmosphere during a transit can then be calculated by integrating the transmittance over all possible paths (or altitudes) through the atmosphere:

$$A = \int_0^{R_0} 2\pi r (1 - T) dr \quad (2.15)$$

This equation constitutes the total starlight blocked by the atmosphere by integrating over the concentric annular rings at different altitudes r . This can be converted to an *effective planetary radius* as:

$$\begin{aligned} A_{\text{eff}} &= \pi R_{\text{eff}}^2 = \pi R_0^2 + A \\ R_{\text{eff}} &= \sqrt{R_0^2 + A/\pi} \end{aligned} \quad (2.16)$$

which gives the effective planetary radius as a function of wavelength, i.e., the transmission spectrum. In addition to absorption by atmospheric species, continuum opacity sources such as clouds and hazes are included in the form of an opaque cloud deck and Rayleigh scattering. Following Gibson et al. (2020), the Rayleigh scattering cross-section of Lecavelier des Etangs et al. (2008) are used, and allow for an increase in abundance (χ_{Ray}) relative to H_2 , to increase the scattering strength (e.g., due to larger scattering particles). To account for clouds, an opaque (gray) cloud deck is assumed, located at a pressure, P_{cloud} , at which the model is truncated. The effect of a gray

cloud deck on transmission spectra is shown in Fig. 2.6, and highlights the aforementioned degeneracy in transmission spectroscopy between the absolute abundance of an atmospheric species and other atmospheric parameters—such as the cloud deck pressure or reference radius/pressure (Benneke & Seager, 2012). By varying the absolute abundance of a species as well as the scattering properties and/or reference pressure, one can produce an identical transmission spectrum (assuming a fixed scale height).

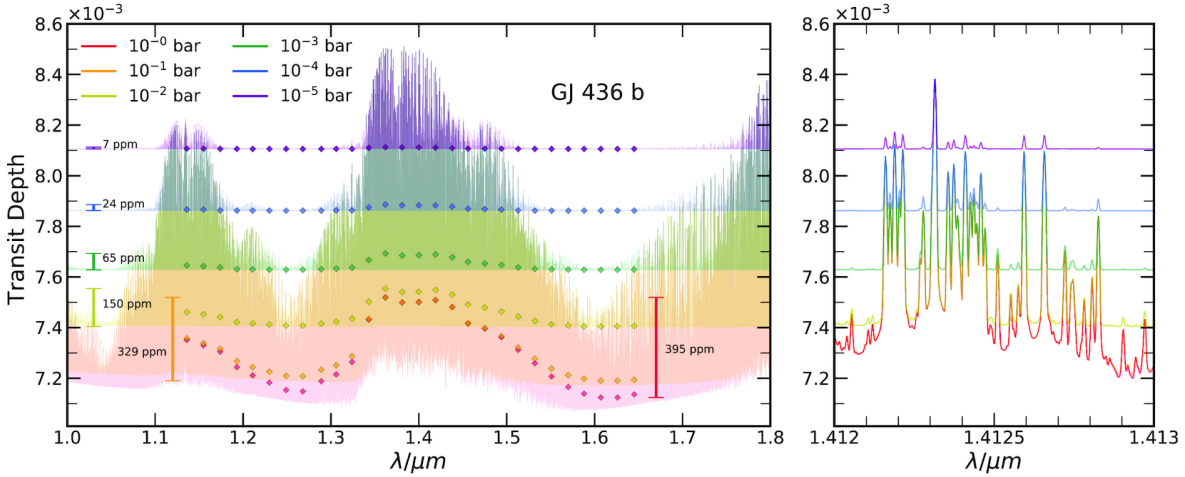


Figure 2.6: High-resolution transmission spectra of the warm Neptune GJ 436b with varying cloud deck pressures, highlighting the degeneracy in transmission spectroscopy between the absolute abundance of an atmospheric species and other atmospheric parameters, such as the cloud deck pressure. The right panel shows the high resolution spectra in a small region around 1.4125 μm . Figure from Gandhi et al. (2020).

2.3.2 Line Broadening

With the one-dimensional transmission spectrum generated, including opacity from atmospheric species as well as Rayleigh scattering and an opaque cloud deck, broadening effects are then included. High-resolution observations are not only sensitive to the positions of individual absorption lines, but also the subtle variations in their line shapes caused by winds and rotation (Seidel et al., 2020; Hoeijmakers et al., 2020). Similar to the spectral lines of a rotating star, which are broadened as light from the receding limb is redshifted and the approaching limb is blueshifted, planetary absorption and emission lines are also broadened by the Doppler shifts of the rotating planet’s receding and approaching limbs. Additionally, the planetary lines present in the observations undergo pressure broadening, broadening due to atmospheric winds, as well

as instrumental broadening due to the intrinsic instrumental profile of the spectrograph. The absorption cross-sections used are pressure broadened across the vertical temperature-pressure structure.

2.3.2.1 Instrumental Broadening

The instrumental line-spread function (LSF) can be assumed to be a Gaussian profile with a full width at half maximum (FWHM) which varies as a function of wavelength, as the resolution of the spectrograph is not constant with wavelength. In order to investigate this variation for ESPRESSO, the full-width at half-maximum (FWHM) was determined by fitting Gaussian profiles to the spectrograph’s calibration source ThAr lines across the full wavelength range of ESPRESSO, from which a linear function of FWHM as a function of wavelength was determined (see Fig. 2.7). It is worth noting that this LSF determination method is hampered by the fact that lines in a ThAr spectrum are unevenly bright, not regularly spaced, and often suffer from blending between thorium and argon lines (Schmidt & Bouchy, 2024).

2.3.3 Rotational Broadening

As the planet transits its host star, the rotating planetary atmosphere causes absorption lines to be broadened. For the analysis of the ultra-hot Jupiter WASP-121b outlined in Chap. 3, it is assumed that this rotational broadening, as well as the instrumental broadening, can be modelled by a single Gaussian broadening kernel, with which the one-dimensional transmission spectrum is convolved. As aforementioned, the instrumental profile varies with wavelength, and thus a more accurate approach would be to model this separately, and perform the convolution after the one-dimensional model had been shifted to the three-dimensional array of the observations (see Sect. 2.3.4). However, this convolution in three dimensions is costly, therefore a single convolution with a Gaussian kernel of width W_{conv} is preferred. This also assumes that, in transit, the planetary atmosphere is a rigid rotating sphere. In reality, as a planet transits its host star, the observations are only sensitive to a thin annulus of the atmosphere

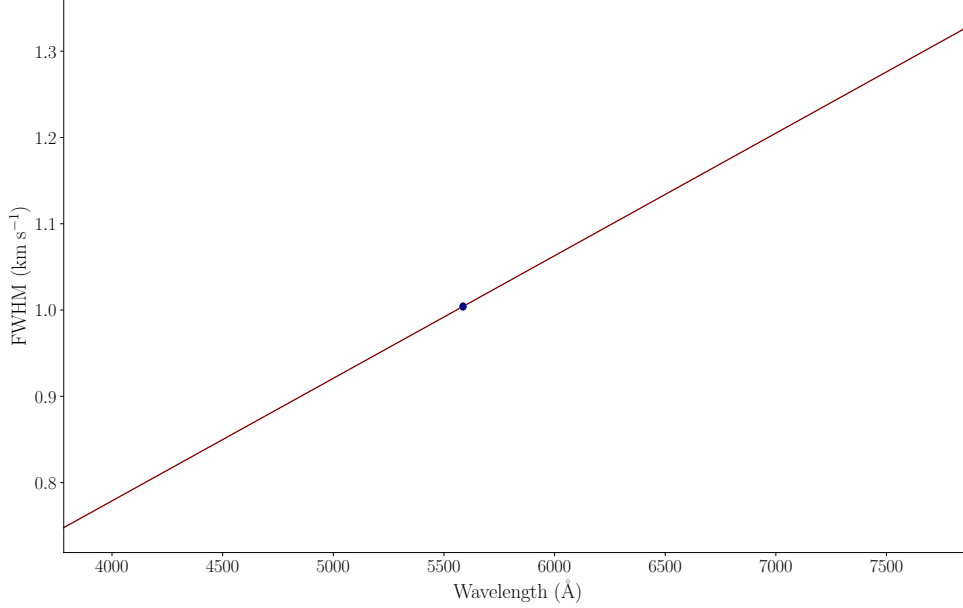


Figure 2.7: The ESPRESSO instrumental profile FWHM as a function of wavelength. The FWHM is determined by fitting Gaussian profiles to the spectrograph’s calibration source ThAr lines across the full wavelength range of ESPRESSO. The mean FWHM value used for the instrumental profile computation is shown as a blue circle.

known as the *terminator*, below which the planet is an opaque disk.

2.3.3.1 Rotating Annulus Broadening Profile

Recent studies have modelled the morning (leading) limb and evening (trailing) limb of a transiting exoplanetary terminator directly with the use of realistic rotational broadening kernels (Gandhi et al., 2023; Boucher et al., 2023). These broadening kernels allow for the morning half of the terminator to be effectively separated from the evening half of the terminator in velocity, by modelling subtle variations in line shape. In practice, each half of the terminator (limb) is modelled separately with its own 1D atmospheric model, and each transmission spectrum is convolved with one half of the broadening kernel derived below. The effect of this convolution is shown in Fig. 4.1. This procedure allows for separate atmospheric parameters, as well as separate rotational velocities Δv_{rot} and thickness d , to be retrieved for each atmospheric limb. This results in four additional parameters for the forward model, two for each limb: d_m ,

d_e , $\Delta v_{\text{rot},m}$, and $\Delta v_{\text{rot},e}$. The subscripts m and e represent the morning and evening limbs, respectively.

For a uniformly irradiated disk projected by a rigid rotating sphere, the broadening kernel $G(\Delta v)$ is given by:

$$G(\Delta v) = \frac{I_\lambda(\Delta v)}{I_\lambda(0)} \quad (2.17)$$

where $I_\lambda(0)$ is the line intensity at the line centre and $I_\lambda(\Delta v)$ is the line intensity after a Doppler shift caused by the line of sight velocity, Δv , at each x coordinate along the disk. For a rigid rotating sphere, such that there is no latitudinal change in rotation rate, all elements on the disk surface along the same x coordinate undergo the same Doppler shift, such that $x = \Delta v / \Delta v_{\text{rot}}$, where Δv_{rot} is the Doppler shift due to the equatorial velocity ($r = r_1$). Eq. 2.17 is given by the ratio of the length of the chord at constant x , to the length of the chord at $x = 0$.

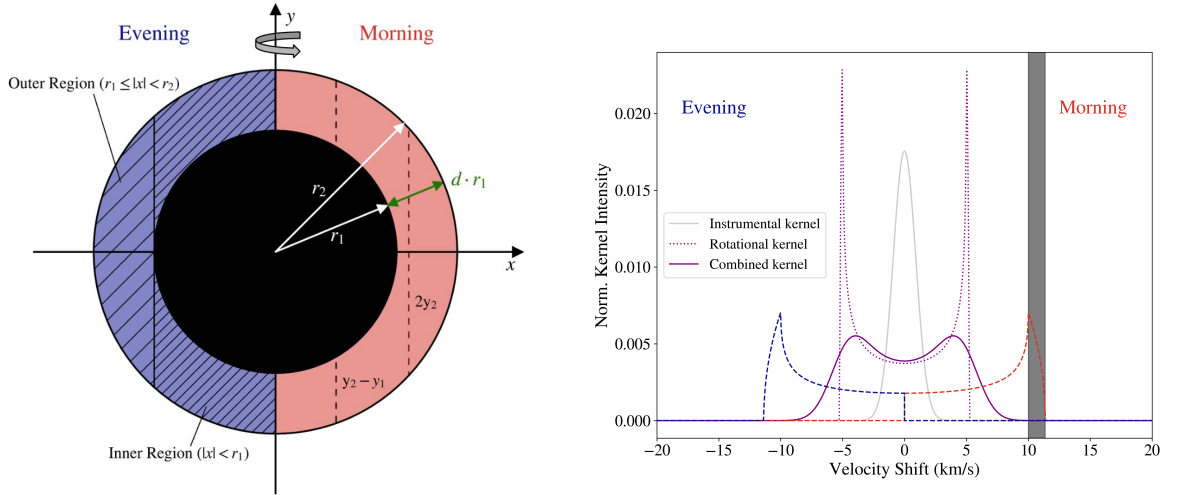


Figure 2.8: (left) Schematic diagram of a rotating annulus of inner radius r_1 and outer radius $r_2 = r_1 + d \cdot r_1$. A portion of the inner and outer regions described in the text is highlighted. Chords at constant x , of length $2y_2$ and $2(y_2 - y_1)$, are also shown. (right) The resultant broadening kernels for varying $d_{m/e}$ and $\Delta v_{\text{rot},m/e}$.

This expression can be adapted for a uniformly irradiated annulus projected by a rigid rotating spherical shell (see Fig. 2.8), such as a planetary atmosphere. Fig. 2.8

shows a rotating annulus with inner radius $r_1 = R_p$. Setting $r_1 = R_p = 1$, such that the outer radius $r_2 = 1 + d$, where d denotes the thickness of the atmosphere *relative* to the planetary radius R_p . Thus, the length of the chord at $x = 0$ is $2d$. See Boucher et al. (2023) for a similar expression with alternative notation, in which the absolute height of the atmosphere $z = d \cdot R_p$. The length of the chord at constant x varies for different regions of the annulus.

Outer region ($r_1 \leq |x| < r_2$):

When $r_1 \leq |x| < r_2$, the outer disk ($r = r_2$) is not occulted by the planetary disk, such that the lines simply undergo rotational broadening due to a rigid rotating disk ranging from $-r_2 \rightarrow r_2$. Therefore the length of the chord at constant x is simply:

$$\begin{aligned} 2y_2 &= 2\sqrt{r_2^2 - x_2^2} \\ &= 2\sqrt{(1 + d)^2 - x_2^2} \end{aligned}$$

As all elements on the disk surface along the same x coordinate undergo the same Doppler shift, this expression becomes:

$$2y_2 = 2\sqrt{(1 + d)^2 - (\Delta v / \Delta v_{\text{rot}})^2}$$

Such that Eq. 2.17 is:

$$\begin{aligned} G(\Delta v) &= \frac{2y_2}{2d} \\ &= \frac{\sqrt{(1 + d)^2 - (\Delta v / \Delta v_{\text{rot}})^2}}{d} \end{aligned} \tag{2.18}$$

Inner region ($|x| < r_1$):

However, when $|x| < r_1$, the outer disk ($r = r_2$) is occulted by the inner disk ($r = r_1$), such that the lines undergo rotational broadening due to a rotating spherical shell of

inner radius r_1 and outer radius r_2 . The length of the chord at constant x is:

$$2(y_2 - y_1) = 2 \left(\sqrt{(1+d)^2 - (\Delta v / \Delta v_{\text{rot}})^2} - \sqrt{1 - (\Delta v / \Delta v_{\text{rot}})^2} \right)$$

Such that:

$$\begin{aligned} G(\Delta v) &= \frac{2(y_2 - y_1)}{2d} \\ &= \frac{\sqrt{(1+d)^2 - (\Delta v / \Delta v_{\text{rot}})^2} - \sqrt{1 - (\Delta v / \Delta v_{\text{rot}})^2}}{d} \end{aligned} \quad (2.19)$$

In summary, Eqs. 2.18 & 2.19 give a broadening profile of:

$$G(\Delta v) = \begin{cases} \frac{a}{d} & , \text{ for } r_1 \leq |x| < r_2 \\ \frac{a - \sqrt{1 - (\Delta v / \Delta v_{\text{rot}})^2}}{d} & , \text{ for } |x| < r_1 \end{cases} \quad (2.20)$$

for a rotating annulus of inner radius r_1 and outer radius $r_2 = r_1 + (d \cdot r_1)$. $a = \sqrt{(1+d)^2 - (\Delta v / \Delta v_{\text{rot}})^2}$, d is the thickness of the annulus relative to r_1 , Δv is the velocity shift of the line at a position x , and Δv_{rot} is the shift due to the equatorial velocity. An example of this rotating annulus broadening kernel, as well as the effect of its convolution with a sodium doublet, is shown in Fig. 4.1, highlighting the separation of the morning and evening contributions to the transmission spectrum in velocity space. This kernel is used extensively in the analysis of WASP-76b (see Sect. 4.2.2).

2.3.4 Model Projection

The dimensions of high-resolution time-series transmission spectroscopy datasets obtained by observing with an echelle spectrograph, such as ESPRESSO, are typically given by *echelle order* $\times$ *time/orbital phase* $\times$ *wavelength*. Thus, in order to compare these observations to the forward models outlined above, one must project the one-dimensional forward model to the three-dimensional array of the data. After the model is broadened with a given broadening kernel, it is interpolated to the wavelength arrays

of each order via linear interpolation. The planetary model is then Doppler shifted for each orbital phase, or exposure, of the observations according to the planetary radial velocity:

$$\mathbf{v}_p = K_p \sin(2\pi \cdot \phi) + \Delta v_{\text{sys}} + \mathbf{v}_{\text{bary}} + \mathbf{v}_{\text{sys}} \quad (2.21)$$

where K_p , ϕ , Δv_{sys} , $\mathbf{v}_{\text{bary}}$, and $\mathbf{v}_{\text{sys}}$ are the planet’s radial velocity semi-amplitude, orbital phase, systemic velocity offset, barycentric velocity, and systemic velocity, respectively. The barycentric velocity is defined as the velocity induced by the motion of the observatory caused by the Earth’s own rotation, as well as the motion of the Earth as it orbits the Sun. The systemic velocity of the star is the observed stellar system’s constant radial velocity relative to the observer, unaffected by planetary-induced oscillations. The systemic velocity offset is any additional offset from the systemic velocity caused by planetary winds or rotation, for example. For the forthcoming analyses, the wavelength solutions have already been corrected for the barycentric velocity by the ESPRESSO Data Reduction Software (DRS). As outlined in Sect. 2.2.2, the observations are shifted to the stellar rest frame using the ESPRESSO pipeline radial velocities, $\mathbf{v}_{\text{sys}}$. Thus, the additional parameters in the forward model are K_p and Δv_{sys} . The projected model is then weighted by a transit model of the given planet, assuming no limb darkening. An example of this projection and weighting is shown in the middle panel of Fig. 4.1.

2.3.5 Model Filtering

The three-dimensional forward model (order $\times$ orbital phase $\times$ wavelength) is now an accurate representation of the real astrophysical signal measured by the spectrograph, with distortions in the line shapes from rotation, winds, varying longitudinal distributions of atmospheric parameters, and instrumental broadening. However, the astrophysical signal undergoes extensive preprocessing, as outlined in Sect. 2.2. As mentioned above, how well the model transmission spectra represent the *measured* ex-

oplanet signal is critical when performing model comparison within Bayesian inference algorithms, in order to retrieve accurate constraints of atmospheric parameters. As outlined in Sect. 2.2.4.1, data preprocessing techniques—such as SYSREM—distort the exoplanet signal, and thus it is important to apply these same processing steps to the forward model, such that it more accurately represents the data. However, SYSREM is an iterative process, and therefore the execution time is too long to be practically folded into an atmospheric retrieval framework (discussed further in Sect. 2.4.3).

Thus, Gibson et al. (2022) introduced a novel model filtering technique, which utilises the output matrices $\mathbf{U}$ and $\mathbf{W}$, containing the column and row vectors $\mathbf{u}$ and $\mathbf{w}$ for each SYSREM iteration (see Sect. 2.2.4.1). In Eq. 2.8, $\mathbf{U}\mathbf{W}^\top$ can be seen as a linear basis model, where $\mathbf{U}$ contains N basis vectors (for each iteration of SYSREM), and $\mathbf{W}$ the corresponding weights. In practice, $\mathbf{U}$ is fit to each order, $\mathbf{M}$ (orbital phase $\times$ wavelength), of the forward model, using a linear least squares to find the best-fit weights:

$$\mathbf{w}' = (\mathbf{U}^\top \mathbf{U})^{-1} \mathbf{U}^\top \mathbf{y} \quad (2.22)$$

for a single column vector $\mathbf{y}$, or:

$$\mathbf{W}' = (\mathbf{U}^\top \mathbf{U})^{-1} \mathbf{U}^\top \mathbf{Y} \quad (2.23)$$

for a 2D orbital phase $\times$ wavelength array $\mathbf{Y}$. The best-fit model, $\mathbf{Y}'$, to the array $\mathbf{Y}$, is then given by the outer product of the best-fit weights, $\mathbf{W}'$, and the basis vectors $\mathbf{U}$, where the term $(\mathbf{U}^\top \mathbf{U})^{-1} \mathbf{U}^\top$, in Eq. 2.23, is the Moore-Penrose inverse, $\mathbf{U}^\dagger$, such that:

$$\mathbf{Y}' = \mathbf{U}\mathbf{U}^\dagger \mathbf{Y} \quad (2.24)$$

However, to account for the data uncertainties, which are accounted for initially when computing $\mathbf{U}$, the mean of the uncertainties over wavelength, $\hat{\sigma}$, are taken for each order, as only the relative weights will affect the best-fit, and it is too slow to provide each array of uncertainties for every wavelength. Therefore, the final fit to the forward model is:

$$\mathbf{M}' = \mathbf{U}(\mathbf{\Lambda}\mathbf{U})^\dagger (\mathbf{\Lambda}\mathbf{M}) \quad (2.25)$$

where $\mathbf{\Lambda}$ is a diagonal matrix of $1/\hat{\sigma}$ terms. $\mathbf{M}'$ is then subtracted from the forward model, $\mathbf{M}$, equivalent to the treatment of the data with the SYSREM model in Sect. 2.2.4.1. The product of this subtraction is the final forward model, ready to be compared to the data. The final forward model, after projection and filtering, is shown in the bottom panel of Fig. 4.1.

The term $\mathbf{U}(\mathbf{\Lambda}\mathbf{U})^\dagger \mathbf{\Lambda}$ depends solely on the SYSREM basis vectors and the data uncertainties, meaning it can be precomputed, allowing Eq. 2.25 to be applied directly for each given forward model. This procedure is computed independently for each order, each with their own basis vectors, in each likelihood calculation of the atmospheric retrieval (see Sect. 2.4.3), and allows for the same preprocessing steps to be applied to the model, as the data, without the expensive computational overhead of iterative processes such as SYSREM. This is also considerably faster than PCA, where $\mathbf{U}$ is also recomputed for each iteration.

2.4 Data Analysis

Armed with the final data products, whose reduction is outlined extensively in Sect. 2.2, and the complete forward model (see Sect. 2.3), in which numerous chemical and dynamical process of the atmosphere have been encoded, the data is ready to be compared to the models. These models have now also been filtered to mimic any distortions said reduction has caused on the real underlying exoplanetary signal, thus they are an

accurate representation of the noiseless data.

2.4.1 Cross-correlation

This residual data (see Fig. 2.2d) contains a planetary signal buried deep beneath the noise of the observations. The individual planetary lines have a low signal-to-noise ratio ($\text{SNR}_{\text{line}} \lesssim 1$). However, at high spectral resolution, each line that is detected increases the total plant signal-to-noise ratio by a factor of $\sqrt{N_{\text{lines}}}$ (Birkby, 2018), following:

$$\text{SNR}_{\text{planet}} = \left(\frac{S_p}{S_\star} \right) \text{SNR}_\star \sqrt{N_{\text{lines}}} \quad (2.26)$$

where $S_p/S_\star$ is the planet-to-star signal ratio, and $\text{SNR}_\star = \sqrt{S_\star}$ is the *photon-limited*, total signal-to-noise of the star. Therefore, this can be leveraged to increase the signal-to-noise by cross-correlating the residuals with the forward model described above. The cross-correlation technique, pioneered by Snellen et al. (2010) for detecting exoplanetary atmospheres, effectively sums the contributions from many individual spectral lines, weighting each by its depth. The optimally-weighted cross-correlation function is given by:

$$\text{CCF}(\Delta v_{\text{sys}}) = \sum_{i=1}^N \frac{f_i m_i(\Delta v_{\text{sys}})}{\sigma_i^2} \quad (2.27)$$

where f_i is the data, σ_i is the uncertainties, and N is the number of datapoints. $m_i(\Delta v_{\text{sys}})$ is the model, Doppler shifted over a range of systemic velocity offsets, Δv_{sys} . The summation occurs over both wavelength and spectral order. This process is repeated for each exposure, or orbital phase, producing a cross-correlation value for each combination of orbital phase, ϕ , and Δv_{sys} . The result is a 2D array of cross-correlation values known as a “ ϕ - Δv_{sys} ” map, or simply, a “cross-correlation” map. An example of a cross-correlation map is shown in Fig. 3.1c. As outlined above, the cross-correlation method is a powerful tool for detecting atmospheric species via template-matching

with an atmospheric forward model. However, this process is only effective if the line positions in the atmospheric template precisely match those in the observations. For this, the line positions at which the cross-sections (σ_{species}), described in Sect. 2.3.1, are calculated must be accurate. Several line list or cross-section/opacity databases exist, including HITRAN (Rothman et al., 2009; Gordon et al., 2017), HITEMP (Rothman et al., 2010), and ExoMol (Tennyson et al., 2016), among others.

The cross-correlation map in Fig. 3.1c shows a visible trail of the planetary signal. However, for weaker signals in which this trail is not visible, and also to constrain the planetary radial velocity semi-amplitude (K_p), it is necessary to integrate the cross-correlation maps over a range of predicted planetary velocities, v_p . In practice, a range of radial velocity semi-amplitude values are chosen, in the vicinity of the predicted value from RV measurements. The cross-correlation function for each orbital phase is then shifted to a new planetary velocity given by Eq. 2.21 for a given K_p , and integrated as a function of time/orbital phase, “collapsing” the signal in time. The collapsed array is stored for each value of K_p , producing a velocity-summed cross-correlation map, known as a “ K_p - Δv_{sys} ” map (see Fig. 3.1d). In order to compute the statistical significance of a detection within a K_p - Δv_{sys} map, the map is typically normalised by subtracting the mean of regions away from the detection peak, before dividing the map by the standard deviation of those regions (Brogi et al., 2012, 2018). However, the regions away from the peak in which the mean/standard deviation of the map is calculated are arbitrarily chosen, and thus the resultant detection significance is not exact. Furthermore, the values within a K_p - Δv_{sys} map are not statistically independent, and are often highly correlated with neighbouring values. Thus, the calculated standard deviation is not a true reflection of the spread of these values. Therefore, one of the limitations of this technique is the conversion of the cross-correlation values into a statistically robust goodness-of-fit estimate, such as a chi-squared statistic or likelihood value, for direct model comparison (Brogi et al., 2016, 2017).

2.4.2 Likelihood Mapping

Although the cross-correlation technique is a powerful tool for detecting atmospheric species, as well as constraining the signal’s radial velocity, it cannot place constraints on the physical parameters (e.g., abundance, temperature, etc.) of the atmospheric species. The cross-correlation to log-likelihood mapping (CC-to-log L), or *likelihood mapping*, introduced by Brogi & Line (2019), aims to leverage the large number of spectral lines available at high resolution and the well-determined planetary radial velocity from the cross-correlation technique. This method converts the cross-correlation signal into a well-defined likelihood function, facilitating Bayesian inference. In exoplanetary atmosphere studies, this process of inferring atmospheric model parameters via Bayesian estimation is commonly referred to as an “atmospheric retrieval” (Madhusudhan & Seager, 2009), although it is essentially traditional model fitting.

2.4.2.1 Brogi & Line (2019)

The idea of mapping a cross-correlation value to a log-likelihood for high-resolution spectroscopy was first presented by Zucker (2003) to determine precise stellar radial velocities. Lockwood et al. (2014) outlined a CC-to-log L framework for high-resolution exoplanet spectroscopy of the non-transiting planet τ Boötis b. However, this framework requires that the change in the planet’s radial velocity during one set of observations is negligible with respect to the instrumental resolution, which is violated by high-resolution spectroscopic observations of close-in exoplanets. Therefore, Brogi & Line (2019) developed a CC-to-log L framework to exploit these characteristics of high-resolution spectroscopic observations of exoplanets, derived below.

Beginning with the data f_i and the Doppler shifted model $m_i(\boldsymbol{\theta})$, they define a Gaussian likelihood function of the form:

$$L = \prod_i^N \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{1}{2} \frac{(f_i - \alpha m_i(\boldsymbol{\theta}))^2}{\sigma^2}\right) \quad (2.28)$$

where α is a model scale factor, which accounts for any uncertainty in the scaling of the atmospheric model, which is often set to unity ($\alpha = 1$). Note the subtle difference in the notation when compared to Eq. 2.27, where $\boldsymbol{\theta}$ represents the vector of all atmospheric model parameters (including Δv_{sys}). Furthermore, σ is no longer explicitly defined over both wavelength and time, but instead is assumed constant for each pixel. This is the most important distinction between this likelihood framework and that of Gibson et al. (2020), outlined in Sect. 2.4.2.2. In practice, however, the natural logarithm of the likelihood, or log-likelihood, is computed:

$$\log L = -N \log \sigma - \frac{1}{2\sigma^2} \sum_i^N (f_i - m_i(\boldsymbol{\theta}))^2 \quad (2.29)$$

Instead of fixing a value for σ , the maximum likelihood estimator $\hat{\sigma}$ is computed by nulling the partial derivative of the log-likelihood:

$$\begin{aligned} \frac{\partial \log L}{\partial \sigma} &= 0 \\ \frac{N}{\hat{\sigma}} &= \frac{1}{\hat{\sigma}^3} \sum_i^N (f_i - m_i(\boldsymbol{\theta}))^2 \\ \hat{\sigma}^2 &= \frac{1}{N} \sum_i^N (f_i - m_i(\boldsymbol{\theta}))^2 \end{aligned} \quad (2.30)$$

substituting $\hat{\sigma}^2$ into Eq. 2.29, neglecting constant terms, and dropping explicit reference to $\boldsymbol{\theta}$ gives:

$$\begin{aligned} \log L &= -N \log \left\{ \sqrt{\frac{1}{N} \sum_i^N (f_i - m_i)^2} \right\} - \frac{N}{2} \\ &= -\frac{N}{2} \log \left\{ \frac{1}{N} \sum_i^N (f_i - m_i)^2 \right\} \\ &= -\frac{N}{2} \log \left\{ \frac{1}{N} \sum_i^N (f_i^2 - 2f_i m_i + m_i^2) \right\} \end{aligned} \quad (2.31)$$

$$= -\frac{N}{2} \log \left\{ \frac{1}{N} \left(\sum_i^N f_i^2 - 2 \sum_i^N f_i m_i + \sum_i^N m_i^2 \right) \right\} \quad (2.32)$$

where the second summation in Eq. 2.32 is the CCF given in Eq. 2.27, for a constant uncertainty σ .

2.4.2.2 Gibson et al. (2020)

Inspired by the approach of Brogi & Line (2019), an alternative CC-to-log L framework was developed by Gibson et al. (2020). This framework will be used exclusively in the forthcoming chapters. Similarly to above, beginning with a Gaussian likelihood of the form:

$$L = \prod_i^N \frac{1}{\sqrt{2\pi(\beta\sigma_i)^2}} \exp\left(-\frac{1}{2} \frac{(f_i - \alpha m_i(\boldsymbol{\theta}))^2}{\beta\sigma_i^2}\right) \quad (2.33)$$

where now the time- and wavelength-dependent uncertainties are accounted for via σ_i . A scaling term for the uncertainties, β , has also been introduced, which accounts for the fact that the scaling may not be accurate. A noise scaling term such as this is standard practice in transit modelling (Winn et al., 2008; Gibson et al., 2008) where the noise in the data is fit rather than imposed directly from photon statistics. Taking the natural logarithm of Eq. 2.33, and again dropping reference to $\boldsymbol{\theta}$, gives:

$$\log L = -\frac{N}{2} \log 2\pi - N \log \beta - \sum_i^N \log \sigma_i - \frac{1}{2} \sum_i^N \frac{(f_i - \alpha m_i)^2}{(\beta\sigma_i)^2} \quad (2.34)$$

In practice, constant terms are dropped from the computation. The final summation gives χ^2 :

$$\chi^2 = \sum_i^N \frac{(f_i - \alpha m_i)^2}{(\beta\sigma_i)^2} \quad (2.35)$$

expanding gives:

$$\chi^2 = \frac{1}{\beta^2} \left[\sum_i^N \frac{f_i^2}{\sigma_i^2} - 2\alpha \sum_i^N \frac{f_i m_i}{\sigma_i^2} - \alpha^2 \sum_i^N \frac{m_i^2}{\sigma_i^2} \right] \quad (2.36)$$

where the second summation gives the optimally-weighted CCF in Eq. 2.27. Both Eqs. 2.32 & 2.34 give alternative approaches of mapping the cross-correlation function to a log-likelihood function, exploiting the power of cross-correlation in a Bayesian framework in a statistically principled manner. Thus, allowing for the inference of atmospheric model parameters via an atmospheric retrieval.

2.4.3 Atmospheric Retrieval

An atmospheric retrieval is simply the inference of atmospheric model parameters from a set of observations, where the atmospheric parameters—and by extension, the atmosphere itself—are ‘retrieved’. Thus, it is simply a model-fitting exercise, in this case using Bayesian inference (Bayes, 1763). Bayes’ theorem states that the posterior probability (i.e., *the posterior*) of particular values of the model parameters—given the data and the model—is proportional to the likelihood of the dataset given these parameter values, multiplied by their prior probability (i.e., *the prior*). It is often stated as:

$$P(\boldsymbol{\theta}|\mathbf{D}) \propto L(\mathbf{D}|\boldsymbol{\theta}) \cdot P(\boldsymbol{\theta}) \quad (2.37)$$

where $\mathbf{D}$ is the data, and $\boldsymbol{\theta}$ is the model parameters, as before. The above expression is typically converted to the natural logarithm, leveraging the logarithmic properties of multiplication to avoid numerical overflow/underflow issues:

$$\log P(\boldsymbol{\theta}|\mathbf{D}) = \log L(\mathbf{D}|\boldsymbol{\theta}) + \log P(\boldsymbol{\theta}) + C \quad (2.38)$$

where C is a constant term. Equipped with the log-likelihood from Eq. 2.34, Eq. 2.38 allows for the calculation of the posterior probability of a given set of model parameters. To explore the prior probability space and build a posterior distribution, numerical sampling methods, such as Markov Chain Monte Carlo (MCMC; Hastings 1970) or nested sampling (Skilling, 2006), can be employed. These techniques iteratively sample the parameter space, evaluating the likelihood and prior probabilities to generate

a set of parameter values that represent the posterior distribution.

In this work, MCMC methods are used to sample the parameter spaces. MCMCs work by creating a chain of samples, where each new step toward a new sample is based on its probability relative to the previous step. Thus, the chains gradually move towards regions of higher probability, allowing for the efficient exploration of the multi-dimensional parameter space. The proposal mechanism, as well as the acceptance criteria, of these steps varies depending on the algorithm of MCMC used. Using the posterior distribution, we can gain insights into the most probable (i.e., *maximum likelihood*) parameter values and their uncertainties. These parameter constraints are the ‘retrieved’ parameter values of the atmospheric model, in this case.

The particular algorithm of MCMC used in this work is the Differential Evolution Markov Chain (DEMC; Ter Braak 2006), which uses multiple chains to sample the parameter space. This method combines the genetic algorithm Differential Evolution (Storn & Price, 1997) for global optimisation with MCMC. The chains may begin in arbitrary regions of the parameter space. As the parameter space is sampled, they will ‘converge’ to the target posterior distribution, from which constraints may be extracted. In order to ensure the chains effectively sample the parameter space, a “burn-in” period is typically run to allow the chains to deviate from their initial position. The resultant samples are then discarded, and the subsequent samples are used estimate the posterior. To assess the chains’ convergence, the Gelman-Rubin (GR) statistic is calculated after a given period. This statistic compares the variance between chains to the variance within chains. If the chains are well-mixed and converged, the GR statistic approaches 1. One may also inspect the convergence of the chains visually, to qualitatively assess if they have converged to a stable distribution. One of the benefits of DEMC is its ability to adaptively scale step sizes by comparing differences between chains, which allows it to explore the parameter space more efficiently. This is particularly useful in large, multimodal, parameter distributions, where more basic MCMC

algorithms may get ‘stuck’ in local minima. This ability to handle complex parameter spaces makes DEMC particularly suited for atmospheric retrievals at high-resolution, where there are often numerous complex and degenerate parameters being sampled simultaneously.

Atmospheric Retrievals of WASP-121b with ESPRESSO

The following chapter details a temporal survey of the atmosphere of the ultra-hot Jupiter (UHJ) WASP-121b via three transit observations with ESPRESSO. This work was published in the *Monthly Notices of the Royal Astronomical Society* (Maguire et al., 2023).

WASP-121b is a UHJ ($R_p = 1.753 \pm 0.036 R_{\text{Jup}}$) orbiting an F6V type star, with an orbital period of $P \sim 1.27$ days and an equilibrium temperature of 2358 ± 52 K (Delrez et al., 2016; Bourrier et al., 2020), on a highly misaligned orbit close to its Roche limit. It has been the subject of extensive observational campaigns, in transmission (Evans et al., 2016, 2018; Salz et al., 2019; Sing et al., 2019; Wilson et al., 2021), emission (Evans et al., 2017; Mikal-Evans et al., 2019; Kovács & Kovács, 2019; Mikal-Evans et al., 2020), as well as with phase curve measurements (Bourrier et al., 2020; Daylan et al., 2021; Mikal-Evans et al., 2022), in an effort to characterise its atmosphere.

As discussed in Sects. 1.2.2.2 & 2.4.1, HRCCS has been developed upon to infer atmospheric dynamics (Snellen et al., 2010; Brogi et al., 2012; Seidel et al., 2020; Wardenier et al., 2021b), as well as map longitudinal variations in the abundance profiles of chemical species (Ehrenreich et al., 2020; Kesseli & Snellen, 2021; Kesseli et al., 2022; Prinoth et al., 2022). It has also been shown that for some UHJs, including WASP-121b, the atmospheric regions probed by transmission spectroscopy studies are different before and after mid-transit, due to the large rotation angles of these planets relative to the “opening angle” of their day-to-night terminator regions (Wardenier et al., 2021a).

The readily accessible absorption signatures of these extreme objects, particularly those of neutral metals which have generally avoided condensation at such high temperatures, have allowed a plethora of species to be identified in the atmosphere of WASP-121b

using this method, among others, alongside traditional low-resolution studies. Such species include neutral atomic species; Fe I, Mg I, Cr I, V I, Ca I, Na I, H I, Ni I, V I, K I, and Li I (Gibson et al., 2020; Hoeijmakers et al., 2020; Borsa et al., 2020; Cabot et al., 2020) and ionic species; Fe II, Mg II, and Ca II (Sing et al., 2019; Ben-Yami et al., 2020; Borsa et al., 2020; Merritt et al., 2021). Lothringer et al. (2021) recently showed that the abundance of these metals, or refractories, relative to that of volatile species such as H₂O and CO, in the form of a “refractory-to-volatile” ratio, could be used to constrain the formation and migration pathway of HJ/UHJs.

Evans et al. (2016) found additional absorption near 1.2 μm in the atmosphere of WASP-121b, tentatively attributed to a combination of strong optical absorbers such as TiO and VO, which aimed to explain the presence of a thermal inversion layer, indicated by the dayside emission of H₂O observed with HST/WFC3 (Evans et al., 2017). This additional absorption attributed to VO could not be confirmed, however, with a joint analysis of this data set and follow-up secondary eclipse observations with the same instrument (Mikal-Evans et al., 2020). Evans et al. (2018) also found no evidence for TiO absorption features in the transmission spectrum of WASP-121b, as well as a strong near-UV (NUV) slope attributed to the SH molecule. The former of which was interpreted as the condensation of Ti-bearing species at higher temperatures compared to V-bearing species. Follow up observations using HRCCS also reported non-detections of TiO, VO, and SH (Merritt et al., 2020; Hoeijmakers et al., 2020), with Hoeijmakers et al. (2020) postulating that absorption by atomic metals is sufficient to explain the NUV slope detected by Evans et al. (2018).

Exospheric Fe II and Mg II, extending beyond the Roche lobe of WASP-121b, has also been detected (Sing et al., 2019), with the presence of Fe II confirmed at high-resolution (Ben-Yami et al., 2020; Borsa et al., 2020). Borsa et al. (2020) also found evidence of H α and Ca II absorption at high altitudes with ESPRESSO, indicative of an evaporating upper atmosphere (see also Cabot et al. 2020; Merritt et al. 2021). A

recent study by Mikal-Evans et al. (2022) revealed a nightside temperature below the condensation temperature of neutral Ca. However, Ca has previously been detected in the gas-phase along the day-night terminator, suggesting that vertical mixing may be operating efficiently in the atmosphere of WASP-121b to prevent day-night “cold trapping” processes.

3.1 ESPRESSO Observations

Two full primary transits of WASP-121b were observed with the ESPRESSO spectrograph (Pepe et al., 2021) at the VLT on the nights of 2021 January 26 and 2021 March 4, as part of the program 106.21R1 (PI: Gibson). ESPRESSO is the extremely stable, fibre-fed, high-resolution, cross-dispersed echelle spectrograph installed at the VLT, described in Sect. 2.1.1. Installed at the inherent combined Coudé focus (ICCF), ESPRESSO is capable of illumination from any one of the unit telescopes (UT) at a time (1-UT mode), as well as all 4 unit telescopes simultaneously (4-UT mode), via the UT Coudé trains. Both transits were observed using the 1-UT mode, achieving a resolution of $R \sim 140,000$. An archival partial primary transit of WASP-121b was also included in the analysis, observed in the 4-UT mode ($R \sim 70,000$) on the night of 2018 November 30 during the commissioning of ESPRESSO, as part of the program 60.A-9128, previously analysed in Borsa et al. (2020). All three datasets cover a wavelength range of approximately 3770–7900 Å. The observed datasets are hereafter labelled T1, T2, and T3 in chronological order. Further details regarding the observations are given in Table 3.1. The data were reduced using the ESPRESSO DRS v2.3.3, and the two-dimensional non-blaze-corrected S2D spectra were extracted. The DRS includes standard reduction procedures for echelle time-series spectra, such as bias and

Table 3.1: A summary of the ESPRESSO observations of WASP-121b.

Dataset	Date	N_{exp} (in-transit)	Seeing	S/N@550nm	Obs. Mode
T1	30-11-18	29 (16)	$0.7'' - 1.1''$	~ 150	4-UT
T2	26-01-21	96 (33)	$0.79'' - 1.35''$	~ 19	1-UT
T3	04-03-21	93 (33)	$0.79'' - 2.15''$	~ 15	1-UT

dark subtraction, flat-field and contaminated pixel correction, as well as wavelength calibration and barycentric velocity correction.

3.1.1 Data Reduction

The extracted spectra were cleaned by subtracting a model from each spectral order. The model was constructed via the outer product of the spectral median (i.e., median over time) and temporal median (i.e., median over wavelength) of each order, weighted by the mean of the spectral median. A 10th order polynomial was then fit to each spectrum of the residual orders, and any 5σ outliers were replaced by their respective polynomial value, before adding the cleaned residual array back to the model. The choice is made here to replace these values with their respective polynomial value, as opposed to a NaN value, as the subsequent data reduction methods involve division by the median time-series spectrum. Thus, replacing with NaNs could lead to invalid operations and potentially cause floating point errors. This procedure replaced approximately 0.05%, 0.03%, and 0.03% of pixels for T1, T2, and T3, respectively.

In order to optimise the information extracted from the time-series spectra, good initial estimates of the time- and wavelength-dependent uncertainties are required. To estimate the uncertainties, the procedure outlined in Sect. 2.2.1 was followed. The resultant spectral orders were then blaze-corrected following Merritt et al. (2020), which is also outlined in Sect. 2.2.2. The original orders and their respective uncertainties were then divided by the resultant smoothed blaze function. This does not remove the blaze distortion, but instead places each order on a common blaze in time. This procedure also reduces the low-frequency ‘wiggle’ pattern seen in ESPRESSO spectra (Allart et al., 2020), which has a period of ~ 30 Å and amplitude of $\sim 1\%$ at 600 nm (Tabernero et al., 2021; Kesseli et al., 2022). There is also a second set of ‘wiggles’ which affect ESPRESSO spectra, with a shorter period of ~ 1 Å, and amplitude of $\sim 0.1\%$ at 600 nm, which was minimised by using a narrower median filter width in the blaze correction, compared previous works. These wiggles are likely caused by an inter-

ference pattern induced by a combination of readout electronics and inhomogeneities in the Coudé train optics (Sedaghati et al., 2021)^{1,2}. After cleaning and blaze correction, the spectra were then Doppler shifted to the stellar rest frame via the stellar radial velocity, computed via Eq. 2.3 and the orbital parameters outlined in Table 3.2.

To ensure these values did not significantly distort the underlying exoplanet signal, injection-recovery tests were performed with an atmospheric model containing neutral Fe, Mg, and Cr, for each dataset. The calculation of this atmospheric model is outlined in Sects. 2.3 & 3.2.1. The model had a negative K_p , to ensure that the injected signal was separated from the real exoplanet signal. The retrieval analysis, similar to that described below in Sect. 3.2.3, was performed on the injected data, and the retrieved model parameters, as well as the retrieved relative abundances and T - P profiles were found to be in agreement with the injected values. These results are outlined in Figs. A1, A2, and A3 for T1, T2, and T3, respectively. In addition to contamination, or spectral distortion such as the blaze, imprinted on the spectra, there is also spectral imprints due to the spatial variation of the stellar spectrum across the stellar disk, whilst a planet is in transit, such as CLVs and the RM effect. These distortions were modelled and removed following the procedure described in Sect. 2.2.3. Without this step, an anomalous ‘Doppler shadow’ is apparent in the cross-correlation maps ($\Delta v_{\text{sys}} \simeq 0 \text{ km s}^{-1}$) of species present in the stellar atmosphere (see Fig. 3.1a). This anomaly was not prominent in the UVES observations of WASP-121b previously outlined in Gibson et al. (2020, 2022) and Merritt et al. (2020, 2021), and due to its small change in velocity relative to WASP-121b in-transit, it was not modelled/removed from these observations (see Gibson et al. 2020 for further details).

With the CLV and RM distortions of the stellar lines modelled and removed, the stellar and telluric lines were (quasi-)stationary in time throughout the data. In order to

¹The ESPRESSO consortium and ESO are working to characterise this effect (Allart et al., 2020).

²See Section 4.3 of the ESPRESSO user manual for details (https://www.eso.org/sci/facilities/paranal/instruments/espresso/ESPRESSO_User_Manual_P109_v2.pdf).

3. ATMOSPHERIC RETRIEVALS OF WASP-121b WITH ESPRESSO

Table 3.2: Physical and orbital parameters of the WASP-121 system.

Parameter	Value	Reference
<i>Stellar parameters</i>		
$R_{\star}$	$1.458 \pm 0.030 R_{\odot}$	Delrez et al. (2016)
$M_{\star}$	$1.353^{+0.080}_{-0.079} M_{\odot}$	Delrez et al. (2016)
T_{eff}	$6460 \pm 140 \text{ K}$	Delrez et al. (2016)
Spectral type	F6V	Delrez et al. (2016)
$\log g \text{ [cgs]}$	$4.242^{+0.011}_{-0.012}$	Delrez et al. (2016)
[Fe/H]	0.13 ± 0.09	Delrez et al. (2016)
$K_{\star}$	$177.0^{+8.5}_{-8.1} \text{ m s}^{-1}$	Bourrier et al. (2020)
$v_{\star} \sin i$	$13.56^{+0.69}_{-0.68} \text{ km s}^{-1}$	Delrez et al. (2016)
v_{sys}	$38.198 \pm 0.002 \text{ km s}^{-1}$	Borsa et al. (2020)
<i>Planetary parameters</i>		
P	$1.27492504^{+1.5 \cdot 10^{-7}}_{-1.4 \cdot 10^{-7}} \text{ days}$	Bourrier et al. (2020)
R_{p}	$1.753 \pm 0.036 R_{\text{Jup}}$	Bourrier et al. (2020)
M_{p}	$1.157 \pm 0.070 M_{\text{Jup}}$	Bourrier et al. (2020)
g_{p}	$9.33^{+0.71}_{-0.67} \text{ m s}^{-2}$	Bourrier et al. (2020)
$R_{\text{p}}/R_{\star}$	$0.12355^{+0.00033}_{-0.00029}$	Bourrier et al. (2020)
$a_{\text{p}}/R_{\star}$	$3.8131^{+0.0075}_{-0.0060}$	Bourrier et al. (2020)
i_{p}	$88.49 \pm 0.16^{\circ}$	Bourrier et al. (2020)
λ	$87.20^{+0.41}_{-0.45}^{\circ}$	Bourrier et al. (2020)

remove the stationary spectral lines, SYSREM (Tamuz et al., 2005) was applied to each order of the data. The SYSREM algorithm, as well as its application to high-resolution time-series observations, is outlined extensively in Sect. 2.2.4.1. Cross-correlation and likelihood mapping analysis was performed for an atmospheric model with multiple species (Fe I, Mg I, Cr I, Ti I, V I, Na I, and Ca I), and the optimum number of SYSREM iterations for each dataset was determined from the resultant detection significance, conditioned on the optimum K_{p} and Δv_{sys} values, outlined in Sect. 3.3.1. Nugroho et al. (2017) separate each order and subsequently determine the optimum number of SYSREM iterations for each order via injection tests. Conversely, in this study, the number of SYSREM iterations were kept constant across all orders. The approach of Nugroho et al. (2017) benefits from the fact that the systematics vary across orders, which is then accounted for by order-based SYSREM optimisation. Also,

SYSREM acts to distort the underlying exoplanet signal, the extent of which is reduced via this approach. However, for a fast model filtering framework (see Sect. 2.3.5), it is more convenient to keep the number of SYSREM iterations constant across all orders. Fixing the number of SYSREM iterations also ensures that the detection is not biased by optimising over each order, which may cause an overfitting of the stellar/telluric spectrum. The optimum number of SYSREM iterations for each dataset was 18, 1, and 4 for T1, T2, and T3, respectively.

3.2 Methods

3.2.1 Modelling WASP-121b

When performing atmospheric retrievals with high-resolution datasets, the computational speed of the underlying forward model, as well as how accurately it represents the exoplanet’s signal, is critical. For this analysis, a 1D transmission spectrum model, IRRADIATOR (Gibson et al., 2022), described in detail in Sect. 2.3, was computed across a wavelength range of 3670–8000 Å, at a constant resolution of $R = 200,000$. In the analysis, absorption cross-sections for neutral atomic species (Fe I, Mg I, Cr I, Ti I, V I, Na I, and Ca I) were used, all of which were previously detected in the atmosphere of WASP-121b at high-resolution, with the exception of Ti I (Gibson et al., 2020; Hoeijmakers et al., 2020; Borsa et al., 2020; Ben-Yami et al., 2020), using the precomputed opacity grids provided by petitRADTRANS¹ (Mollière et al., 2019). 70 atmospheric layers were defined, equidistant in log space, ranging from 10^2 bar to 10^{-12} bar, across which a T - P profile was computed using the parametric model from Guillot (2010) with input parameters T_{irr} , T_{int} , κ_{IR} , and γ (see Eq. 2.9), corresponding to the irradiation temperature, internal temperature, mean infrared opacity, and the ratio of visible-to-infrared opacity, respectively. After computing the vertical extent of the atmosphere assuming hydrostatic equilibrium, and accounting for varying temperature and gravity in each layer, the radiative transfer equations were solved by computing the opacity

¹<https://petitradtrans.readthedocs.io/en/latest/>

of each predefined layer of the atmosphere, weighing each species' cross-sections on their respective volume mixing ratios (VMRs), χ_{species} , and integrating through the grazing geometry. The computed optical depth for each layer was then converted to an effective planetary radius. Any values below the corresponding radius of a given cloud deck pressure, P_{cloud} , were masked to account for an opaque cloud deck. In addition, a H_2 VMR, χ_{ray} , along with H_2 opacities from Dalgarno & Williams (1962), were included to account for Rayleigh scattering, with the minimum prior limit corresponding to Jupiter's H_2 abundance. The truncated transmission spectrum was then converted from an effective planetary radius to a differential flux (ΔF) value.

The one-dimensional model was broadened via convolution with a Gaussian kernel (see Sect. 2.3.3), and linearly interpolated to the 2D wavelength grid of the data (order $\times$ wavelength). For each order, the 2D forward model was then Doppler shifted to a planetary velocity given by Eq. 2.21. This resulted in a 3D shifted forward model, $\mathbf{M}$ (time/phase $\times$ order $\times$ wavelength). As mentioned above, how well the model transmission spectra represent the underlying exoplanet signal is critical when performing model comparison within Bayesian inference algorithms, in order to retrieve accurate constraints of atmospheric parameters. As outlined in Sect. 2.2.4.1, data preprocessing techniques – such as SYSREM – distort the exoplanet signal, and thus it is important to apply these same processing steps to the 3D forward model, such that it more accurately represents the data. As described in Sect. 2.3.5, the output matrices $\mathbf{U}$ and $\mathbf{W}$, containing the column and row vectors $\mathbf{u}$ and $\mathbf{w}$ for each SYSREM iteration were used to ‘filter’ the data. From Eq. 2.25, $\mathbf{M}'$ was then subtracted from the forward model, $\mathbf{M}$, equivalent to the treatment of the data with the SYSREM model in Sect. 2.2.4.1.

3.2.2 Cross-correlation

Equipped with the data, free of spectral distortions and stellar and telluric contamination, as well as the Doppler shifted model, filtered to mimic the effect of the data preprocessing steps, traditional cross-correlation analysis (e.g., Snellen et al. 2010;

Ehrenreich et al. 2020; Gibson et al. 2020; Hoeijmakers et al. 2020; Merritt et al. 2020, 2021) could now be performed. This procedure is outlined in detail in Sect. 2.4.1, and summarised briefly here. The data and the shifted model were multiplied, before summing their products over both wavelength and spectral order, in order to produce a cross-correlation function (CCF). This is mathematically equivalent to a dot product, such that:

$$\text{CCF}(\Delta v_{\text{sys}}) = \sum_{i=1}^N \frac{f_i m_i(\Delta v_{\text{sys}})}{\sigma_i^2} \quad (3.1)$$

where the product is weighted on the variance of the data, σ_i^2 , and the summation occurs over both wavelength and spectral order. Eq. 3.1 produces cross-correlation values for each combination of orbital phase, ϕ , and Δv_{sys} , via Eq. 2.21, referred to as a “ ϕ – Δv_{sys} ” map, or simply, a “cross-correlation” map.

The cross-correlation map in Fig. 3.1c shows a visible trail of the planetary signal. However, for weaker signals in which this trail is not visible, and also to constrain the planetary orbital velocity, it is necessary to integrate the cross-correlation maps over a range of predicted planetary velocities, v_p . In practice, a range of radial velocity semi-amplitude values, K_p , were chosen, in the vicinity of the predicted value from RV measurements. The cross-correlation function for each orbital phase was then shifted to a new planetary velocity given by Eq. 2.21 for a given K_p , and integrated as a function of time/phase, “collapsing” the signal in time. The collapsed array was stored for each value of K_p , producing a velocity-summed cross-correlation map, known as a “ K_p – Δv_{sys} ” map (see Fig. 3.1d). In order to place constraints on the detection significance of a given species within a K_p – Δv_{sys} map, the map was subtracted by the mean of the noise in regions away from the peak, before dividing the map by the standard deviation of the noise away from the peak (Brogi et al., 2012, 2018). However, the regions away from the peak in which the mean/standard deviation of the noise was calculated are arbitrarily chosen, and thus the resultant detection significance is not exact. Therefore,

one of the limitations of this technique is the conversion of the cross-correlation values into a statistically robust goodness-of-fit estimate, such as a chi-squared statistic or likelihood value, for direct model comparison (Brogi et al., 2016, 2017).

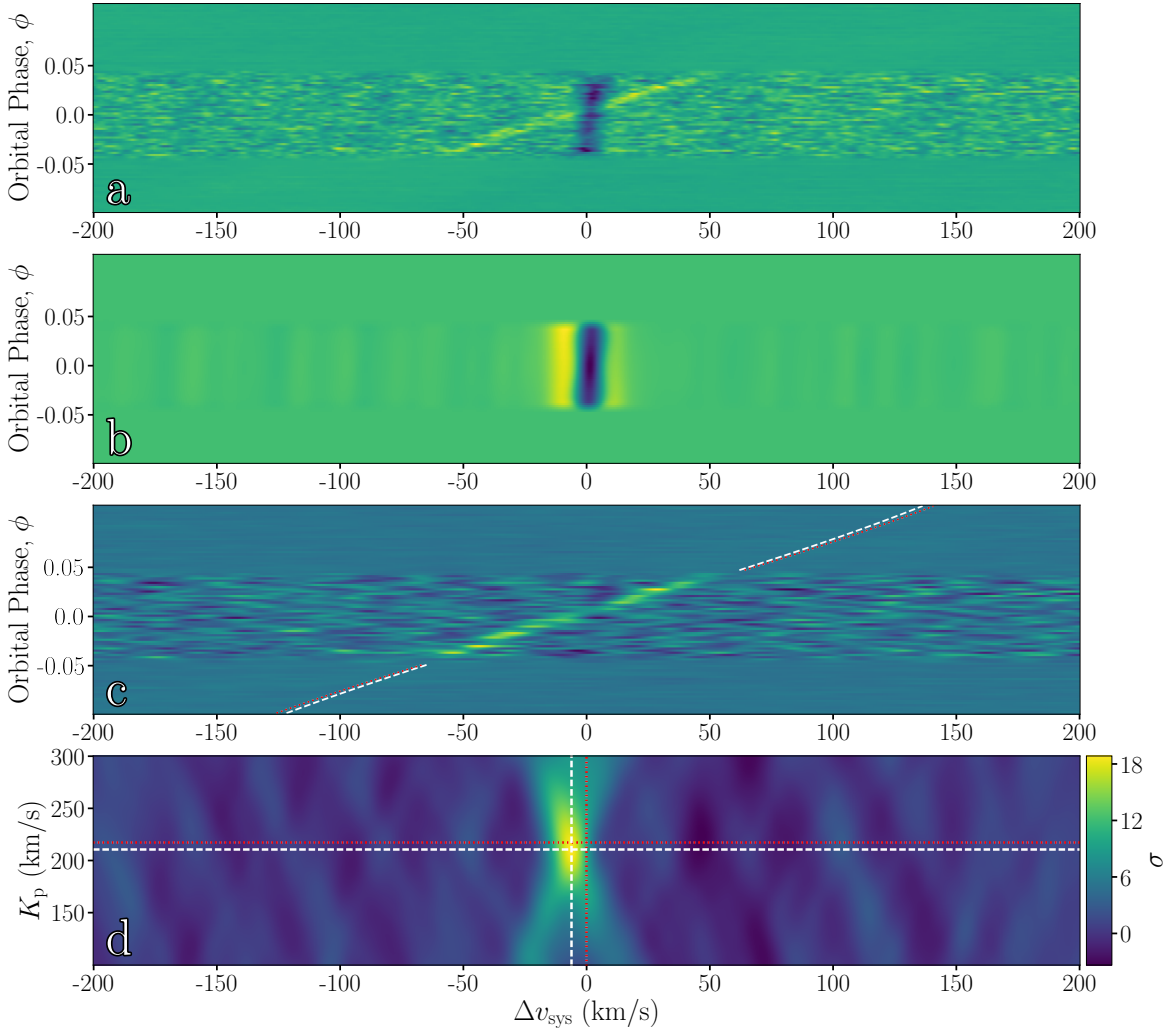


Figure 3.1: The planetary signal detected via cross-correlation analysis of T2 with the combined (Fe I, Mg I, Cr I, Ti I, V I, Na I, and Ca I) atmospheric model. **(a)** Cross-correlation map before the removal of CLM and RM distortions, weighted proportional to the transit light curve. **(b)** The ‘Doppler shadow’ produced by cross-correlating the CLM and RM distortions with the model. **(c)** Cross-correlation map after the removal of CLM and RM distortions. The red dotted curve shows the expected planetary velocity trail from RV measurements, whereas the white dashed curve shows the planetary velocity trail corresponding to the maximum K_p and Δv_{sys} values. **(d)** The final K_p - Δv_{sys} map, showing an 18.8σ detection near the expected planetary velocity.

3.2.3 Atmospheric Retrieval

Brogi & Line (2019) first introduced a method to ‘map’ cross-correlation values of a given atmospheric model to a likelihood value. An alternative, yet similar method was developed by Gibson et al. (2020) using a full Gaussian likelihood function, which allows for time- and wavelength-dependent uncertainties to be accounted for. These methods are discussed in detail in Sect. 2.4.2. Eqs. 2.34 & 2.35 allow for the computation of the log-likelihood directly from the CCF, and thus the ability to perform model comparison and direct atmospheric retrievals from high-resolution observations whilst utilising the power of the cross-correlation method.

In order to perform a full retrieval analysis on the datasets, a forward model must be computed for a given set of model parameters $\boldsymbol{\theta}$. $\boldsymbol{\theta}$ is comprised of $\{\alpha, \beta, K_p, \Delta v_{\text{sys}}, W_{\text{conv}}\}$, where W_{conv} is the width of the Gaussian broadening kernel in pixels, as well as the IRRADIATOR input parameters $\{T_{\text{irr}}, T_{\text{int}}, \kappa_{\text{IR}}, \gamma, P_{\text{cloud}}, \chi_{\text{ray}}, \chi_{\text{species}}\}$ (see Sect. 2.3).

Adopting uniform prior distributions, each spectrum of the forward model was divided by its median value, to imitate the blaze correction, and then filtered, as described in Sect. 2.3.5. The log-posterior was computed by computing the log-prior and adding the log-likelihood for a given set of model parameters. This can then be folded into an MCMC framework, in order to sample the posterior, and retrieve an estimate of the posterior distributions of the model parameters for each dataset. A Differential-Evolution Markov Chain (DEMC) (Ter Braak, 2006; Eastman et al., 2013) was used, running an MCMC chain with 192 walkers, with a burn-in length of 200 and a chain length of 300, resulting in 96,000 samples of the posterior, of which 38,400 were discarded. In each of the retrievals, T_{int} is fixed at 200 K, and the remaining parameters were fit. Fixing T_{int} at 200 K should have minimal influence on the T - P structure of UHJs observed via transmission spectroscopy, where we are sensitive to

lower pressures. The chains' convergence were checked via the Gelman-Rubin statistic, after splitting each chain into four separate subchains. The chains were also divided into groups of independent walkers, and the 1D and 2D marginal distributions overplotted in different colours, in order to visualise the convergence of the MCMC (see Fig. 3.2).

3.3 Analysis

3.3.1 Cross-correlation and Likelihood Mapping

Cross-correlation analysis was performed with a model transmission spectrum, containing neutral Fe, Mg, Cr, Ti, V, Na, and Ca, for each of the reduced observations, T1, T2, and T3, using the best-fit model parameters from the atmospheric retrieval. A cross-correlation map before the removal of the CLV and RM distortions in-transit is shown in Fig. 3.1a. The anomalous 'Doppler shadow' produced by these spectral distortions after cross-correlation with a model template is shown in Fig. 3.1b, with the final 'corrected' cross-correlation map of the model template shown in Fig. 3.1c. This corrected cross-correlation map was then shifted to a range of planetary velocities and collapsed over time, producing a K_p - Δv_{sys} map, shown in Fig. 3.1d. A formal detection significance of 40.5σ , 18.8σ , and 11.4σ was computed for the best-fit atmospheric models, as outlined in Sect. 3.2.2, for the T1, T2, and T3 datasets, respectively. It is worth noting that the significance of these values is difficult to interpret statistically, as they are sensitive to arbitrary choices. The detection significance of each best-fit model was also computed using the likelihood distribution of the model scale factor, α , conditioned on the optimum K_p and Δv_{sys} values, similar to the approach of Gibson et al. (2020). The mean and standard deviation of α was extracted from this conditional distribution, and the mean was divided by the standard deviation to get a detection significance. This method, therefore, does not rely on different regions of the K_p - Δv_{sys} map when calculating the noise properties and thus the detection significance, as before. Using this method, a detection significance of 71.3σ , 23.9σ , and 15.2σ

was calculated for the T1, T2, and T3 datasets, respectively. While it is difficult to interpret and compare these values, it is clear that strong detections of the atmospheric models were obtained for each of the datasets.

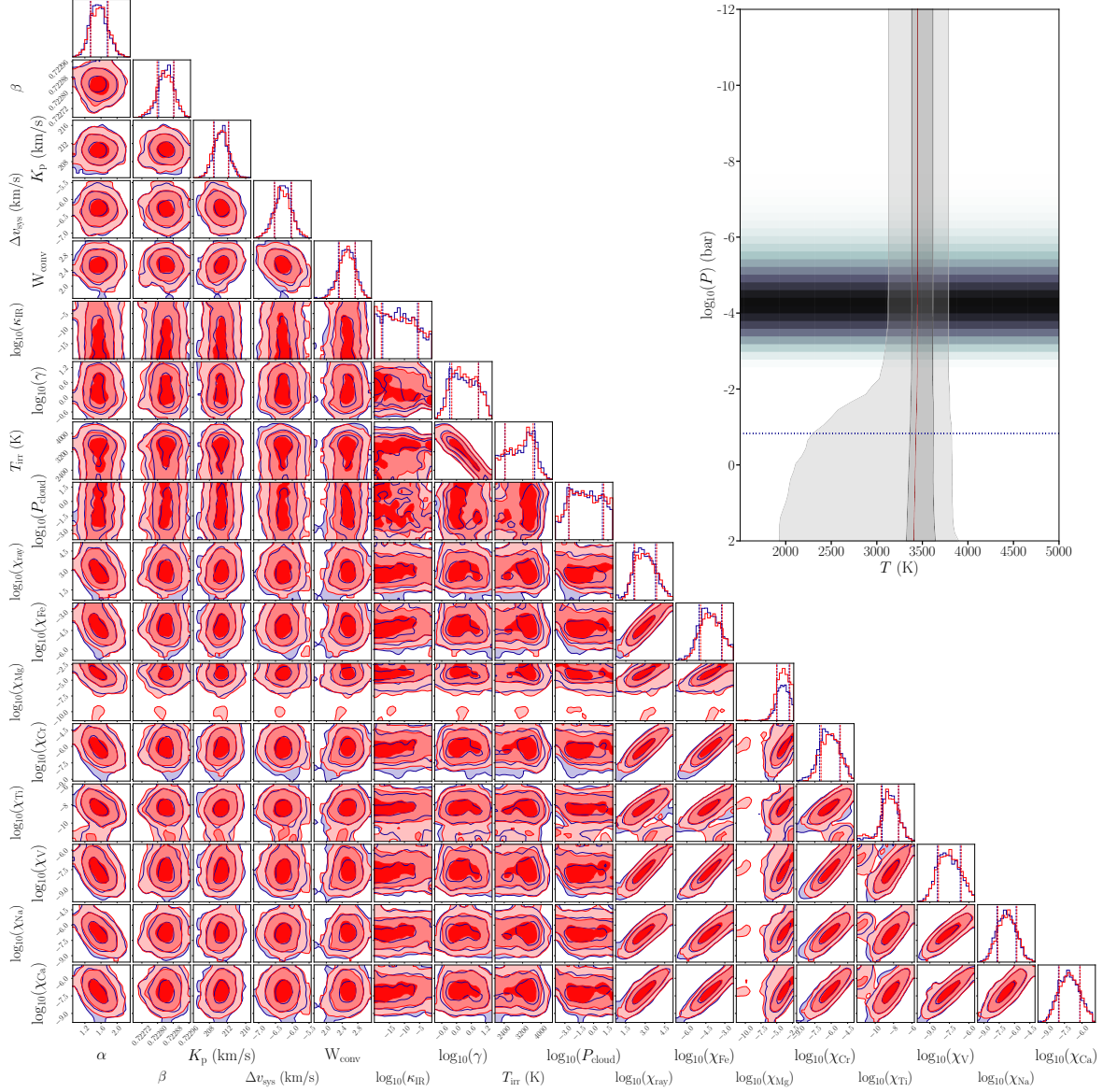


Figure 3.2: A summary of the retrieval results for T2, with the 1D and 2D marginalised posterior distributions of each of the model parameters displayed within a corner diagram. The red and blue posterior distributions represent independent subchains, of the same MCMC chain, both converging to similar distributions. The correlations in the retrieved abundances are evident in the lower right panels of the corner diagram. The T - P profile on the right was computed from 10,000 random samples of the MCMC, where the red curve shows the median profile, and the grey and lighter grey shaded regions show the 1σ and 2σ contours, respectively. The blue horizontal dotted line is the median retrieved cloud deck pressure, $\log_{10}(P_{\text{cloud}})$, below which the model spectrum is truncated. Also plotted is the mean contribution function for the ESPRESSO wavelength range. This corner diagram was generated using CORNER (Foreman-Mackey, 2016).

3.3.2 Relative Abundance Constraints

The retrieved parameters from the ESPRESSO observations T1, T2, and T3 were then compared, alongside a previous transit of WASP-121b observed on the night of 2016 December 26 with the UVES spectrograph (see Gibson et al. 2020, 2022; Merritt et al. 2020, 2021 for further details regarding this dataset). A summary of the retrieval results for T2 is shown in Fig. 3.2, whereas the retrieval results for T1, and T3 are given in Appendix A (Figs. A4 & A5, respectively).

The retrieval framework also allows the absolute abundances of each species to be constrained, however, the transmission spectra lack an absolute normalisation, resulting in broad constraints on the absolute abundances, with significant correlations. The relative abundances, however, are constrained more precisely (see Fig. 3.3) for each of the observations, from the relative line strengths of each species.

The retrieved relative abundance constraints for each dataset is shown in Fig. 3.3. The relative abundance constraints retrieved from the UVES observations (Gibson et al., 2022) are shown as black histograms, however neutral Na and Ca were not included in this analysis, whereas they have been included here.

3.3.3 The Search for Exospheric Species

$H\alpha$, Fe II, Mg II, and Ca II have previously been reported to exist at high altitudes in the exosphere of WASP-121b. These recent detections motivated the search for potentially exospheric species, using the likelihood mapping method outlined in Sect. 2.4.2. This search was conducted solely using the T1 dataset, due to the higher S/N and lower resolution data, resulting in a faster likelihood evaluation. Although the underlying atmospheric model assumes hydrostatic equilibrium, an assumption which ultimately breaks down in a hydrodynamically outflowing envelope, the existence of these species can be mapped via the artificial ‘scaling up’ of the model absorption features via the

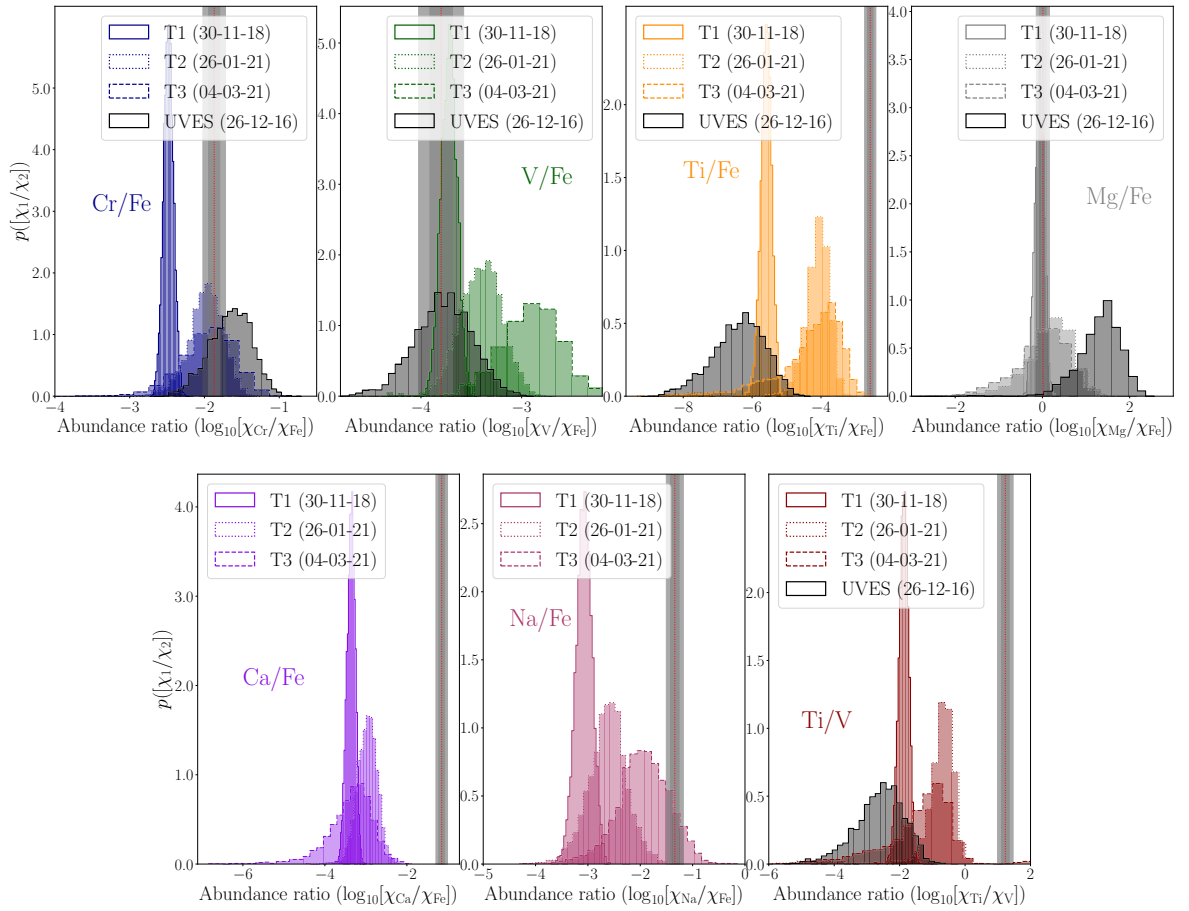


Figure 3.3: Comparison of the relative abundance constraints from the atmospheric retrievals for each of the observations. The vertical red dotted lines, and the grey shaded regions, represent the relative abundance ratio of WASP-121, and their respective 1σ and 2σ contours, calculated using elemental abundances from Polanski et al. (2022) and solar elemental abundances from Asplund et al. (2009).

model scale factor, α . As outlined in Fig. 3.2, retrieving an α value close to 1 reaffirms the assumption of hydrostatic equilibrium, which is valid for species lower in the atmosphere. However, retrieving a relatively large α value, orders of magnitude greater than 1, would be explained by species in an extended upper atmosphere. For this reason, these species were excluded from previous retrievals, due to a varying α value between species in different layers of the atmosphere.

A full atmospheric retrieval was performed for each individual exospheric species, similar to that outlined in Sect. 3.2.3 – with the exception of Mg II, which was not detected in this dataset. The best-fit model parameters were used to generate model transmission spectra of H α , Fe II, and Ca II individually, from which a likelihood map and a

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conditional likelihood distribution of α was computed, shown in Fig. 3.4. 10,000 random samples of the MCMC were then drawn, for each individual species, and model transmission spectra were generated. From this, the median and standard deviation of the scaled transmission spectra were computed, and the resultant effective planetary radius values, R_p , were found from the *strongest absorption lines* of each transmission spectra. From this, one can map the extent of these absorption signals in the upper atmosphere (see Fig. 3.5). The scaled transmission spectra resulted in absorption features extending up to $1.54 \pm 0.04 R_p$, $1.17 \pm 0.01 R_p$, and $2.52 \pm 0.34 R_p$, for H α , Fe II, and Ca II, respectively.

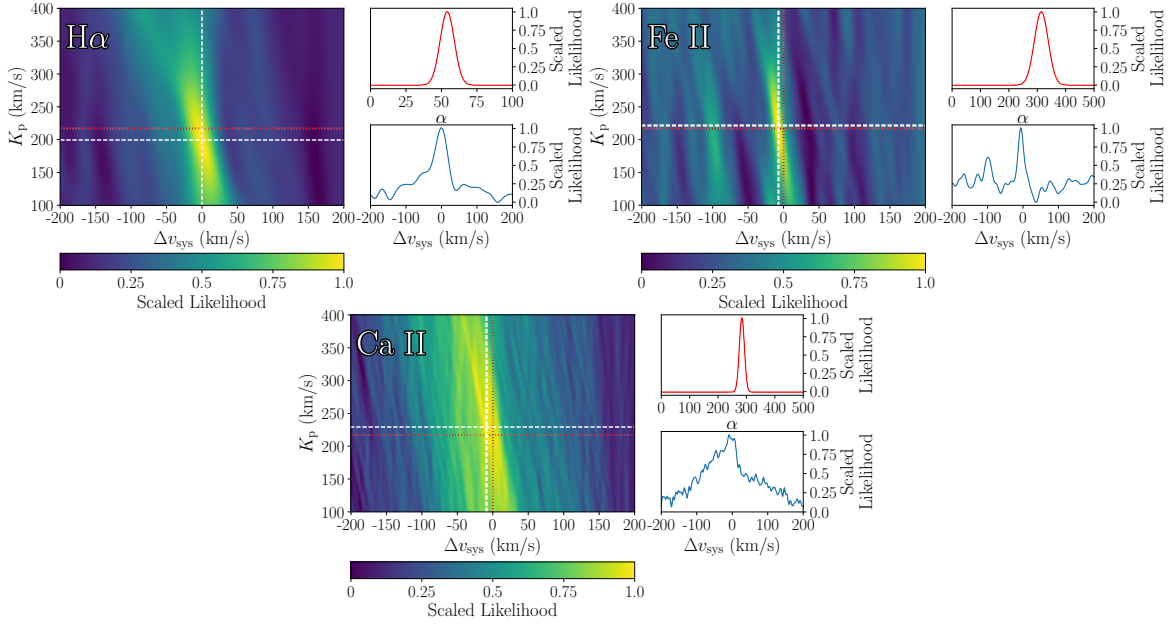


Figure 3.4: The likelihood maps and conditional likelihood distributions of α for the potential exospheric species, for T1 only. **(left subpanel)** The maximum likelihood map, normalised between 0 and 1 for ease of visualisation. The red dotted lines show the expected planetary velocity values, whereas the white dashed lines show the maximum K_p and Δv_{sys} values. **(upper right subpanel)** The conditional distribution of α (red), normalised between 0 and 1, fitted with a Gaussian function (blue). **(lower right subpanel)** The likelihood function at the maximum K_p value, outlining the various Δv_{sys} values for each species. The multi-peaked, ‘diamond-like’ shape of the Ca II signal may also be evidence of Ca II present in two different atmospheric limbs of the planet.

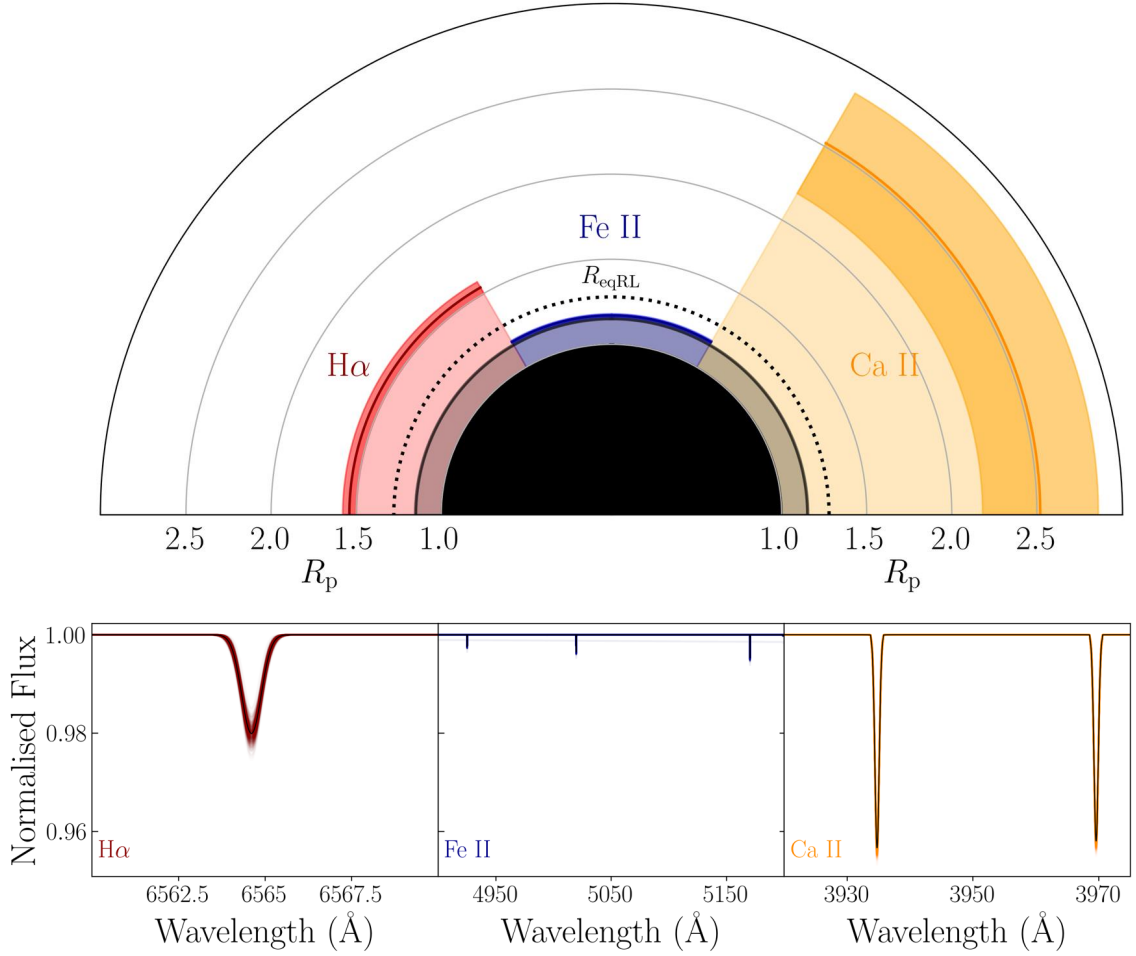


Figure 3.5: (upper) A schematic diagram showing the extent of potential exospheric species via the artificial ‘scaling up’ of their transmission spectra with the model scale factor, α . The dark shaded regions represent the 1σ contours. The transit equivalent Roche limit, R_{eqRL} , is shown as a black dotted line. The black shaded region highlights the maximum vertical extent of the best-fit combined atmospheric model for T1 (see Fig. A4). This diagram is not indicative of any real latitudinal variation in the extent of these species. (lower) Scaled model transmission spectra, generated from 10,000 random samples of the MCMC, centred around the strongest line(s) for each of the exospheric species. The median transmission spectra are shown in black.

3.4 Discussion

The cross-correlation analysis outlined above clearly detects the combined transmission spectrum model containing neutral Fe, Mg, Cr, V, Ti, Na, and Ca, with a detection significance of 40.5σ , 18.8σ , and 11.4σ for the T1, T2, and T3 datasets, respectively. The transmission spectrum model was produced using IRRADIATOR (Gibson et al., 2022), outlined in Sect. 2.3, which accounts for pressure-dependent cross-sections, Rayleigh scattering in the form of H_2 opacities combined with a H_2 VMR, and an opaque cloud

deck. This result was produced after the removal of CLV and RM distortions from the ESPRESSO datasets. The forward model was then filtered using a novel model filtering technique (Gibson et al., 2022), which acts to reproduce the distortion of iterative algorithms such as SYSREM on the underlying observed exoplanet signal. The cross-correlation value can also be mapped to a likelihood value, outlined in Sect. 2.4.2, and a direct likelihood evaluation then enables a full retrieval framework. Thus, the absolute abundances of each individual species may be constrained, as well as the velocity shifts, T - P structure, line broadening parameters, and vertical extent of the atmosphere.

From the T - P profile constraints (Fig. 3.2), the temperature in the upper atmosphere, at pressures $> 10^{-2}$ bar, is approximately 3450 ± 160 K, which is consistent within 2σ across all datasets, as well as with previous UVES observations of WASP-121b (Gibson et al., 2020, 2022). Significantly higher temperatures were retrieved, however, than those inferred for the nightside of the planet from low-resolution studies (Bourrier et al., 2020; Evans et al., 2018; Wilson et al., 2021; Mikal-Evans et al., 2022), and the dayside temperature of 2870 ± 50 K inferred from TESS phase curve measurements (Bourrier et al., 2020). Similar temperatures to the dayside temperature of ~ 3200 K were retrieved, obtained by Mikal-Evans et al. (2022). This could be explained by high-resolution studies probing higher up in the atmosphere, where higher temperatures would be expected due to the previously reported thermal inversion (Evans et al., 2017), which is hinted at by the existence of ionised species in the upper atmosphere. The existence of ionised species at high altitudes, however, could also be explained by a lower electron pressure, which acts to significantly ionise, as well as photoionisation at lower pressures. Deeper in the atmosphere, the T - P structure was not constrained well, which is expected, where emission studies would be more sensitive to the temperature structure of the deeper atmosphere. It is important to note that transmission studies are typically not very sensitive to the T - P structure of the atmosphere, despite the stringent constraints. Furthermore, the parameterisation of the T - P profile may also bias the retrieved values. Therefore, care must be taken not to overinterpret the

retrieved profiles.

The constrained atmospheric dynamic parameters, such as K_p and Δv_{sys} , from which the planetary orbital velocity was calculated, v_p , were also consistent across all observations, with a net blueshift of $\Delta v_{\text{sys}} \sim 6 \text{ km s}^{-1}$ for the combined model, similar to previous results from high-resolution transmission spectroscopy studies of WASP-121b (Gibson et al., 2020, 2022; Hoeijmakers et al., 2020; Merritt et al., 2020, 2021; Borsa et al., 2020). The constraints on the planetary orbital velocity, v_p , are outlined in Fig. A6, where it is evident that this quantity is well constrained in-transit. The width of the Gaussian broadening kernel, W_{conv} , was also constrained to 2.82 ± 0.07 pixels, 2.54 ± 0.20 pixels, and 1.50 ± 0.68 pixels, for T1, T2, and T3, respectively. For an atmospheric model computed at a resolution of $R = 200,000$, or velocity of $\approx 1.5 \text{ km s}^{-1}$, these broadening kernel widths convert to FWHM of $9.89 \pm 0.25 \text{ km s}^{-1}$, $8.91 \pm 0.70 \text{ km s}^{-1}$, and $5.26 \pm 2.39 \text{ km s}^{-1}$, for T1, T2, and T3, respectively. As the equatorial rotational velocity of WASP-121b is 7.4 km s^{-1} ($\approx 15 \text{ km s}^{-1}$ peak-to-peak), assuming it's tidally locked, the measurements of the broadening do not indicate clear evidence of broadening beyond rotation in the lower atmosphere. However, this analysis would benefit from a full modelling of planetary wind patterns.

Due to the degeneracies between the chosen reference transit radius and the reference pressure of the atmosphere, the transmission spectra lack an absolute normalisation (Heng & Kitzmann, 2017), limiting the ability to place stringent constraints on the *absolute* abundance of each of the model species. The constraints on the absolute abundances are quite broad, with strong correlations, which can be seen in the lower right panels of the corner diagram in Fig. 3.2. However, the *relative* abundances can be constrained much more precisely, as although information is lost regarding the absolute abundances, the relative abundance is constrained from the relative line strengths, assuming a well-mixed, hydrostatic atmosphere (Benneke & Seager, 2012).

3. ATMOSPHERIC RETRIEVALS OF WASP-121b WITH ESPRESSO

The retrieved relative abundance ratios were compared with the relative abundance ratios of WASP-121, calculated using elemental abundances from Polanski et al. (2022) and solar elemental abundances from Asplund et al. (2009). In the upper left panel of Fig. 3.3, the retrieved abundance ratio $\log_{10}(\chi_{\text{Cr}}/\chi_{\text{Fe}})$ is consistent across each of the ESPRESSO observations within 1σ , and is also consistent with stellar values for the T2, T3, and UVES observations, whereas T1 deviates from stellar. For $\log_{10}(\chi_{\text{V}}/\chi_{\text{Fe}})$, consistent values are retrieved across all observations, with T1 and T3 consistent within 2σ . These values also agree with stellar values, within 1σ , however T3 is consistent within 2σ . Fe and V have been previously detected in transmission in the atmosphere of WASP-121b (Gibson et al., 2020; Hoeijmakers et al., 2020), and have a relatively large number of spectral lines in the observed wavelength range, which makes their relative abundances an ideal target for this analysis. The $\log_{10}(\chi_{\text{Mg}}/\chi_{\text{Fe}})$ relative abundance ratio is also in agreement across all observations, within 1σ , and is consistent with stellar values. The relative abundance ratios which include Ti, $\log_{10}(\chi_{\text{Ti}}/\chi_{\text{Fe}})$ and $\log_{10}(\chi_{\text{Ti}}/\chi_{\text{V}})$, are broadly consistent between the observations, however are inconsistent with stellar, which can be explained by a depletion of Ti in each of the datasets. Also, Evans et al. (2018) proposed that TiO undergoes nightside condensation and rain-out, in order to explain the absence of TiO in their transmission spectrum. This would result in the depletion of Ti, as chemical equilibrium would drive the remaining Ti to TiO until all remaining Ti bearing species are condensed out (Hoeijmakers et al., 2020; Hoeijmakers et al., 2024). Thus, if Ti were present, the relative abundances, $\log_{10}(\chi_{\text{Ti}}/\chi_{\text{Fe}})$ and $\log_{10}(\chi_{\text{Ti}}/\chi_{\text{V}})$, would be expected to be substellar, as all Ti bearing species in the atmosphere of WASP-121b would have condensed out of the gas phase. The $\log_{10}(\chi_{\text{Na}}/\chi_{\text{Fe}})$ abundance ratio is in agreement across each of the ESPRESSO observations, within 1σ , with T3 consistent with stellar values. $\log_{10}(\chi_{\text{Ca}}/\chi_{\text{Fe}})$ is also consistent across each of the ESPRESSO observations, however is lower than stellar values. This could be explained by the model assuming a hydrostatic, well-mixed atmosphere, whereas these species are likely impacted by an escaping upper atmosphere, as Fe II and Ca II have previously been detected at high altitudes (Sing et al., 2019;

Borsa et al., 2020). $\log_{10}(\chi_{\text{Ca}}/\chi_{\text{Fe}})$ is significantly lower than the reported stellar value, however the absolute abundance of Fe is similar to the stellar value, whereas the absolute abundance of Ca is less than the reported stellar value. With Ca II extending to much greater altitudes than Fe II (Fig. 3.5), this result suggests that Ca could possibly undergo greater ionisation than Fe in the atmosphere of WASP-121b. A similar result could be inferred from the inconsistency of $\log_{10}(\chi_{\text{Na}}/\chi_{\text{Fe}})$ with stellar values for T1, T2, and UVES, where the absolute abundance of Na is also less than stellar. Alkali metals such as Na have a relatively low ionisation energy with only one free valence electron, and thus Na would be more readily ionised relative to Fe, driving this inconsistency.

Mikal-Evans et al. (2022) recently obtained an overall metallicity value of $[\text{M}/\text{H}] = 0.76^{+0.30}_{-0.62}$, which is approximately $1\text{--}10\times$ solar. This result, however, is difficult to directly compare to the results of the analysis, as in their study, the overall heavy metal enrichment is allowed to vary, whilst they fix the relative abundance ratios of the included species to solar values. It is important to note that the analysis would greatly benefit from a more sophisticated atmospheric model, in order to constrain and interpret the relative abundance values more precisely, and to directly compare with works such as Mikal-Evans et al. (2022) and future results.

The vertical extent of species previously reported at high altitudes in the atmosphere of WASP-121b was also probed, namely $\text{H}\alpha$, Fe II, and Ca II, using the T1 dataset. Sing et al. (2019) first detected exospheric Fe II and Mg II extending beyond the Roche lobe of WASP-121b in the UV using HST/STIS, at $\sim 2.7R_p$ and $\sim 2.5R_p$, respectively. This detection led to multiple follow-up campaigns at high-resolution, in search of potentially exospheric metal ions. Fe II was then detected in the optical with HARPS (Ben-Yami et al., 2020). Cabot et al. (2020) also detected $\text{H}\alpha$ with HARPS, up to $\sim 1.5R_p$, again attributed to an extended upper atmosphere. Finally, Borsa et al. (2020) confirmed the detection of Fe II with ESPRESSO in the 1-UT mode, and also found both $\text{H}\alpha$

and Ca II, present beyond the Roche lobe of WASP-121b, at $\sim 1.4 R_p$ and $\sim 2 R_p$, respectively. The results are summarised in Fig. 3.4. Each exospheric species, with the exception of Mg II, was detected near the expected planetary velocity of WASP-121b, with each model spectrum requiring a significantly larger model scale factor, α , than 1, which hints at their existence in an extended/outflowing upper atmosphere. This is similar to results obtained by Ben-Yami et al. (2020), where Fe II required a higher weighted absorption strength relative to species in the lower atmosphere (Fe I, Cr I, and V I). Similarly, Hoeijmakers et al. (2020) detected neutral Mg in the atmosphere of WASP-121b, which required a significantly greater line amplitude in comparison to other species, which is consistent with the expectation of an outflowing atmosphere. The ‘scaled up’ transmission spectra were converted to an effective planetary radius, displayed in Fig. 3.5, with H α extending to $1.54 \pm 0.04 R_p$, Fe II to $1.17 \pm 0.01 R_p$, and Ca II to $2.52 \pm 0.34 R_p$, where the transit equivalent Roche limit $R_{\text{eqRL}} \sim 1.3 R_p$ (Sing et al., 2019). Furthermore, there is a clear variability in the systemic velocity offset, Δv_{sys} , and the width of the Gaussian broadening kernel, W_{conv} , between the exospheric species. H α , Fe II, and Ca II were detected at a Δv_{sys} of -1.8 km s^{-1} , -7.7 km s^{-1} , and -16.2 km s^{-1} , respectively. At a model resolution of $R = 200,000$, or velocity of $\approx 1.5 \text{ km s}^{-1}$, the retrieved W_{conv} values, converted to a FWHM, are $26.95 \pm 2.01 \text{ km s}^{-1}$, $10.74 \pm 0.92 \text{ km s}^{-1}$, and $61.21 \pm 3.89 \text{ km s}^{-1}$, for H α , Fe II, and Ca II, respectively. The variability in the velocity constraints of the exospheric species, relative to one another, as well as to species detected lower in the atmosphere ($\alpha \simeq 1$), hints at species existing in different dynamical regions of the atmosphere (Prinoth et al., 2022). The broad, ‘diamond-like’ shape of the Ca II signal (see Fig. 3.4) explains the significantly large broadening of Ca II, and may be evidence of Ca II present in two different atmospheric limbs of the planet (Nugroho et al., 2020b; Wardenier et al., 2021b).

A long-standing goal of exoplanet studies is to link the observed bulk composition of an exoplanet to that planet’s formation pathway and evolution history. Previous studies have placed constraints on the atmospheric C/O ratio, which can be used to

map the formation mechanism and migration pathway of HJ/UHJs (Öberg et al., 2011; Madhusudhan et al., 2014). Recent work by Lothringer et al. (2021) has shown that refractory elements, such as Fe, Mg, and Si, can also be used to map the formation and migration pathways of UHJs, via their “refractory-to-volatile” ratio. These species are thought to condense into solids at $T < 2000$ K, and thus are unobservable via transmission spectroscopy. However, in hotter objects with $T > 2000$ K, such as WASP-121b, these species avoid condensation, such that constraints can be placed on their abundance, allowing their abundance ratios relative to volatile species, such as H_2O , CO , and CO_2 , to be computed. The relative abundance constraints obtained in this study are solely for refractory species, with similar condensation temperatures, meaning that alone they are not ideal in tracing the formation history of the planet. However, the consistency and precision of these constraints, across timescales of months to years between transits, shows great promise for future measurements of relative abundances from high-resolution transmission spectroscopy, which can then be used to constrain the refractory-to-volatile ratio and infer planet formation and evolution processes. For example, $\log_{10}(\chi_{\text{Fe}}/\chi_{\text{V}})$ is constrained to 3.72 ± 0.08 , 3.40 ± 0.21 , and 2.98 ± 0.51 for T1, T2, and T3, respectively. This is equivalent to 0.15 ± 0.12 dex, -0.17 ± 0.23 dex, and -0.59 ± 0.52 dex, respectively, emphasising the importance of these results alongside low-resolution efforts in the era of JWST.

The importance of the “hierarchy of models” (Fortney et al., 2021) used in retrievals of exoplanet transmission/emission spectra cannot be understated. With the ever increasing data quality provided by advanced space- and ground-based observatories, it is necessary to consider the three-dimensional nature of HJ/UHJs when modelling their spectra (MacDonald & Lewis, 2022). It has been shown that abundance gradients across the morning and evening limbs can result in biased inferences when using 1D models (Pluriel et al., 2022), therefore caution must be taken when interpreting retrieved atmospheric properties from 1D retrievals, as these assumptions inherently result in non-negligible biases in the retrieved parameters. The computational cost of

complex 3D forward models, particularly when folded into a retrieval framework with high-resolution data, must also be considered, in order to optimise the information content of the rich datasets on the horizon.

Recent discoveries outlining the spatial asymmetry in the atmospheres of HJ/UHJs must also be taken into account when constraining the atmospheric composition of these objects, with a longitudinal variation in the abundance of Fe I proposed in the atmosphere of WASP-76b (Ehrenreich et al., 2020; Kesseli & Snellen, 2021). However, Savel et al. (2022) have modelled the atmosphere of WASP-76b with three-dimensional Global Circulation Models (GCMs), in which a combination of Fe condensation, optically thick clouds, and a small nonzero eccentricity is needed to replicate the findings of Ehrenreich et al. (2020). Borsa et al. (2020) also found variations in the velocity shift of the Fe I signal in the atmosphere of WASP-121b, between the beginning ($-2.80 \pm 0.28 \text{ km s}^{-1}$) and end ($-7.66 \pm 0.16 \text{ km s}^{-1}$) of transit, alluding to different dynamical regions being probed during transit. Wardenier et al. (2021a) also showed that transmission spectroscopy studies of some UHJs, including WASP-121b, observe different atmospheric regions before and after mid-transit, due to the relatively large rotation angle of these planets during transit. Prinoth et al. (2022) also found evidence for chemical inhomogeneity in the atmosphere of WASP-189b, using high-resolution cross-correlation spectroscopy, again emphasising the importance of 3D effects in interpreting the nature of UHJs.

In addition to the multidimensional nature of WASP-121b, the complex dynamics of an outflowing upper atmosphere must also be considered, and a full exospheric treatment with vertically outflowing winds could also be implemented, outlined in previous works using transmission spectroscopy at high-resolution (Seidel et al., 2020; Dos Santos et al., 2022), in order to map the extent of these species, and infer the physical and dynamical properties of these regions.

3.5 Conclusions

In this chapter, multiple high-resolution transmission spectroscopy observations of the UHJ WASP-121b have been presented, using the ESPRESSO echelle spectrograph installed at the VLT, across several months/years. The removal of spectral distortions caused by the CLV and RM effect was demonstrated, as well as the removal of (quasi-)stationary stellar and telluric spectral lines with SYSREM.

- From these observations, consistent relative abundance constraints of neutral metals in the atmosphere of WASP-121b were obtained, which were broadly consistent with literature stellar values, across several high-resolution instruments/instrument modes, including previous relative abundance constraints obtained with VLT/UVES.
- The T - P structure of WASP-121b was also consistently constrained across multiple observations, which were in agreement with previously reported values at high-resolution.
- The atmospheric dynamic parameters, such as the planetary orbital velocity and broadening of spectral features were also constrained, and were consistent with previous results across each of the observations.
- The retrieval framework was also implemented to map the vertical extent of ionised metals which have been previously detected in the exosphere of WASP-121b, via the model scale factor, α . This artificial scaling up resulted in the absorption features of these species extending to the similar high altitudes as reported in the literature. These exospheric species also showed clear variability in their velocity constraints, which hints further at their existence in different dynamical regions of the atmosphere.

This study is a strong validation of the model filtering and retrieval framework, as well as the stability of the atmosphere of WASP-121b over the observed timescales. Studies

such as this, coupled with low-resolution efforts in the era of JWST and high-resolution efforts in the near-infrared/infrared (NIR/IR), as well as advanced atmospheric modelling, will place further constraints on these quantities, bridging the gap between the observed composition of these objects and their formation mechanism and evolution history.

Multidimensional Atmospheric Retrievals of WASP-76b with ESPRESSO

The following chapter describes a survey of the atmosphere of the UHJ WASP-76b via three transit observations with ESPRESSO. These transits, which are separated on the timescale of months/years, were used to monitor potential asymmetries in atmospheric parameters across the morning (leading) and evening (trailing) limbs of the atmosphere. This work was published in *Astronomy & Astrophysics* (Maguire et al., 2024).

Close-in, tidally-locked objects such as WASP-76b undergo significant rotation during transit, such that we are sensitive to distinct longitudinal regimes of the atmosphere as a function of orbital phase (Wardenier et al., 2021a). The potential variation in abundance and dynamical properties of these species as a function of orbital phase has opened a new avenue in the characterisation of these objects, by exploring their intrinsic three-dimensional nature. Their tidally-locked orbits also ensure a permanently irradiated dayside, and a cooler nightside, with drastically differing chemical and dynamical properties, which is expected to drive asymmetries in the chemical abundance and T - P profile across the limbs of the planet. This effect was first observed in the atmosphere of WASP-76b, in which an apparent “kink” in the cross-correlation trail of Fe was observed, hinting at the existence of an asymmetric Fe abundance in the atmosphere across the limbs of the planet, as different regions rotated into and out of view (Ehrenreich et al., 2020). However, Savel et al. (2022) have shown that this apparent discrepancy in the Fe abundance across the limbs of the planet is likely explained by a global effect, such as asymmetric cloud formation or a longitudinal temperature asymmetry. This hypothesis gains further support from the presence of a similar kink in the CC trails of similar neutral atomic species in the atmosphere of WASP-76b (Kesseli et al., 2022; Pelletier et al., 2023). These species form at similar altitudes as Fe, but

have a range of condensation temperatures, suggesting that a global process is likely influencing their common apparent radial velocity offsets.

Similar asymmetries have also been found in other UHJs. Prinoth et al. (2022) found absorption signals from a range of neutral and ionised metals in the atmosphere of WASP-189b, with line positions which varied significantly between species, suggesting an inhomogeneity in their spatial distributions. Offsets in velocity between species were also detected in the atmosphere of WASP-121b, particularly for ionised calcium (see Sect. 3.3.3), which is thought to exist as part of an extended outflowing envelope, such that it is present in a different dynamical regime to the aforementioned neutral species. This outflowing envelope of ionised species is further supported by the existence of artificially “scaled-up” Fe II features relative to Fe, suggesting the model assumption of hydrostatic equilibrium has broken down for Fe II. Further analysis of this data set by Seidel et al. (2023) found a potential asymmetric super-rotating Na jet, which stems from the planet’s hotter dayside post mid-transit. However, as this is only a partial transit of WASP-121b, further analysis is required to rule out its existence as part of a global day-to-night flow.

Recently, this varying longitudinal representation of an exoplanetary atmosphere has been modelled directly at high-resolution with the combination of advanced rotational broadening kernels (Gandhi et al., 2022; Boucher et al., 2023), and distinct transit light curves for the *leading* morning limb and *trailing* evening limb. As a planet transits its host star, the morning limb passes the stellar disk before the evening limb. For tidally-locked planets, the morning limb is permanently redshifted, whereas the evening limb is permanently blueshifted. This process is, however, further complicated by the existence of complex wind patterns, such as super-rotational equatorial jets or radially outflowing winds, which are often degenerate with planetary rotation. This information can be used to separate the morning and evening contributions of planetary absorption lines in velocity space and separately model each limb. Thus, constraining

the atmospheric properties (abundances, T - P profiles, dynamics, etc.) of the morning and evening limb separately.

Gandhi et al. (2023, hereafter G2023) recently utilised this technique to constrain the atmospheric abundance of multiple metals across the limbs of WASP-76b. The abundances were found to be broadly consistent longitudinally, supporting the aforementioned hypothesis present by Savel et al. (2022) which suggested any asymmetry in a species' CC-trail is likely caused by a global effect, as opposed to a longitudinally varying abundance. This technique is discussed extensively in Sect. 2.3.3.

Pelletier et al. (2023, hereafter P2023) recently utilised MAROON-X observations to retrieve a broadly stellar composition of refractory elements for WASP-76b. However, they found substellar abundances relative to Fe for alkali metals, as well as V and Cr, suggesting that a combination of chemical processes is depleting the abundance of several species. They also detect VO in the atmosphere of WASP-76b with both ESPRESSO and MAROON-X observations, which has long been theorised as a thermal inversion agent which drives high-altitude temperature inversions in the upper atmospheres of UHJs, but has until now remained elusive.

Similarly to the spatially-resolved, high-resolution analysis of exoplanetary atmospheres, first presented by Gandhi et al. (2022), it has been demonstrated that the distinct transit light curves caused by asymmetric limbs enable the extraction of separate transmission spectra for morning and evening limbs directly from low-resolution transit time-series measurements (Espinoza & Jones, 2021; Grant & Wakeford, 2022). Multi-dimensional observations of exoplanetary atmospheres have previously been reserved for eclipse/phase curve measurements, however, these updated modelling approaches will enable the characterisation of the three-dimensional nature of these objects at both low- and high-resolution directly from transmission spectroscopy observations. Coupled with the enhanced sensitivity offered by the next generation space telescopes

and ultra-stable ground-based echelle spectrographs, this will also provide a more detailed understanding of the intricate chemical and physical processes at play in their atmospheres.

4.1 ESPRESSO Observations

One full primary transit of WASP-76b was observed with the ESPRESSO spectrograph at the VLT on 2019 October 18, hereafter referred to as O3. In addition to this observation, two further archival primary transits were included, observed on 2018 September 2 and 2018 October 30, respectively. These archival transits of WASP-76b were first analysed by Ehrenreich et al. (2020), and have been analysed extensively in the subsequent years (Tabernero et al., 2021; Seidel et al., 2021; Gandhi et al., 2022; Kesseli et al., 2022; Gandhi et al., 2023; Pelletier et al., 2023). They are hereafter referred to as O1 and O2, respectively. Further details regarding these observations are given in Table 4.1. The data were reduced using the ESPRESSO DRS v3.1.0, and the non-blaze-corrected S2D spectra were extracted.

Table 4.1: A summary of the ESPRESSO observations of WASP-76b.

Dataset	Date	Obs. Mode	N _{exp} (in-transit)	Exp. Time	S/N@550nm
O1	02-09-18	1-UT (UT3)	35 (21)	600 s	~94
O2	30-10-18	1-UT (UT3)	69 (37)	300 s	~75
O3	18-10-19	1-UT (UT3)	117 (71)	150 s	~45

4.1.1 Data Reduction

The S2D spectra were then cleaned and blaze corrected following Merritt et al. (2020), which is also outlined in Sects. 2.2.2 & 3.1.1. Similarly to Sect. 3.1.1, the residual array in the blaze correction was smoothed with a narrower filter than in previous works (a median filter with a width of 101 pixels and a Gaussian filter with a standard deviation of 200 pixels) in order to minimise the effects caused by the ‘wiggles’ pattern seen in ESPRESSO spectra (Allart et al., 2020). To ensure these wiggles—alongside the

relatively aggressive preprocessing steps and stellar and telluric removal procedures—didn’t inadvertently distort the underlying exoplanetary signal, conducted extensive injection and recovery tests (see Sect. 4.3.1 for further details).

The CLV and RM effect was modelled following Sect. 2.2.3 and removed in a similar manner as described in Sect. 3.1.1. It is worth noting that the efficacy of this procedure relies heavily on a precise estimate of the projected spin-orbit angle, λ , which has a relatively large uncertainty (see Table B1). In addition to the in-transit distortions caused by the RM and CLV effects, the contamination caused by stellar and telluric lines was also removed. Firstly, each spectrum was shifted into the stellar rest frame via the stellar radial velocity, computed via the orbital parameters outlined in Table B1. This ensures that the stellar and telluric lines are (quasi-)stationary in time. These (quasi-)stationary features were then fit with the iterative algorithm SYSREM (see Sect. 2.2.4.1). Before applying SYSREM, each order was divided by its median spectrum, after which the SYSREM model is then subtracted from the data. This procedure is akin to fitting the data directly with SYSREM and dividing through by the resultant model, however subtraction allows for a faster model filtering procedure, outlined in Sect. 2.3.5, whilst retaining the accuracy required for the analysis (Gibson et al., 2022). This model filtering procedure then in turn replicates any distortions caused by SYSREM on the atmospheric model (see Fig. 4.1).

In order to determine the ‘optimum’ number of SYSREM iterations for each dataset, an atmospheric model, including all species outlined in Sect. 4.2.1, was injected with a negative K_p value, where K_p is the planet’s radial velocity semi-amplitude, such that it was well separated from the real exoplanet signal. A likelihood mapping analysis was performed, and the number of iterations which resulted in the optimum detection significance was chosen. In order to compute the detection significance, a log-likelihood distribution (see Sect. 4.3.2) was computed as a function of the model scale factor α , conditioned on the optimum β , K_p , and Δv_{sys} values, where β and Δv_{sys} are the noise

scale factor and the systemic velocity offset, respectively. The expected value, or mean, of this distribution was computed, and divided by its standard deviation, resulting in a detection significance. This, in essence, computes the number of standard deviations the maximum signal deviates from an alpha of 0 (i.e., a non-detection). The optimum number of SYSREM iterations for each dataset was 16, 18, and 22 for O1, O2, and O3, respectively. It is worth noting that this procedure is highly sensitive to the injected model, as a model with many absorption lines in orders dominated by stellar/telluric lines will, in theory, require a higher number of iterations to optimally extract the exoplanet signal. Furthermore, separating each order and subsequently determining the optimum number of SYSREM iterations per order would also minimise the inevitable distortion caused by SYSREM on the exoplanet’s signal (Nugroho et al., 2017).

4.2 Methods

4.2.1 Modelling WASP-76b

For each of the transits, traditional cross-correlation analysis was performed, as well as a full atmospheric retrieval, with 1D atmospheric models computed using IRRADIATOR (Gibson et al., 2022), described in Sect. 2.3, including cross-sections from a number of atomic and molecular species (Fe, V, Cr, Mg, Na, and VO). The cross-sections for Fe, V, Cr, and Mg were obtained via the Kurucz line list (Kurucz & Bell, 1995)¹. Similarly, the Na cross-sections were obtained via the VALD line list (Piskunov et al., 1995), whereas the VO cross-sections were obtained via the ExoMol line list (McKemmish et al., 2016). Similarly to the modelling description of WASP-121b in Sect. 3.2.1, 70 atmospheric layers were predefined, equidistant in log space, ranging from 10^2 bar to 10^{-12} bar, across which a T - P profile was computed using the parametric model from Guillot (2010) with input parameters T_{irr} , T_{int} , κ_{IR} , and γ , corresponding to the irradiation temperature, internal temperature, mean infrared opacity, and the ratio of visible-to-infrared opacity, respectively. After solving for hydrostatic equilibrium, with

¹These cross-sections were obtained from petitRADTRANS via Keeper.

variable gravity, the opacity of each predefined layer of the atmosphere was computed by weighing each species' cross-section on their respective VMRs, χ_{species} , assuming a constant VMR with altitude. As described in Sect. 2.3.1, a H_2 VMR, χ_{ray} , was included along with H_2 opacities from Dalgarno & Williams (1962), to account for Rayleigh scattering, as well as a further continuum opacity source caused by an opaque cloud deck at a pressure level P_{cloud} , below which the transmission spectrum model was truncated. In practice, the logarithms of strictly positive parameters were fit in the retrieval analysis, with the exception of temperature. Therefore, in total, the 1D transmission spectrum model has $6 + N_{\text{species}}$ input parameters (T_{irr} , T_{int} , $\log_{10}(\kappa_{\text{IR}})$, $\log_{10}(\gamma)$, $\log_{10}(P_{\text{cloud}})$, $\log_{10}(\chi_{\text{ray}})$, $\log_{10}(\chi_{\text{species}})$).

4.2.2 Broadening Kernel

Recent studies have modelled the varying longitudinal representation of an exoplanetary atmosphere directly with the use of realistic rotational broadening kernels (Gandhi et al., 2022; Boucher et al., 2023). At high-resolution, we are not only sensitive to the positions of individual absorption lines, but also the subtle variations in their line shapes caused by winds and rotation (Seidel et al., 2020; Hoeijmakers et al., 2020). In transit, observations are only sensitive to a thin annulus of the planet's atmosphere, i.e., the terminator. For a rotating annulus of inner radius r_1 and outer radius $r_2 = r_1 + (d \cdot r_1)$, the broadening profile can be modelled by a kernel given by Eq. 2.20. This kernel is shown in Fig. 2.8 (see Sect. 2.3.3 for a full derivation).

This broadening kernel allows for the morning half of the terminator to be effectively separated from the evening half of the terminator in velocity, via subtle variations in the line shape. In practice, each half of the terminator (limb) was modelled separately with its own 1D atmospheric model and each transmission spectrum was convolved with one half of the above broadening kernel. The effect of this convolution is shown in Fig. 4.1. This procedure allows for separate atmospheric parameters, as well as separate rotational velocities Δv_{rot} and thickness d , for each atmospheric limb to be

retrieved. This results in four parameters for the kernel, two for each limb: d_m , d_e , $\Delta v_{\text{rot},m}$, and $\Delta v_{\text{rot},e}$. The subscripts m and e represent the morning and evening limbs, respectively.

In practice, d_m and d_e were fixed to a constant value equivalent to $5H_s$ following Boucher et al. (2023), where H_s is the atmospheric scale height. Each half of the kernel was also normalised to 0.5, such that each 1D model contributed to half the total absorption. This also ensured that any asymmetry in line/transit depth retrieved from the data is caused solely by physical effects, such as an increase in scale height due to a temperature asymmetry between the morning/evening limbs. This asymmetry, or lack thereof, can then be interpreted via varying physical parameters retrieved for the limbs' individual atmospheric models.

After convolution with the broadening kernels, the independent atmospheric models were summed and linearly interpolated to the 2D wavelength grid of the data (order $\times$ wavelength). For each order, the 2D forward model was then Doppler shifted to a planetary velocity given by Eq. 2.21. This resulted in a 3D shifted forward model with the same dimensions as the data (time/phase $\times$ order $\times$ wavelength). The middle panel of Fig. 4.1 shows a single order of the model after this projection. The forward model was then filtered using the SYSREM basis vectors via the procedure outlined in Sect. 2.3.5 and Gibson et al. (2022). The result of this model filtering is shown in the bottom panel of Fig. 4.1.

4.3 Analysis

4.3.1 Injection and Recovery Tests

Before conducting a full retrieval using the atmospheric model, it is imperative that injection and recovery tests are conducted. These tests ensure that the preprocessing steps applied in Sect. 4.1.1 do not inadvertently distort the underlying exoplanetary

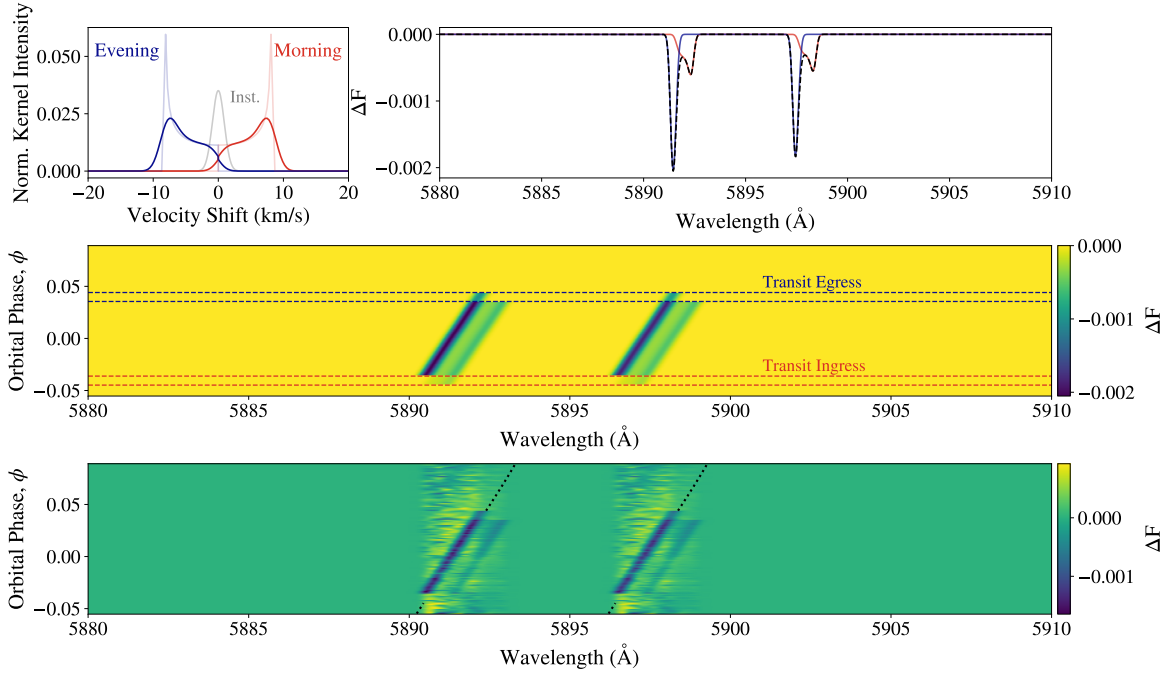


Figure 4.1: (**upper left**) The rotational broadening kernel outlined in Eq. 2.20. The solid lines red/blue show the final morning/evening halves, after convolution with an instrumental profile, shown in grey. (**upper right**) An asymmetric Na model, with varying broadening and atmospheric parameters between the morning and evening limbs. The combined model is overplotted with a black dashed line. (**middle**) The one-dimensional model projected to a two-dimensional orbital phase $\times$ wavelength array for a single ESPRESSO order. This array is then weighted by the limb-darkening model described in Gandhi et al. (2022). This ensures solely morning/evening contributions during ingress/egress, respectively. (**lower**) The two-dimensional orbital phase $\times$ wavelength array after SYREM model filtering, highlighting the distortions of the planetary lines after preprocessing. The black dotted curve shows the planetary radial velocity to which the model is projected.

signal, biasing the retrieved constraints and subsequent interpretations. Furthermore, to constrain any asymmetric signals stemming from the morning/evening limbs, it is essential to ensure that the retrieval framework is sensitive to subtle variations in line shapes, which are already deep beneath the noise of the observations. Thus, typically individual line shapes are unable to be measured directly in order to observe these variations. For each of the datasets, an asymmetrically broadened atmospheric model was injected into a subset of ESPRESSO orders¹, prior to the cleaning and blaze correction steps outlined in Sect. 4.1.1. This injected model included cross-sections from Fe, Na, V, and VO. The retrieval analysis was then performed on the injected data, similar to that outlined in Sect. 4.3.2, and the retrieved model parameters, T - P

¹The number of ESPRESSO orders in the injection tests were reduced for increased computational efficiency and speed.

4. MULTIDIMENSIONAL ATMOSPHERIC RETRIEVALS OF WASP-76b WITH ESPRESSO

Table 4.2: The parameters of the atmospheric model of WASP-76b. $\mathcal{U}(a, b)$ represents a uniform prior from a to b . The various parameters for the morning and evening limbs are shown, with a separate $\log_{10}(\chi_{\text{species}})$ for each species.

Parameter, θ	Units	Prior Range
<i>Global:</i>		
α	-	1 (fixed)
β	-	$\mathcal{U}(0.1, 2)$
K_p	km s ⁻¹	$\mathcal{U}(150, 250)$
Δv_{sys}	km s ⁻¹	$\mathcal{U}(-20, 20)$
<i>Morning:</i>		
d_m	R_p	0.062 (fixed)
$\Delta v_{\text{rot},m}$	pixels	$\mathcal{U}(0, 50)$
$\log_{10}(\kappa_{\text{IR}})$	-	$\mathcal{U}(-4, 4)$
$\log_{10}(\gamma)$	-	$\mathcal{U}(-4, 2)$
T_{irr}	K	$\mathcal{U}(1000, 4500)$
T_{int}	K	200 (fixed)
$\log_{10}(P_{\text{cloud}})$	bar	$\mathcal{U}(-4, 2)$
$\log_{10}(\chi_{\text{ray}})$	-	$\mathcal{U}(-0.068, 10)$
$\log_{10}(\chi_{\text{species}})$	-	$\mathcal{U}(-15, -2.3)$
<i>Evening:</i>		
d_e	R_p	0.062 (fixed)
$\Delta v_{\text{rot},e}$	pixels	$\mathcal{U}(0, 50)$
$\log_{10}(\kappa_{\text{IR}})$	-	$\mathcal{U}(-4, 4)$
$\log_{10}(\gamma)$	-	$\mathcal{U}(-4, 2)$
T_{irr}	K	$\mathcal{U}(1000, 4500)$
T_{int}	K	200 (fixed)
$\log_{10}(P_{\text{cloud}})$	bar	$\mathcal{U}(-4, 2)$
$\log_{10}(\chi_{\text{ray}})$	-	$\mathcal{U}(-0.068, 10)$
$\log_{10}(\chi_{\text{species}})$	-	$\mathcal{U}(-15, -2.3)$

profiles, and broadening kernels were found to be in agreement with those injected (see Figs. B1 – B3).

4.3.2 Atmospheric Retrieval

In order to perform a full atmospheric retrieval analysis on each of the datasets, a forward model, m_i , must be computed for a given set of model parameters, θ , outlined in Table 4.2. Assuming uniform priors, the log-posterior was computed by adding the log-prior to the log-likelihood given in Eq. 2.34. This was then folded into an Markov Chain Monte Carlo (MCMC) framework in order to retrieve posterior distributions for each of the model parameters, for each of the datasets. A DEMC (see Sect. 2.4.3) was used, running an MCMC chain with 128 walkers, with a burn-in length of 300 and a chain length of 600, unless stated otherwise. This resulted in 115,200 samples of the posterior, of which 38,400 were discarded. The chains' convergence was assessed via the Gelman-Rubin (GR) statistic, after splitting each chain into four independent subchains. The chains were also split into groups of independent walkers, and the 1D and 2D marginal distributions were overplotted, in order to visualise the convergence of the MCMC. The results of each of the retrievals are shown in Figs. B6 – B8.

The retrieved *absolute* abundances were compared across each of the transits for the morning (Fig. B4) and evening (Fig. B5) limbs. These results were also compared with stellar values, for species with measured stellar abundances (Tabernero et al., 2021), as well as with solar abundances, where measured (Asplund et al., 2009).

The morning/evening abundance constraints were also compared with the constraints presented by G2023. Due to the relatively large rotation angle of close-in planets such as WASP-76b during transit, G2023 opt to retrieve varying regions of the morning/evening limbs before and after mid-transit (see Gandhi et al. (2022) for further details). The simultaneous retrieval of both limbs were compared with the weighted mean of regions A and B (evening), and C and D (morning) from G2023, respectively. It is also worth noting that the constraints obtained by G2023 are from a joint retrieval of O1 and O2, whereas both datasets were fit individually in this study.

Similarly to previous studies, the *relative* abundances of the atmospheric species were also compared, and these values were found to be better constrained (see Figs. 4.3 & 4.4). This is due to degeneracies in model transmission spectra, as well as the normalisation of high-resolution spectra during preprocessing, which removes sensitivity to the true continuum of the planet (Birkby, 2018).

4.3.3 Cross-correlation

The individual presence of each species included in the atmospheric model was confirmed via traditional cross-correlation analysis. The atmospheric models were calculated using the optimum parameters from the various atmospheric retrievals. The results of which can be seen in Appendix B. The novel detection of VO in the atmosphere of WASP-76b by P2023 was confirmed in datasets O2 and O3, independently detecting VO in O3 (see Fig. B9). As this is the first analysis of the O3 dataset, an investigation was also conducted into the apparent kink in the cross-correlation trail first shown by Ehrenreich et al. (2020) for O1 and O2 (see Fig. B11). This apparent kink has previously been independently confirmed via reanalysis of these transits (Kesseli et al., 2022), as well as additional analysis from subsequent observations using HARPS (Kesseli & Snellen, 2021) and MAROON-X (P2023).

Traditional cross-correlation analysis also allows for the investigation of any apparent asymmetry in the abundance of individual species between the morning and evening limbs. The data was first cross-correlated with an *unbroadened* model, Doppler shifted over a range of Δv_{sys} values. The cross-correlation function (CCF) for each orbital phase was then shifted to a new planetary velocity given by Eq. 2.21 for a range of K_p values, and integrated as a function of time/phase. The CCF was then plotted at the optimum K_p value, an example of which is shown in Fig. 4.2. As the model is unbroadened (i.e., it is not convolved with the broadening kernel, but still includes its natural line widths from thermal/pressure broadening) the distribution of the CCF

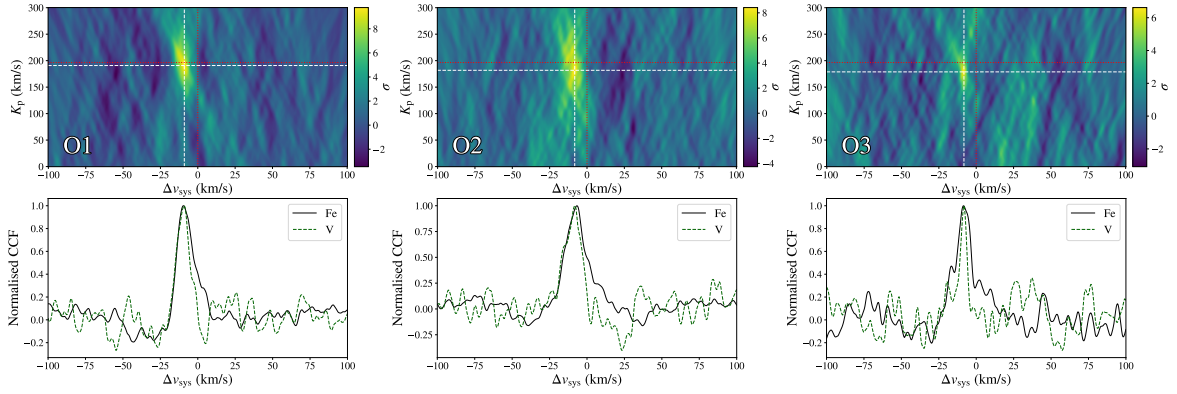


Figure 4.2: (*Upper*) K_p - Δv_{sys} maps of V, for O1, O2, and O3. The V atmospheric models were calculated using the optimum parameters from the various atmospheric retrievals, however, they were unbroadened. The red dotted lines shows the expected planetary velocity values, whereas the white dashed lines shows the maximum K_p and Δv_{sys} values. (*Lower*) A comparison of the CCF of Fe and V, at their optimum K_p value. As the models were unbroadened, this distribution may be used as a proxy for the average line shape of each species in the data, highlighting any apparent asymmetries in the species' longitudinal distributions.

may be used as a proxy for the average line shape in the data, after rotational and instrumental broadening. In other words, the cross-correlation is a convolution of the intrinsic line shape in the data with the unbroadened model. By comparing the shape of the cross-correlation function of Fe, previously detected in both limbs (Gandhi et al., 2022, 2023), with that of other species, an empirical search can be conducted for any apparent asymmetry in their CCF as a function of Δv_{sys} . This asymmetric CCF could potentially be caused by an asymmetric distribution in their abundance between the blueshifted evening limb and redshifted morning limb (Wardenier et al., 2023). Cross-correlation trails which deviate from the planet's Keplerian velocity curve, such as that first seen in Ehrenreich et al. (2020), can also often result in a 'diamond' feature in the K_p - Δv_{sys} maps, as a warped CC-trail summed in time will result in multiple peaks in the map localised at the expected K_p and Δv_{sys} values (Nugroho et al., 2020c; Wardenier et al., 2021b; Maguire et al., 2023). Fig. 4.2 shows the results of this test for Fe and V, in which a narrower CCF for V is seen relative to Fe, for both O1 and O3, caused by a predominantly blueshifted V line shape.

4.4 Discussion

4.4.1 Abundance Constraints

The abundance constraints were directly compared with stellar values (Tabernero et al., 2021) where measured (i.e., Fe, Cr, Mg, Na), as well with solar values (Asplund et al., 2009) where measured. The individual constraints obtained for the morning and evening limbs were also compared with a similar spatially-resolved analysis of WASP-76b, conducted by G2023, for specific species (i.e., Fe, V, Mg, Cr). For species such as Na and VO, where previous spatially-resolved constraints are not available, the results are compared with those obtained by P2023. It's important to note that, unlike the approach presented here, P2023 modelled the terminator as a whole. The relative abundance constraints for the morning and evening limbs are shown in Figs. 4.3 & 4.4, respectively. Whereas, the absolute abundance constraints for the morning and evening limbs are shown in Figs. B4 & B5, respectively.

Fe

Across all three transits, consistent Fe abundance constraints are found in both the morning and evening limbs and the abundances are found to be consistent across the limbs of the atmosphere for each of the individual transits. This suggests a stable uniform longitudinal distribution of Fe in the atmosphere of WASP-76b, which is consistent with previous spatially-resolved constraints by Gandhi et al. (2022, 2023). This uniform distribution of Fe indicates that a global process, such as an uneven cloud deck or temperature asymmetry, is likely responsible for the asymmetric CC trail previously found (Ehrenreich et al., 2020; Savel et al., 2022). This is further supported by the asymmetric CC trails found for a multitude of species with varying condensation temperatures (Kesseli et al., 2022; Pelletier et al., 2023).

Furthermore, both the morning and evening Fe abundance constraints are consistent

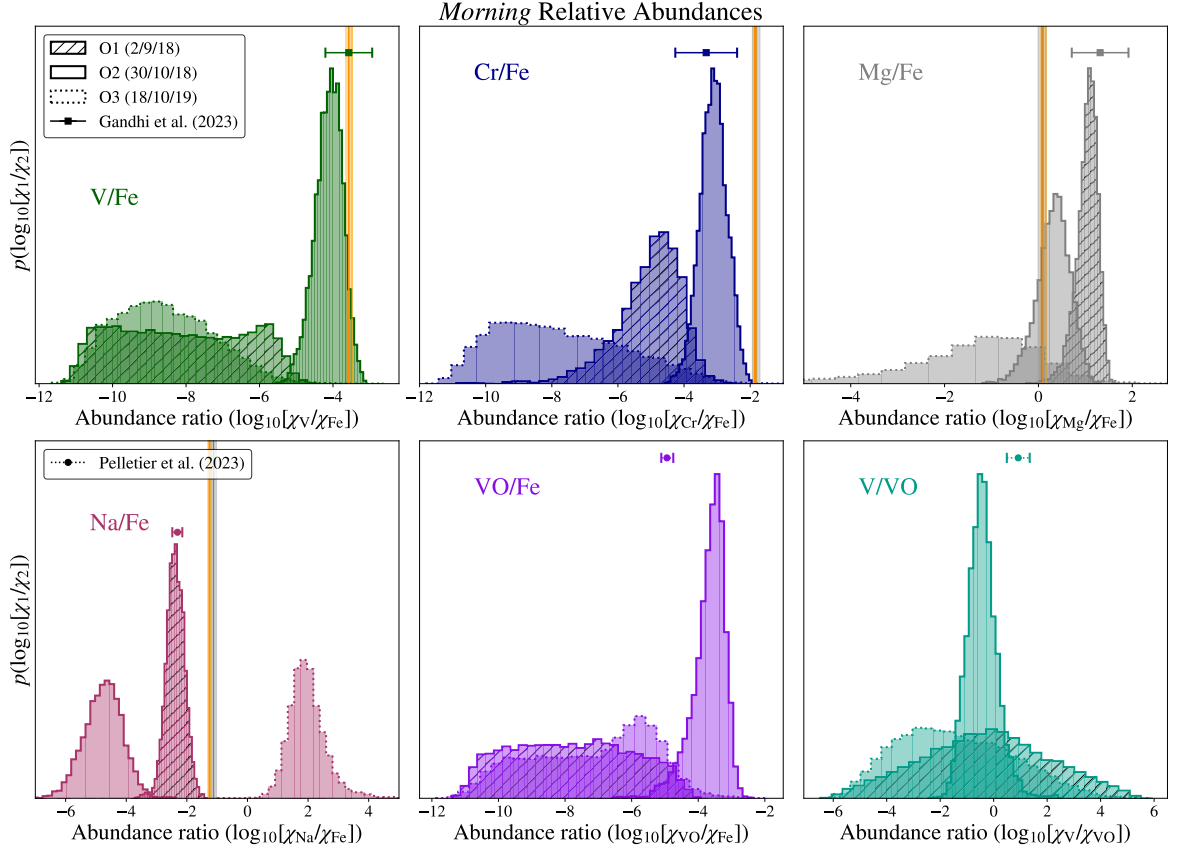


Figure 4.3: Relative abundance comparison across each of the three transits, for the *morning* limb. The stellar values from Tabernero et al. (2021) are shown as a grey vertical line with their 1σ contours shaded, where measured. The solar values from Asplund et al. (2009) are shown as an orange vertical line with their 1σ contours shaded. The weighted mean of the retrieved relative abundances in regions C and D (morning) from G2023 are also shown, where measured. Otherwise, the relative abundances measured for the whole terminator from P2023 are shown.

with stellar values, which suggests a uniform atmospheric composition similar to that of its parent protoplanetary disk. This is consistent with the findings of G2023, in which Fe/H values of a range of UHJs—corrected for the stellar metallicity of each system—were found to be consistent with their host star values. P2023 also found a similar trend for the abundances of refractory metals in the atmosphere of WASP-76b.

V & VO

V is consistent with solar values and G2023 for O2. Similarly, VO is also consistent with constraints obtained by P2023 for O2 in the morning limb. Both V and VO are unconstrained in the morning limb for both O1 and O3, with upper limits consistent with O2.

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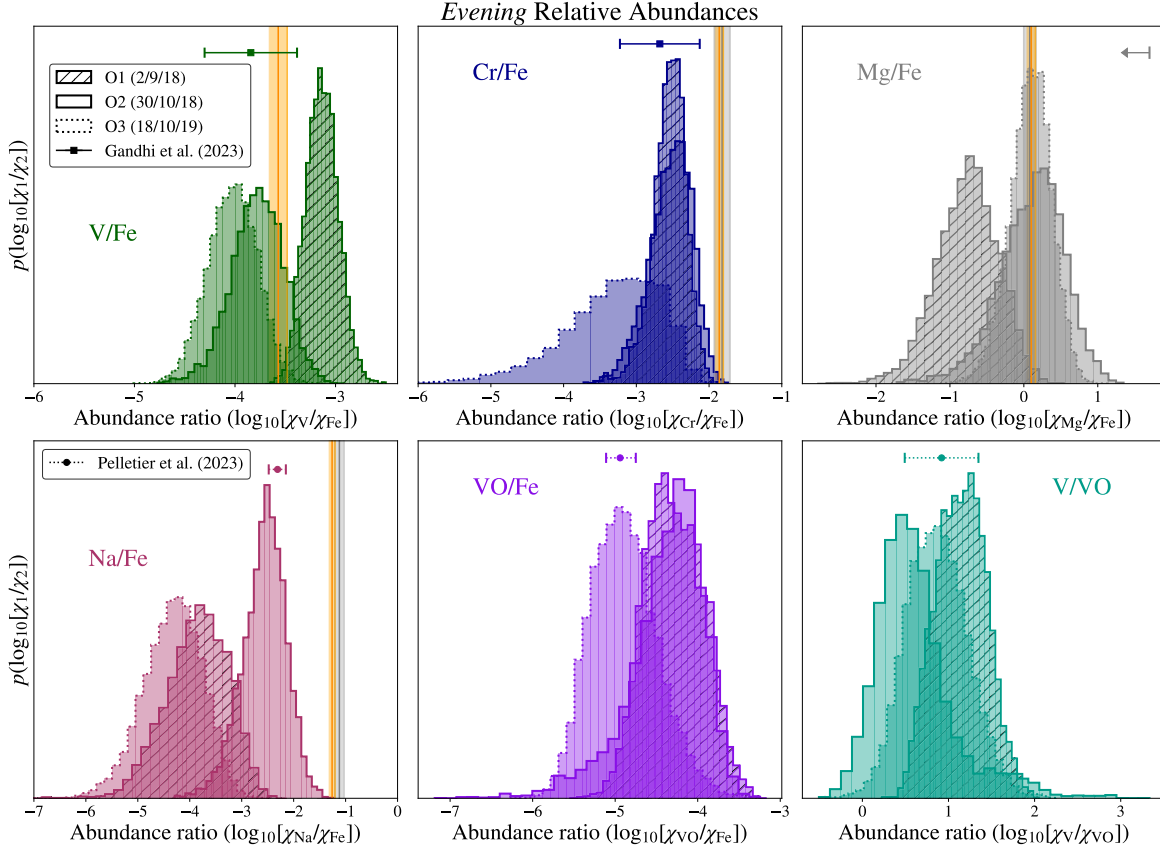


Figure 4.4: Relative abundance comparison across each of the three transits, for the *evening* limb. Shaded regions are as in Fig. 4.3. The weighted mean of the retrieved relative abundances in regions A and B (evening) from G2023 are also shown, where measured.

In the evening limb, all three transits are consistent, aligning with solar values as well as with both G2023 and P2023. Where constrained, V and VO abundances are found to be consistent across the limbs of the planet.

There is an interesting discrepancy between the morning and evening constraints for both V and VO. For O2, both species are constrained across both limbs. However, for O1 and O3, only the species in the evening limb are constrained. This leads the V/Fe ratio in the morning limb for both O1 and O3 (see Fig. 4.3) to be subsolar. Gandhi et al. (2022) found that, overall, the combined signal is dominated by the more blueshifted evening limb, which is in agreement with previous GCM predictions (Wardenier et al., 2021b). However, signals from irradiated terminator regions (regions A & D of G2023) typically dominate the combined signal in their respective phase ranges due to larger temperatures and, thus, scale heights. G2023 was also unable to constrain V in the

dayside morning region (D). These dominant signals result in tighter constraints for these regions, making it surprising that V is no longer constrained. All three of the observations are of similar quality, with comparable S/N ratios when adjusted for the varying exposure times. The integrated water vapour (IWV) was monitored between observations and no significant trend was found which may impact the reliability of the data. This is further supported by the similar constraints shown between each of the injection tests (see Figs. B1 – B3). The variation in airmass was also monitored between observations, where an increase in airmass was found for O1 and O3 during ingress, which could explain the dampened morning V/VO signal. However, such an effect would likely reduce the quality of the constraints in the morning limb uniformly across all species, which is not the case, and thus a decrease in data quality for O1 and O3 relative to O2, which might explain worse V/VO constraints in the morning limb, seems unlikely. It is possible that both the V and VO signals are dampened in the cooler morning limb for O1 and O3, due to a combination of recombination and condensation at lower temperatures. However, as the upper limits are consistent with those of O2, as well as G2023, their presence in the morning limb cannot be ruled out entirely.

The search for the dampened V signal in the morning limb for both O1 and O3 relative to O2 can be approached more empirically. In Fig. 4.2, a slice through the optimal K_p value is shown for both Fe and V. The figure shows CCFs of *unbroadened* models that peak at similar Δv_{sys} values. Fe has been previously detected in both limbs of the planet by Gandhi et al. (2022), as well as in this work. Thus, in order to identify any asymmetries in the line profile of V, the CCFs of Fe and V were compared. For O2, the CCFs of both Fe and V exhibit a similar shape, characterised by a relatively broad profile. This broad shape is due to contributions from both the blueshifted (evening) and redshifted (morning) components of the line profile. In contrast, for both O1 and O3, the CCF of V is notably narrower relative to Fe and is primarily dominated by the blueshifted (evening) component, perhaps indicating a more localised contribution to the line profile.

Although the origin of this asymmetry in the V and VO distributions across the morning and evening limbs for O1 and O3 is unclear, if present, its discrepancy with the well-constrained V and VO abundances measured for both limbs for O2 indicates an atmosphere with clear variable chemistry, in which a combination of recombination/condensation is altering the V and VO abundances at the cooler morning limb over the course of months/years.

Although the VO line list used (VOMYT; McKemmish et al. (2016)) has resulted in detections of VO in the atmosphere of WASP-76b (e.g., P2023 & Fig. B9), it has previously led to non-detections of VO in the atmosphere of WASP-121b at high-resolution (Hoeijmakers et al., 2020; Merritt et al., 2020). These non-detections were reported as inconclusive, and this line list was shown to be insufficient in recovering injected VO signals from UVES transmission spectroscopy data of WASP-121b (de Regt et al., 2022). Recently, Bowesman et al. (2024) presented an updated MARVEL-ised (Measured Active Rotational-Vibrational Energy Levels; Császár et al., 2007) line list for VO (HyVO), which includes hyperfine splitting effects and should facilitate more reliable high-resolution detections and abundance constraints of VO.

A cross-correlation analysis was conducted with the updated line list, with cross-sections computed at $T = 2800$ K and $P = 0.1$ mbar, shown in Fig. B10. In order to determine the optimum parameters for this cross-correlation analysis, an MCMC similar to that outlined in Sect. 4.3.2 was performed, using a simple one-dimensional Gaussian broadening kernel, and an isothermal T - P profile. VO has now been detected in O1 via cross-correlation. However, the previous detection of VO in O2 has now shifted to a significantly lower Δv_{sys} and K_p . The O3 detection significance has increased with the updated line list. It is difficult to assess the accuracy of these new detections/non-detections without performing a full atmospheric retrieval, with a varying T - P profile and two-dimensional broadening kernel. As the updated cross-sections

are not readily available across the full T - P grid, an atmospheric retrieval akin to that presented above is impracticable at this time. A quantitative assessment of the updated line list is beyond the scope of this work; however, it is required to ensure its reliability for exoplanetary studies at high-resolution going forward. Despite this added uncertainty in terms of a VO detection, the results still show a potentially variable V abundance, with which there is no uncertainty regarding line list accuracy and, alongside this VO analysis, provides an interesting insight into the chemistry of V-bearing species.

Cr

The Cr/Fe constraints obtained are also consistent between transits, as well as with G2023, for both the morning and evening limbs. Similarly to V and VO, however, Cr/Fe is found to be depleted relative to stellar for O1 and O3 in the morning limb, potentially due to partial recombination/condensation of Cr to other compounds, such as CrH, which has previously been detected in the atmosphere of WASP-31b (Braam et al., 2021; Flagg et al., 2023). P2023 also constrain the abundance of CrH in their 1D retrieval of WASP-76b, however were unable to detect it via cross-correlation. Both P2023 and G2023 also found substellar Cr/Fe ratios, within 1σ , consistent with these findings.

Relative abundances are compared as these constraints are typically more accurate and reliable at high-resolution, and in general for transmission spectra. This is due to the well-known degeneracy between the absolute abundance, χ_{species} , and opaque cloud deck pressure, P_{cloud} , and/or reference pressure, such that a model with a higher χ_{species} and lower P_{cloud} could, in principle, produce identical features as a model with a lower χ_{species} and higher cloud deck pressure P_{cloud} (Benneke & Seager, 2012). This degeneracy can be clearly in Fig. 2.6. Furthermore, the normalisation of high-resolution spectra during preprocessing limits sensitivity to absolute line strengths above the planetary continuum, making relative line strengths, and consequently, relative abundance

constraints, more precise (Birkby, 2018; Gibson et al., 2020).

Mg

Similarly to Fe, the Mg abundance constraints are consistent with both stellar values and G2023 across all three transits. They are also consistent across the limbs of the atmosphere for each of the individual transits. Interestingly, the absolute abundance of Mg is consistent with the upper prior limit (see Table 4.2) for both the morning (O1 and O2) and evening (O2 and O3) limbs. Similar behaviour has been seen previously in high-resolution analysis of WASP-121b with UVES and ESPRESSO (Gibson et al., 2022; Maguire et al., 2023). As Mg II has previously been detected in the upper atmosphere of WASP-121b (Sing et al., 2019), it is thought that Mg may be part of an extended, non-hydrostatic envelope, such that the model assumption of hydrostatic equilibrium breaks down. To account for this, the model would artificially increase the abundance of Mg, increasing its line strengths. It is difficult to say if this is also the case for WASP-76b, as Mg II has not yet been detected in its atmosphere. Furthermore, Mg has relatively few lines in the ESPRESSO wavelength range, which could also explain its poorer abundance constraints.

Na

A substellar Na abundance relative to Fe is found in the evening limb across all three transits. This is in agreement with P2023, who find substellar abundances for alkali metals (Li, Na, K), suggesting their lower ionisation energies cause a greater degree of ionisation at the temperatures and pressures probed, driving a decrease in the abundance of neutral alkaline atoms. Similar behaviour was found in the atmosphere of WASP-121b, where the abundance of both Na and Ca relative to Fe were typically lower than their stellar counterparts, alongside the presence of high-altitude Ca II indicates a greater degree of ionisation (Maguire et al., 2023). It is also worth noting that G2023 were unable to constrain Na in both the morning and evening limbs of WASP-76b via an independent joint retrieval of O1 and O2.

The morning Na abundances relative to Fe are also found to be substellar for both O1 and O2, consistent with the evening limb and continuing the trend mentioned above. However, for O3, a drastically higher Na/Fe ratio is found, driven by an anomalously high Na abundance. It is possible that Na is also part of an extended outer envelope, similar to Mg, becoming more readily ionised in the upper atmosphere, which is accounted for on the morning limb by an artificial increase in abundance. Another possible explanation is the existence of a high-altitude cloud deck on the morning limb, or similar continuum opacity source such as H^- opacity, which is not accounted for in the model. This artificially increases the Na abundance, in order to create a pseudo-continuum. In order to ensure this artificially high Na abundance does not affect the abundances of the other species in the O3 retrieval, the retrieval was re-run without the presence of Na. It was found to have minimal impact on the retrieved abundances, however, it significantly alters the morning T - P profile constraints. This is to be expected, as a higher Na abundance with a smaller uncertainty would result in a lower temperature with tighter constraints.

4.4.2 Temperature Constraints

For O1, the morning and evening temperatures at 0.1 mbar, $T_{0.1\text{mbar}}$, vary at the 1σ level (see Table 4.3 and Fig. B6). These morning and evening temperature constraints are consistent with the spatially-resolved temperature constraints of Gandhi et al. (2022). Above the high-altitude morning cloud deck, a morning T - P profile which is cooler than that of the evening limb is found, which is inverted above ~ 0.1 mbar.

For O2, a cooler evening T - P profile is found, which varies from that of the morning limb at the 2σ level at 0.1 mbar (see Table 4.3 and Fig. B7). The evening temperature at 0.1 mbar is consistent with that of Gandhi et al. (2022). For O2, the $T_{0.1\text{mbar}}^{\text{Morn}}$ is significantly higher than that of Gandhi et al. (2022), and at high pressures, it reaches unphysically high values for WASP-76b. This discrepancy between the morning limb

with both previous transits presented in this study, as well as with previous studies, is also likely explained by the presence of V and VO in the morning limb, whereas it's unconstrained for O1 and O3, as VO is known to be a thermal inversion agent which drives high-altitude temperature inversions in the upper atmospheres of UHJs. It is worth noting that transmission spectroscopy studies are typically not very sensitive to the T - P structure of the atmosphere, and therefore caution must be taken not to overinterpret the constraints. For O3 (see Table 4.3 & Fig. B8), a hotter evening T - P

Table 4.3: Temperature constraints for O1, O2, and O3 compared to Gandhi et al. (2022).

Transit	$T_{0.1\text{mbar}}^{\text{Morn}}$ (K)	$T_{0.1\text{mbar}}^{\text{Eve}}$ (K)
O1	2820^{+140}_{-50}	2240^{+530}_{-170}
O2	3650^{+120}_{-60}	3060^{+180}_{-70}
O3	1360^{+130}_{-60}	2120^{+810}_{-460}
Gandhi et al. (2022)	2615^{+266}_{-275}	2950^{+111}_{-156}

profile is found, which is inverted above ~ 0.1 mbar, similar to O1. The evening temperature at 0.1 mbar is consistent with that of Gandhi et al. (2022), and varies from the morning limb within 1σ . The $T_{0.1\text{mbar}}^{\text{Morn}}$ is significantly lower than that of Gandhi et al. (2022). This adverse decrease in temperature could be due to the model neglecting the presence of H^- opacity, whose presence is known to cool the atmosphere in this pressure regime (Parmentier et al., 2018). As mentioned in Sect. 4.4.1, this temperature discrepancy is also driven by the presence of an anomalously high Na abundance on the morning limb of O3. When Na is excluded from the retrievals, a much broader morning temperature constraint of $T_{0.1\text{mbar}}^{\text{Morn}} = 1950^{+990}_{-380}$ K is found, which is consistent with that found in Gandhi et al. (2022). The evening T - P profile does not change significantly.

4.4.3 Atmospheric Dynamics

For O1, a $K_p = 185.48 \pm 1.22$ km/s and $\Delta v_{\text{sys}} = -7.70 \pm 0.82$ km/s is retrieved, for O2: $K_p = 175.48 \pm 1.33$ km/s and $\Delta v_{\text{sys}} = -8.77 \pm 0.44$ km/s, and for O3: $K_p = 181.33 \pm 2.14$

km/s and $\Delta v_{\text{sys}} = -7.88 \pm 0.66$ km/s. Although different values are constrained for each of the transits, the planetary orbital velocities, given Eq. 2.21, were computed using 10,000 random samples from the posterior distributions of K_p and Δv_{sys} , and v_p was found to be consistent within 1σ in-transit. There is also a degeneracy between the global systemic velocity offset, Δv_{sys} , and the blueshifted component of the rotational velocity, $\Delta v_{\text{rot,e}}$, with the latter ideally accounting for subtle variations in the individual line shapes caused by additional wind patterns and rotation. When accounting for a broadening of an atmospheric model with $R=200,000$, broadening parameters of $v_{\text{rot,m}} = 1.24 \pm 1.16$ km/s and $v_{\text{rot,e}} = 2.97 \pm 1.61$ km/s for O1 are obtained. For O2, $v_{\text{rot,m}}$ and $v_{\text{rot,e}}$ were obtained as 2.50 ± 1.45 km/s and 0.99 ± 0.72 km s⁻¹, respectively. For O3, $v_{\text{rot,m}}$ and $v_{\text{rot,e}}$ were found to be 5.77 ± 2.62 km s⁻¹ and 1.33 ± 0.94 km s⁻¹. It's important to note that these distributions are non-Gaussian, and therefore, the constraints may not be accurately represented by the median value and standard deviation alone. The combination of these broadening parameters with a constant blueshifted offset of ~ 8 km/s is in agreement with previous high-resolution studies of WASP-76b (Ehrenreich et al., 2020; Pelletier et al., 2023; Gandhi et al., 2022, 2023).

The treatment described above also assumes a single K_p , Δv_{sys} , $\Delta v_{\text{rot,m}}$, and $\Delta v_{\text{rot,e}}$ value governs the dynamics of each of the atmospheric species. In reality, as seen in previous high-resolution studies (Prinoth et al., 2022; Wardenier et al., 2023), velocity offsets *between* species can occur. In reality, each species is likely to exist in different dynamical regimes, particularly when considering differing atmospheric limbs and/or an extended upper atmosphere. A more robust modelling approach would involve the individual treatment of each species' dynamics (i.e, varying K_p , Δv_{sys} , $\Delta v_{\text{rot,m}}$, and $\Delta v_{\text{rot,e}}$ for each species), which is left as an avenue for future research.

Recent studies using low-resolution transmission spectroscopy with JWST have also allowed us to investigate the three-dimensional nature and varying chemistry across the limbs of these objects. For example, Rustamkulov et al. (2023) found a wavelength-

dependent central transit time for WASP-39b, suggesting an asymmetric distribution of atmospheric species across the terminator. Furthermore, it has been shown that by probing the varying transit light curves of each atmospheric limb, particularly during ingress and egress, one can retrieve separate transmission spectra for each half of the terminator (Espinoza & Jones, 2021; Grant & Wakeford, 2022). These techniques at low-resolution, coupled with analysis such as that provided in this study, highlight the enormous promise of utilising low- and high-resolution transmission spectroscopy observations to investigate the three-dimensional nature of close-in exoplanets, a regime which until now was accessible only with eclipse/phase curve measurements.

4.5 Conclusions

In this chapter I have presented multiple high-resolution transit observations of the atmosphere of the UHJ WASP-76b, monitored across several months/years, with the ESPRESSO spectrograph at the VLT. The morning (leading) and evening (trailing) limbs of the atmosphere have been modelled separately with the use of realistic rotational broadening kernels, allowing for separate atmospheric abundances, T - P profiles, and dynamical parameters to be retrieved for each atmospheric limb via an atmospheric retrieval framework.

- The presence of VO, recently discovered in the atmosphere of WASP-76b by Pelletier et al. (2023), has been confirmed via cross-correlation in both T2 and T3 of the observations, with a detection significance of 4.0σ and 7.2σ , respectively.
- A uniform longitudinal distribution of Fe and Mg across the limbs of the atmosphere, for each of the transits, was found, consistent with previous works as well as stellar abundances.
- Cr/Fe and Na/Fe ratios were constrained, and were found to be broadly consistent between the limbs of the atmosphere for each of the transits, with the exception of Na/Fe in the morning limb for T3. These abundance ratios were also found to

be substellar in both the morning and evening limbs, hinting at possible depletion of Cr and Na due to recombination and ionisation, respectively, as suggested in previous works.

- The V/Fe and VO/Fe ratios were also found to be consistent between the limbs of the atmosphere for each of the transits, with V/Fe also consistent with solar in the evening limb. V and VO were, however, unconstrained in the morning limb for T1 and T3, suggesting possible depletion due to recombination and condensation. This is further supported by an apparent asymmetric CCF for V relative to Fe for both T1 and T3.

The consistent results obtained across multiple observations spanning months or years, as well as with previous studies using different modelling and retrieval frameworks and/or instruments, affirms the efficacy of high-resolution atmospheric retrieval frameworks. Spatially-resolved temporal atmospheric surveys such as this, coupled with low-resolution efforts in the era of JWST, will allow us to place further constraints on the time-varying dynamics and chemistry of these worlds, allowing us to infer how they evolved to their current climate.

Assessing Telluric Removal Methods on High-resolution Exoplanetary Transmission Spectra

In the following chapter, the efficacy of two of the most common high-resolution telluric removal methods, SYSREM and MOLECFIT (see Sects. 2.2.4.1 & 2.2.4.2), was compared. Simulated planetary transmission spectra were injected into three high-resolution optical observations taken with ESPRESSO. These planetary signals were injected at orbital periods of $P = 2$ days and $P = 12$ days, resulting in differing changes in radial velocity during transit. The various injected atmospheric model parameters were retrieved in order to determine the efficacy of the telluric removal methods, as well as their effect on the transmission spectra of exoplanets with varying orbital architectures. This work is currently under review in *Astronomy & Astrophysics*.

Observing from the ground poses significant challenges, not least the removal of contamination by numerous telluric absorption and emission lines caused by the Earth's atmosphere. In the past, a telluric standard star would be observed alongside the target star, in order to correct for telluric contamination. This method, however, is costly, as it would require valuable telescope time to observe the telluric star, which would otherwise be used for other scientific observations (Smette et al., 2015). In more recent years, it has become common practice to model the telluric spectra directly, with tools such as MOLECFIT (Sect. 2.2.4.2; Smette et al. 2015; Kausch et al. 2015) and TELFIT (Gullikson et al., 2014), which combine line-by-line radiative transfer calculations with on-site meteorological data to estimate the transmission spectrum of the Earth's atmosphere across the wavelength range of the observations. This method also accounts for the temporal variation of airmass above the telescope over the course of an observation, and has been successfully implemented in removing telluric contam-

ination of high-resolution exoplanetary spectra (Sedaghati et al., 2021). This telluric removal method has also been shown to be more effective in removing the contamination on high-resolution X-Shooter spectra when compared to correcting with a telluric reference star (Kausch et al., 2015). It has also been shown to be more effective in removing the contamination on exoplanetary spectra when compared to obtaining a telluric reference spectrum directly from the data, assuming telluric line strength varies linearly with airmass (Langeveld et al., 2021).

Another common method of telluric removal is constructing a model of the observed spectra directly using Principal Component Analysis (PCA) algorithms and removing this model from the observations. Many PCA-like algorithms have been successfully implemented to treat high-resolution spectroscopy observation of exoplanetary atmospheres, such as singular value decomposition (de Kok et al., 2013), eigenvalue decomposition (Damiano et al., 2019), and SYSREM (Sect. 2.2.4.1; Tamuz et al. 2005; Birkby et al. 2013). In contrast to PCA, for example, SYSREM can account for time- and wavelength-based uncertainties when modelling systematic trends. The modelling and removal of telluric contamination from high-resolution exoplanetary spectra using SYSREM was first implemented by Birkby et al. (2013), and has since become common practice for both transmission and emission observations (e.g., Gibson et al., 2020; Nugroho et al., 2021). These methods model the stellar and telluric lines which are (quasi-)stationary in wavelength, as a function of time, which can then be subsequently removed from the observations. However, these algorithms can often be overly aggressive in their removal, as there exists no obvious halting criterion, and thus run the risk of inadvertently distorting the underlying exoplanet signal (Birkby et al., 2017). There are also other emerging techniques to model time-varying systematics on high-resolution spectra which are worth noting.

Meech et al. (2022) modelled the telluric and planetary components of high-resolution dayside emission spectra using Gaussian process (GP) regression, and successfully re-

covered injected planetary signals. They also showed that traditional telluric removal frameworks, such as linear airmass regression and SYSREM, significantly truncate planetary atmospheric features in comparison to their GP methodology. Recent work by Cabot et al. (2024) and Cheverall & Madhusudhan (2024) successfully recovered a simulated signal of the temperate sub-Neptune TOI-732c from IGRINS data using PCA-based telluric removal, showing the feasibility of these detrending methods at low radial velocities changes during transit. Cheverall & Madhusudhan (2024) conclude that due to the high number of out-of-transit spectra observed, the planetary signal does not form a principal component of the spectra, and thus the planetary signal is prevented from being removed by the detrending algorithm.

When performing model comparison, in the form of an atmospheric retrieval or otherwise, it is imperative that the inevitable distortion on the underlying exoplanetary signal is taken into account, such that the forward model is an accurate representation of the noiseless data. If the distortions caused by these detrending algorithms are not accounted for, they may bias the retrieved atmospheric parameters (Brogi & Line, 2019). Previous studies have addressed this issue by filtering the forward model in the same way as the data (Brogi & Line, 2019; Pelletier et al., 2021). However, due to the need to interpolate the 1D model to the 3D data array (order $\times$ time/phase $\times$ wavelength) and then reprocess each forward model for each likelihood calculation in an atmospheric retrieval framework, these methods generally require a large amount of computing resources. Gibson et al. (2022) recently implemented a fast model filtering technique, which uses the SYSREM model basis vector(s) to reproduce these distortions on the atmospheric forward model. This model filtering technique is outlined extensively in Sect. 2.3.5. This technique can also be applied where standard PCA algorithms have been used to detrend the data.

The precise removal of telluric contamination of ground-based spectra, whilst also preserving the faint underlying exoplanet spectra, is of the utmost importance to the

exoplanet community. This will allow for the optimum extraction of the information-rich datasets on the horizon.

5.1 Methods

5.1.1 ESPRESSO Observations

The injection and recovery tests detailed henceforth were performed on three time-series observations of the UHJ host MASCARA-4 (Dorval et al., 2020) with ESPRESSO. These observations were taken on the nights of 2022 February 4, 2022 February 6, and 2022 February 9 as part of Program ID 106.21BV.005 (PI: Pino). These datasets are hereafter referred to as DS1, DS2, and DS3, respectively. These datasets were chosen in order to simulate realistic time-series observations of an UHJ host star. These observations were performed for the purpose of measuring the planet’s emission spectrum, and are therefore free of any transit signatures in the high-resolution spectra. These signatures typically include spectral artefacts on the in-transit stellar lines due to the inhomogeneity of the stellar disk as the planet transits, caused by the centre-to-limb variation (CLV) and the Rossiter-McLaughlin (RM) effect (Rossiter, 1924; McLaughlin, 1924). This choice was made to minimise the post-processing steps, focusing solely on the effects of telluric removal methods. As they are emission spectroscopy observations, they also minimise contamination from a potentially transiting exoplanet’s signal, as found in similar time-series observations. MASCARA-4 is an A-type star, thus these datasets were chosen as the star has very broad absorption lines (see Figs. 5.1 & 5.2), allowing for precise modelling of telluric lines. The data were reduced using the ESPRESSO Data Reduction Software (DRS) v2.4.0, with the extracted non-blaze-corrected S2D spectra (`ESO_PRO_CATG = S2D_BLAZE_A`) being used for further analysis. It must be noted that the decision was made not to use the sky-subtracted spectra, to avoid adding unnecessary noise into the spectra. However, this has the disadvantage of not removing the few sky emission lines (mainly from O₂ and OH) present in the wavelength range of ESPRESSO. This, however, has implications for the retrieved

relative abundances of OH, which is discussed further in Sect. 5.3.2.

5.1.2 Forward Model

For the injected signal, two scenarios were assumed; a Jupiter-like planet with an orbital period of 2 and 12 days, hereafter referred to as P2 and P12, respectively. The stellar/planetary parameters of the injected models are given in Table 5.1.

For the injected forward models, 1D transmission spectra were generated using the IRRADIATOR code, described in detail in Sect. 2.3.1, computed across a wavelength range of 3670–8000 Å, at a constant resolution of $R = 200,000$. Multiple atmospheric opacity sources were included, both molecular and atomic, with significant absorption in the given wavelength range. These included Fe, V, Na, OH, and H₂O. The cross-sections for Fe and V were obtained via the Kurucz line list (Kurucz & Bell, 1995). Similarly, the Na cross-sections were obtained via the VALD line list (Piskunov et al., 1995). The OH and H₂O cross-sections were obtained via the MoLLIST (Bernath, 2020) and POKAZATEL (Polyansky et al., 2018) line lists, respectively. These opacity sources are assumed to have a constant volume mixing ratio (VMR) with altitude, whilst assuming a vertical temperature-pressure (T - P) profile parameterised using the treatment outlined in Guillot (2010). This treatment requires four distinct parameters: T_{irr} , T_{int} , $\log_{10}(\kappa_{\text{IR}})$, $\log_{10}(\gamma)$, corresponding to the irradiation temperature, internal temperature, mean infrared opacity, and the ratio of visible-to-infrared opacity, respectively. A H₂ VMR, χ_{ray} , was also included, along with H₂ opacities from Dalgarno & Williams (1962), to account for Rayleigh scattering, as well as a further continuum opacity source caused by an opaque cloud deck at a pressure level P_{cloud} , below which the transmission spectrum model is truncated. Thus, for the one-dimensional atmospheric model, there are $6 + N_{\text{species}}$ input parameters (T_{irr} , T_{int} , $\log_{10}(\kappa_{\text{IR}})$, $\log_{10}(\gamma)$, $\log_{10}(P_{\text{cloud}})$, $\log_{10}(\chi_{\text{ray}})$, $\log_{10}(\chi_{\text{species}})$). The transmission spectra for each injection scenario are shown in Fig. C1. For each injection scenario the planet’s irradiation temperature, T_{irr} , was calculated from Eq. 1 of Guillot (2010), assuming a circular orbit.

These transmission spectra were then convolved with a number of convolution kernels to imitate the astrophysical and instrumental effects which change the shapes of the final observed spectral lines. Firstly, the spectra were convolved with a box kernel whose width was determined from the *maximum* velocity shift between subsequent exposures over the course of the observations to simulate signal ‘smearing’. Secondly, the spectra were convolved with the mean instrumental profile of ESPRESSO, the full-width at half-maximum (FWHM) of which was determined by fitting Gaussian profiles to the spectrograph’s calibration source ThAr lines across the full wavelength range of ESPRESSO (see Fig. 2.7). Finally, to account for solid-body rotational broadening, the spectra were convolved with another Gaussian kernel with a FWHM equal to the planetary rotational velocity, v_{rot} , assuming a tidally-locked planet. The final assumption of a Gaussian rotational broadening kernel is not entirely accurate, as a rotating atmosphere is not a sphere but an annulus with a distinct rotational broadening kernel, which has been studied extensively in recent works (e.g., Chap. 4, Gandhi et al. 2022, 2023; Boucher et al. 2023; Maguire et al. 2024; Nortmann et al. 2024). However, for the purposes of this study, a simplified rotational kernel is preferred for simplicity. After this point, the signals were injected into the observed data in slightly different manners, depending on the final treatment of the tellurics, outlined below.

5.1.3 Model Injection

For the MOLECFIT procedure, for each orbital phase, ϕ , the 1D convolved transmission spectra were Doppler shifted by the injected planetary velocity given by Eq. 2.21, where $\mathbf{v}_{\text{sys}}$ is the systemic velocity, which is corrected for in Sects. 5.1.4 & 5.1.5. This 2D grid (time/phase $\times$ wavelength) is then directly injected into the raw, merged S1D ESPRESSO spectra, which MOLECFIT uses to compute the telluric model. Injecting into the S1D spectra is a necessary additional step for the MOLECFIT preprocessing since this is the data product MOLECFIT utilises. Therefore, to replicate any effects MOLECFIT may impose on a planetary signal, the model must also be injected into the S1D data product before running MOLECFIT.

Table 5.1: Injected stellar and planetary parameters.

Parameter	P2	P12
$R_{\star}$	1.0 $R_{\odot}$	1.0 $R_{\odot}$
$M_{\star}$	1.0 $M_{\odot}$	1.0 $M_{\odot}$
T_{eff}	5780 K	5780 K
P	2.0 days	12.0 days
R_{p}	1.25 R_{Jup}	1.25 R_{Jup}
M_{p}	0.75 M_{Jup}	0.75 M_{Jup}
$a_{\text{p}}/R_{\star}$	6.68	22.06
K_{p}	-104.10 km s^{-1}	-57.29 km s^{-1}
T_{irr}	2236.31 K	1230.69 K
$R_{\text{p}}/R_{\star}$	0.1541	0.1541
e	0.0	0.0
i	0.0°	0.0°

For both the MOLECFIT and SYSREM procedures, the 1D convolved transmission spectra were also linearly interpolated to the 2D wavelength grid of the data (order $\times$ wavelength). For each order, the 2D forward models were Doppler shifted to the injected planetary velocity given by Eq. 2.21. This 3D (order $\times$ time/phase $\times$ wavelength) model array was then injected into the raw S2D ESPRESSO spectra. These are the final datasets which undergo the respective telluric removal procedures, outlined below.

5.1.4 Spectral Preprocessing with MOLECFIT

To remove the telluric absorption signature with MOLECFIT, the S1D (stitched and resampled) spectra from the pipeline were used. The atmospheric models were also injected into these S1D spectra, as outlined above. The MOLECFIT (v. 4.2.3) routines were run on esoreflex platform independently for each spectrum. Telluric absorption lines were modelled with a line by line radiative transfer model, using the atmospheric pressure profile that MOLECFIT estimated from the temperature and humidity profiles that it obtains from the Global Data Assimilation System (GDAS) database. These

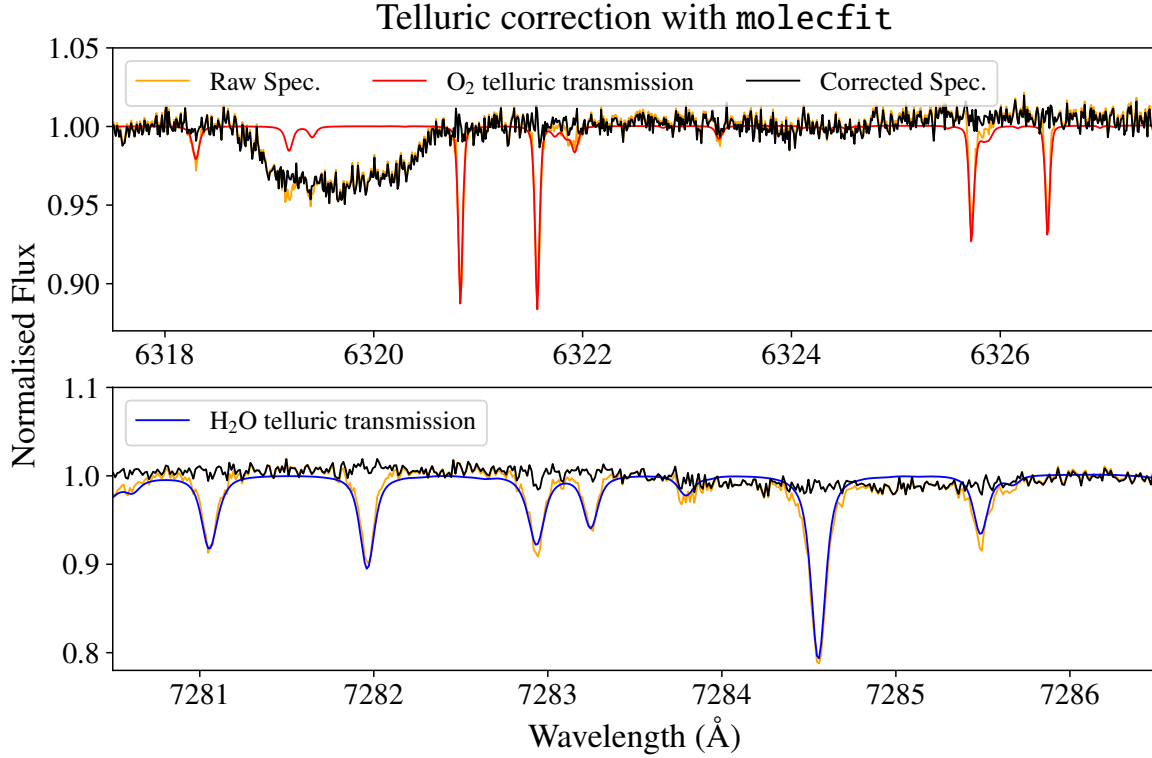


Figure 5.1: An example of telluric absorption correction with MOLECFIT on ESPRESSO S1D spectra. The top panel shows an O₂ region, including a broad stellar absorption line. The bottom panel shows a H₂O region. The final telluric model was used to correct the raw ESPRESSO S2D spectra (see Sect. 5.1.4).

profiles were used as starting point in a minimisation algorithm that finds the best fit model to the telluric absorption lines for those molecules input by the user. In the case of ESPRESSO’s wavelength coverage, only O₂ and H₂O were included in the modelling. For a detailed explanation of the MOLECFIT modelling procedure, see Sect. 2.2.4.2. In this modelling procedure, the parameters of a variable kernel (a Voigt profile) describing line shapes, a first order polynomial describing the local continuum at the location of the selected absorption lines and the abundances of the two selected species, were fit. From the results produced by MOLECFIT, the normalised telluric transmission model was used to remove the telluric contamination from the spectra, details of which are given below. An example of this procedure is shown in Fig. 5.1. Future processing by MOLECFIT would likely gain by using the updated ESPRESSO instrumental Line Spread Function (LSF) determined by Schmidt & Bouchy (2024).

Apart from applying the respective telluric correction routines, MOLECFIT or SYSREM (see Sect. 5.1.5 below), the data reduction employs identical steps:

- (1) The time- and wavelength-dependent uncertainties of the raw S2D data are estimated assuming Poisson noise, following the procedure outlined in Sect. 2.2.1.
- (2) A telluric model of the S1D (time/phase $\times$ wavelength) data was generated using v4.2.3 of MOLECFIT. This model was then linearly interpolated to the S2D grid (order $\times$ time/phase $\times$ wavelength), before dividing it out of the *model-injected* S2D data.
- (3) The paired echelle slices, being the result of ESPRESSO’s Anamorphic Pupil Slicing Unit (APSU), are merged into single orders.
- (4) These merged spectra are then shifted to the stellar rest frame using the ESPRESSO pipeline radial velocities, $\mathbf{v}_{\text{sys}}$.
- (5) The orders are placed on a common blaze function, by firstly dividing each order by its mean spectrum. The resultant residual array was then smoothed with a median filter to remove outliers, followed by a Gaussian filter. The original orders and their respective uncertainties were then divided by these resultant smoothed residuals. This procedure places each spectrum on a common blaze function in time.
- (6) Each order is divided by a master stellar spectrum, which is created using the mean of the out-of-transit spectra in each order.

5.1.5 Spectral Preprocessing with SYSREM

Steps (1), and (3)–(6) are performed identically for the SYSREM correction. For each SYSREM iteration, each order is decomposed into two column vectors, $\mathbf{u}$ and $\mathbf{w}$, where the SYSREM model for each order is given by their outer product, $\mathbf{uw}^\top$. This model is then subtracted from the input array(s), to get the processed array(s), and the procedure is repeated on the processed array(s) for the next iteration. Dividing through by the median spectrum in each order first and then subsequently subtracting

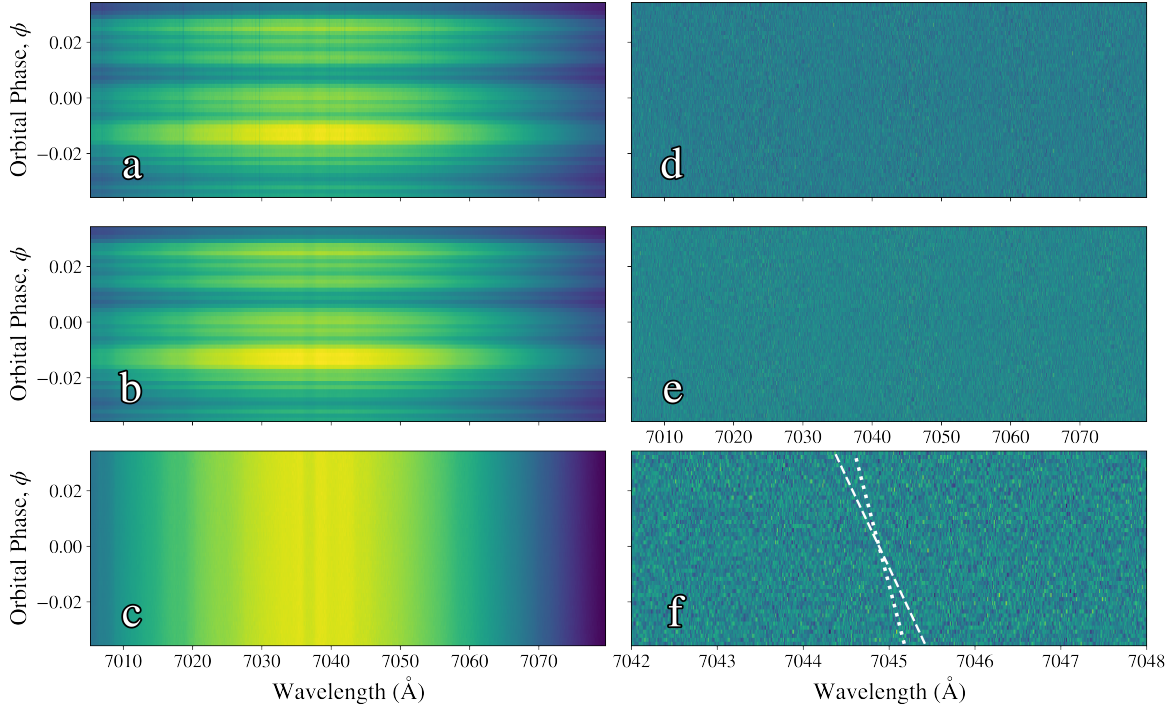


Figure 5.2: The various reduction steps applied for an individual ESPRESSO order of DS1. **(a)** Before telluric removal with MOLECFIT. **(b)** After telluric removal with MOLECFIT and shifted to the stellar rest frame. **(c)** Each spectrum is placed on a common blaze function (see Sect. 5.1.4). **(d)** Residuals after division through by the mean out-of-transit spectrum, weighted on their uncertainties. This panel shows the final data product used in the MOLECFIT preprocessing analysis. **(e)** Residuals after division through by the mean out-of-transit spectrum, weighted on their uncertainties, and subtraction of the SYSREM model. This panel shows the final data product used in the SYSREM preprocessing analysis. It is worth noting that for this procedure, no preceding telluric removal was performed (i.e., Sect. 5.1.4, Step (2)). **(f)** A magnification of panel (e) showing the wavelength shifts caused by each injected model. The planetary velocity curve for P2 is shown as a white dashed curve, whereas the slower moving planet's (P12) velocity curve is shown as a white dotted curve.

the SYSREM model allows for a faster model filtering process in each likelihood calculation (Gibson et al., 2022). It is worth noting that a more accurate approach would be to perform SYSREM on the unnormalised data, and divide by the resultant model, however this difference is expected to be negligible here. The effects of each of the preprocessing steps outlined above on a single ESPRESSO order are highlighted in Fig. 5.2.

For each of the datasets, and each of the injected models, the number of SYSREM iterations was optimised following the procedure outlined in Sect. 2.3 of Maguire et al. (2023). The optimum number of SYSREM iterations for each dataset was determined from the resultant detection significance of the injected model, using the likelihood

distribution of the model scale factor, α , conditioned on the injected K_p , and Δv_{sys} values. The expected value, or mean, of this distribution was computed, and divided by its standard deviation, resulting in a detection significance. This, in essence, computes the number of standard deviations the maximum signal deviates from an α of 0 (i.e., a non-detection). For DS1, the optimum number of iterations was found to be 13 and 10 for P2 and P12, respectively. Likewise, for DS2 the optimum number of iterations were found to be 3 and 1 for P2 and P12, respectively. Finally, for DS3, the optimum number of iterations were found to be 8 and 8 for P2 and P12, respectively. Although there is no consensus on an optimum stopping criterion for PCA-like telluric removal methods, this method is preferred here as it does not suffer from biases introduced by noise amplification, as the detection significance is determined from the likelihood as a function of alpha directly, conditioned on the injected K_p , and Δv_{sys} . These biases are seen for detection significances computed directly from cross-correlation functions (CCF) and their resultant K_p - Δv_{sys} maps (Cheverall et al., 2023). The problem of determining a stopping criterion at which the ‘optimum’ number of iterations is reached via injection-recovery tests is completely model-dependent. Furthermore, in principle this optimum number would change order-by-order depending on the severity of the telluric contamination, as well as additional systematics, present in each order.

5.2 Analysis

5.2.1 Injection and Recovery Tests

In the past, the efficacy of the removal of telluric contamination on high-resolution exoplanetary absorption/emission spectra has been determined in a variety of manners. A typical approach performs classic cross-correlation analysis with the injected forward model, and attempts to determine the telluric removal process which results in the highest ‘detection significance’ of the injected signal (Cheverall et al., 2023). Typically, in order to calculate the detection significance of a given model within a K_p - Δv_{sys} map, the mean of the noise in the map in regions away from the peak is

5. ASSESSING TELLURIC REMOVAL METHODS ON HIGH-RESOLUTION EXOPLANETARY TRANSMISSION SPECTRA

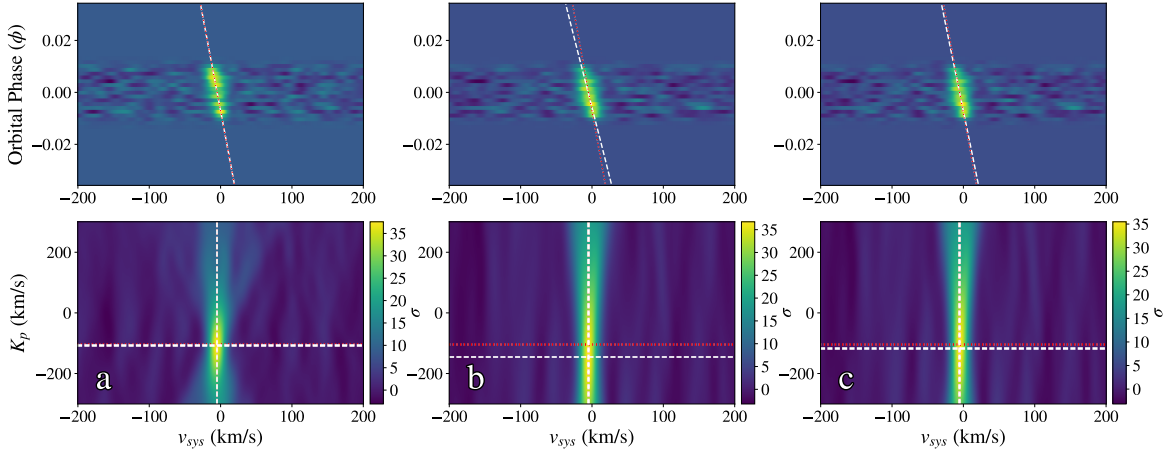


Figure 5.3: Cross-correlation and $K_p - \Delta v_{\text{sys}}$ maps for a planetary signal injected with $P = 2$ days injected into DS1 (P2). Red dotted lines/curves show the injected velocity values, whereas white dashed lines/curves show the recovered values (i.e., the values at which there was a maximum in the CCF). **(a)** Data reduced using the SYSREM telluric removal method. Forward model also reprocessed using SYSREM filtering technique (Gibson et al., 2022). **(b)** Data reduced using the MOLECFIT telluric removal method. Forward model also reprocessed by division of mean out-of-transit spectrum (see panel (c)). If this step was omitted, an anomalous offset was found from the injected K_p value.

subtracted, before dividing the map by the standard deviation of the noise away from the peak (Brogi et al., 2012, 2018). However, the regions away from the peak in which the mean/standard deviation of the noise is calculated are arbitrarily chosen, whilst also assuming the noise in these regions follow a Gaussian distribution (which is not always the case), and thus the resultant detection significance is not exact. Another method is to measure the line profiles of the atmospheric absorption/emission lines, and compare with the injected values (Meech et al., 2022) or compare the consistency of the atmospheric line profiles over the course of multiple observations (Langeveld et al., 2021).

With the recent introduction of Bayesian inference frameworks to high-resolution exoplanetary spectroscopy studies (Brogi & Line, 2019; Gibson et al., 2020), in the form of CC-to-likelihood mapping, the forward model can be directly compared to the data, after the aforementioned reduction steps, thus allowing for direct atmospheric retrievals of the injected signal. These “injection and recovery” tests not only allow us to test the efficacy of the telluric removal routines, but also can highlight any biases which may

be introduced as a result of the various reduction procedures. This method also has the advantage of effectively averaging over the line profiles of multiple injected species, in order to assess any distortions caused by the telluric removal processes across the full wavelength range of the observations.

5.2.2 Cross-correlation

Traditional cross-correlation analysis (Snellen et al., 2010) was initially performed in order to recover the injected signal after both reduction procedures. This involves Doppler shifting an atmospheric model across a range of systemic velocity offsets, Δv_{sys} , and cross-correlating with each of the time-series exposures. This effectively creates a two-dimensional time/orbital phase vs Δv_{sys} map, referred to as a “ ϕ - Δv_{sys} ” map, or simply, a “cross-correlation” map. This map will display the planetary cross-correlation trail projected to the injected orbital velocity given by Eq. 2.21 with parameters outlined in Table 5.1. This cross-correlation map can also be shifted across a range of orbital velocities with varying K_p values and collapsed in time. This creates a map of cross-correlation values for each combination of K_p and Δv_{sys} , known as a K_p - Δv_{sys} map, which should reach a maximum at the injected values.

5.2.3 Model Filtering

In order to accurately retrieve the injected model, the forward model with which one performs cross-correlation or likelihood analyses must be a representation of the noiseless data (Gibson et al., 2022). Therefore, any distortions caused by the aforementioned reduction methods must be accounted for in the computation of the forward model. In the SYSREM/PCA case, this includes performing a full SYSREM/PCA filtering to the forward model, as outlined in (Gibson et al., 2022). Whereas, in the MOLECFIT pre-processing case, this means simply dividing the forward model by a master spectrum (ignoring the initial division of the telluric model). It was found that employing these model filtering methods was imperative, even for traditional cross-correlation analysis,

in order to recover the injected signal accurately.

5.2.4 Atmospheric Retrieval

In order to recover the injected signal via an atmospheric retrieval analysis on each of the datasets, a forward model, m_i , must be computed for a given set of model parameters, θ . Assuming uniform priors, the log-posterior is computed by adding the log-prior to the log-likelihood given by Eq. 2.34. The parameter space was sampled using a Markov Chain Monte Carlo algorithm, specifically DEMC (see Sect. 2.4.3), running an MCMC chain with 128 walkers, with a burn-in length of 500 and a chain length of 1000. Each chains' convergence was assessed via the Gelman-Rubin (GR) statistic, after splitting each chain into four independent subchains. The chains were also split into groups of independent walkers, and overplot their 1D and 2D marginal distributions, in order to visualise the convergence of the MCMC. The retrieved abundances of each of the injected species relative to the abundance of Fe were compared, as the relative abundance constraints are typically more precise than those of the absolute abundances. This is due to a well-known degeneracy between the absolute abundances and other model parameters, such as the cloud deck pressure (Benneke & Seager, 2012; Heng & Kitzmann, 2017). Due to the reduction methods, the planetary continuum is lost, leaving sensitivity only to the relative line strengths above the planet's continuum. This allows for more precise constraints on the relative abundances, provided that the reduction methods are accounted for when computing the forward model (See Sect. 5.2.3).

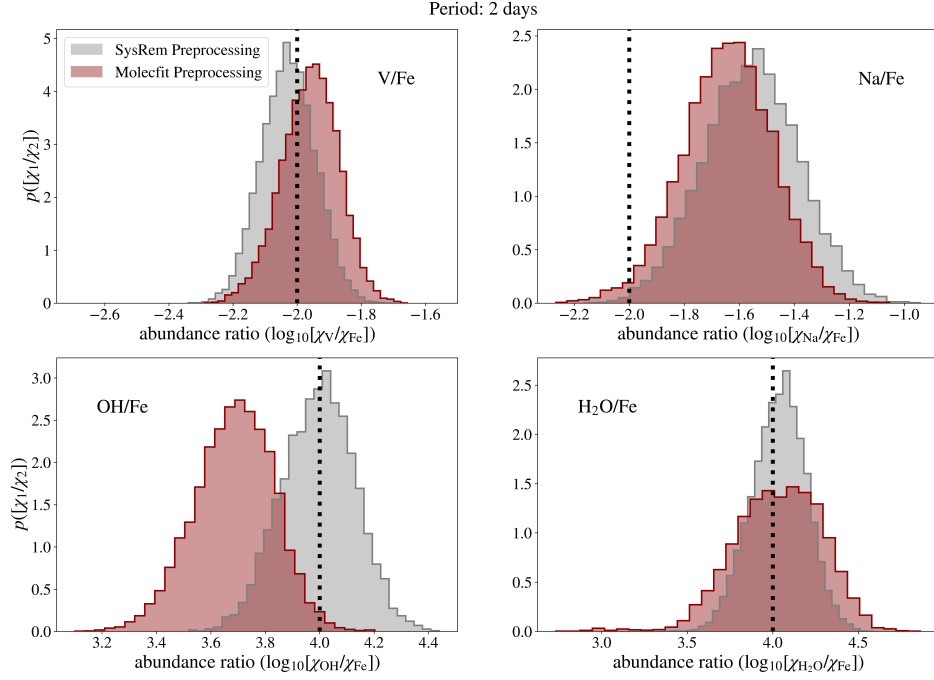


Figure 5.4: Relative abundance comparison for DS1, for P2. Injected relative abundance values shown as a vertical black dotted line. The posterior distributions for both the SYSREM and MOLECFIT preprocessing methods are shown in grey and red, respectively.

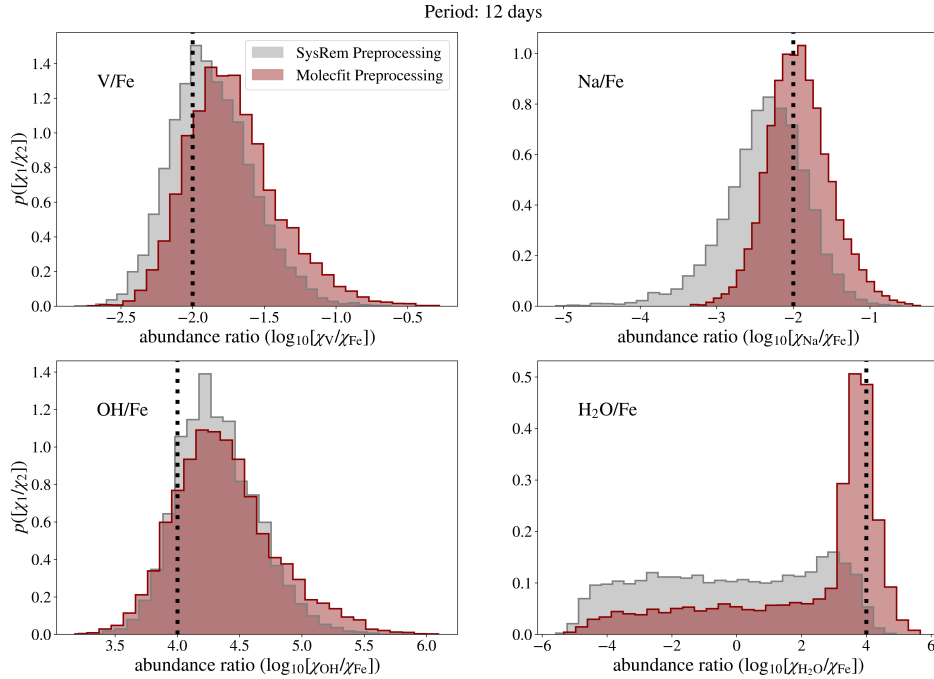


Figure 5.5: Relative abundance comparison for DS1, for P12. Injected relative abundance values shown as a vertical black dotted line. The posterior distributions for both the SYSREM and MOLECFIT preprocessing methods are shown in grey and red, respectively.

5.3 Discussion

5.3.1 Model Filtering

The necessity for proper model filtering is highlighted when computing the forward model. This ensures that the forward model accurately represents the noiseless data, and thus allows for the accurate retrieval of injected model parameters. This model filtering is also necessary for the accurate retrieval of real planetary signals. For the injected data preprocessed with SYSREM, a full SYSREM filtering was performed to the forward model (Gibson et al., 2022) each time log-likelihood was computed for a given set of model parameters within the MCMC. Similarly, the division by the median out-of-transit spectrum for the injected data preprocessed with MOLECFIT also distorted the injected signal, and must be accounted for. The division of the planetary signal by stellar lines caused a distortion in the line shape/position, which materialised as an anomalous offset from the injected K_P value (see Fig. 5.3). Therefore, without accounting for this step in the computation of the forward model, one risks an inaccurate retrieval of the injected parameters.

5.3.2 Atmospheric Retrieval Comparison

P = 2 days

For DS1, both reduction methods resulted in accurate recovered values for the atmospheric species' abundances relative to Fe (see Fig. 5.4). However, both methods also caused the recovery of a slightly higher Na/Fe value, despite still having overlapping probability mass with the injected value. The MOLECFIT preprocessing method also caused a decrease in the recovered OH/Fe abundance with respect to the injected value, caused by a lower recovered OH abundance. OH appears in the Earth's atmosphere as emission, where MOLECFIT does not correct for atmospheric emission, which explains any biases introduced by its non-removal. This issue would potentially be resolved with

the use of the sky-subtracted products provided by the DRS. Furthermore, the $\text{H}_2\text{O}/\text{Fe}$ abundance is broader for the MOLECFIT case, which could be due to SYSREM’s ability to model and remove additional systematics present in the data, which also effect the exoplanetary signal, and thus ultimately provide better constraints on the injected abundances. Both methods also recovered the injected vertical T - P profile accurately (see Figs. C6 & C8). It is worth noting that the forward model is truncated below the cloud deck pressure (P_{cloud}), thus the atmospheric retrieval is unable to constrain an accurate T - P profile below this value (see Fig. C6 for reference).

For DS2, an accurate recovery of the injected model parameters is seen for both data reduction methods (see Fig. C2). The SYSREM preprocessing method did, however, cause a slightly higher OH/Fe value to be recovered, due to an underestimation of the injected Fe abundance, though still consistent with the injected value with 2.5σ (see Fig. C10). Both methods again recovered the injected vertical T - P profile accurately (see Figs. C10 & C12).

Finally, for DS3, the injected model parameters were accurately recovered, with each reduction method performing similarly. There was, however, broad constraints on the $\text{H}_2\text{O}/\text{Fe}$ ratio for the MOLECFIT preprocessing method, with a local maxima in the posterior distribution consistent with the injected value. In contrast, the SYSREM preprocessing method recovers a well-constrained $\text{H}_2\text{O}/\text{Fe}$ posterior at the injected value (see Fig. C4). Both reduction methods also caused the injected T - P profiles to be recovered within 2σ (see Figs. C14 & C16), with the SYSREM preprocessing resulting in more precise constraints on the T - P profile overall.

P = 12 days

For DS1, the MOLECFIT preprocessing method resulted in an accurate recovery of the abundances, as well as the T - P profile (see Figs. 5.5 & C9). The recovered H_2O abundance shows broad constraints, with a local maxima at the injected value. However,

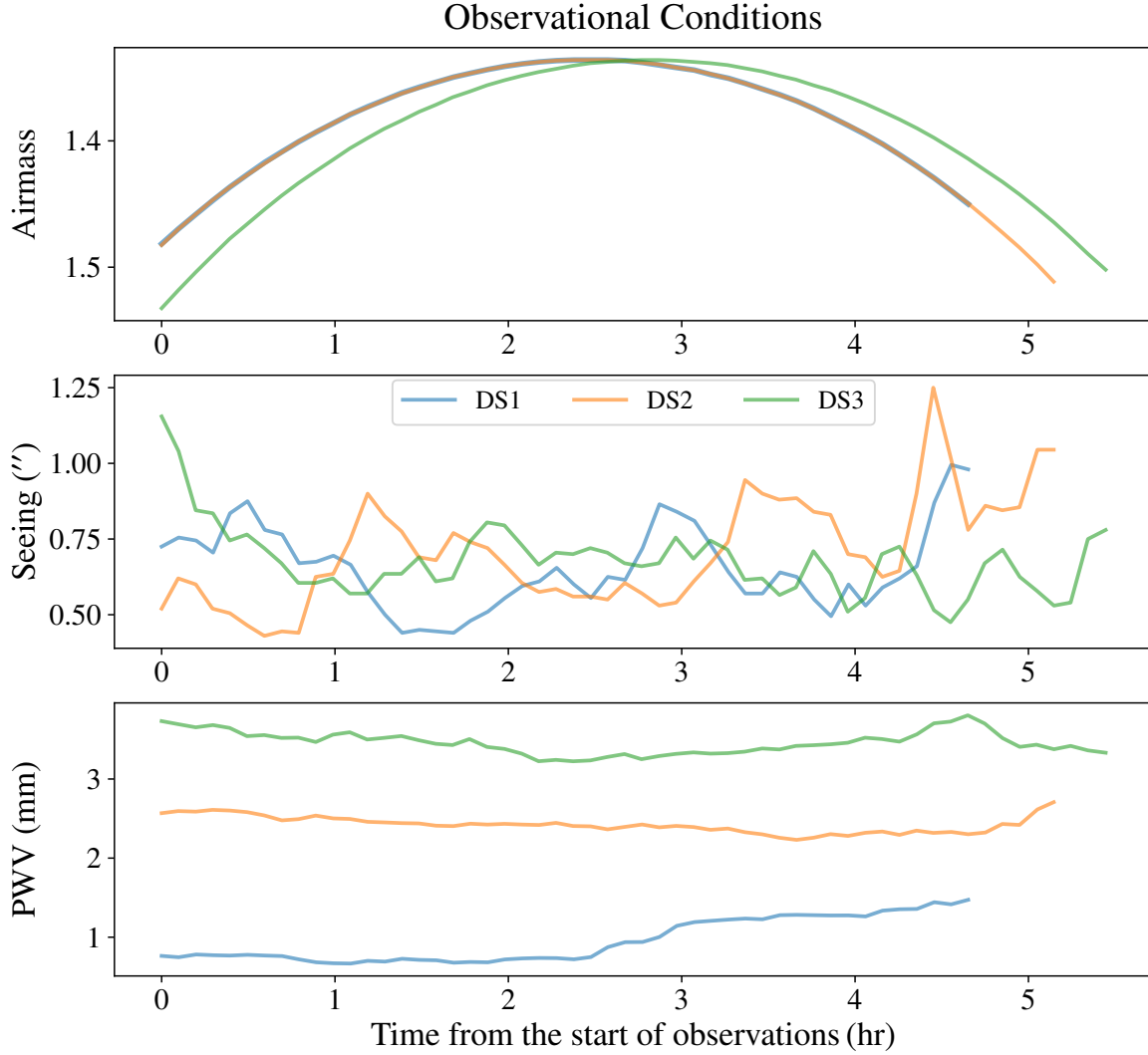


Figure 5.6: The various observational conditions of each of the datasets. The top panel shows the airmass variation throughout the observations. The middle panel shows the seeing variation throughout the observations. The bottom panel shows the precipitable water vapour (PWV) variation throughout the observations.

for the SYSREM preprocessing case, an unconstrained $\text{H}_2\text{O}/\text{Fe}$ value is found, caused by an unconstrained posterior for the H_2O abundance. This is likely due to the fact that the planetary H_2O lines exist at locations close to the telluric H_2O lines, albeit shifted by Δv_{sys} and drifting in time due to v_p (see Eq. 2.21). Therefore, as a PCA-like algorithm such as SYSREM fits these regions with many telluric lines, it inadvertently fits/removes the planetary lines as well. This is particularly true in this case of P12 ($|K_p| = 57.29 \text{ km s}^{-1}$), as the slow-moving planetary signal’s wavelength shift during a transit is less prominent (i.e., it is more stationary with respect to time), causing it to be ‘targeted’ more effectively by these fitting algorithms. It is also worth noting

that the optimum number of SYSREM iterations (10) was greater for this injection and recovery test when compared to DS2 and DS3, despite the fact that DS1 benefited from the lowest amount of precipitable water vapour (PWV) of all three nights of observations (see Fig. 5.6). This also caused the recovered T - P profile to differ from the injected value by greater than 3σ in this case (see Fig. C7). This injection scenario and dataset was also tested with a fewer number of SYSREM iterations (5) in order to mitigate this issue, however the unconstrained $\text{H}_2\text{O}/\text{Fe}$ posterior remained.

For DS2, both reduction methods performed similarly, likely due to the relatively low number of SYSREM iterations used. For both, V/Fe , OH/Fe , and $\text{H}_2\text{O}/\text{Fe}$ values are recovered slightly higher than, but still in agreement with, the injected value, due to an Fe abundance recovered below the injected value (see Fig. C3). Despite this, both methods recovered the injected T - P profile accurately (see Figs. C11 & C13).

Similarly to the P2 forward model injected into DS3, a broad heavy-tailed $\text{H}_2\text{O}/\text{Fe}$ distribution was found for the MOLECFIT preprocessing case, with a prominent local maxima at the injected value (see Fig. C5). The SYSREM preprocessing method, however, resulted in a more precise $\text{H}_2\text{O}/\text{Fe}$ value at the injected value, albeit less accurate than the MOLECFIT value. The more precise abundance constraints provided by SYSREM with respect to MOLECFIT in this dataset, for both injection scenarios, hinted at potential additional systematics present in the data which were affecting the injected exoplanet signal, and which were then modelled and removed more effectively by SYSREM. Furthermore, the PWV measured for this dataset was the highest of all three nights of observations. The remaining injected abundances were also recovered accurately by both reduction methods. Both also recovered the injected T - P profile accurately, with the MOLECFIT method providing slightly more stringent constraints (see Figs. C15 & C17).

5.4 Conclusions

In this chapter I have presented numerous injection and recovery tests of exoplanetary signals in transmission, on two distinct orbital periods of $P = 2$ and $P = 12$ days. The purpose of these distinct orbital architectures was to test the limitations of the typical high-resolution reduction methods used on planetary signals with very different orbital velocities and thus different Doppler shift of their respective signals in-transit. Primarily, the aim was to assess and compare the efficacy of the two most common telluric removal methods used in the literature—PCA-like algorithms such as SYSREM and the telluric modelling software MOLECFIT, and their effects on the retrieval of atmospheric parameters.

For a Jupiter-like planet injected at $P = 2$ days, the two telluric removal methods performed similarly, providing accurate recovery of the exoplanetary signal with precise constraints. However, SYSREM typically performed better for species that are also present in the Earth’s atmosphere. For the $\text{H}_2\text{O}/\text{Fe}$ abundance, a slightly more precise constraint was found when the data was preprocessed with SYSREM across all three datasets. This is notably true for DS3, where the heavy-tailed H_2O abundance seen for the MOLECFIT reduction causes broad, heavy-tailed constraints on $\text{H}_2\text{O}/\text{Fe}$.

Furthermore, for a Jupiter-like planet injected at $P = 12$ days, a well constrained $\text{H}_2\text{O}/\text{Fe}$ value was seen for DS1 in the MOLECFIT case, whereas for SYSREM, the H_2O signal was effectively removed, causing an unconstrained $\text{H}_2\text{O}/\text{Fe}$ posterior. This behaviour is expected, as a slower moving planetary signal will be targeted and distorted more effectively by PCA-like algorithms, as they appear more stationary in time relative to the slower moving, close-in planetary signals. However, this behaviour was not ubiquitous across all three datasets investigated, and in the case of DS3, a more precise but less accurate $\text{H}_2\text{O}/\text{Fe}$ constraint was seen when SYSREM was used to treat the tellurics. This result is consistent with the findings of Cheverall & Madhusud-

han (2024) where they found it possible to recover injected signals of the sub-Neptune TOI-732c from Immersion GRating INfrared Spectrometer (IGRINS) data when using a PCA-based telluric removal method, despite the planet’s low radial velocity shift during transit. Both methods performed similarly for DS2, with accurate and precise retrievals of the injected signals.

Considering the results and conclusions presented, it can be stated that there is no definitive, “one size fits all” method for modelling/removing telluric contamination from high-resolution optical datasets. The delicate and often aggressive nature of high-resolution data filtering means that the utmost care must be taken in ensuring real exoplanetary signals are not only preserved, but any inevitable distortions caused by these reduction methods must be minimised and accounted for in computing the forward model. This is evident even for cross-correlation analysis (see Sect. 5.3.1). Ideally, the impact, or lack thereof, of high-resolution reduction frameworks on real exoplanetary data would be highlighted via injection and recovery tests on a case-by-case basis. Furthermore, a technique which was not explored as part of this study, but would potentially be of interest in the future, is the combination of multiple telluric modelling/removal methods. This would be straight forward to implement in the framework outlined in this work, with radiative transfer modelling such as MOLECFIT handling dominant telluric contamination, and PCA-like algorithms such as SYSREM handling additional time-invariant systematics.

Although this study presented analysis of an idealised test case, free from additional in-transit contamination such as the RM and CLV effects, it nonetheless provides a test bed from which to extrapolate the different biases introduced by the most common telluric removal methods on various atomic and molecular absorption signals in the optical wavelength regime. Going forward, a similar study in the NIR/IR with instruments on the VLT such as the upgraded Cryogenic high-resolution InfraRed Echelle Spectrograph (CRIRES+) would also be of great interest. At these wavelengths, tel-

luric contamination—particularly from H_2O —dominates and can often saturate the absorption spectrum. However, modelling and removing these telluric bands are of the utmost importance in the search for telluric signatures in exoplanetary atmospheres from the ground.

Future Work and Conclusions

The primary goals of this thesis were to observe the atmospheres of UHJs via high-resolution, ground-based transmission spectroscopy. From these observations, atmospheric chemistry and dynamics were extracted with the aim of furthering our knowledge of these extreme, complex objects, of which there is no Solar System analogue. Firstly, ESPRESSO was used to observe three transits of the UHJ WASP-121b over the course of months/years, to investigate the stability of the relative abundances of various neutral metals. From these observations, dynamical information such as winds and rotation, as well as the vertical temperature structure, could also be extracted and compared via advanced atmospheric retrieval frameworks recently introduced in Gibson et al. (2020). This work was presented in Chap. 3 and was also published in *Monthly Notices of the Royal Astronomical Society* as Maguire et al. (2023). Secondly, a novel rotational broadening kernel was developed to extract the relative abundances of neutral metals, dynamics, and vertical temperature structure across the morning and evening limbs of the UHJ WASP-76b. Three transits of this object were also observed with ESPRESSO over the course of months/years, allowing for these quantities to be monitored as a function of both time and longitude. This broadening kernel allows for the morning and evening limbs to be separated in velocity, such that their individual line contributions may be modelled and retrieved independently. This work was outlined in Chap. 4 and was published in *Astronomy & Astrophysics* as Maguire et al. (2024). Finally, as the aim of this thesis was to further our knowledge of these worlds using ground-based spectroscopy, an investigation into the most common telluric removal methods was presented in Chap. 5. This study focussed on two of the most common telluric modelling and removal frameworks used by the high-resolution community for extracting insights into exoplanetary atmospheres. By modelling and injecting signals into real ESPRESSO observations, and recovering the injected model parameters via an atmospheric retrieval, the efficacy of the various telluric removal methods and their effect on the underlying exoplanet signal could be determined and

compared. Finally, I will draw this thesis to a close with some final conclusions of each of the studies presented, as well as remarks on future avenues of research.

6.1 Primary Scientific Objectives

6.1.1 WASP-121b

The study of WASP-121b, presented in Chap. 3 and published in *Monthly Notices of the Royal Astronomical Society* as Maguire et al. (2023) was conducted with the aim of retrieving the relative abundances of neutral metals which have been vapourised in the extreme temperature of an UHJ. These relative abundance constraints were compared with previous relative abundance constraints of WASP-121b obtained with VLT/UVES and published in Gibson et al. (2022). These constraints were consistent across each of the observations. The T - P structure of WASP-121b was also consistently constrained across multiple observations, which were also in agreement with previously reported values at high-resolution. The atmospheric dynamical parameters, such as the planetary orbital velocity and broadening of spectral features were also constrained, and were consistent with previous results across each of the observations. This highlights the stability of the atmospheric chemistry of the terminator of WASP-121b across months/years, where these quantities remain unchanged. Furthermore, this consistency across multiple instruments and instrument modes is a strong validation of the model filtering and retrieval frameworks introduced in Gibson et al. (2020) and Gibson et al. (2022), respectively. The retrieval framework was also implemented to map the vertical extent of ionised species ($H\alpha$, Fe II, Ca II) which have been previously reported in the exosphere of WASP-121b, with artificial scaling up of their absorption features resulting in these species extending to the similar high altitudes as reported in the literature.

6.1.2 WASP-76b

The atmosphere of WASP-76b was also studied using the ESPRESSO spectrograph, which is presented in Chap. 4 and published in *Astronomy & Astrophysics* as Maguire et al. (2024). Similarly to the study of WASP-121b, three WASP-76b transits were observed with ESPRESSO, with the aim of monitoring its atmospheric chemistry across multiple observations. Additionally, a novel rotational broadening kernel was developed to separate the morning and evening limbs of the planet in transit, such that their individual abundances, T - P profiles, and dynamical properties could be obtained. A uniform longitudinal distribution of Fe and Mg across the limbs of the atmosphere, for each of the transits, was found, consistent with previous works as well as stellar abundances. Cr/Fe and Na/Fe ratios were constrained, and were found to be broadly consistent between the limbs of the atmosphere for each of the transits, with the exception of Na/Fe in the morning limb for T3. These abundance ratios were also found to be substellar in both the morning and evening limbs, hinting at possible depletion of Cr and Na due to recombination and ionisation, respectively, as suggested in previous works. The presence of VO, recently discovered in the atmosphere of WASP-76b by Pelletier et al. (2023), has been confirmed via cross-correlation in both T2 and T3 of the observations. The V/Fe and VO/Fe ratios were also found to be consistent between the limbs of the atmosphere for each of the transits, with V/Fe also consistent with solar in the evening limb. V and VO were, however, unconstrained in the morning limb for T1 and T3, suggesting possible depletion due to recombination and condensation. This is further supported by an apparent asymmetric CCF for V relative to Fe for both T1 and T3. The broad consistency of these quantities both between each observation as well as across the limbs of the planets highlights the stability of this atmosphere over these timescales. It also supports the argument presented by Savel et al. (2022) which suggested any asymmetry in a species' CC-trail, first seen in Ehrenreich et al. (2020), is likely caused by a global effect, as opposed to a longitudinally varying abundance.

6.1.3 Telluric Removal

With the ultimate goal of pushing these observations to Earth-like analogues that have the potential to harbour life, it is essential that the various data reduction methods used are tested and compared. This ensures that the observations on the horizon are optimised for detecting these slow-moving, subtle signals. With this in mind, the study presented in Chap. 5 used two of the most common methods for modelling and removing telluric absorption from high-resolution, ground-based, time-series spectra: SYSREM and MOLECFIT. To do so, two simulated exoplanetary atmospheres, with orbital periods of $P = 2$ days and $P = 12$ days, respectively, were injected into three real ESPRESSO datasets to test the limitations of the typical high-resolution reduction methods used on planetary signals with very different orbital velocities and thus different Doppler shift of their respective signals in-transit. These datasets were reduced using two distinct frameworks—one which used SYSREM to treat tellurics, and the other which used MOLECFIT. From these reduced datasets, these signals were recovered via atmospheric retrievals, in order to compare the efficacy of these telluric removal methods, and their effect on the exoplanetary signals. For a Jupiter-like planet injected at $P = 2$ days, the two telluric removal methods performed similarly, providing accurate recovery of the exoplanetary signal with precise constraints. However, SYSREM typically performed better for species that are also present in the Earth’s atmosphere. For a Jupiter-like planet injected at $P = 12$ days, a well constrained $\text{H}_2\text{O}/\text{Fe}$ value was seen for DS1 in the MOLECFIT case, whereas for SYSREM, the H_2O signal was effectively removed, causing an unconstrained $\text{H}_2\text{O}/\text{Fe}$ posterior. This behaviour is expected, as a slower moving planetary signal will be targeted and distorted more effectively by PCA-like algorithms, as they appear more stationary in time relative to the slower moving, close-in planetary signals. However, this behaviour was not ubiquitous across all three datasets investigated. This work is currently under review for publication in *Astronomy & Astrophysics*.

6.2 Future Work

6.2.1 Combining Multiwavelength High-resolution Observations

As shown in this study, the methods used to reduce and analyse high-resolution observations of exoplanetary atmospheres are robust, and are consistent across multiple instruments and instrument modes over various timescales. Furthermore, these methods have been used to place narrow constraints on the relative abundances of neutral metals in these atmosphere. To fully leverage the power of these methods, and make more conclusive statements about the origin, evolution, and current states of these worlds, multiple observations across a broad wavelength regime must be taken. This is particularly true at high-resolution, where there is currently both a high-resolution optical (ESPRESSO) and NIR/IR (CRIRES+) spectrograph mounted on the VLT, for example. Furthermore, there are numerous high-resolution spectrographs (e.g., HARPS, IGRINS, MAROON-X, SPIROU) whose data can be combined to paint a more complete picture of these objects. By constraining the chemical makeup of a planetary atmosphere, we hope to link its current composition to its formation and evolution pathway, addressing the open question of how the diverse population of planetary systems observed were formed. This is particularly true for ultra-hot Jupiters, where their atmospheric composition is thought to be representative of the planet's bulk composition, as under these high temperatures, most species have not condensed out of the atmosphere. The C/O ratio of a planet's atmosphere has long been used as a proxy for the planet's formation location (Öberg et al., 2011). However, carbon- and oxygen-bearing molecules are often elusive, particularly when observed from the ground using high-resolution spectrographs, where telluric contamination distorts the exoplanet's signal. Instead, it has been shown that by constraining a hot Jupiter's refractory-to-volatile ratio, as well as isotope ratios, we can also trace its formation and evolution pathway (Mollière et al., 2019; Lothringer et al., 2021). Therefore, by combining high-resolution optical observations, such as those outlined in this thesis,

which are sensitive to gaseous refractory species, with NIR/IR observations, which are sensitive to volatile species, it is possible to constrain the C/O ratio, metallicity (Fe/H), refractory-to-volatile ratio, and isotope ratios of these objects directly by combining ground-based optical and NIR data.

6.2.2 Combining High-resolution and Low-resolution Observations

As outlined in Sect. 1.2.2, observations of exoplanetary atmospheres at both low- and high-resolution have their own set of drawbacks and advantages. Therefore, it is natural to deduce that by combining these observations, one can get a more complete picture of exoplanetary atmospheres across a broader pressure range, as these two sets of observations are sensitive to different pressure/altitude regimes. This has been done by Smith et al. (2024), where a combined atmospheric retrieval of the HJ WASP-77Ab was performed using both ground-based IGRINS observations and space-based JWST/NIRSpec, where both observations consistently conclude a subsolar metallicity.

Traditionally, uncovering the multidimensional nature of exoplanetary atmospheres was only possible through phase curve and secondary eclipse observations. However, the work presented in Chap. 4 probes the multidimensional nature of these close-in giant planets during transmission, by separating their morning/evening contributions in velocity. Thus, a separate transmission spectrum may be retrieved for both the morning and evening limbs. In a similar fashion, recent work by Espinoza et al. (2024) has shown that we can also detect longitudinal variations in these atmospheres during transmission by mapping the subtle changes in the shape of transit light curves during a planet’s ingress and egress, caused by asymmetries across the atmospheric limbs (see Fig. 6.1). This split-terminator method can also be parameterised using “transmission strings” (Grant & Wakeford, 2022), which also allows for more complexity by incorporating additional harmonics into these ‘strings’, defining more intricate shapes for the

obscuring disk/terminator. By combining these low-resolution techniques with the multidimensional high-resolution method outlined in Chap. 4, varying atmospheric physics as a function of planetary longitude could be inferred with unprecedented precision.

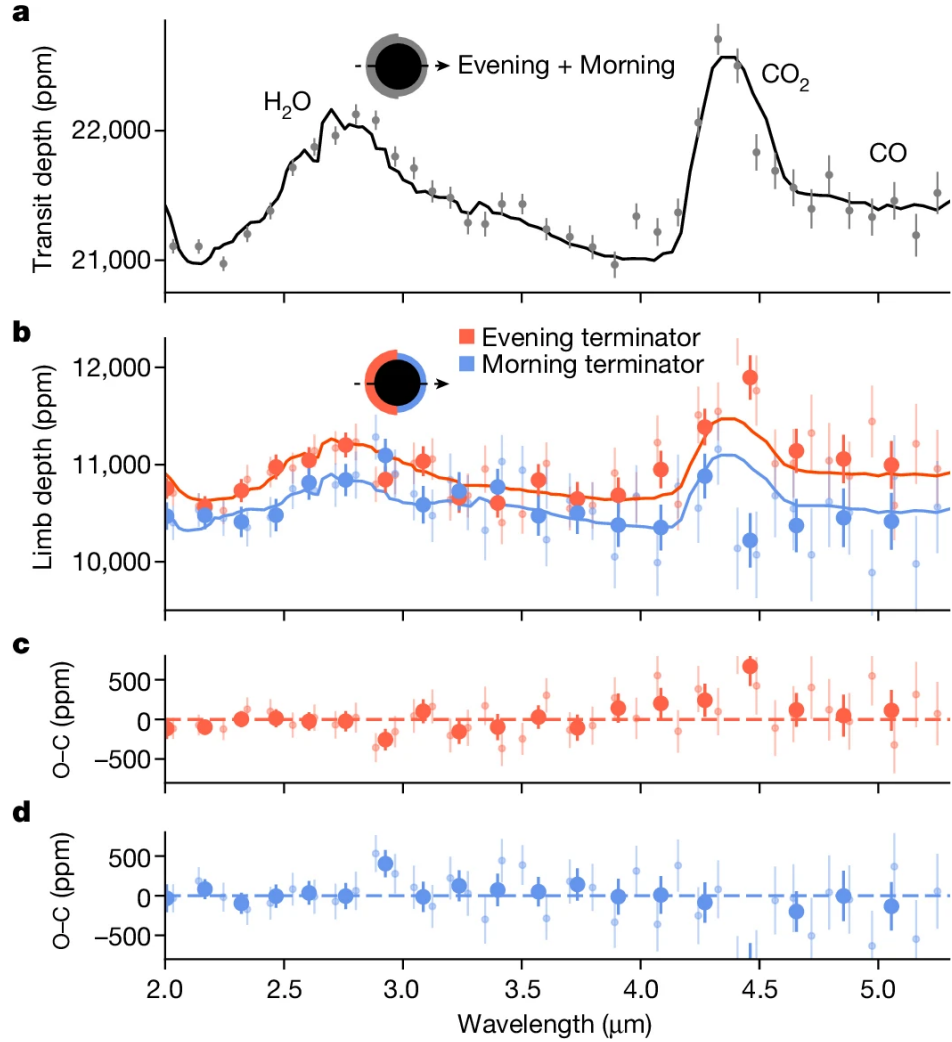


Figure 6.1: (a) The total transmission spectrum of WASP-39b, combining the morning and evening spectra. (b) The retrieved best-fit morning (blue) and evening (red) transmission spectra of WASP-39b from NIRSpec/PRISM observations. The big datapoints are observations binned at $R = 30$, and the small points at $R = 100$. (c) The residuals from the best-fit evening model and data. (d) The residuals from the best-fit morning model and data. Figure from Espinoza et al. (2024).

6.2.3 Future Observatories and Instrumentation

At the time of writing, the Extremely Large Telescope (ELT) is currently under construction at Cerro Armazones, Chile. With planned first light by 2028 (Padovani & Cirasuolo, 2023), the ELT's 39 m primary mirror will offer astronomical observations

at an unprecedented level of precision. The ELT will also be equipped with a high-resolution spectrograph, the ArmazoNes high Dispersion Echelle Spectrograph (ANDES), which will cover a broad wavelength range of $\sim 0.4 - 1.8 \mu m$, and will provide a detailed view of planets across the full optical-NIR regime (Palle et al., 2023). The telescopes increased sensitivity also means that the techniques outlined in this thesis, which until now have been reserved for the large signals of close-in, giant planets, may be applied to smaller Earth-like analogues on larger orbital separations. The study of rocky exoplanet atmospheres, with the potential for detections of ‘biomarkers’, is driving the instrumental design of ANDES.

Furthermore, during the lifetime of ELT/ANDES, ESA will also launch two complementary space-telescopes, whose primary science cases are the detection and characterisation of exoplanets and their atmospheres. Scheduled for launch in 2026, the PLANetary Transits and Oscillations of stars (PLATO) mission will survey the night sky, and use the transit method to discover and characterise exoplanets, particularly Earth-like planets, in orbit around Sun-like stars. Similarly, launching in 2029, the Atmospheric Remote-sensing Infrared Exoplanet Large-survey (ARIEL) will survey roughly 1000 exoplanets, analysing their atmospheres in the optical and NIR. These observatories, coupled with the ground-breaking research being conducted at current ground- and space-based facilities, will aid astronomers in answering fundamental questions about these worlds. With the postulations of Ancient Greece answered regarding the existence of extrasolar planets, we may go one step further, answering: What are exoplanets made of? What physical processes shape planetary atmospheres? How did planets and planetary systems form and evolve to their current state? And finally, are there potentially habitable planets?

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Appendices

Appendix A

We have included additional plots regarding the injection and recovery tests detailed in Sect. 3.1.1 below. Additional 1D and 2D posterior distributions, similar to Fig. 3.2, for T1 and T3 have also been included. A table of best-fit atmospheric model parameters found for each data set is also given in Table A1 below.

Injection and Recovery Tests

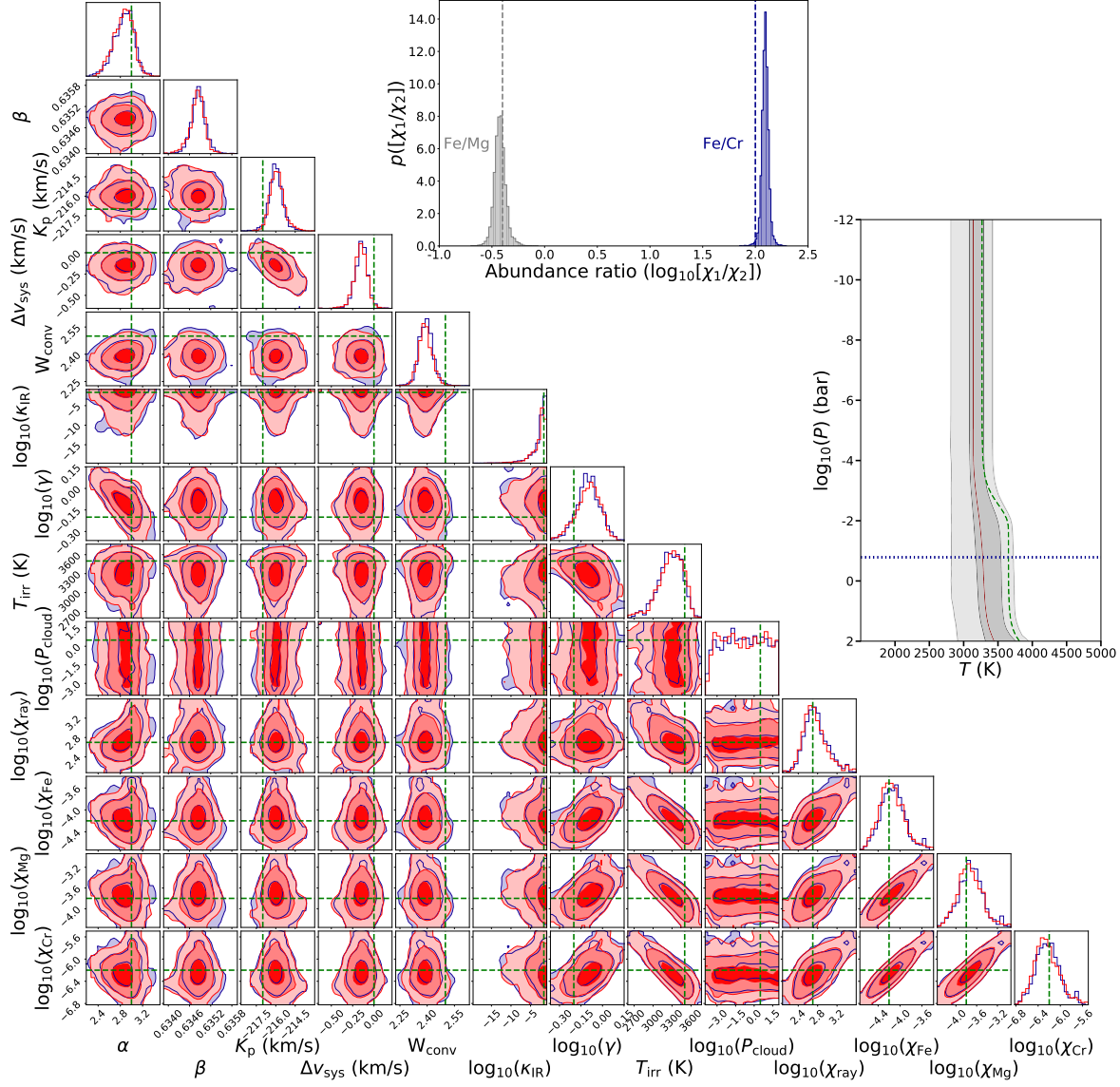


Figure A1: The results of the injection tests described in Sect. 3.1.1, for T1. (*left subpanel*) 1D and 2D marginalised posterior distributions of each of the model parameters, with the injected values shown as green dashed lines in each. (*upper mid subpanel*) The retrieved relative abundance constraints, $\log_{10}(\chi_{\text{Fe}}/\chi_{\text{Mg}})$ and $\log_{10}(\chi_{\text{Fe}}/\chi_{\text{Cr}})$, and their injected values highlighted as vertical dashed lines. (*right subpanel*) The retrieved T - P profile, and its injected value shown as a green dashed curve. The blue horizontal dotted line is the median retrieved cloud deck pressure, $\log_{10}(P_{\text{cloud}})$, below which the model spectrum is truncated.

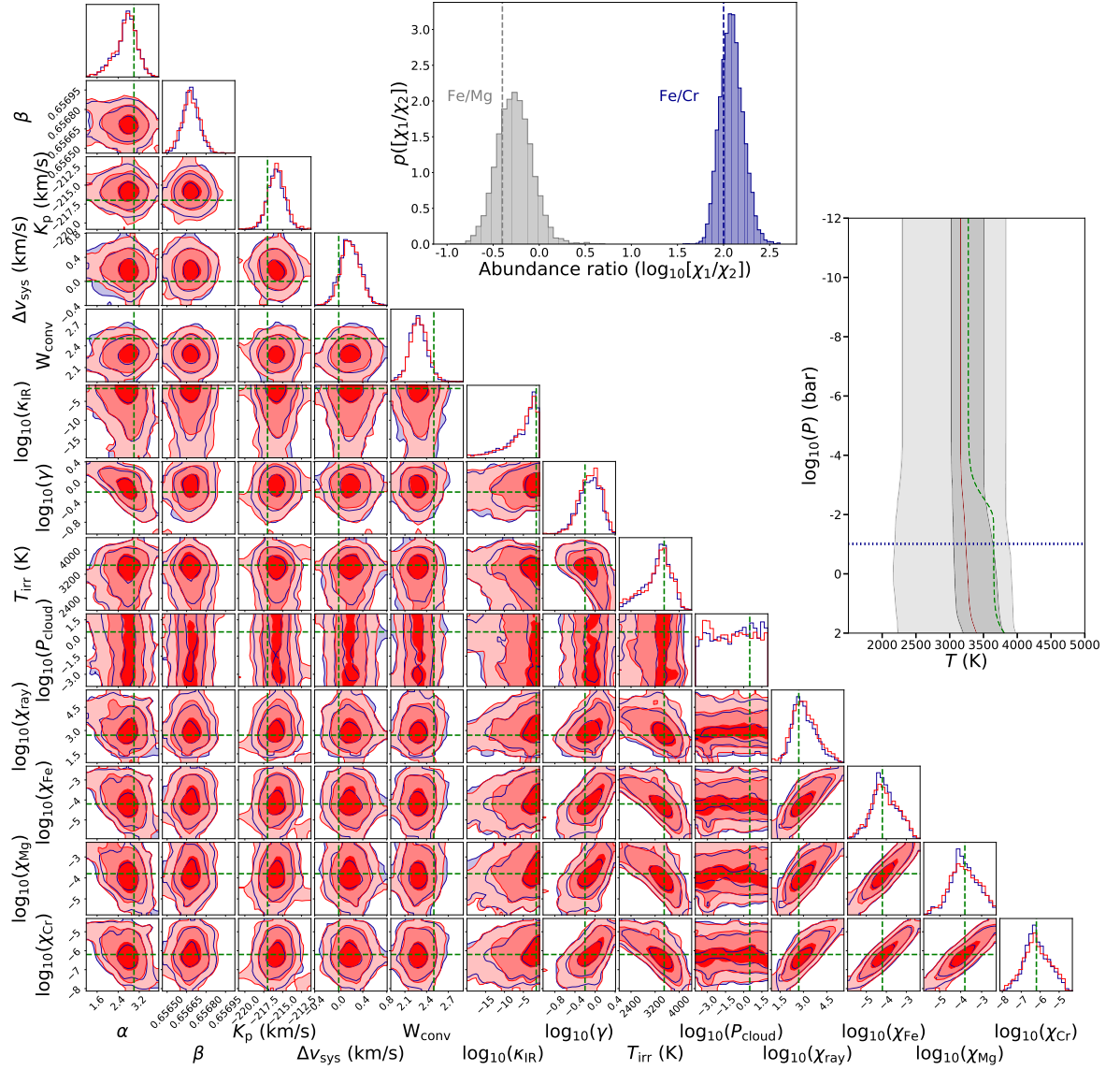


Figure A2: Similar to Fig. A1, but for T2.

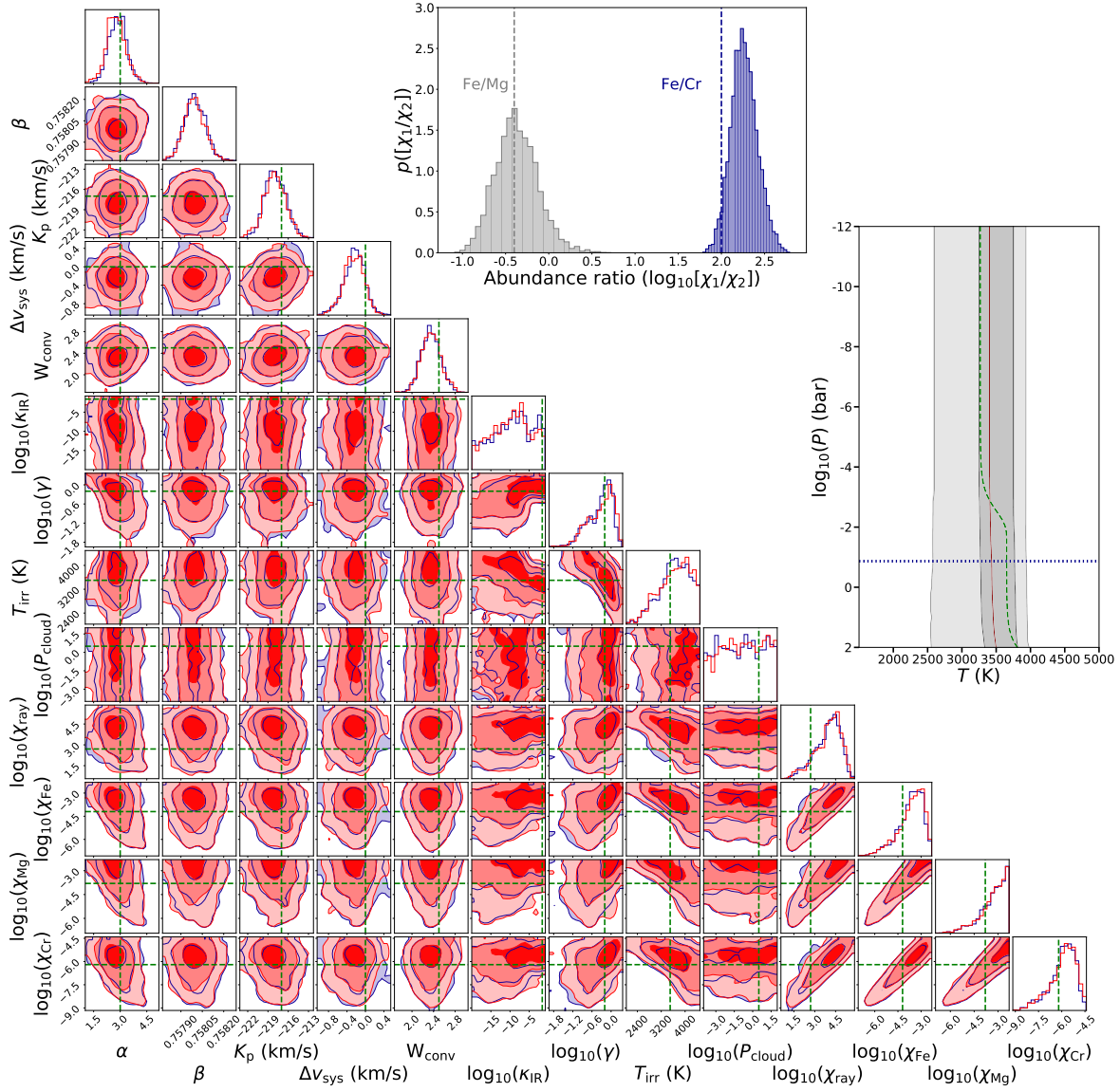


Figure A3: Similar to Fig. A1, but for T3.

Atmospheric Retrieval Results

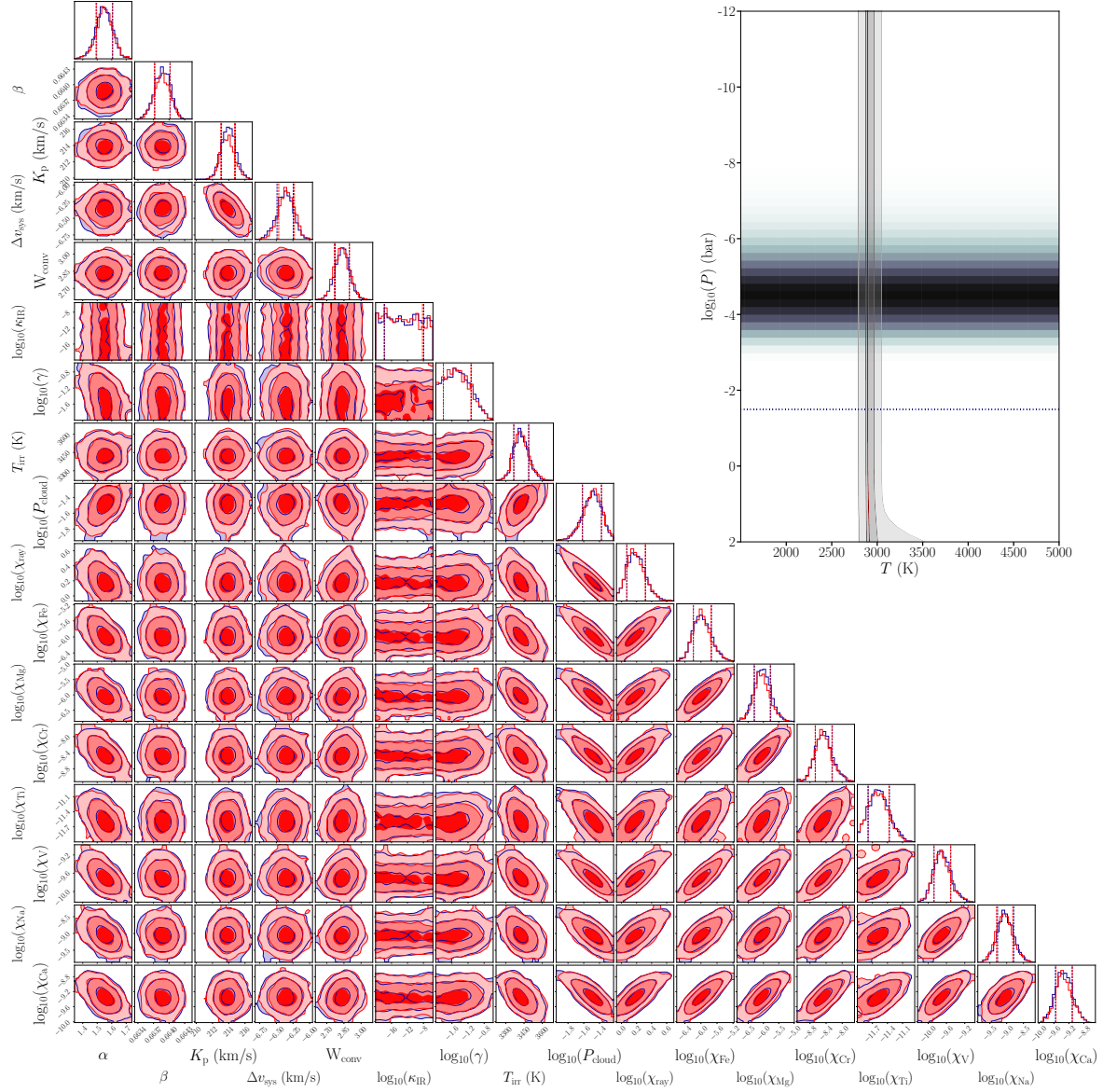


Figure A4: Similar to Fig. 3.2, but for T1.

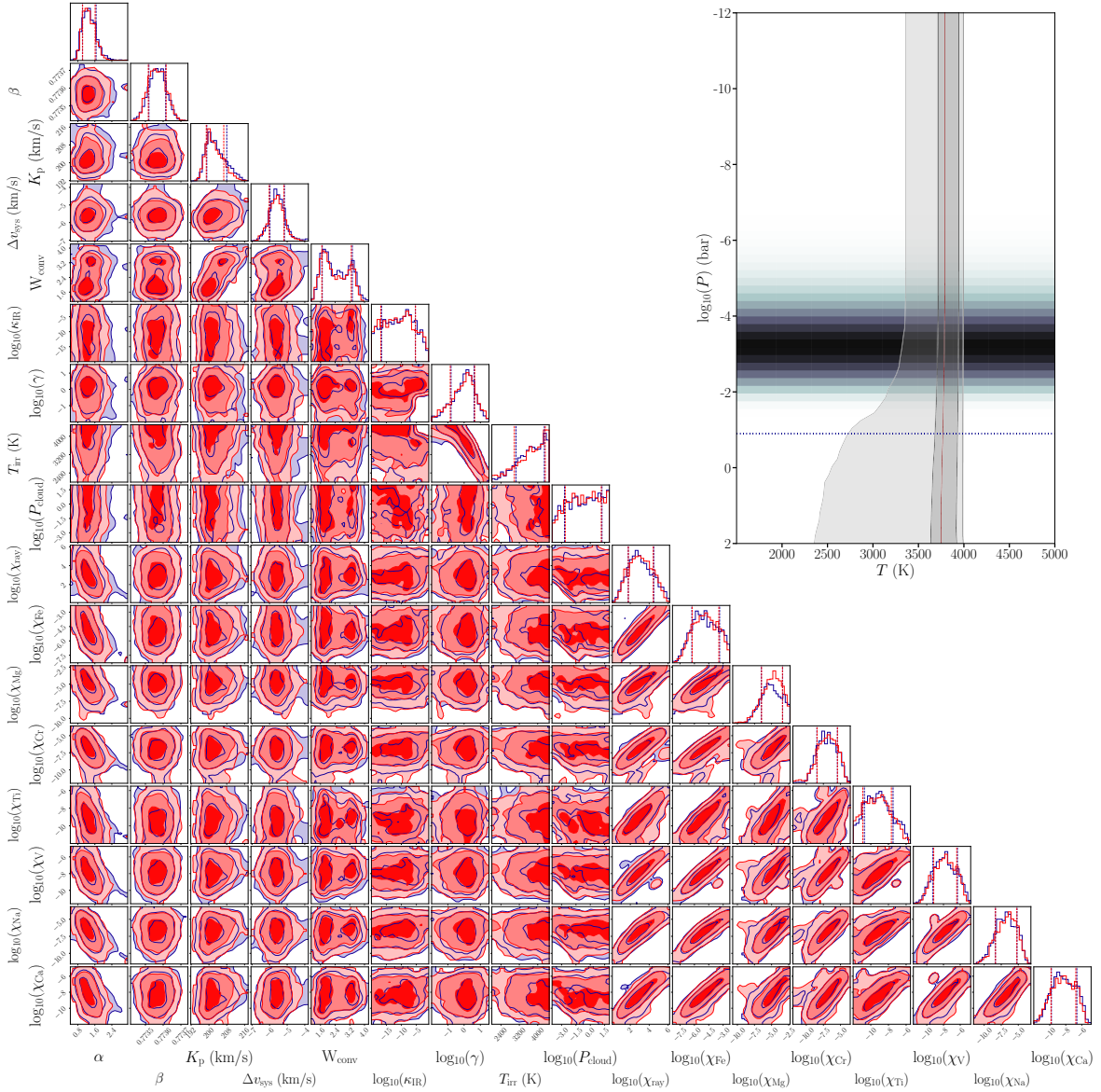


Figure A5: Similar to Fig. 3.2, but for T3.

Table A1: Best-fit model parameters for each of the atmospheric retrievals of WASP-121b.

Parameter	T1	T2	T3
α	1.59 ± 0.06	1.51 ± 0.22	1.54 ± 0.32
β	$0.66 \pm 1.42 \cdot 10^{-4}$	$0.72 \pm 4.23 \cdot 10^{-5}$	$0.77 \pm 4.72 \cdot 10^{-5}$
K_p (km s $^{-1}$)	213.61 ± 0.88	208.80 ± 1.65	197.67 ± 4.24
Δv_{sys} (km s $^{-1}$)	-6.35 ± 0.12	-6.26 ± 0.26	-5.92 ± 0.45
W_{conv} (pixels)	2.82 ± 0.07	2.54 ± 0.20	1.50 ± 0.68
$\log_{10}(\kappa_{\text{IR}})$	-9.48 ± 4.18	-1.58 ± 5.18	-15.92 ± 4.80
$\log_{10}(\gamma)$	-1.42 ± 0.31	-0.21 ± 0.51	-0.14 ± 0.76
T_{irr} (K)	3417.12 ± 61.19	3688.82 ± 573.53	3937.438 ± 609.25
$\log_{10}(P_{\text{cloud}})$ (bar)	-1.45 ± 0.12	0.52 ± 1.57	-2.04 ± 1.67
$\log_{10}(\chi_{\text{ray}})$	0.14 ± 0.13	2.71 ± 0.80	1.23 ± 1.23
$\log_{10}(\chi_{\text{Fe}})$	-6.05 ± 0.22	-4.40 ± 0.83	-6.69 ± 1.27
$\log_{10}(\chi_{\text{Mg}})$	-6.10 ± 0.27	-4.18 ± 1.06	-6.58 ± 1.40
$\log_{10}(\chi_{\text{Cr}})$	-8.54 ± 0.21	-6.41 ± 0.86	-8.51 ± 1.36
$\log_{10}(\chi_{\text{Ti}})$	-11.72 ± 0.20	-8.20 ± 1.01	-10.81 ± 1.47
$\log_{10}(\chi_{\text{V}})$	-9.77 ± 0.18	-7.72 ± 0.82	-10.13 ± 1.30
$\log_{10}(\chi_{\text{Na}})$	-8.98 ± 0.24	-7.10 ± 0.91	-9.23 ± 1.45
$\log_{10}(\chi_{\text{Ca}})$	-9.38 ± 0.22	-7.22 ± 0.87	-10.59 ± 1.40

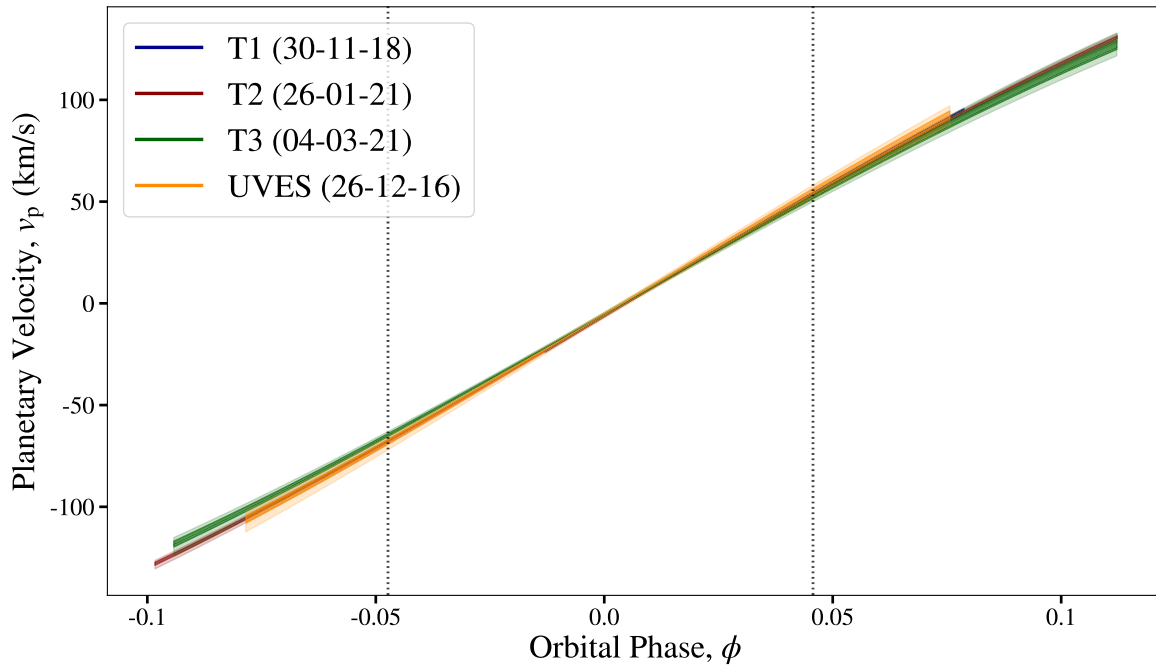


Figure A6: The retrieved planetary orbital velocity from each of the observations, computed from 10,000 random samples of the MCMC, where the solid curves show the median value, and the shaded regions show the 1σ contour. The vertical dotted lines indicate the orbital phases of ingress and egress.

Appendix B

Stellar Parameters

Table B1: Physical parameters of WASP-76. Values adopted from Ehrenreich et al. (2020).

Parameter	Value
$R_{\star}$	$1.756 \pm 0.071 \text{ R}_{\odot}$
$M_{\star}$	$1.458 \pm 0.021 \text{ M}_{\odot}$
T_{eff}	$6329 \pm 65 \text{ K}$
Spectral type	F7V
$\log g \text{ [cgs]}$	4.196 ± 0.106
[Fe/H]	0.366 ± 0.053
$K_{\star}$	$116.02^{+1.29}_{-1.35} \text{ m s}^{-1}$
$v_{\star} \sin i$	$1.48 \pm 0.28 \text{ km s}^{-1}$
v_{sys}	$-1.11 \pm 0.050 \text{ km s}^{-1}$
λ	$61.28^{+7.61}_{-5.06} \text{ deg}$

Injection and Recovery Tests

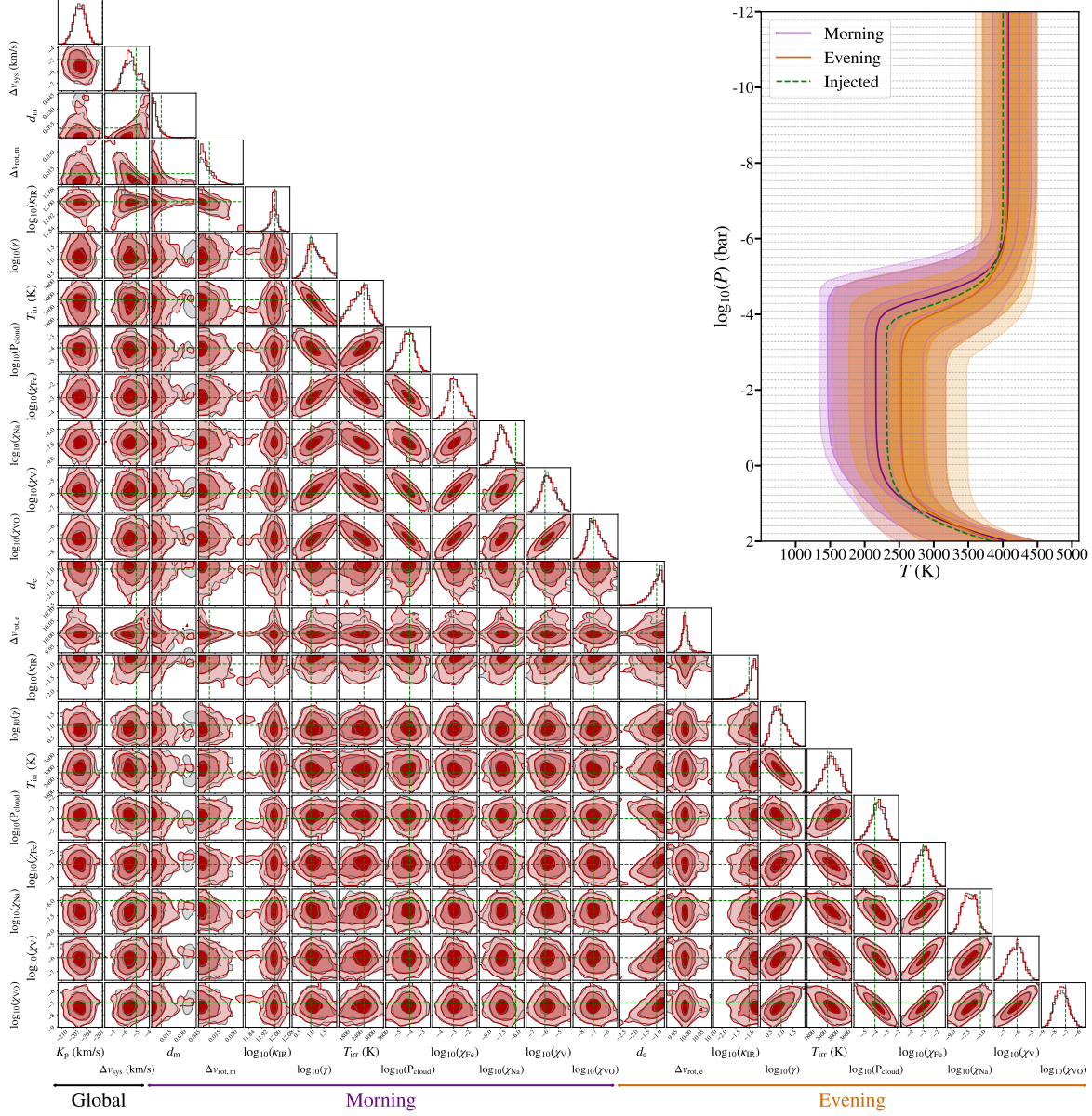


Figure B1: A summary of the injection and recovery tests for O1 outlined in Sect. 4.3.1, with the 1D and 2D marginalised posterior distributions of each of the model parameters displayed. The red and grey posterior distributions represent independent subchains, of the same MCMC chain, both converging to similar distributions, with the injected values highlighted by horizontal/vertical dashed green lines. The various global, morning, and evening parameters are highlighted. The T - P profiles on the right were computed from 10,000 random samples of the MCMC, where the solid curve shows the median profile, and the shaded regions show the 1 σ , 2 σ , and 3 σ contours, for both the morning and evening limbs. The dashed green curve shows the injected T - P profile. This corner diagram was generated using CORNER (Foreman-Mackey, 2016).

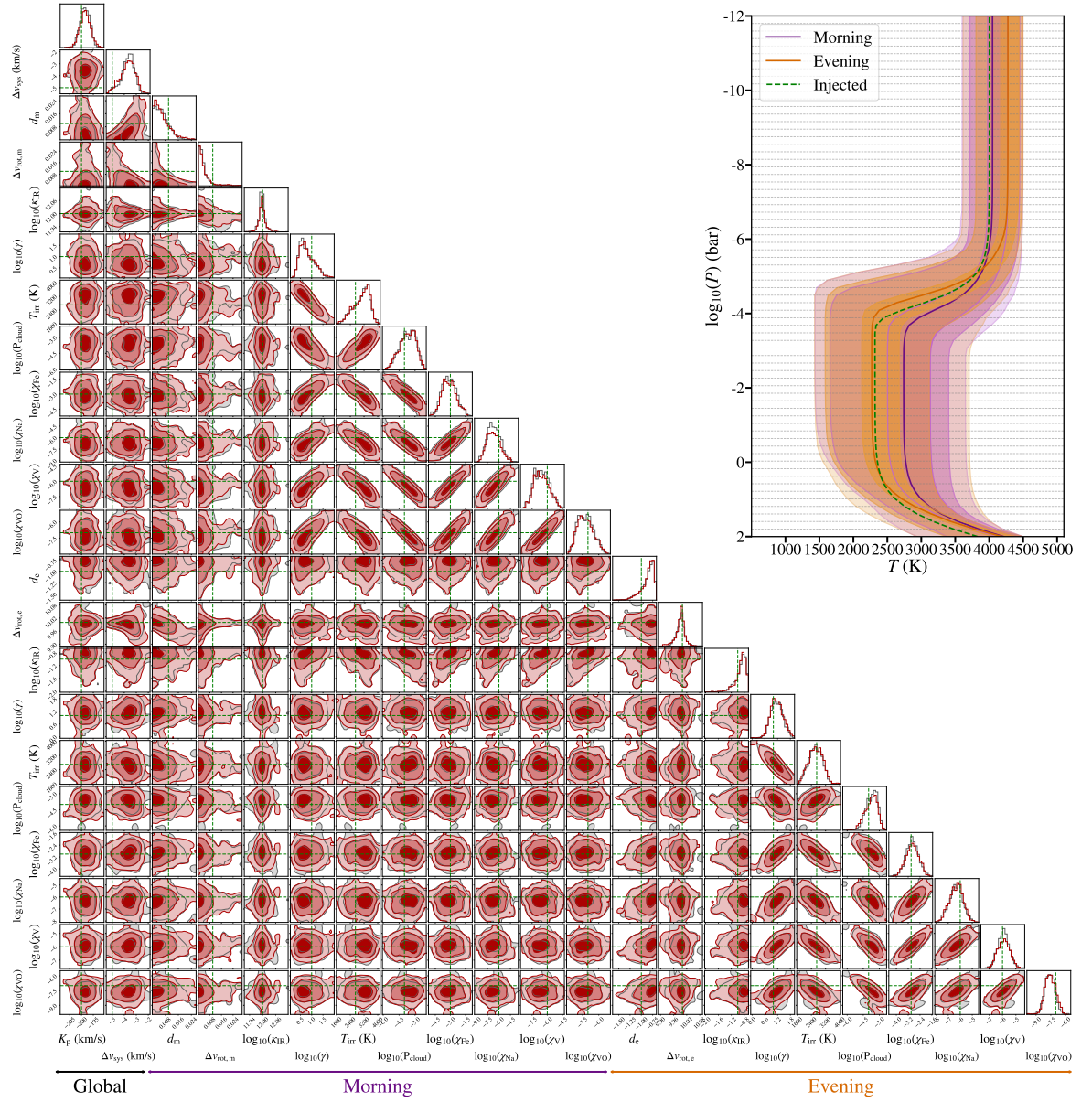


Figure B2: Similar to Fig. B1, for O2.

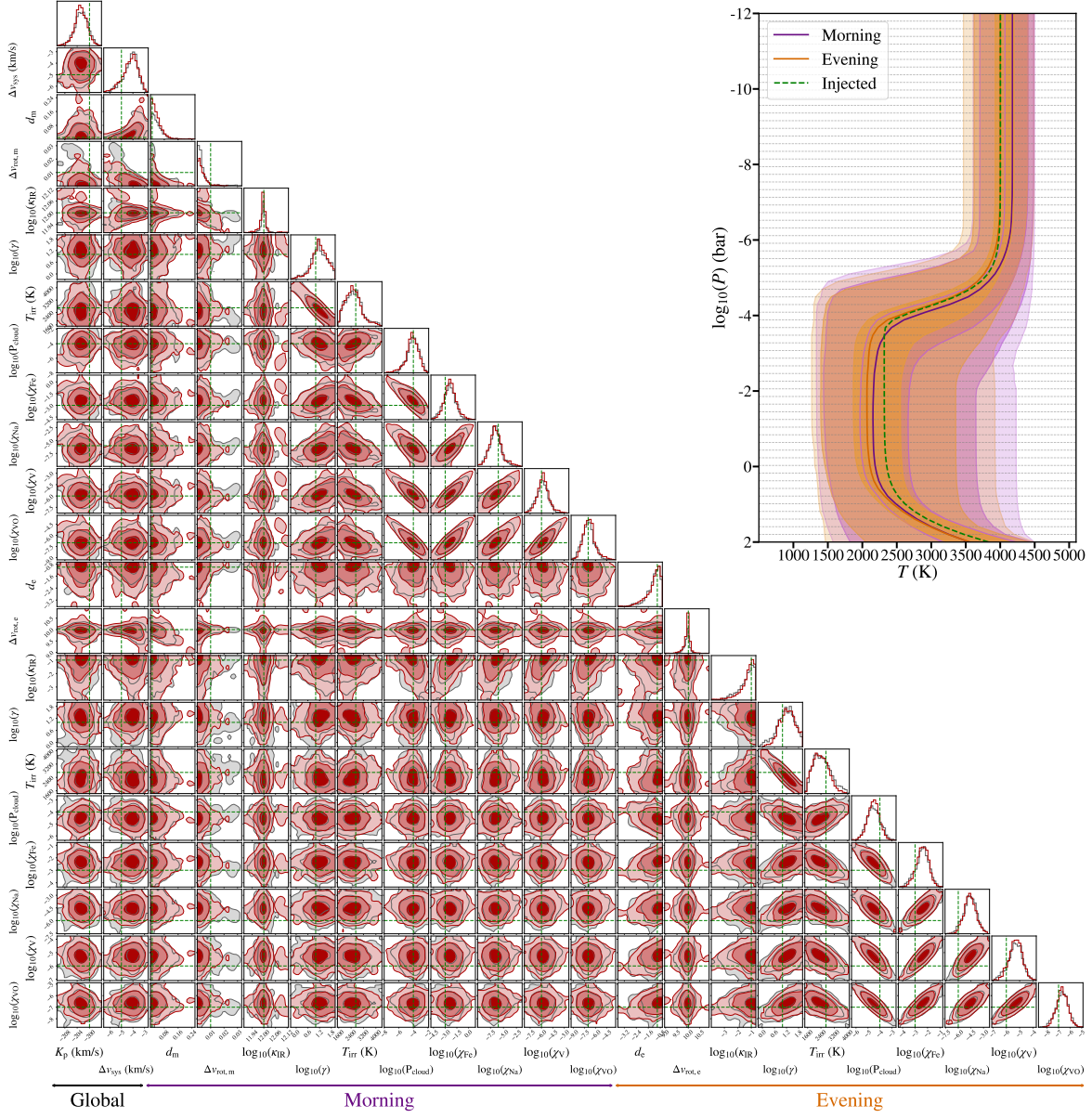


Figure B3: Similar to Fig. B1, for O3.

Atmospheric Retrieval Results

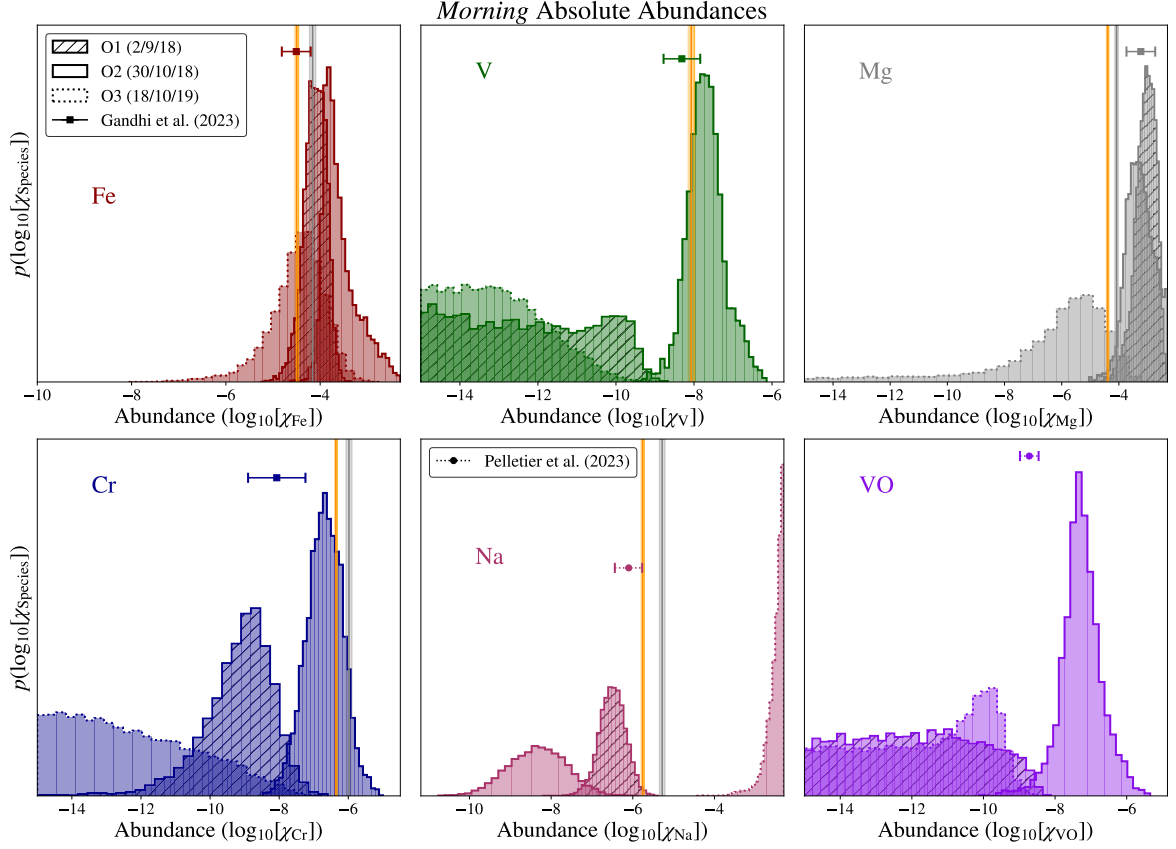


Figure B4: Absolute abundance comparison across each of the three transits, for the *morning* limb. The stellar values from Tabernero et al. (2021) are shown as a grey vertical line with their 1σ contours shaded, where measured. The solar values from Asplund et al. (2009) are shown as an orange vertical line with their 1σ contours shaded. The weighted mean of the retrieved abundances in regions C and D (morning) from G2023 are also shown, where measured. Similarly, the retrieved abundances for the whole terminator from P2023 are also shown for Na and VO.

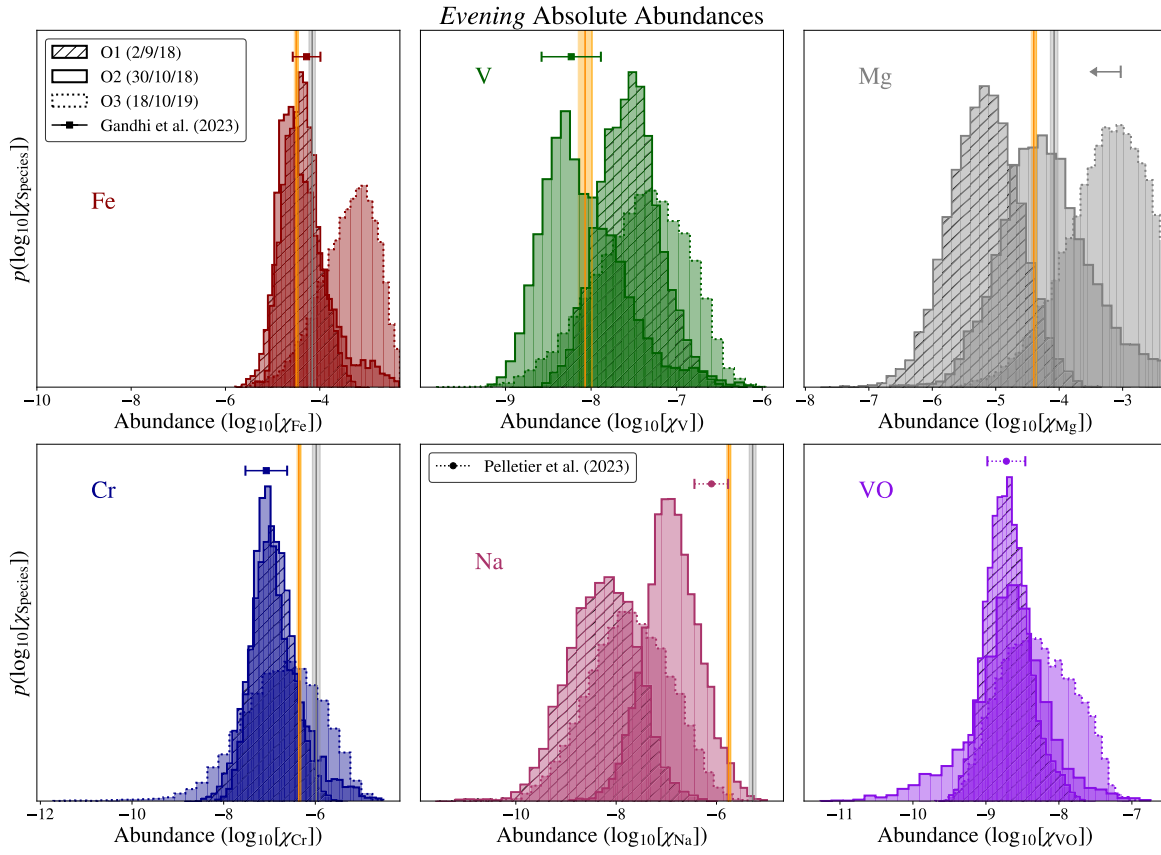


Figure B5: Absolute abundance comparison across each of the three transits, for the *evening* limb. The shaded regions are as in Fig. B4. The weighted mean of the retrieved abundances in regions A and B (evening) from G2023 are also shown, where measured.

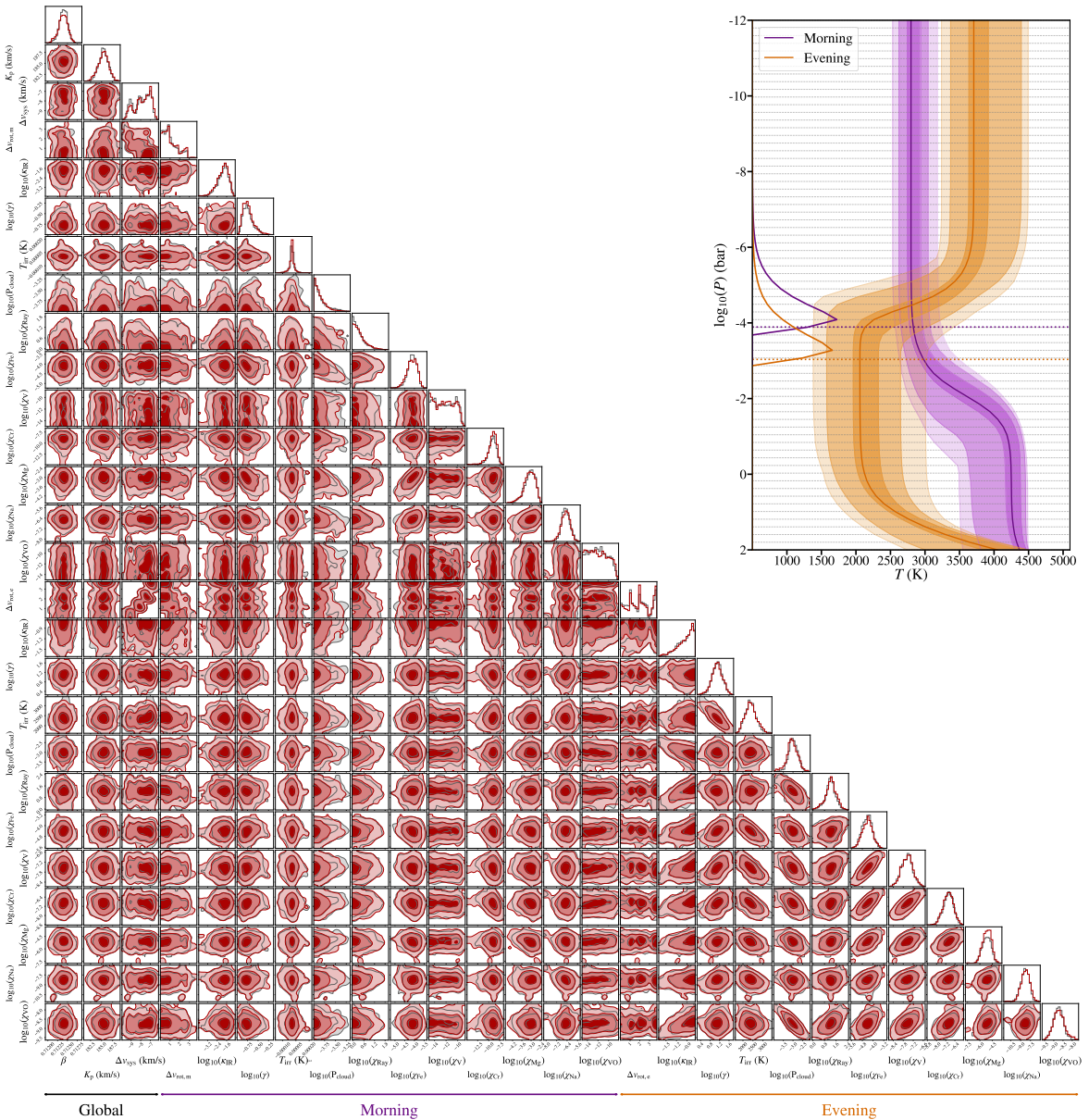


Figure B6: A summary of the atmospheric retrieval results for O1 outlined in Sect. 4.3.2, with the 1D and 2D marginalised posterior distributions of each of the model parameters displayed. The red and grey posterior distributions represent independent subchains, of the same MCMC chain, both converging to similar distributions. The various global, morning, and evening parameters are highlighted. The T - P profiles on the right were computed from 10,000 random samples of the MCMC, where the solid curve shows the median profile, and the shaded regions show the 1σ , 2σ , and 3σ contours, for both the morning and evening limbs. The horizontal dotted lines are the median retrieved cloud deck pressures, $\log_{10}(P_{\text{cloud}})$, below which the model spectrum is truncated. Also plotted are the mean contribution functions for the ESPRESSO wavelength range. This corner diagram was generated using CORNER (Foreman-Mackey, 2016).

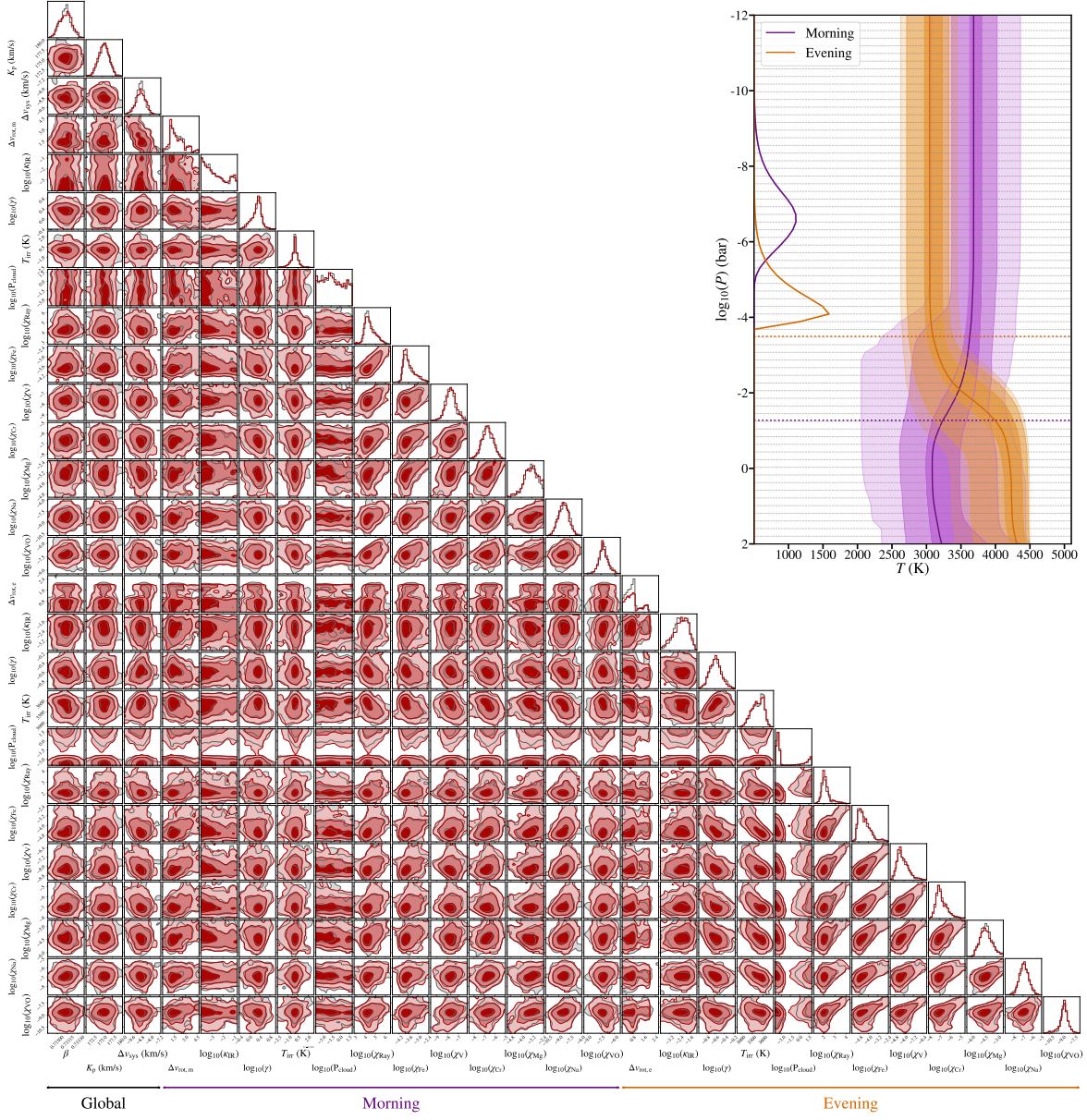


Figure B7: Similar to Fig. B6, for O2.

Cross-correlation

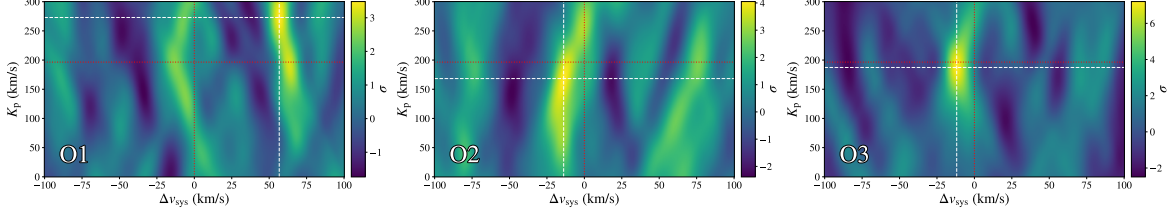


Figure B9: K_p - Δv_{sys} maps of VO, for O1, O2, and O3, confirming the novel detection of VO by Pelletier et al. (2023). The VO atmospheric models were calculated using the optimum parameters from the various atmospheric retrievals and broadened with the respective optimum broadening parameters, using the broadening kernel given by Eq. 2.20. The red dotted lines shows the expected planetary velocity values, whereas the white dashed lines shows the maximum K_p and Δv_{sys} values.

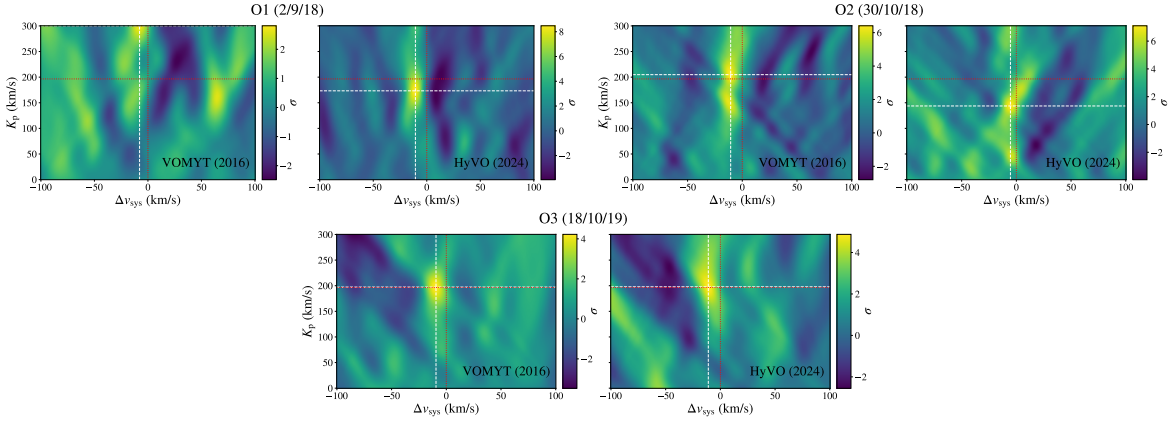


Figure B10: K_p - Δv_{sys} maps of VO, for O1, O2, and O3, using both the VOMYT (McKemmish et al., 2016) and HyVO (Bowesman et al., 2024) line lists. The VO cross-sections were calculated at $T = 2800$ K and $P = 0.1$ mbar. The transmission spectra were computed using an isothermal T - P profile, and convolved with a 1D Gaussian kernel. The red dotted lines shows the expected planetary velocity values, whereas the white dashed lines shows the maximum K_p and Δv_{sys} values.

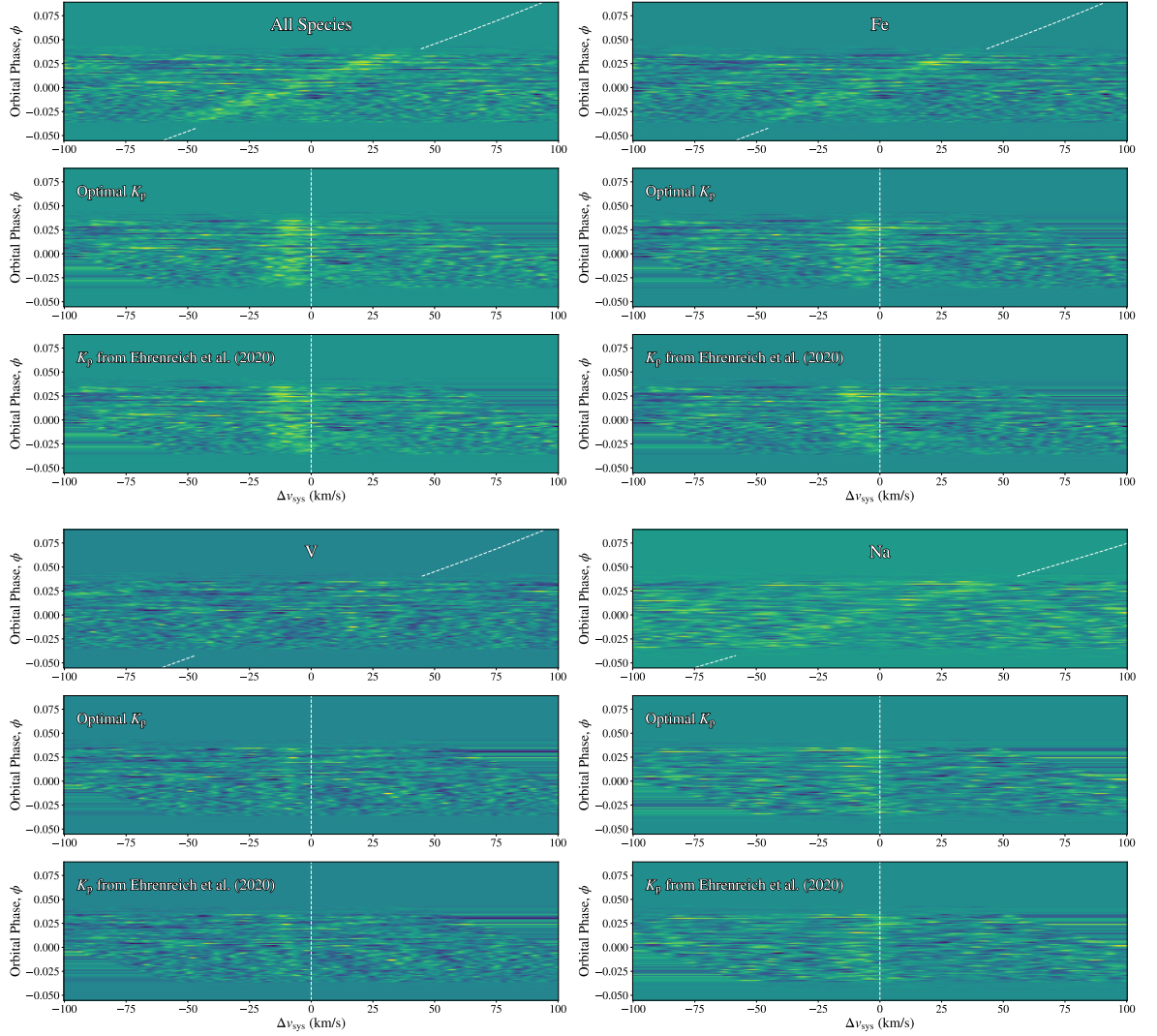


Figure B11: The CC trails of various species for O3, shifted to the optimum K_p values, as well as to the K_p value from Ehrenreich et al. (2020), in order to visualise any apparent “kink”. The atmospheric models were calculated using the optimum parameters from the various atmospheric retrievals, however, were unbroadened, in order to aid visualisation of any deviation from the planet’s Keplerian velocity curve. For clarity, we only plot species in which there was a clearly visible CC trail.

Appendix C

Injected Transmission Spectra

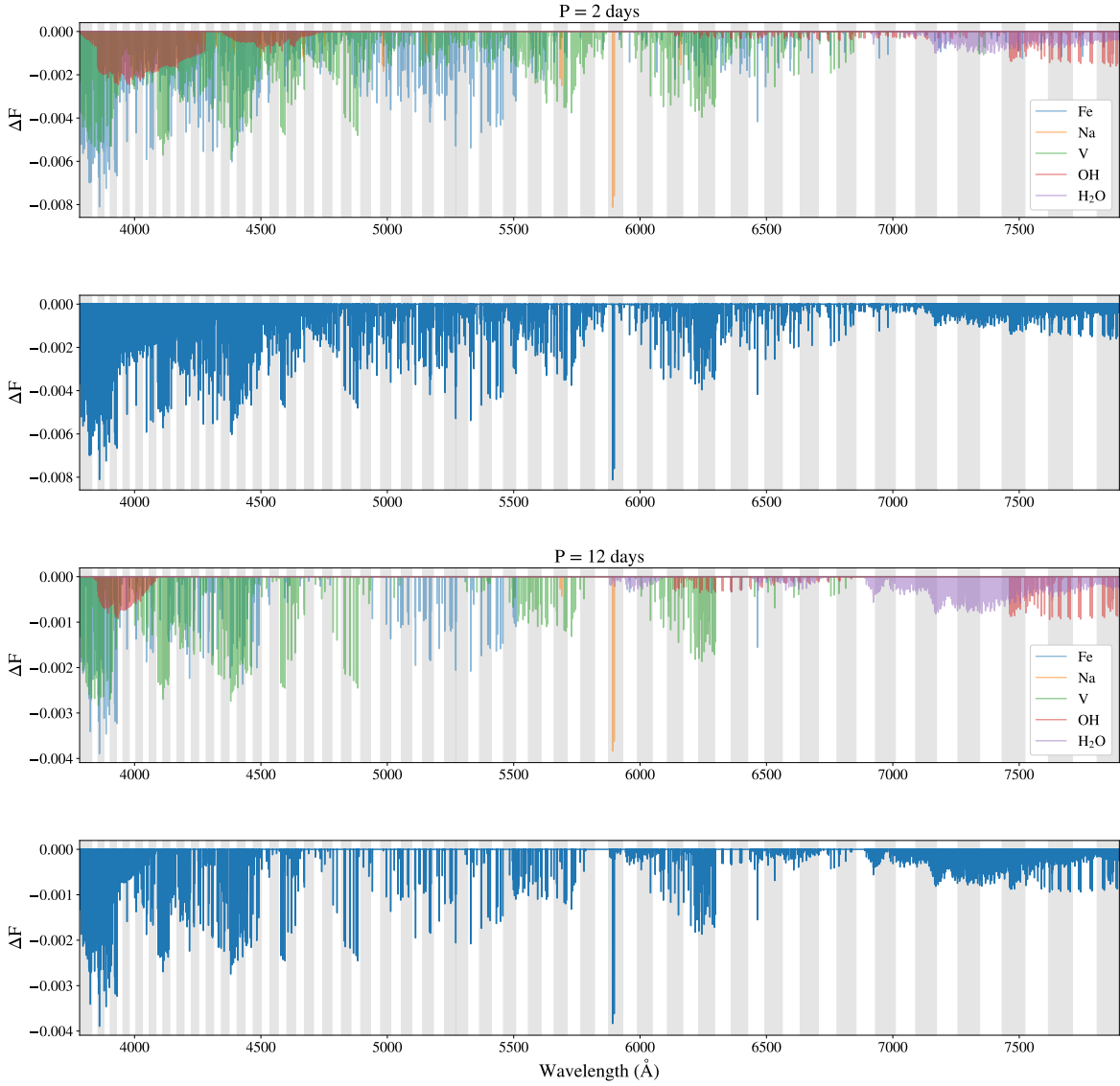


Figure C1: The model transmission spectra injected into each of the datasets. The top two panels show both the individual species' contributions, as well as the total unbroadened spectrum for $P = 2$ days. The bottom two panels show both the individual species' contributions, as well as the total unbroadened spectrum for $P = 12$ days. The alternating white and grey shaded regions in each of the panels are the individual ESPRESSO orders after pairing, described in Sect. 5.1.4.

Additional Relative Abundance Comparisons

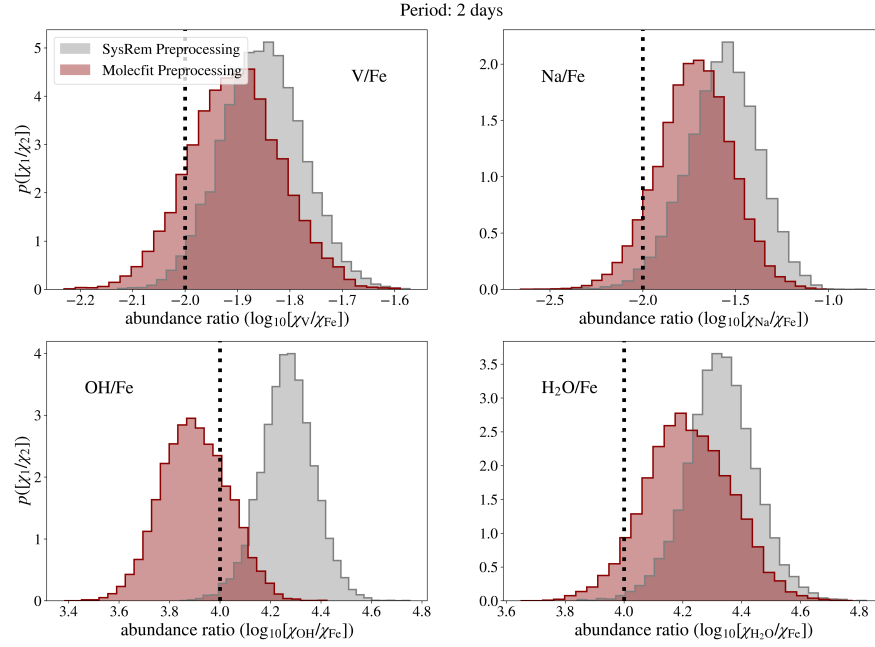


Figure C2: Similar to Fig. 5.4, for DS2.

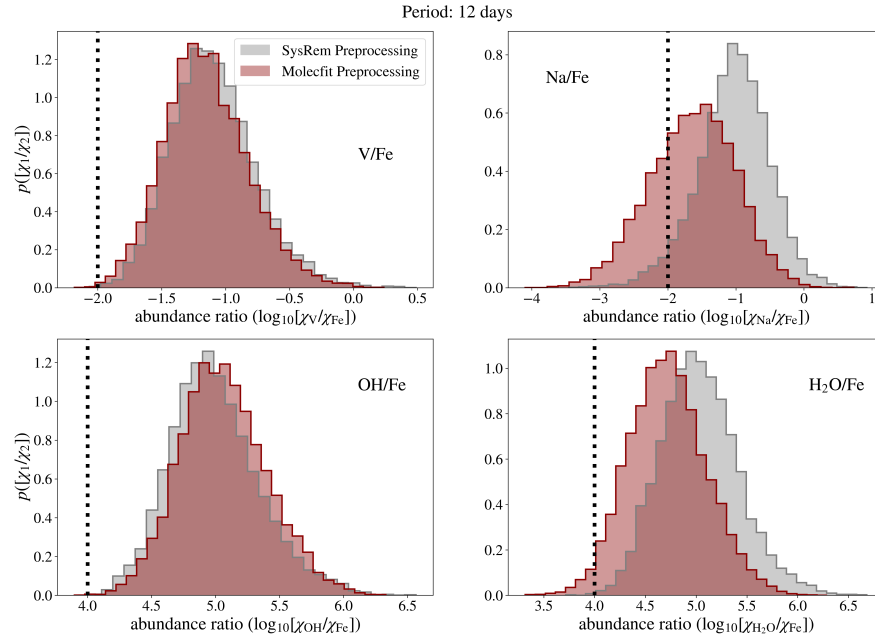


Figure C3: Similar to Fig. 5.5, for DS2.

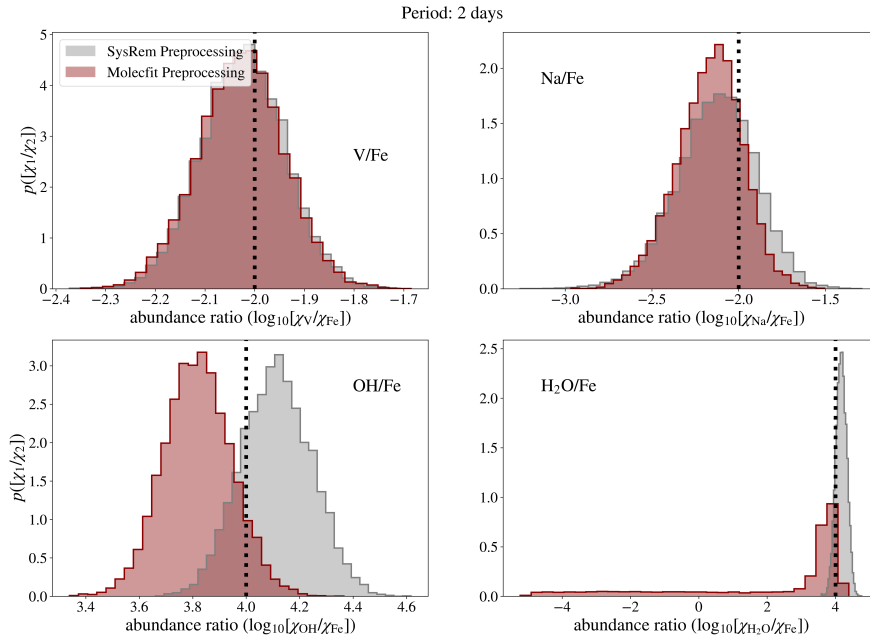


Figure C4: Similar to Fig. 5.4, for DS3.

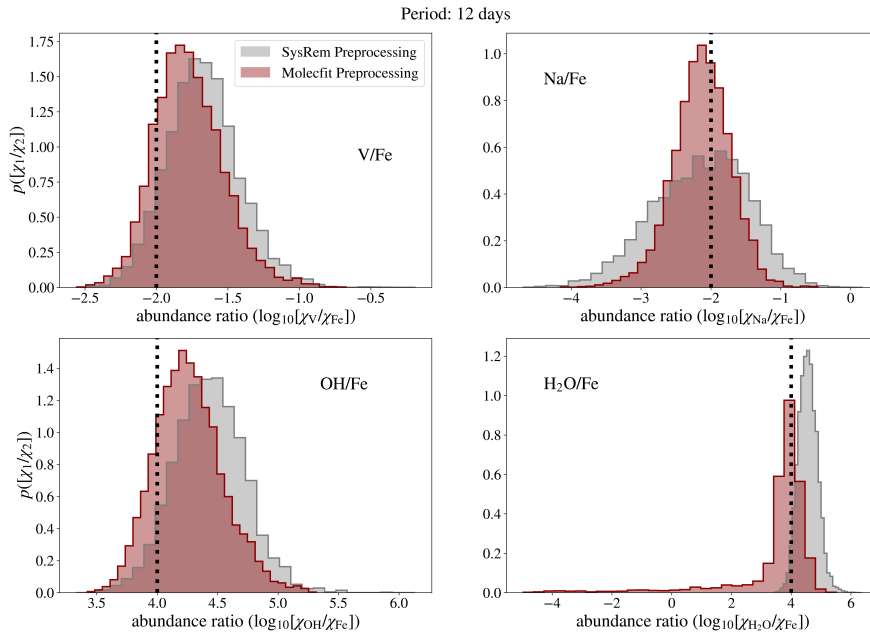


Figure C5: Similar to Fig. 5.5, for DS3.

Atmospheric Retrieval Corner Plots

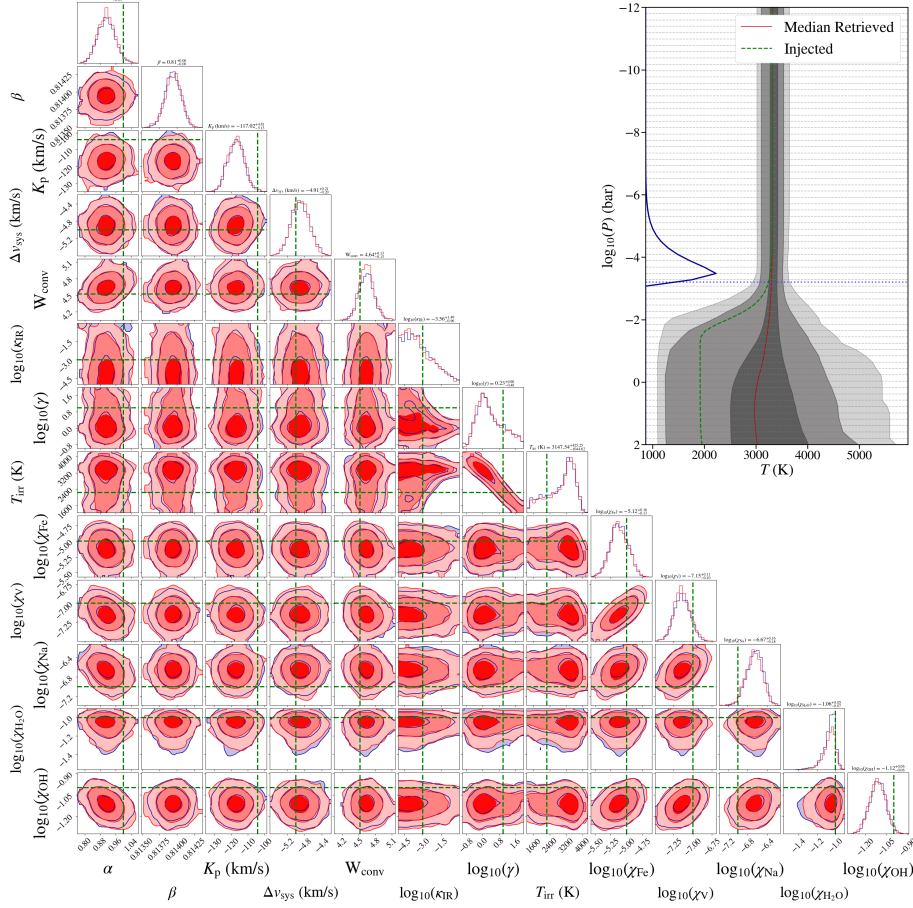


Figure C6: The atmospheric retrieval results for P2 injected into DS1 and preprocessed with SYSREM, with the 1D and 2D marginalised posterior distributions of each of the model parameters displayed. The red and blue posterior distributions represent independent subchains, of the same MCMC chain, both converging to similar distributions. The injected values are shown as green vertical/horizontal dashed lines. The T - P profile shown on the right was computed from 10,000 random samples of the MCMC, where the solid red curve shows the median profile, and the grey shaded regions show the 1σ , 2σ , and 3σ contours. The injected profile is shown as a green dashed curve. The cloud deck, located at $\log_{10}(P_{\text{cloud}})$ is highlighted as a blue dotted line. Below this value, the model is truncated, and thus the model inference breaks down. The contribution curve is also shown in blue.

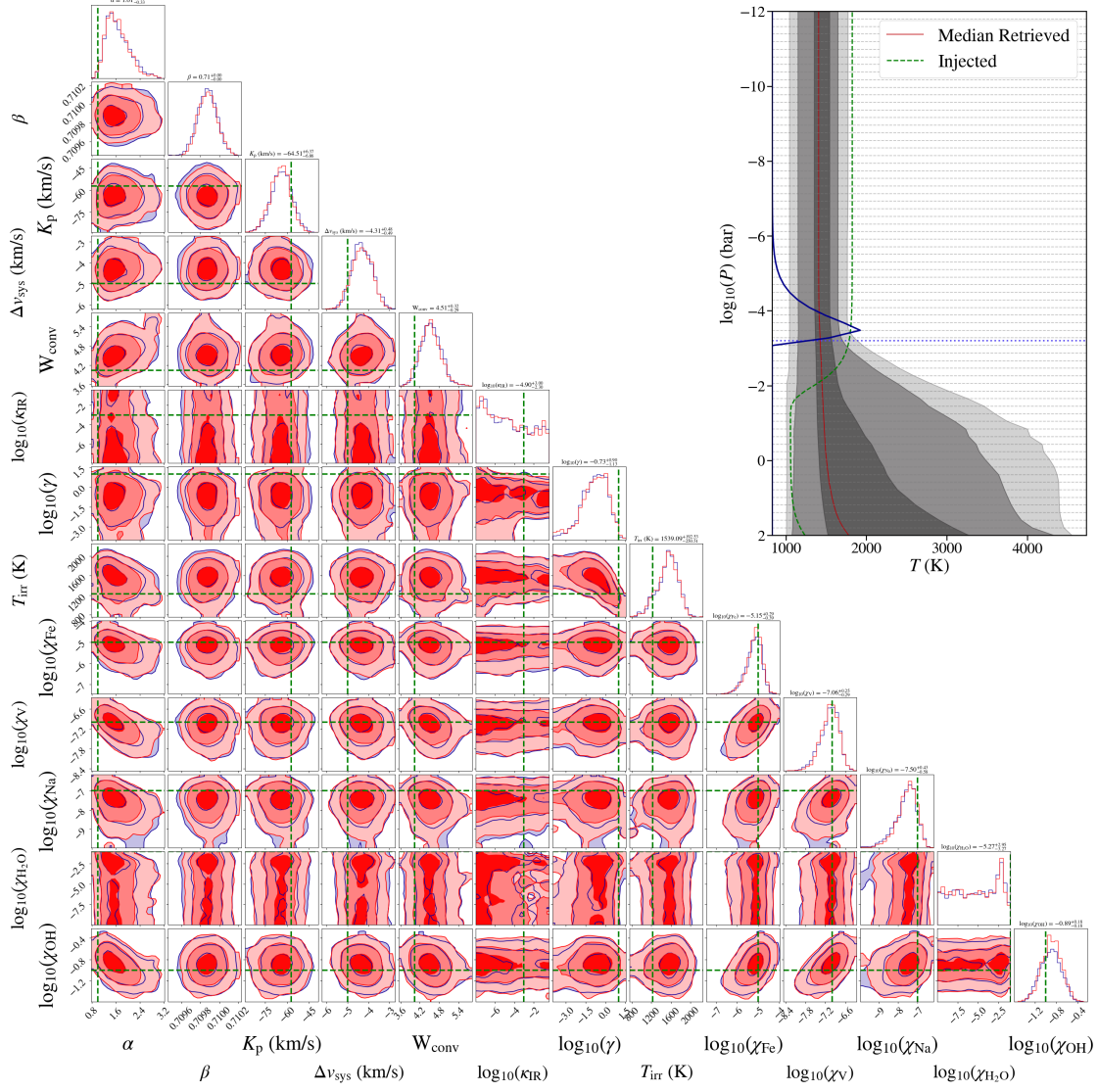


Figure C7: Similar to Fig. C6, for P12.

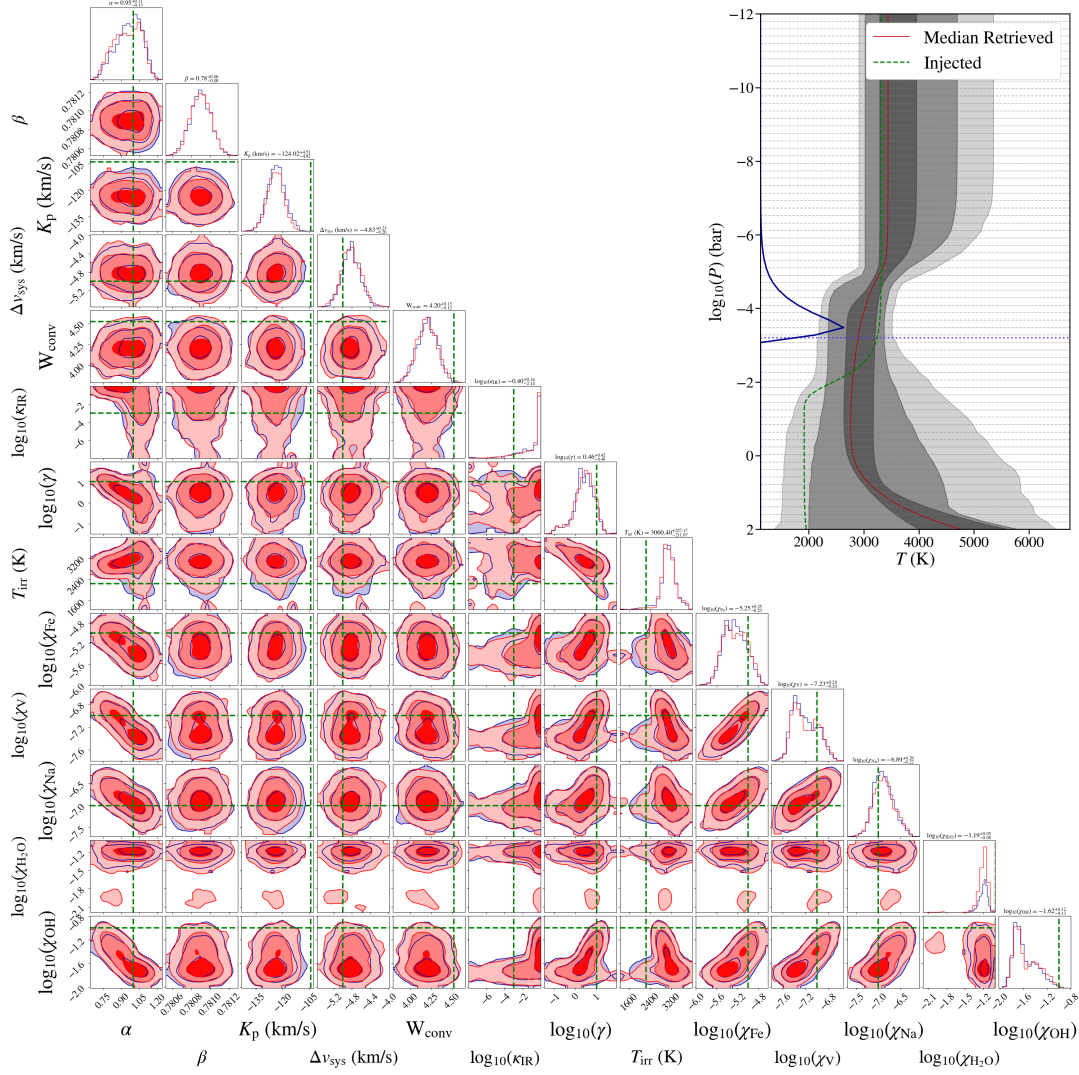


Figure C8: The atmospheric retrieval results for P2 injected into DS1 and preprocessed with MOLECFIT, with the 1D and 2D marginalised posterior distributions of each of the model parameters displayed. The red and blue posterior distributions represent independent subchains, of the same MCMC chain, both converging to similar distributions. The injected values are shown as green vertical/horizontal dashed lines. The T - P profile shown on the right was computed from 10,000 random samples of the MCMC, where the solid red curve shows the median profile, and the grey shaded regions show the 1σ , 2σ , and 3σ contours. The injected profile is shown as a green dashed curve. The cloud deck, located at $\log_{10}(P_{\text{cloud}})$ is highlighted as a blue dotted line. Below this value, the model is truncated, and thus the model inference breaks down. The contribution curve is also shown in blue.

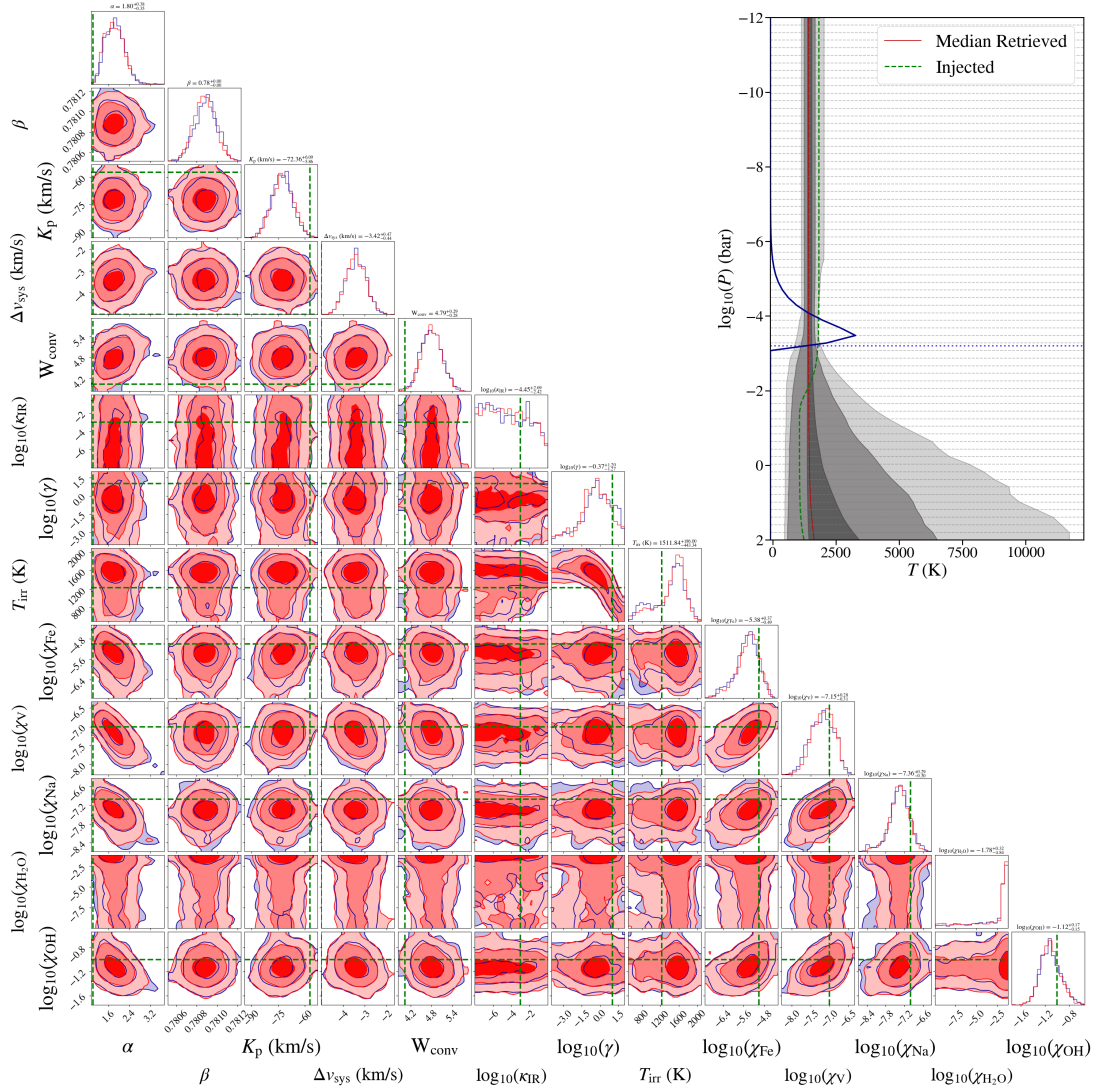


Figure C9: Similar to Fig. C8, for P12.

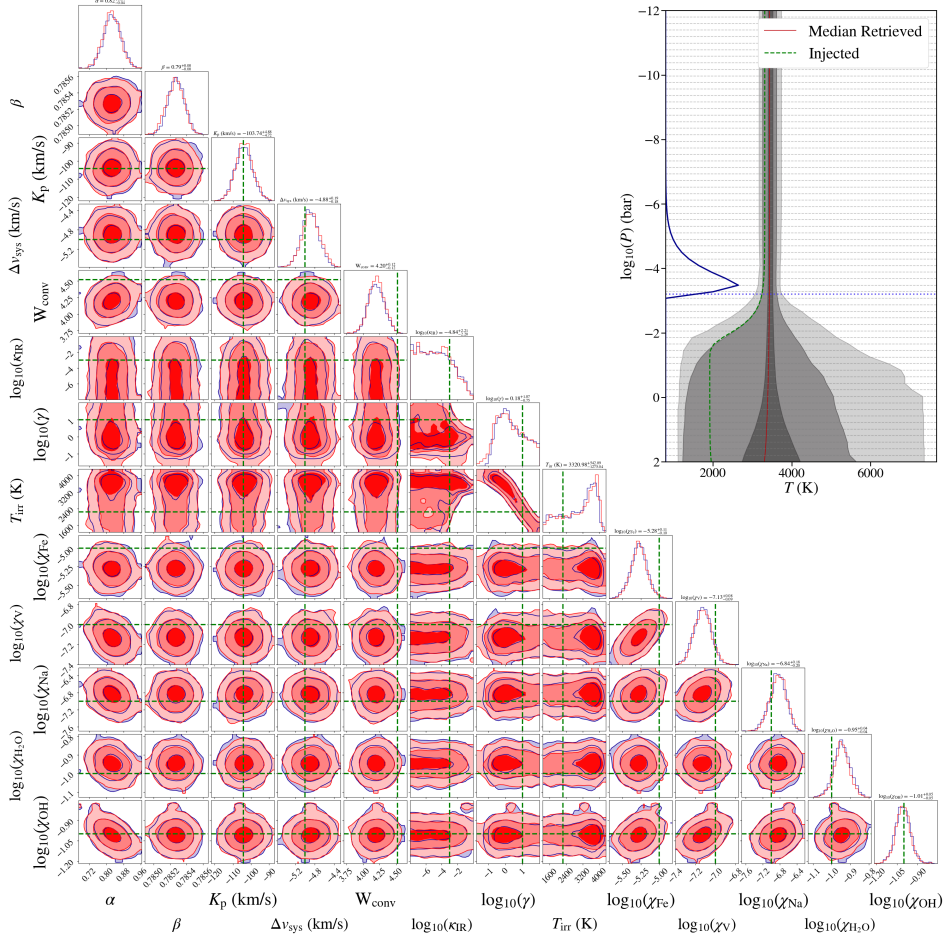


Figure C10: The atmospheric retrieval results for P2 injected into DS2 and preprocessed with SYSREM, with the 1D and 2D marginalised posterior distributions of each of the model parameters displayed. The red and blue posterior distributions represent independent subchains, of the same MCMC chain, both converging to similar distributions. The injected values are shown as green vertical/horizontal dashed lines. The T - P profile shown on the right was computed from 10,000 random samples of the MCMC, where the solid red curve shows the median profile, and the grey shaded regions show the 1σ , 2σ , and 3σ contours. The injected profile is shown as a green dashed curve. The cloud deck, located at $\log_{10}(P_{\text{cloud}})$ is highlighted as a blue dotted line. Below this value, the model is truncated, and thus the model inference breaks down. The contribution curve is also shown in blue.

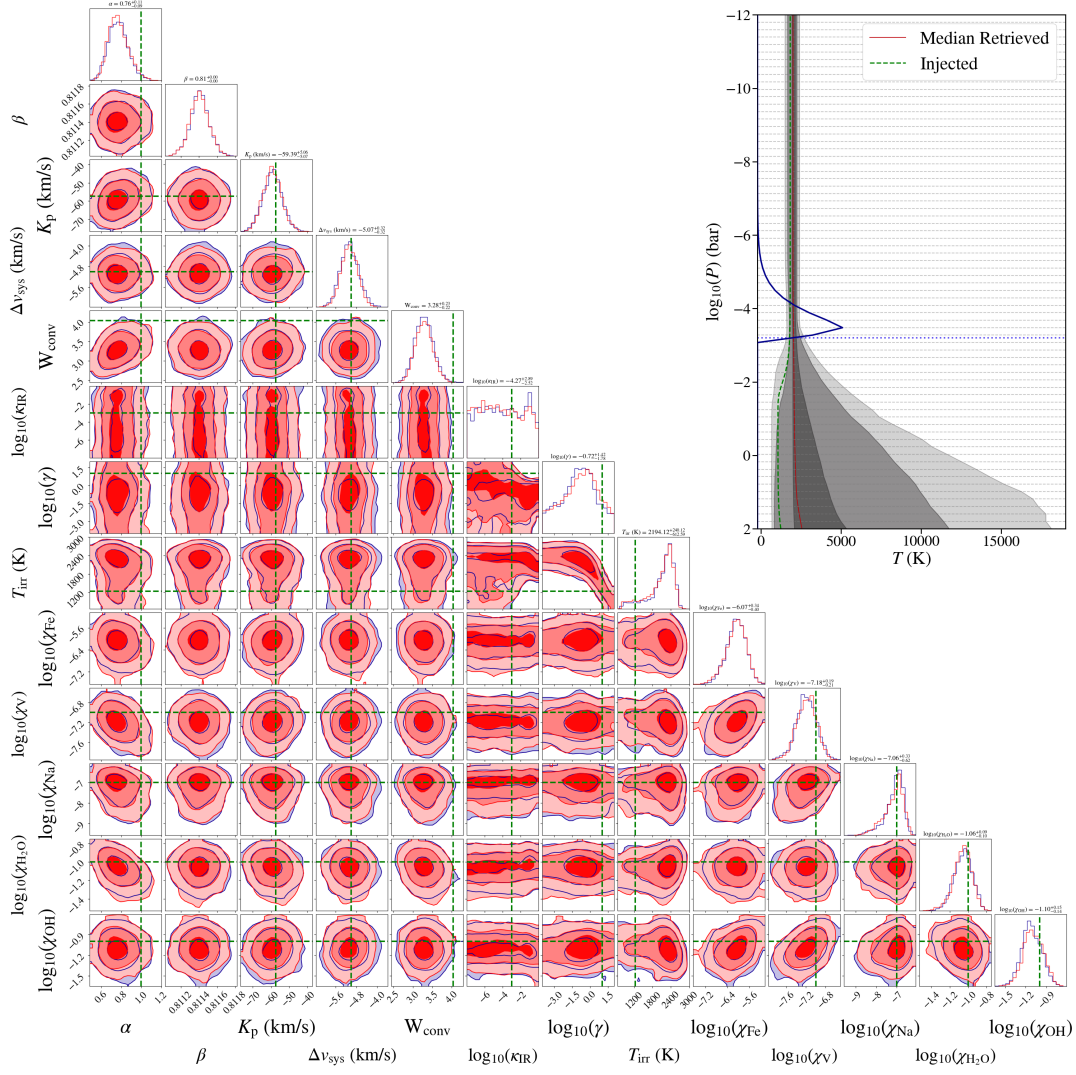


Figure C11: Similar to Fig. C10, for P12.

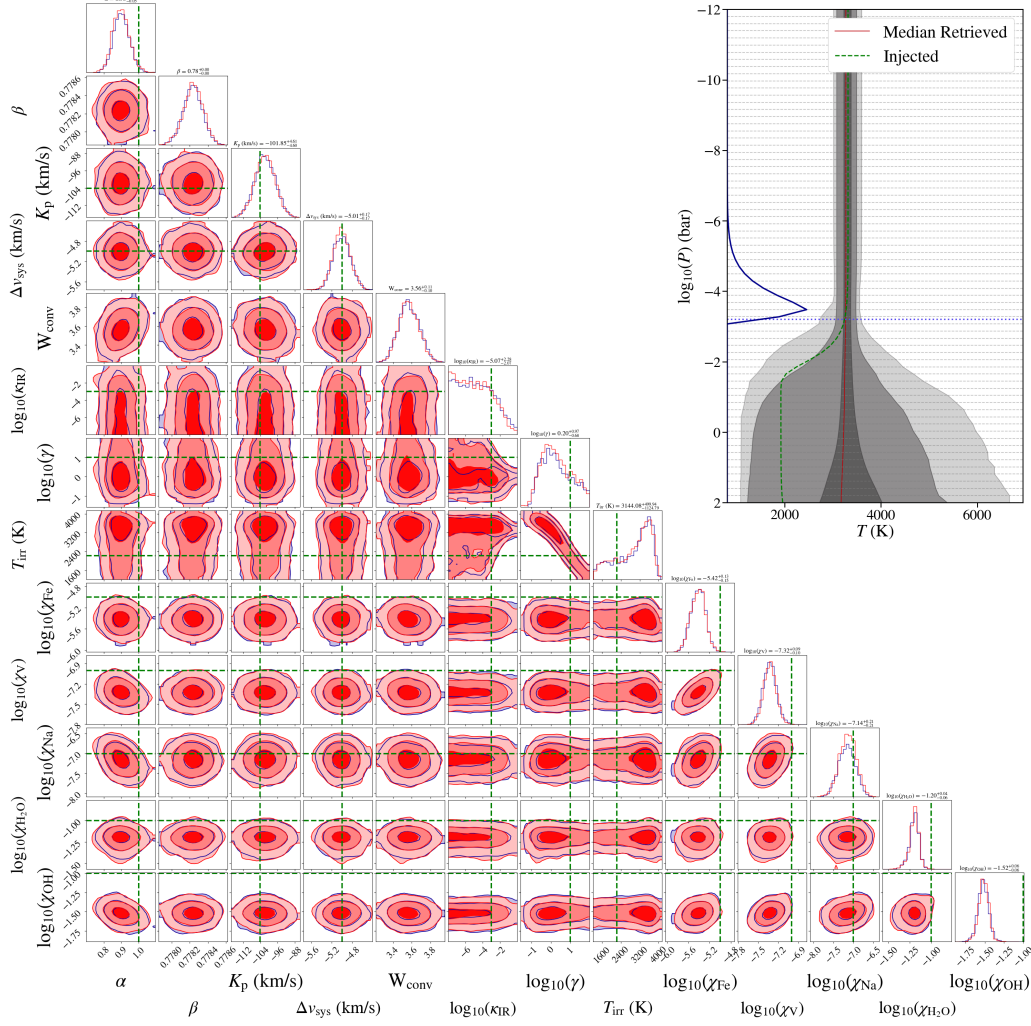


Figure C12: The atmospheric retrieval results for P2 injected into DS2 and preprocessed with MOLECFIT, with the 1D and 2D marginalised posterior distributions of each of the model parameters displayed. The red and blue posterior distributions represent independent subchains, of the same MCMC chain, both converging to similar distributions. The injected values are shown as green vertical/horizontal dashed lines. The T - P profile shown on the right was computed from 10,000 random samples of the MCMC, where the solid red curve shows the median profile, and the grey shaded regions show the 1σ , 2σ , and 3σ contours. The injected profile is shown as a green dashed curve. The cloud deck, located at $\log_{10}(P_{\text{cloud}})$ is highlighted as a blue dotted line. Below this value, the model is truncated, and thus the model inference breaks down. The contribution curve is also shown in blue.

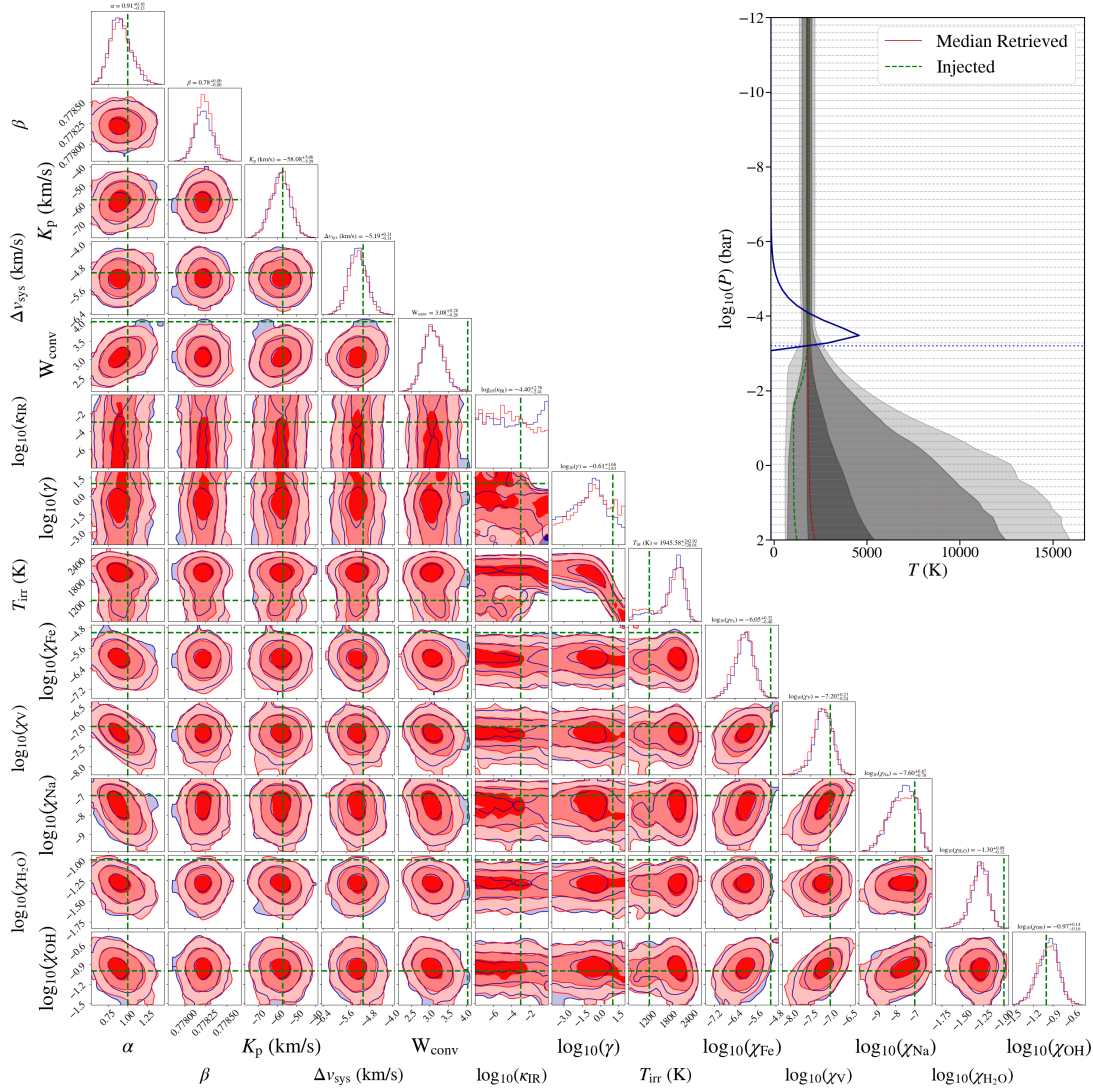


Figure C13: Similar to Fig. C12, for P12.

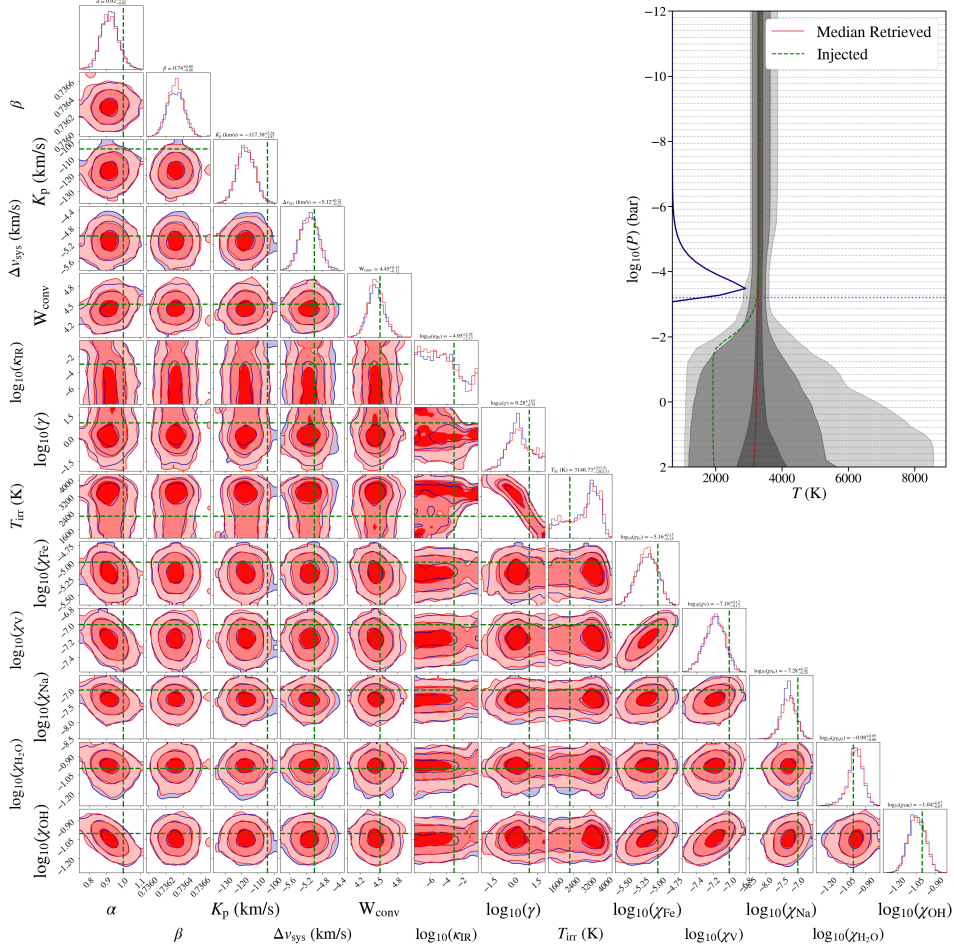


Figure C14: The atmospheric retrieval results for P2 injected into DS3 and preprocessed with SYSREM, with the 1D and 2D marginalised posterior distributions of each of the model parameters displayed. The red and blue posterior distributions represent independent subchains, of the same MCMC chain, both converging to similar distributions. The injected values are shown as green vertical/horizontal dashed lines. The T - P profile shown on the right was computed from 10,000 random samples of the MCMC, where the solid red curve shows the median profile, and the grey shaded regions show the 1σ , 2σ , and 3σ contours. The injected profile is shown as a green dashed curve. The cloud deck, located at $\log_{10}(P_{\text{cloud}})$ is highlighted as a blue dotted line. Below this value, the model is truncated, and thus the model inference breaks down. The contribution curve is also shown in blue.

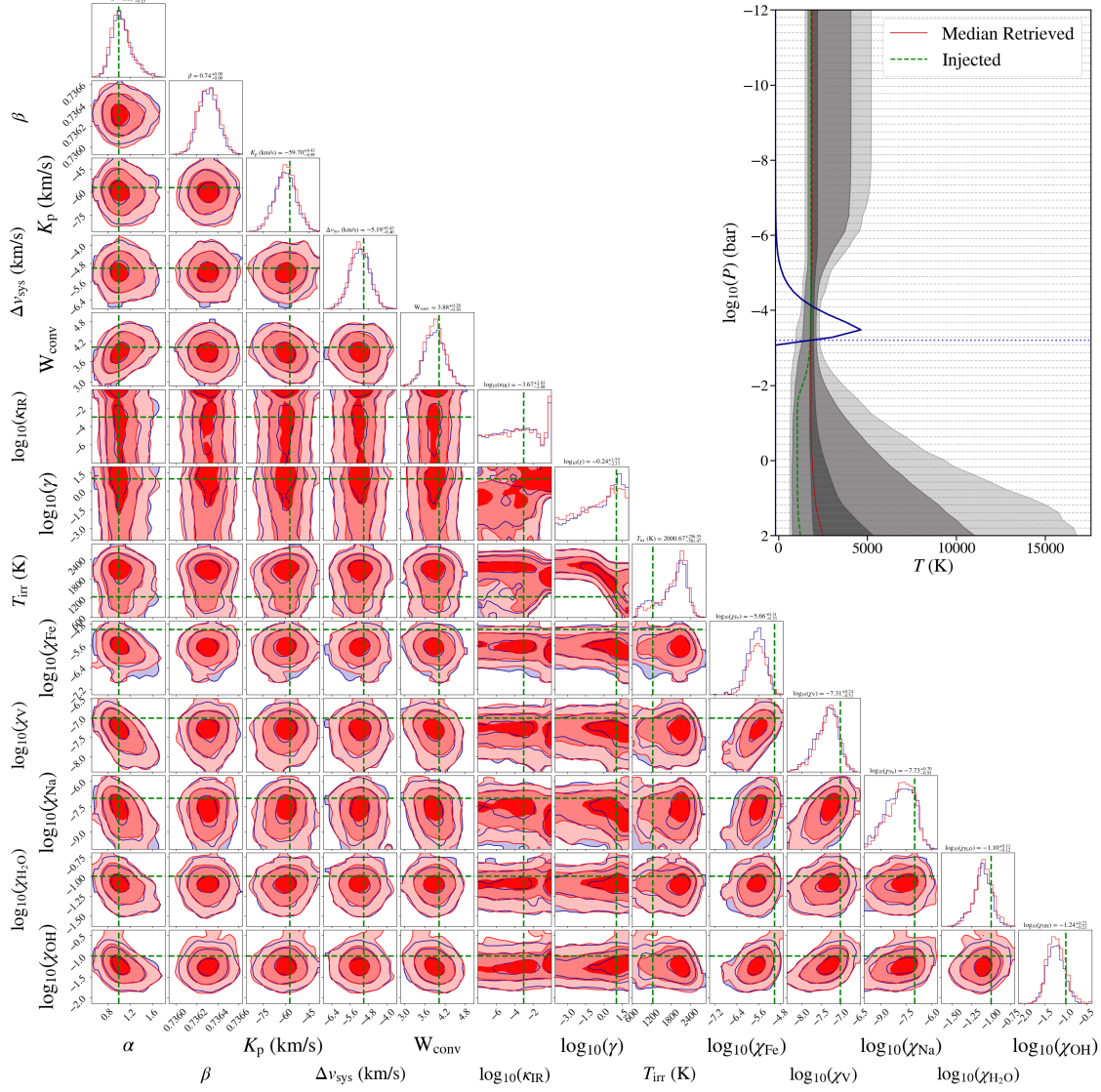


Figure C15: Similar to Fig. C14, for P12.

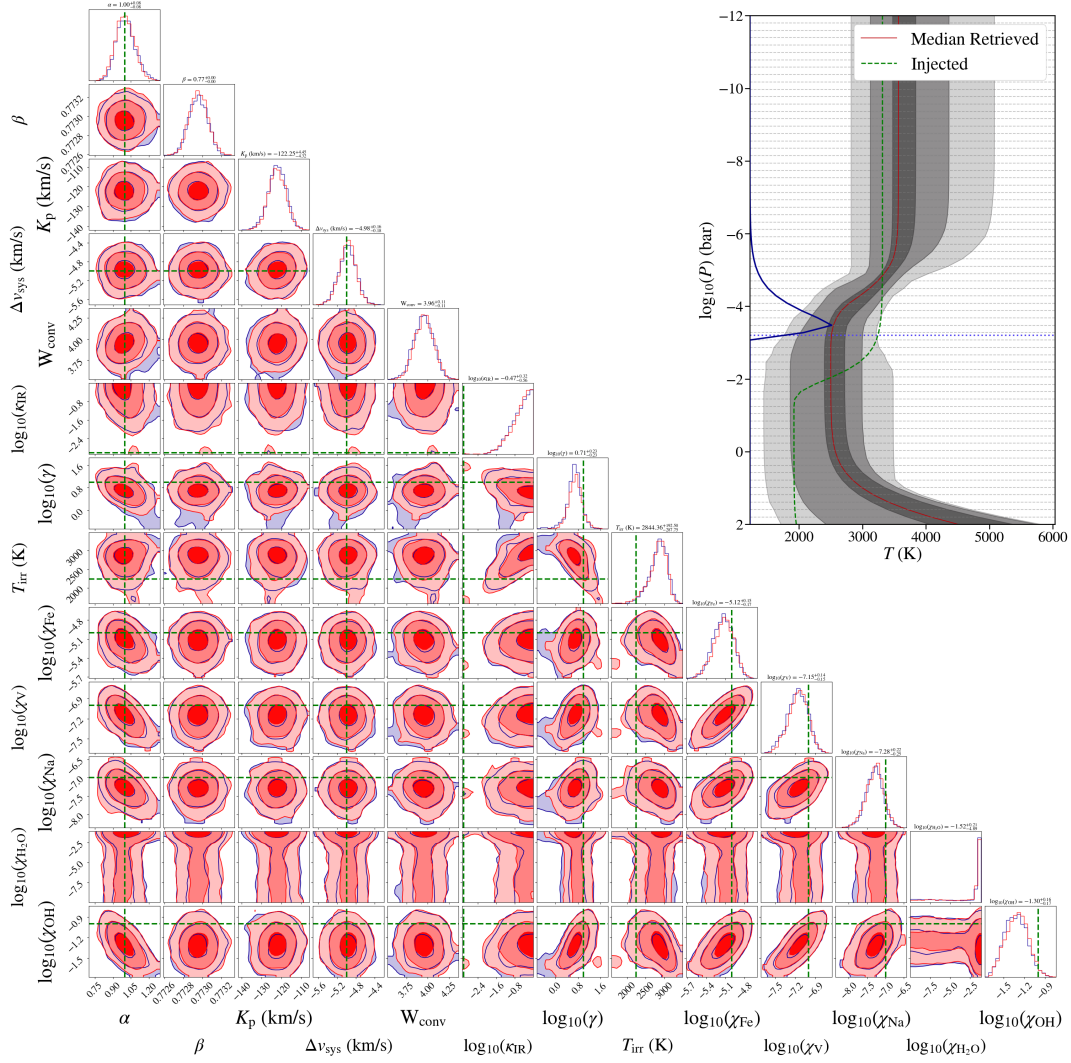


Figure C16: The atmospheric retrieval results for P2 injected into DS3 and preprocessed with MOLECFIT, with the 1D and 2D marginalised posterior distributions of each of the model parameters displayed. The red and blue posterior distributions represent independent subchains, of the same MCMC chain, both converging to similar distributions. The injected values are shown as green vertical/horizontal dashed lines. The T - P profile shown on the right was computed from 10,000 random samples of the MCMC, where the solid red curve shows the median profile, and the grey shaded regions show the 1σ , 2σ , and 3σ contours. The injected profile is shown as a green dashed curve. The cloud deck, located at $\log_{10}(P_{\text{cloud}})$ is highlighted as a blue dotted line. Below this value, the model is truncated, and thus the model inference breaks down. The contribution curve is also shown in blue.

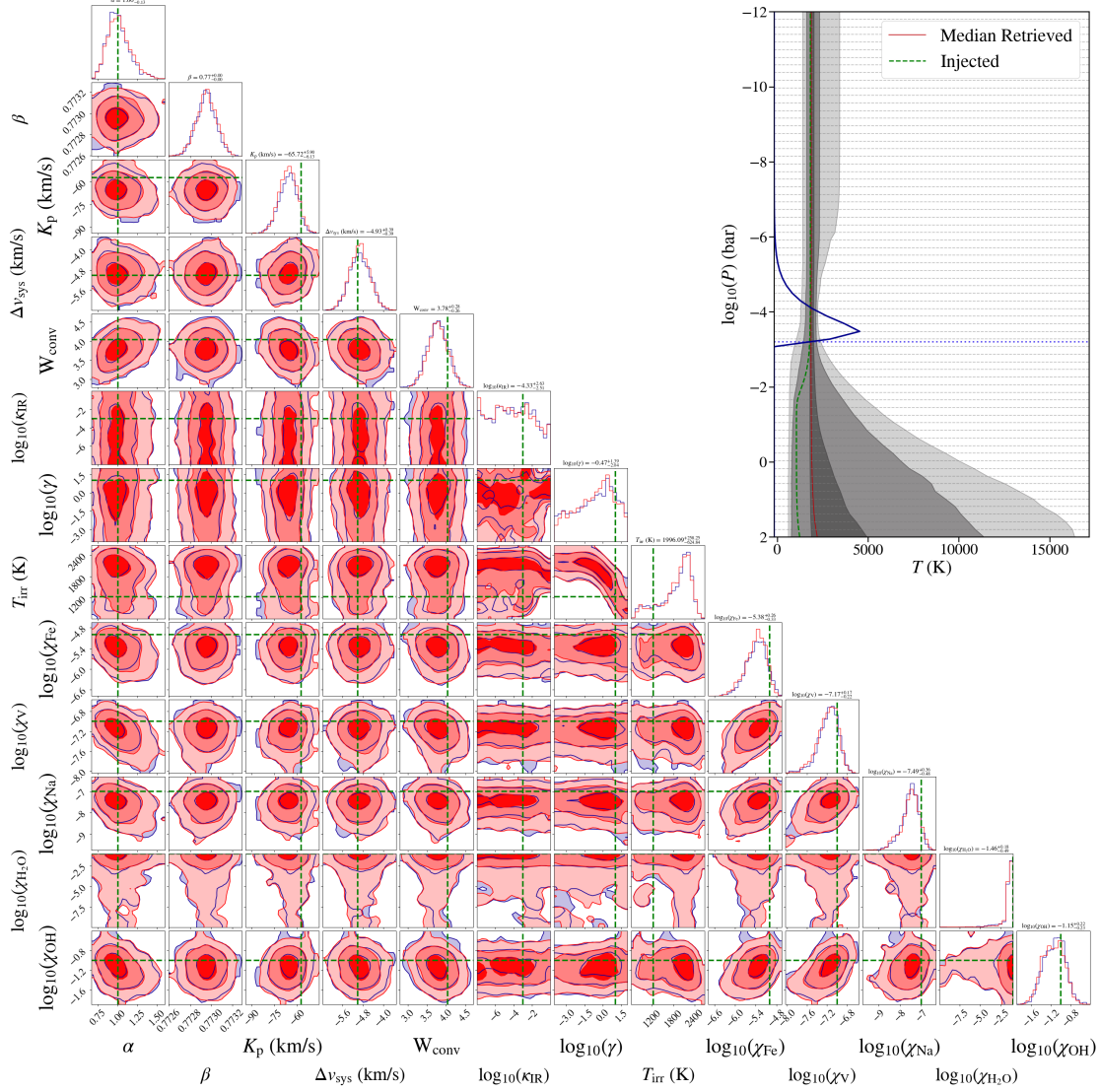


Figure C17: Similar to Fig. C16, for P12.

