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Bridging Ground-based High-resolution and JWST Low-resolution Spectroscopy for In-depth Exoplanet Atmosphere Analysis

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of the requirements for the degree of
Doctorate of Philosophy in Physics.

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Abstract

Since the first extrasolar planet was discovered orbiting a Solar-type star, spectroscopy has been a prominent method for finding and studying exoplanets and their atmospheres. In particular, hot Jupiters are an interesting category. Because of their proximity to their host star and large diameter, they are great targets for precise spectroscopic observations.

Various instruments are used for exoplanet spectroscopy, providing us with different types of data. Low-resolution spectroscopy ($R \lesssim 1,000$), often used in space-based observations (such as with the James Webb Space Telescope), provides us with broad spectral coverage. Low-resolution spectroscopy is used for the study of the spectral continuum and detection of the most dominant species. To study the individual lines in detail and detect atmospheric winds and rotation, we need high-resolution spectroscopy ($R \gtrsim 10,000$). Ground-based facilities are used for this type of observation, as the large instruments are necessary, often supplemented with adaptive optics for higher precision (for example, ESPRESSO and CRIRES spectrographs on the ESO/VLT or HARPS on La Silla 3.6m telescope).

Combining space-based low-resolution and ground-based high-resolution spectroscopy offers a powerful way to probe exoplanetary atmospheres in greater depth, as the two techniques are sensitive to different atmospheric layers and physical processes. This combined approach has the potential for ground-breaking discoveries, similar to when combining spectroscopic and photometric observations at the beginning of the 21st century led to the determination of the mass of exoplanets. Bridging the high- and low-resolution spectroscopy can lead to detecting less dominant species and potentially a discovery of biomarkers indicating the possibility of life.

This work focuses on developing a framework for the simultaneous analysis of JWST and ground-based high-resolution spectroscopic data, with the aim of providing tighter constraints on atmospheric properties. To validate this framework, archival low- and high-resolution spectra of the ultra-hot Jupiter WASP-121b are analysed. This report presents an overview of the methodology and the first results.

Keywords: Exoplanets, Transmission spectroscopy, Atmospheric retrievals, High-resolution, Low-resolution, JWST

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1. Introduction and Overview of the Literature

Research of extrasolar planets – that is, planets found outside of our Solar System – is one of the leading fields in astronomy in the 21st century. In just over three decades, it has captivated both professional and amateur astronomers as well as many enthusiasts from the general public. State-of-the-art ground based observatories and space telescopes are used to search for new exoplanets and further study the already-known planetary systems. With 6,153 confirmed exoplanets (NASA Exoplanet Archive [1]) and new research published daily, exoplanets are set to be in astronomical focus for decades to come.

In 2019, the Nobel prize in Physics was awarded to Michel Mayor and Didier Queloz for “the discovery of the first exoplanets orbiting a solar-type star”¹. This award served as a recognition of the exoplanet research – of its revolutionary findings and a huge impact it had on our understanding of the universe and our place in it.

As discussed in [2], there are several reasons to study exoplanets. First of all, we are learning more about the formation and evolution of our Solar System. Prior to the discovery of the first exoplanets (Wolszczan & Frail 1992 [3], Mayor & Queloz 1995 [4]), our knowledge of planetary systems was limited to our own. Although it has eight planets, hundreds of moons, and well over a million asteroids², the Solar System is missing various types of planets we observe in our Galaxy (e.g., hot Jupiters and fast orbiting planets, lava worlds, etc.). New discoveries allow us to study young systems in different stages of their evolution. As we compare new findings with our system, we learn more about its past. This can lead to better predictions about the future of the Earth, Solar System, and life in it.

Searching for extraterrestrial life is another objective of exoplanet research. Since the beginning, mankind has been fascinated by the question of life in the universe. We haven’t found life anywhere else in space yet. However, there are places even in our Solar System where the conditions could allow for its existence (e.g., Jupiter’s moon Europa³). Discovery of thousands of exoplanets broadened our search for habitable worlds further into outer space. While first discoveries often led to planets where we do not expect to find any signs of life, modern surveys focus on selecting targets that could have habitable

¹The prize was co-awarded to James Peebles for “theoretical discoveries in physical cosmology”. Taken as of 2026-04-01 from <https://www.nobelprize.org/prizes/physics/2019/summary/>

²Retrieved on 2026-04-01 from <https://science.nasa.gov/solar-system/asteroids/>

³Retrieved as of 2026-04-01 from source <https://science.nasa.gov/mission/europa-clipper/why-europa-ingredients-for-life/>

conditions. Thanks to the powerful research facilities and recent advancements in data analysis we are able to study Earth-like rocky planets or sub-Neptune sized exoplanets. Launch of the James Webb Space Telescope (JWST) in 2021 gave us the opportunity to better characterize these planets and to look for signatures of possible biomarkers in their atmospheres (Seager et al. 2025 [5]).

1.1 A Brief History of Exoplanet Research

1.1.1 The idea of extrasolar planets

The idea of planets existing outside of the Solar System has been fascinating humans for millennia. Notable is the theory of cosmic pluralism introduced by ancient Greek philosophers Democritus of Abdera (460 – 370 BC) and Epicurus (341 – 270 BC). Although they did not think directly about exoplanets, they imagined there are numerous solar systems in the universe, some similar to ours, some very different, and some probably inhabited by alien civilizations (Čeman & Pittich: Slněčná sústava [6], Kolinski [7]). However, their theory was not accepted at that time. It was almost two thousand years later when an Italian friar Giordano Bruno (1548 – 1600 AD) brought it back. He correctly described that the Milky Way – a light belt visible on a dark night sky – is the light from thousands and thousands of stars similar to our Sun [6]. He proclaimed that each one of these stars has its own “earths” (he probably became the first person to claim that stars are the same objects as our Sun). He suggested the universe is infinite with an infinite amount of “suns” (Rowland, Giordano Bruno: Philosopher/Heretic [8]). He also believed many of these distant worlds are inhabited by humans and animals.

The true scientific breakthrough came in the 20th century. A known universe was already much bigger (thanks to the discoveries of many galaxies other than our own Galaxy), and the idea of exoplanets orbiting other stars became widely accepted. Radial velocity (RV) measurements and photometry of transits were used for observations of binary systems. In 1952, Otto von Struve [9] discussed the possibility of exoplanet detection using available instruments. He concluded that the detection of a hot Jupiter-sized planet was feasible with expected RV oscillations in the range of $\pm 200 \text{ ms}^{-1}$. He also suggested the possibility of transits observation of such a planet.

1.1.2 First discoveries

The first confirmed discovery, though, came quite unexpectedly. In 1992, Aleksander Wolszczan and Dale Frail discovered irregularities in the timing variation of the millisecond pulsar PSR B1257+12 [3]. They concluded that two planet-like objects are orbiting the pulsar. Later, the third planet was confirmed in the system (Wolszczan 1994

[10]). All three planets are terrestrial (Konacki & Wolszczan 2003 [11]). One of them, PSR B1257+12 b, with its mass of $0.02 M_{\oplus}$ is considered to be the least massive exoplanet known⁴. A pulsar, a rapidly rotating neutron star, is just a remnant of a dead star which died in a massive supernova explosion. Before this discovery, it was believed to be impossible for planets to exist in such systems.

The first extrasolar planet orbiting a Sun-like star was discovered not long after. In 1995, Michel Mayor and Didier Queloz discovered an exoplanet orbiting the star 51 Pegasi using the method of RV measurements (Mayor & Queloz 1995 [4]). It is a Jupiter-like planet orbiting very close to its host star with a semi-major axis only 0.0527 AU. This proximity to the star warms its atmosphere to more than 1200 K. Therefore, the category of giant gas exoplanets orbiting close to their stars was named hot Jupiters (HJ). Soon after the discovery of 51 Pegasi b, more exoplanet detections followed. In many cases, exoplanets have been confirmed in the previously observed data (e.g., the discovery of 47 Ursae Majoris b, Butler & Marcy 1996 [12]).

Another important milestone was the first observation of transit of exoplanet HD 209458 b using transit photometry (Henry et al. 2000 [13], Charbonneau et al. 2000 [14]). The first detection of this hot Jupiter was done in 1999, just a few months after the exoplanet was discovered via RV measurements. A combination of two different detection methods made it possible to properly characterise HD 209458 b, as it would not be possible to calculate planetary mass based on only one of these methods. Two years later, thanks to the observations made with the Hubble Space Telescope (HST), a signature of planetary atmosphere was detected (Charbonneau et al. 2002 [16]). It was the first time the exo-atmosphere was confirmed. Since this discovery, numerous studies have been published focusing on its atmosphere.

1.1.3 An era of the space telescopes

With the beginning of the 21st century, the number of confirmed exoplanets has been rapidly increasing⁵. However, most of the discoveries were made by observing a single target, usually using the RV method. Though it was precise, especially at the beginning of exoplanet research, and the most successful discovery method, astronomers were keen to target more stars per observation. Transit photometry was an ideal method for this purpose. Various surveys were conducted from the ground based observatories. For example, well known is WASP or Wide Angle Search for Planets (Pollacco et al. 2006 [17]), which discovered almost 200 exoplanets⁶. However, to detect a transit of a potential

⁴According to the NASA Exoplanet Archive, retrieved 2026-04-02 from <https://exoplanetarchive.ipac.caltech.edu/cgi-bin/TblView/nph-tblView?app=ExoTbls&config=PSCompPars>

⁵The last year when no exoplanet was confirmed was 1997.

⁶Retrieved on 2026-04-03 from <https://wasp-planets.net/wasp-planets/>

exoplanet with an unknown orbital period, it is necessary to observe the target star for as long as possible. Naturally, ground based surveys are limited by the available night-time window and the weather conditions. This limitation paved the way for space-based survey observations.

The first mission dedicated to exoplanet research was CoRoT, launched in 2006. Its objective was to search for exoplanets with short orbital periods, especially seeking the large terrestrial planets (Baglin et al. [18], Monteiro et al. [19]). During its operational time⁷ CoRoT discovered around 30 exoplanets.

A truly ground-breaking mission was the following mission of the Kepler Space Telescope. Launched in 2009, Kepler focused on a single field of view (FOV), continuously monitoring more than 170,000 stars at once via photometric observation (Borucki et al. 2016 [20]). This allowed it to detect even the transits of exoplanets on Earth-like orbits (≈ 1 year orbital periods). To discover an exoplanet candidate, at least two transit detections were necessary. After a malfunction of two out of four reaction wheels in 2013, Kepler had to change its mission. The second mission, named K2, had to change its FOV approximately every month to ensure the telescope's stability (it used solar wind for the stabilization in its orbit). Kepler remained active until October 2018, when its fuel ran out. Up to that point, the Kepler/K2 mission has yielded 3,332 confirmed exoplanets to this date [1].

While Kepler/K2 was an incredibly successful mission, it was not optimized for ground based follow-up observations, which are necessary for candidate confirmation and proper characterization of discovered exoplanets. The biggest issue was the brightness of target stars, which reached magnitudes only a handful of ground based telescopes could observe with reasonable signal-to-noise ratios (SNR). Building up on these findings is mission TESS (Transiting Exoplanet Survey Satellite) launched in 2018 (Ricker et al. 2015 [21]). Its scanned area is almost 400 times larger than Kepler's, as its objective is to cover most of both hemispheres, as it gradually observes large slices of sky. Up to this date TESS, discovered almost 8,000 candidates out of which 765 have been confirmed [1].

Another, even more brave mission is scheduled to launch at the end of this year. PLATO (PLANetary Transits and Oscillations of stars) will study up to one million stars, mostly Sun-like yellow dwarf stars, red dwarfs, and subgiant stars, to detect transiting exoplanets (PLATO Definition study report, ESA 2017 [22]).

Apart from the photometric surveys, space telescopes such as HST or the Spitzer Space Telescope have been used for in-depth follow-up observations and characterization of exoplanets. Some examples are the aforementioned detection of atmosphere of HD 209458 b

⁷CoRoT mission ended in 2013 due to a malfunction.

(Charbonneau et al. 2002 [16]), characterization of ϵ Eridani b (Benedict et al. 2006 [23]), a precise radius calculation of HD 149026 b (Nutzman et al. 2009 [24]), a transit detection of HD 219134 b, a close-to-Earth rocky planet (Motalebi et al. 2015 [25]), discovering and detailed studying of five new exoplanets in the multi-planetary system TRAPPIST-1 (Gillon et al. 2017 [26]) and many more. These space facilities benefit from the view unobstructed by the Earth’s atmosphere, thus they can observe in the near-infrared and infrared parts of the spectrum. In this wavelength range (HST can observe up to $2.5\,\mu\text{m}$ while Spitzer was able to reach wavelengths of $180\,\mu\text{m}$), signatures of various molecular species can be observed in exoplanet spectra, allowing for detailed physical and chemical characterisation.

Huge advancements are being made by the James Webb Space Telescope (JWST), which was launched at the end of 2021. The mission was already planned to be heavily used for exoplanet research and has several upgrades from its predecessor, HST. Apart from the larger primary mirror, it has instruments specialized for near- and mid-infrared observations. Webb is also stationed at Earth’s L2 Lagrange point, where it has an unobstructed view for long observation runs (in comparison with Hubble, which has a more limited view in Earth’s orbit). High-precision JWST spectroscopy (both transmission and emission) allows us to detect key molecules in the exoplanet spectra, such as H_2O , CO_2 , CO , CH_4 , and to characterize exoplanet atmospheres – their physical structure and chemical composition in great depth (Greene et al. 2016 [27], Stevenson et al. 2022 [28]).

1.2 Methods of Exoplanet Research

Various methods are used for the detection and characterization of exoplanets. Most of the methods use indirect effects of planets on their host star, such as pulsar timing, astrometry, or gravitational microlensing. However, in recent years, almost 100 exoplanets were discovered by direct imaging ([1]). Well-known examples are β Pic b (Lagrange et al. 2009 [29] or the HR 8799 system (Marois et al. 2008 [30]).

1.2.1 RV Measurements

The first discoveries were mostly achieved using the RV measurements. It is an indirect method using the Doppler shifts in the stellar spectra. When an exoplanet orbits the star, they are actually both moving around the star-planet barycentre. Stellar movement creates the Doppler shift of the spectral lines detected as the change of radial velocity of the star (Mayor & Queloz 1995 [4]). The RV amplitude depends on the planetary mass and can be calculated as

$$K = \left(\frac{2\pi G}{P} \right)^{\frac{1}{3}} \frac{M_p \sin i}{(M_p + M_*)^{\frac{2}{3}}} \frac{1}{(1 - e^2)^{\frac{1}{2}}}, \quad (1.1)$$

where P is orbital period, i and e are orbital inclination and eccentricity, G is gravitational constant and M_p , M_* are mass of the planet and star respectively. From the spectroscopic observations alone, the orbital inclination cannot be computed; the mass of the exoplanet can be expressed only as $M_p \sin i$ (Fischer et al. 2016 [31]).

1.2.2 Transit Photometry

Transit photometry is historically the most successful exoplanet discovery method [1]. When an extrasolar planet orbits its parent star on an orbit aligned with our line of sight, it periodically crosses the stellar disk, covering it partially. This planetary transit causes the stellar brightness to decrease. As it is possible to do high-precision photometry of many targets at once, this method is ideal for long-term sky surveys. Modest requirements for photometric observations make them accessible for astronomers with almost any type of telescope and simple CCD cameras.

From the shape of the light curve much information can be found. First of all, from the time between two transits, an orbital period P can be determined directly. Using Newton's gravitational law and Kepler's third law, the semi-major axis a can be calculated from period P . From the transit depth δ given by the ratio of in-transit drop of flux ΔF to out-of-transit flux F we can calculate the planet-to-star radius ratio R_p/R_* as

$$\delta = \frac{\Delta F}{F} \simeq \left(\frac{R_p}{R_*} \right)^2, \quad (1.2)$$

assuming a uniform surface brightness of the parent star (Seager & Mallén-Ornelas 2003 [32]). For higher precision, we need to consider the effect of limb darkening in our calculations (Mandel & Agol 2002 [33]). When the stellar parameters are known, the exoplanet radius can be directly calculated from the R_p/R_* ratio. Other obtainable parameters are transit duration τ and the transit latitude on the stellar disk d , using which the orbital inclination i can be derived. Therefore, when we combine RV measurements with transit photometry, using inclination we can calculate mass of the exoplanet.

1.2.3 Transmission Spectroscopy

Mass calculation is not the only advantage of combining spectroscopic and transit observations. When a transiting exoplanet passes in front of its host star, a fraction of the stellar light is transmitted through its atmosphere, imprinting wavelength-dependent absorption features. Therefore, the transit depth is a function of the wavelength $\delta(\lambda)$ and

the same goes for the effective planet radius $R_p(\lambda)$. Substituting this into Eq. (1.2) yields the transmission spectrum

$$\delta(\lambda) = \left(\frac{R_p(\lambda)}{R_\star} \right)^2. \quad (1.3)$$

This method can provide a wide range of information about the planet’s atmosphere, such as molecular composition, atmospheric scale height, bulk properties, or temperature-pressure (T-P) profile (Seager & Sasselov 2000 [34]). Transmission spectroscopy probes only the limb of the planet’s atmosphere, as the observed radius corresponds to the altitude where the atmosphere becomes optically thick, which may be set by a cloud deck or gas opacity. This technique is most effective for highly irradiated planets such as hot Jupiters and ultra-hot Jupiters, where large atmospheric scale heights lead to enhanced transmission signals (Madhusudhan 2012 [35]).

Depending on the instrumentation, two regimes can be distinguished: low-resolution spectroscopy usually conducted with space-based telescopes (e.g., JWST or HST) and high-resolution spectroscopy using ground-based facilities (e.g., ESPRESSO spectrograph on VLT or HARPS on La Silla).

1.2.4 Low-Resolution Spectroscopy

Typically, space-based facilities are used for low- to medium-resolution spectroscopy with resolving power up to $R \sim 3,000$. James Webb Space Telescope is currently leading the field with moderate spectral resolution and wide wavelength range in the near to mid-infrared part of the spectrum across several instruments (e.g. $0.6 - 5.3\mu\text{m}$ for NIRSpec, $5 - 28\mu\text{m}$ for MIRI, Greene et al. 2016 [27]).

Low-resolution spectroscopy can provide a broad spectral coverage ideal for studying the continuum. It can be used for the detection of the most dominant species (although it cannot resolve individual lines). An important advantage of space-based observations is the absence of telluric line contamination from the Earth’s atmosphere, providing us with optimal precision for smaller planets. It can also be used for the study of exoplanets’ T-P profile and climate, e.g., Ahrer et al. 2023 [36], Rustamkulov et al. 2023 [37], Smith et al. 2024 [38]. However, it is not capable of resolving individual lines, and thus we cannot study their shapes or positions. It is also less sensitive in the optical part of the spectrum and is sensitive to systematic effects and stellar contamination affecting absolute transit depth measurements (Rackham et al. 2018 [39]).

1.2.5 High-Resolution Spectroscopy

High-resolution spectroscopy utilizes the high resolving power of ground-based stable spectrographs ($R \sim 50,000 - 100,000$), such as HARPS at ESO/La Silla or ESPRESSO, CRIRES, or UVES at ESO/VLT. The method is based on Doppler-resolved spectroscopy, studying radial velocity shifts of the planetary signal embedded in the observed spectra. At high spectral resolution, it is possible to resolve individual lines in exoplanet transmission spectra. Thanks to the relatively large radial velocity difference between the planet and the host star, planetary spectral lines can be detected against the background of stellar spectra. This is achieved using the cross-correlation method, which combines the signal from numerous spectral lines into a single detection by correlating the data with a model template. This allows the detection of species that would otherwise be undetectable due to weak spectral signatures. The detection is typically performed in the two-dimensional (K_p, v_{sys}) space, where the signal is maximized when the model matches the planetary orbital motion. It is also possible to study the shapes of individual lines (Snellen et al. 2010 [40], Brogi et al. 2012 [41], Gibson et al. 2020 [42]).

This method is useful for the study of atmospheric composition and dynamics, i.e., winds or jet streams (Smith et al. 2024 [38]). It is primarily sensitive to the upper atmosphere where spectral lines are formed. On the other hand, the spectra must be carefully cleaned of telluric contamination from the Earth’s atmosphere. The exoplanet spectrum cannot be inspected directly, and only limited information about the continuum is available.

1.2.6 Combining High- and Low-Resolution Spectroscopy

Combining space-based low-resolution with the ground-based high-resolution spectroscopy provides a complementary approach to probing exoplanetary atmospheres, as the two techniques are sensitive to different atmospheric layers and physical processes (Smith et al. 2024 [38]). This synergy allows for improved constraints of atmospheric composition and structure. It can lead to detecting less dominant species and potentially a discovery of biomarkers indicating the possibility of life.

The first step towards this approach is the development of a framework for the simultaneous analysis of JWST time-series spectra and ground-based high-resolution spectroscopic data. The aim of this framework is to provide tighter constraints on atmospheric properties. For its validation, archival low- and high-resolution spectra of hot and ultra-hot Jupiters are ideal due to their strong irradiation and well-characterized atmospheres. In this work, a benchmark ultra-hot Jupiter WASP-121b is used. This report presents an overview of the methodology and the initial steps towards the joint analysis.

2. Methods and Results

For creating a framework for combining high- and low-resolution retrievals, it is necessary to prepare separate pipelines for each method first. As stated in section 1.2.6, we chose WASP-121b as a reference target. It is a benchmark ultra-hot Jupiter with a solid database of acquired data from ground-based high-resolution spectrographs such as ESPRESSO, CRIRES+, and UVES, as well as the space telescopes (Spitzer, HST, JWST). A broad overview of the available datasets is presented in Table A.1 of Attachment A. WASP-121b orbits an F-type star at an approximate distance of 270 ly (Delrez et al. [43]) with a period of 1.2749255 days. It was discovered in 2015 by the WASP-South survey, in close collaboration with the Euler and TRAPPIST telescopes.

2.1 Low-Resolution Spectroscopy

For low-resolution spectroscopy, we use a WASP-121b transit observed as part of the phase-curve observations done by the JWST program GO-1729 (PI: Mikal-Evans, co-PI: Kataria). For the observation, the NIRSpec/G395H instrument was used. The resulting time-series spectra cover the wavelength range between 2.86 and 5.18 μm . There is a gap in wavelengths from 3.72 to 3.82 μm caused by the division of the NIRSpec instrument into two detectors, NRS1 and NRS2. We worked with the pre-processed data reduced according to Mikal-Evans et al. [44]. For our analysis, we used only part of the phase curve with the transit – approximately 2 hours before and after the transit.

2.1.1 Transit Fitting

To extract a transmission spectrum, the time-series spectra (Figure A.1) were binned into 10-pixel wavelength channels, which we used to construct the spectral light curves. These were subsequently fitted with a transit model. We adopted the same binning scheme as Gapp et al. 2025 [45] to enable a direct comparison of the resulting transmission spectra. For 10-pixel channels, we get 127 points for NRS1 and 204 points for NRS2. This corresponds to the spectral resolution $R \sim 600$ varying with the wavelength. We initially tested 2-pixel channels as well, giving us $R \sim 3000$. However, in this case, we got the transmission spectrum with a significantly lower signal-to-noise ratio. For this reason, we decided to use a 10-pixel bin, as it is sufficient for the purpose of our framework tests. After this point, we combined channels from both detectors into one dataset for fitting.

Before fitting the spectroscopic light curves, we fitted the white light curve to better constrain the global transit parameters (Figure 2.1). These were then used for fitting

each channel, providing a better starting position for spectroscopic light curves fitting. Using this approach, typically, no more than one channel fit failed to converge.

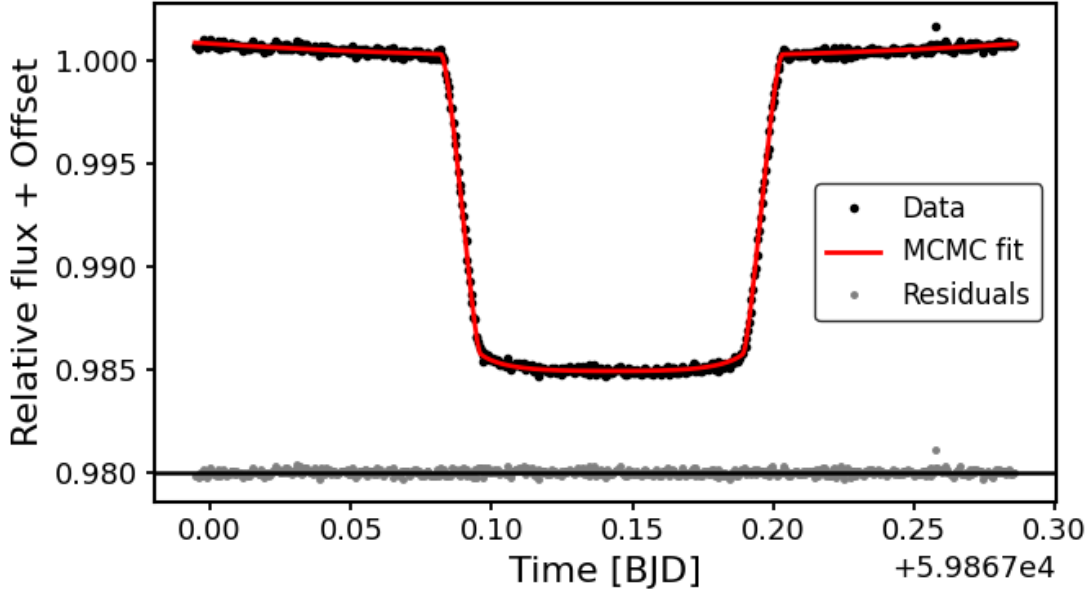


Figure 2.1: MCMC best fit of the white light transit curve with residuals.

We model the transit light curves using an analytic formula for a planet on a circular orbit with quadratic limb darkening. The free parameters of the model are the central transit time (T_0), scaled semi-major axis ($a/R_\star$), a planet-to-star radius ratio ($R_p/R_\star$), impact parameter (b), two stellar limb-darkening parameters (c_1 and c_2), with out-of-transit flux normalisation (f_{oot}), and linear and quadratic baseline trends (T_{grad} , T_{grad2}). The orbital period P is fixed during the white light curve fit. For fitting the spectroscopic light curves we additionally fixed the central transit time (T_0), scaled semi-major axis ($a/R_\star$), and impact parameter (b). Therefore, the parameter vector for fitting was $(R_p/R_\star, c_1, c_2, f_{\text{oot}}, T_{\text{grad}}, T_{\text{grad2}})$.

In order to retrieve posterior distributions of the model parameters, we used a Markov chain Monte Carlo (MCMC) framework. However, as this algorithm can be sensitive to the initial guess of parameter space, we fitted the model first using a least-squares optimisation with the Levenberg–Marquardt (LM) algorithm. We then used the best-fit parameters from LM optimisation to initialise the MCMC algorithm.

The likelihood function was defined assuming independent Gaussian uncertainties with a free white-noise parameter (σ). The log-likelihood is given by the equation

$$\ln \mathcal{L} = -\frac{1}{2} \sum_{i=1}^N \frac{(f_i - m_i)^2}{\sigma^2} - N \ln \sigma - \frac{N}{2} \ln(2\pi), \quad (2.1)$$

where f_i are the fluxes (i.e. data) and m_i is the model. We adopted uniform priors with

physically motivated bounds as we require positive orbital and noise parameters. We also require standard conditions ($c_1 \geq 0$, $c_1 + c_2 \leq 1$, $c_1 + 2c_2 \geq 0$) on the quadratic limb-darkening parameters.

We used Differential-Evolution Markov Chain (DEMC) (Eastman et al. 2013 [46]) for posterior distribution sampling, running the MCMC chain with 256 walkers in parallel with an initial burn-in length of 1000 steps to facilitate an effective exploration of parameter space. Then we performed walker culling and redraw followed by the second burn-in with a length of 100 steps and the main chain with a length of 200 steps. This setup was used for both white light curve and spectroscopic light curves.

The MCMC analysis gives us a posterior distribution of the model parameters for each of the spectral channels. Both input prior values and result posteriors are presented in Table 2.1. From the value of planet-to-star radius ratio we can obtain using Eq. (1.3) a transit depth $\delta(\lambda)$ to construct a transmission spectrum. The resulting spectrum is presented in Figure 2.2.

Parameter	Description	Prior	Posterior
T_0	Mid-transit time	$\mathcal{U}(-\infty, \infty)$	59867.14260 ± 0.00002
P	Orbital period (days)	fixed	1.2749255
$a/R_\star$	Scaled semi-major axis	$\mathcal{U}(0, \infty)$	3.770 ± 0.011
$R_p/R_\star$	Planet-to-star radius ratio	$\mathcal{U}(0, \infty)$	0.12193 ± 0.00011
b	Impact parameter	$\mathcal{U}(0, \infty)$	0.183 ± 0.019
c_1	Linear limb-darkening coefficient	see text	0.006 ± 0.008
c_2	Quadratic limb-darkening coefficient	see text	0.152 ± 0.018
f_{oot}	Out-of-transit flux normalisation	$\mathcal{U}(-\infty, \infty)$	1.00020 ± 0.00002
T_{grad}	Linear baseline trend	$\mathcal{U}(-\infty, \infty)$	$(-2.87 \pm 2.63) \times 10^{-6}$
$T_{\text{grad}2}$	Quadratic baseline trend	$\mathcal{U}(-\infty, \infty)$	$(5.25 \pm 0.23) \times 10^{-5}$
σ	White-noise parameter	$\mathcal{U}(0, \infty)$	$(1.32 \pm 0.04) \times 10^{-4}$

Table 2.1: Inputs and results for the model parameters for fitting the white light curve using MCMC.

2.1.2 Atmospheric Model for Transmission Spectrum

For the atmospheric retrieval of the transmission spectrum, we need a 1D forward atmospheric model for WASP-121b. We constructed this model for our low-resolution retrieval using the Python package **IRRADIATOR** (Gibson et al. 2022 [47]). The model follows a numerical framework in which transmission spectra are computed via radiative transfer in transmission geometry using wavelength-dependent opacity cross-sections.

We set the pressure grid to 80 layers with logarithmic range from 10^2 to 10^{-12} bar. The temperature-pressure profile was computed using the parametric model from Guillot

2010 [48]. This model is parametrized by mean infrared opacity (κ_{IR}), ratio of visible-to-infrared opacity (γ), irradiation temperature (T_{irr}), and internal temperature (T_{int}) as free parameters.

To describe the atmospheric composition, we assumed an H_2 -dominated atmosphere with a fixed mean molecular weight (see Table 2.2 with other fixed system parameters), and we set the volume mixing ratios (VMRs) χ_{species} as free parameters for each species. We included H_2O and CO as absorbing species for these test retrievals. We also used a reference pressure level (P_0) to anchor the planetary radius. To parametrize a grey cloud deck (below which the atmosphere is assumed to be opaque), we set a grey cloud-top pressure (P_{cloud}). We also included a fixed scaling parameter for Rayleigh scattering opacity (χ_{Ray}) to account for enhanced scattering in the atmosphere affecting the spectral slope.

We are using pre-tabulated opacity cross-sections computed with **petitRADTRANS** (Molliere et al. 2019 [49]), interpolated to the local temperature and pressure in each atmospheric layer. The transmission spectrum is computed by evaluating the absorption of stellar light along paths through the planetary limb, including contributions from all atmospheric layers and species.

The resulting transmission spectra are calculated across a wavelength range of $2.7\text{--}5.3\mu\text{m}$ at a constant resolution of $R \approx 200,000$ of the wavelength grid. This resolution is significantly higher than required for our low-resolution spectrum; however, we used it to test our framework for future incorporation into joint retrievals with high-resolution datasets. Calculated spectra are subsequently binned to the observational wavelength grid for comparison with the data.

Parameter	Description	Value	Source
$R_\star$	Stellar radius	$1.458 R_\odot$	Delrez et al. 2016 [43]
$R_p/R_\star$	Planet-to-star radius ratio	0.1228	Gapp et al. 2025 [45]
R_p	Planet radius	derived	this work
M_p	Planet mass	$1.184 M_J$	Delrez et al. 2016 [43]
$T_\star$	Stellar effective temperature	6460 K	Delrez et al. 2016 [43]
g	Surface gravity	derived	this work
μ	Mean molecular weight	2.33	Guillot 2010 [48]

Table 2.2: Fixed system and atmospheric parameters adopted in the atmospheric forward model.

2.1.3 Low-Resolution Retrieval

Performing an atmospheric retrieval means that we let the forward model compute transmission spectra based on a given set of parameters. The retrieval then explores the parameter space in order to identify models that agree with the data set of given transit depths. Similar to the transit fitting, we performed an atmospheric retrieval using an MCMC algorithm. The likelihood was defined assuming Gaussian-distributed residuals between the observed and modelled transmission spectra function. The log-likelihood function was created on the same basis as Eq. (2.1)

$$\ln \mathcal{L} = -\frac{1}{2\beta^2} \sum_{i=1}^N \frac{(d_i - m_i)^2}{\sigma_i^2} - N \ln \beta, \quad (2.2)$$

where d_i stands for observed transit depths, m_i are the model values, σ_i are observational uncertainties, and we also included a fitted noise scaling parameter β . We used uniform priors and imposed hard bounds on all model parameters defined by lower and upper limits. Additionally, we constrained the atmospheric temperature for T-P profile to the range of 1,000 – 4,000K as this is physically sufficient condition. If any parameter violated these conditions, it was rejected and assigned with a zero value of the prior probability.

The posterior distribution was sampled using the Metropolis–Hastings (MH) algorithm with 4 parallel chains. They were initialized around the initial parameter vector (κ_{IR} , γ , T_{irr} , T_{int} , P_0 , P_{cloud} , χ_{Ray} , $\chi_{\text{H}_2\text{O}}$, χ_{CO} , β) with 2 fixed parameters T_{int} and χ_{Ray} and total of 8 free parameters. We sampled parameters spanning multiple orders of magnitude in logarithmic scale, i.e., in log 10, with uniform priors defined in this space (see Table 2.3). To secure a valid starting point, we scaled down the expected parameter uncertainties.

We used the burn-in phase with 10,000 steps followed by a main chain with the same length of 10,000 steps. No walker culling or redrawing was applied during the sampling. This setup of the MCMC framework proved to be the best in terms of convergence and efficiency.

As we show in the Figure 2.2, our model, calculated with MCMC best fit parameters, fits well the transmission spectrum as it sits within the observed data uncertainties. For the final model, we are using best-fit parameters corresponding to the maximum posterior solution. The retrieved posterior distributions are presented in Table 2.3 (also shown in Figure A.4). They indicate the constraints on the atmospheric parameters and molecular abundances for H₂O and CO. We took 1,000 MCMC samples of T-P profiles are shown in Figure 2.4 with median sample and 2σ percentiles.

Parameter	Description	Prior	Value
$\log_{10}(\kappa_{\text{IR}})$	Mean infrared opacity	$\mathcal{U}(-2, 6)$	-1.95 ± 1.53
$\log_{10}(\gamma)$	Visible-to-infrared opacity ratio	$\mathcal{U}(-2, 20)$	-1.50 ± 0.95
T_{irr}	Irradiation temperature (K)	$\mathcal{U}(1200, 4000)$	1222 ± 254
T_{int}	Internal temperature (K)	fixed	20
$\log_{10}(P_0)$	Reference pressure (bar)	$\mathcal{U}(-12, 2)$	-1.56 ± 0.79
$\log_{10}(P_{\text{cloud}})$	Grey cloud-top pressure (bar)	$\mathcal{U}(-2, 10)$	3.45 ± 3.04
$\log_{10}(\chi_{\text{Ray}})$	Rayleigh scattering scaling	fixed	1
$\log_{10}(\chi_{\text{H}_2\text{O}})$	H ₂ O mixing ratio	$\mathcal{U}(-10, -1.5)$	-5.44 ± 1.13
$\log_{10}(\chi_{\text{CO}})$	CO mixing ratio	$\mathcal{U}(-10, -2)$	-2.82 ± 1.48
β	Noise scaling parameter	$\mathcal{U}(-10, 10)$	1.0031 ± 0.0001

Table 2.3: Inputs and results for atmospheric parameters of WASP-121b retrieved from the transmission spectrum.

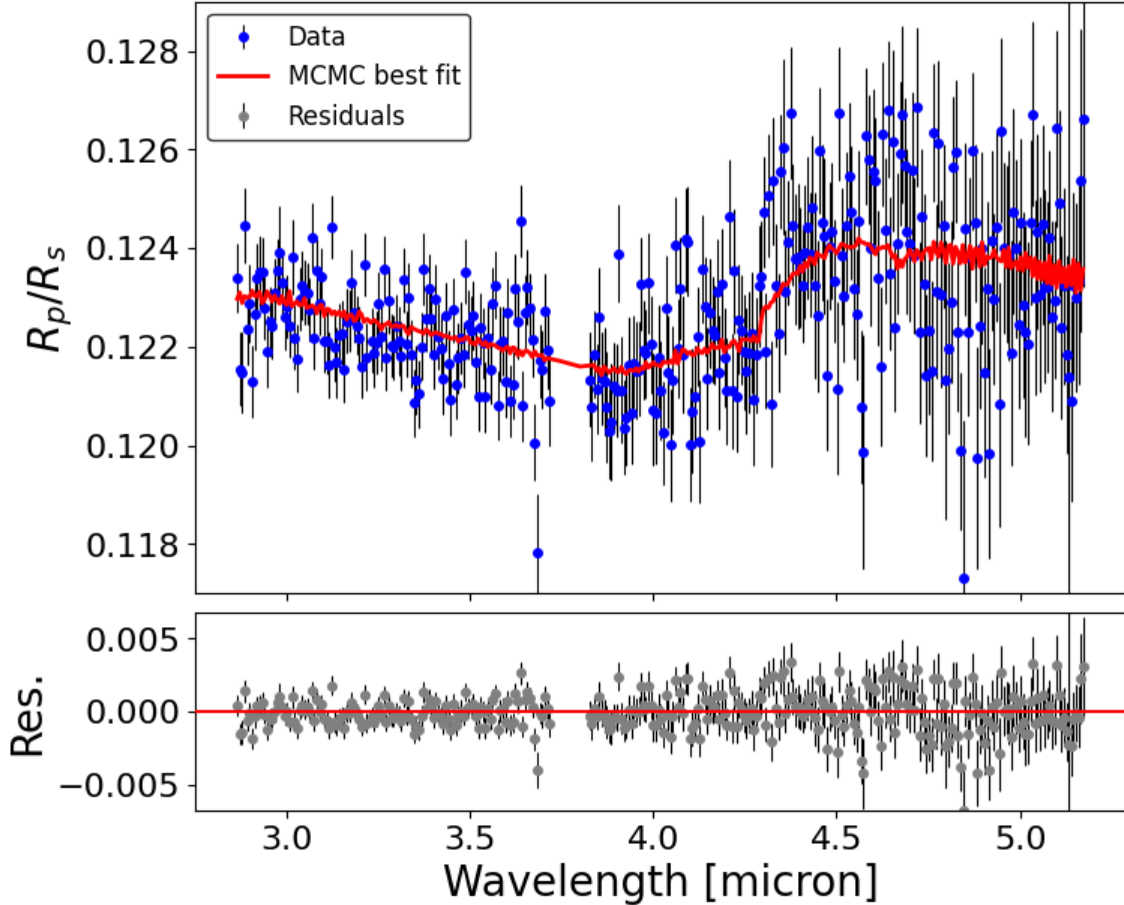


Figure 2.2: Transmission spectrum of WASP-121b plotted with model using MCMC best fit parameters (*top panel*), and residuals (*bottom panel*).

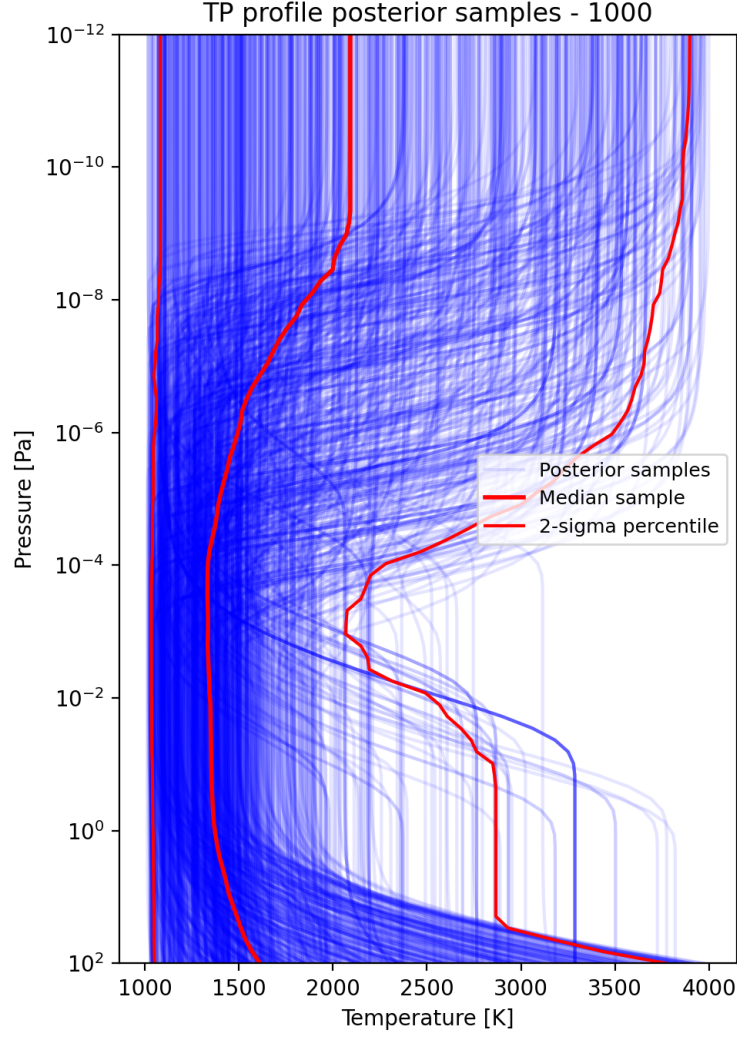


Figure 2.3: T-P profiles retrieved from the transmission spectrum. We present 1000 MCMC samples with a median sample of T-P profile and 2σ percentiles.

2.2 High-Resolution Spectroscopy

High-resolution retrievals were performed on WASP-121b data obtained by the UVES spectrograph mounted at the ESO VLT Unit Telescope 2 as part of program 098.C-0547 (PI: Gibson). Two transits were observed. In this work, we use only the blue arm with a central wavelength of 437 nm, from the transit on December 25, 2016. This is sufficient for our framework testing. The echelle spectra were taken with a set-up giving resolution $R \sim 80,000$ in wavelength range $\approx 3770 - 4950 \text{ \AA}$ over 29 spectral orders. They were taken with an exposure time of 100 seconds and a readout time of approximately 24 seconds, which gave a cadence of 124 seconds. In total, 137 exposures were taken in ≈ 4.7 hours, out of which 3 had not been used due to the lost guidance, leaving us with 134 time points. The first 28 were taken before ingress, 80 in transit, and 26 after egress.

For this work, we used pre-processed data that were treated with basic calibration and blaze correction. The extracted time-series spectra were aligned in the rest frame of the star (as outlined in Gibson et al. 2019 [51] and Gibson et al. 2020 [42]). The dataset includes associated uncertainties derived from the pre-processing statistics, which are adopted in our analysis.

The Rossiter-McLaughlin has been detected in transit of WASP-121b, with amplitude of approximately $100 \text{ m} \cdot \text{s}^{-1}$ (with $\nu \sin i = 13.6 \text{ km} \cdot \text{s}^{-1}$), and its orbit is nearly-polar with projected obliquity of 258° (Delrez et al. 2016 [43]). Generally, the RM effect can impact the spectra; it can affect the removal of stellar spectra or cause planet-like features to appear. However, as discussed in Gibson et al. 2020 [42], the change in planet velocity for WASP-121b during the transit is far greater (more than $100 \text{ km} \cdot \text{s}^{-1}$), thus the RM effect can have only a limited impact in this case.

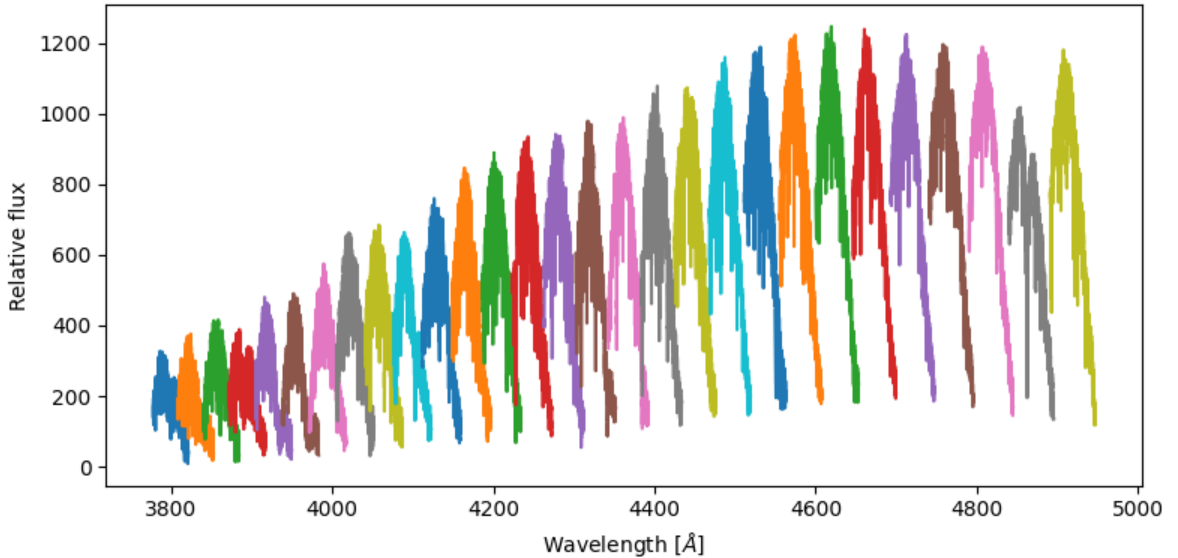


Figure 2.4: UVES echelle spectrum of WASP-121b consisting of 29 orders, used for the high-resolution retrievals.

2.2.1 Stellar and Telluric Lines Removal with SysRem

As the planet is orbiting the star, its signal in the spectra is revealed as the Doppler-shifted signatures. Ground-based observations are also affected by telluric absorption lines originating in the Earth’s atmosphere (caused primarily by molecules of H_2O , O_2 , and CO_2). These features, together with stellar absorption lines, remain approximately stationary in wavelength during an observing sequence, whereas the planetary signal shifts by more than 100 km s^{-1} during transit. Therefore, we need to remove these stationary or quasi-static trends in time. For their removal, we employed the **SysRem** algorithm (Tamuz et al. 2005 [52]), which is well applicable for high-resolution spectroscopy (Birkby et al.

2017 [53]). The algorithm is conceptually similar to a weighted principal component analysis (PCA).

Before the application of **SysRem**, we normalised our spectra by dividing through each order by its median spectrum, removing the dominant continuum structure and placing the data on a relative scale. During this process, the uncertainties were scaled accordingly.

We then applied the **SysRem** to each order. The algorithm determines a model representation of the 2D data array (time $\times$ wavelength) as an outer product of two column vectors, determined for each iteration. After one iteration, the model is subtracted from the data, and it is used for the next **SysRem** iteration. However, rather than using the end product (subtracted residuals), we sum the **SysRem** models for each iteration, creating a global model. As the final step, each order of the dataset is subtracted by this global model. This approach helps to preserve the Doppler-shifted planetary signal while allowing the algorithm to clean the data of telluric and instrumental variations (Gibson et al. 2020 [42]). Within our pipeline, we performed 10 **SysRem** iterations, which proved sufficient to remove the dominant stationary signals while preserving the planetary signal. The results are shown in Figure 2.5

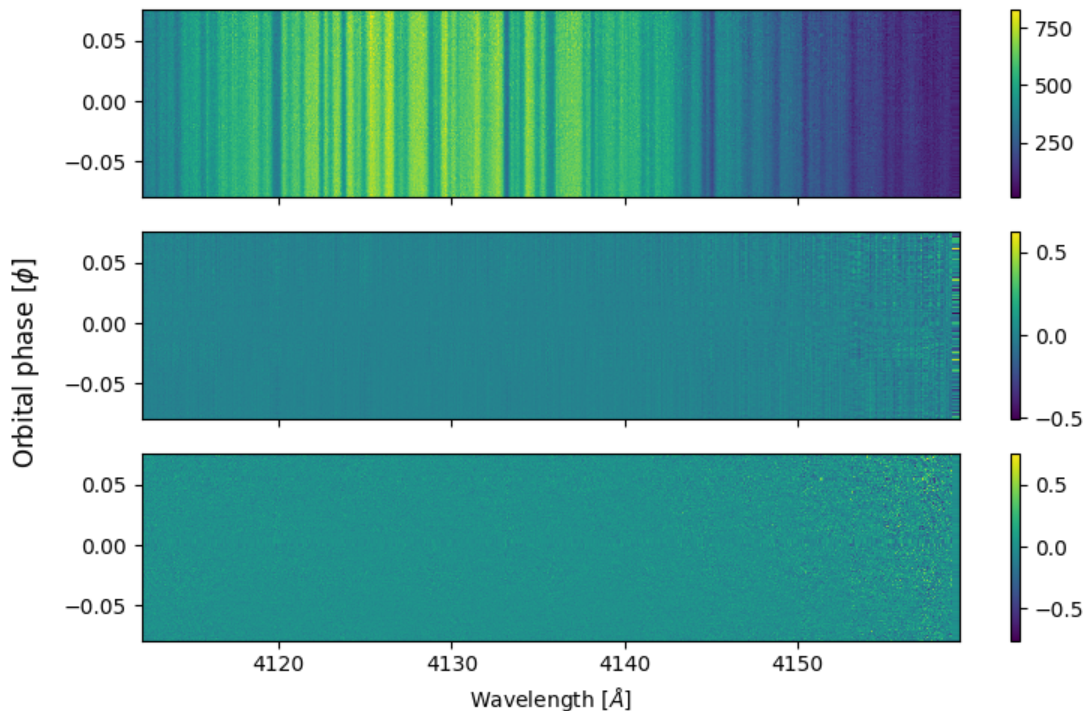


Figure 2.5: Single order of the pre-processed echelle spectrum (*top panel*), SysRem global model for given order (*middle*), and processed data – residuals (*bottom*).

2.2.2 Parameter Space for High-Resolution Retrievals

A high-resolution transmission spectrum was generated from the forward model described in Section 2.1.2, and used as a template in the Doppler cross-correlation analysis. We used the same atmospheric structure, opacity setting, and parametrization as in the low-resolution case (see Table 2.2). We only changed the wavelength grid range for calculation of the template spectra to 370–870nm. For computational efficiency of our test retrievals, we used a slightly lower constant resolution of the wavelength grid at $R \approx 100,000$. Nonetheless, it is still adequate for cross-correlation analysis. We chose a neutral iron FeI as the absorbing species for our test retrievals, as it has been well detected in the atmosphere of WASP-121b (Gibson et al. 2020 [42]).

When comparing models to the data, it is necessary to apply to the model the same processing techniques as used on the data. This includes applying the same **SysRem** filtering using the derived basis vectors, and convolving the forward model with a Gaussian kernel of width W_{conv} , to account for additional line broadening (this could be caused by winds or rotation in the atmosphere). However, as **SysRem** is an iterative and computationally expensive process, we do not re-run it during the modelling. Instead, the filtering is performed using the fixed basis vectors derived from the data, reducing the procedure to a linear basis model fit, which is computationally efficient. The filtered model template is then Doppler-shifted according to the planet’s orbital motion, given by

$$v_p = K_p \sin(2\pi\phi) + v_{\text{sys}} , \quad (2.3)$$

where K_p is the amplitude of planet’s orbital velocity, v_{sys} is the systemic velocity, and ϕ is the planet’s orbital phase. We can ignore the barycentric velocities, as our data have already been shifted to the system’s rest frame. The Doppler-shifted model is then interpolated onto the data before being used in the cross-correlation analysis. The cross-correlation function (CCF) is created by multiplying the (residual) data (f_i) and the shifted model template (m_i), and summing over spectral orders and wavelengths. The product is weighted by the variance (σ_i^2), thus taking into account the noise. The CCF then stands as

$$\text{CCF}(v) = \sum_{i=1}^N \frac{f_i m_i}{\sigma_i^2} . \quad (2.4)$$

For high-resolution retrievals, we had to expand the parameter vector used for the low-resolution retrieval in order to incorporate parameters describing the cross-correlation model. Among the included parameters are K_p , v_{sys} , and W_{conv} as defined above. We also included a scaling parameter (α) that controls the amplitude of the cross-correlation

signal, a (β) parameter describing the uncertainty scaling (analogous to the low-resolution, and actually used instead of that parameter for high-resolution retrievals), and the flux offset parameter δf .

Taking all the parameters into account, we got the full parameter vector for high-resolution retrievals as $(\alpha, \beta, K_p, v_{\text{sys}}, \delta f, W_{\text{conv}}, \kappa_{\text{IR}}, \gamma, T_{\text{irr}}, T_{\text{int}}, P_0, P_{\text{cloud}}, \chi_{\text{Ray}}, \chi_{\text{Fe}})$. Out of these 14 parameters, 11 were used as free parameters for fitting, and 3 were fixed (δf , T_{int} , and $\log_{10}(\chi_{\text{Ray}})$).

2.2.3 High-Resolution Retrieval

High-resolution retrieval is the determination of atmospheric and orbital parameters by fitting Doppler-shifted model spectra to the data using a cross-correlation-based likelihood. We adopted the same Gaussian likelihood function as in the low-resolution case, with additional scaling and offset parameters, and evaluated it using the cross-correlation. This enables constraints on atmospheric composition and structure from the resolved spectral line information. Similar to low-resolution retrieval, we imposed uniform priors on all model parameters with hard-set bounds. The parameter values falling outside these ranges are assigned zero probability. We also added physically-based priors to the T-P profile, requiring the computed temperatures to remain within the range 1,000 – 4,000 K. All the parameters and their corresponding prior distributions are shown in Table 2.4.

Same as for the low-resolution retrievals, we used the MCMC algorithm to explore the posterior distribution of the model parameters. Prior to running the MCMC, we perform a maximum-likelihood optimisation to obtain an improved starting point for the chains, while keeping fixed parameters unchanged. After that, we run the MCMC with 32 walkers. We scaled down the expected parameter uncertainties to ensure walkers have a valid starting point. The burn-in phase was initiated with 200 steps, after which we performed walker culling and redraw, followed by the second burn-in phase with 200 steps to reinitialize the low-probability walkers. Then we ran the main chain with 1,000 steps. Posterior distributions are obtained from the converged chains, from which we derive the best-fit parameters and their associated uncertainties. Results are presented in Table 2.4 and also shown in Figure A.5.

After the retrieval, we evaluated the detection significance and velocity constraints for the studied species. We first constructed a model template using the maximum posterior (best-fit) parameters obtained from the retrieval, and cross-correlated this template with the data over a range of systemic velocities (in this case from -250 to $+250 \text{ km} \cdot \text{s}^{-1}$), after which we performed a summation over all spectral orders. This produced a cross-correlation map (CC map) – a 2D matrix of $(\phi \times v_{\text{sys}})$, where, if strong enough, we can spot a trace of a Doppler-shifted planetary signal. As we can see in Figure 2.6,

the signal of WASP-121b is visible there. The finite width of the cross-correlation peak (propagated to the CC map as the width of the signal – diagonal line) is caused by the instrumental resolution and the intrinsic broadening of the planetary absorption lines, which may include contributions from atmospheric winds and planetary rotation. We then summed the CC map along the expected radial velocity value to generate a K_p – v_{sys} map, which localises the signal in velocity space.

Based on the results of test high-resolution retrieval we can show a possible detection of neutral iron Fe I with the significance 7.1σ and peak location at $v_{\text{sys}} \approx -4.5 \text{ km}\cdot\text{s}^{-1}$ and $K_p \approx 204 \text{ km}\cdot\text{s}^{-1}$. These values are consistent with those obtained from the MCMC posterior distributions.

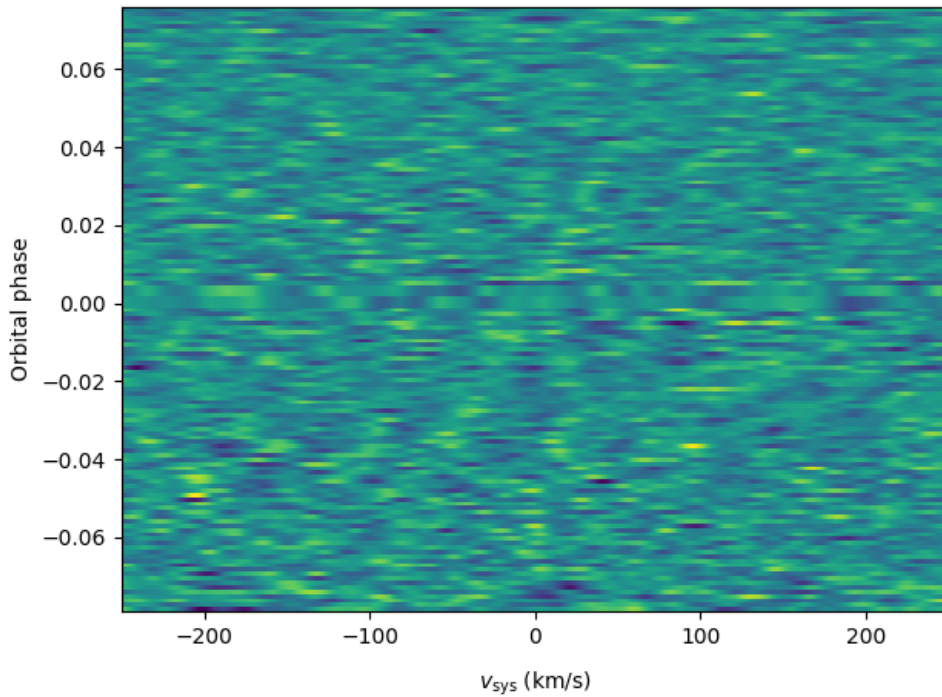


Figure 2.6: A cross-correlation map for neutral iron Fe I. A Doppler-shifted planetary signal is visible as a diagonal line going from bottom left to top right.

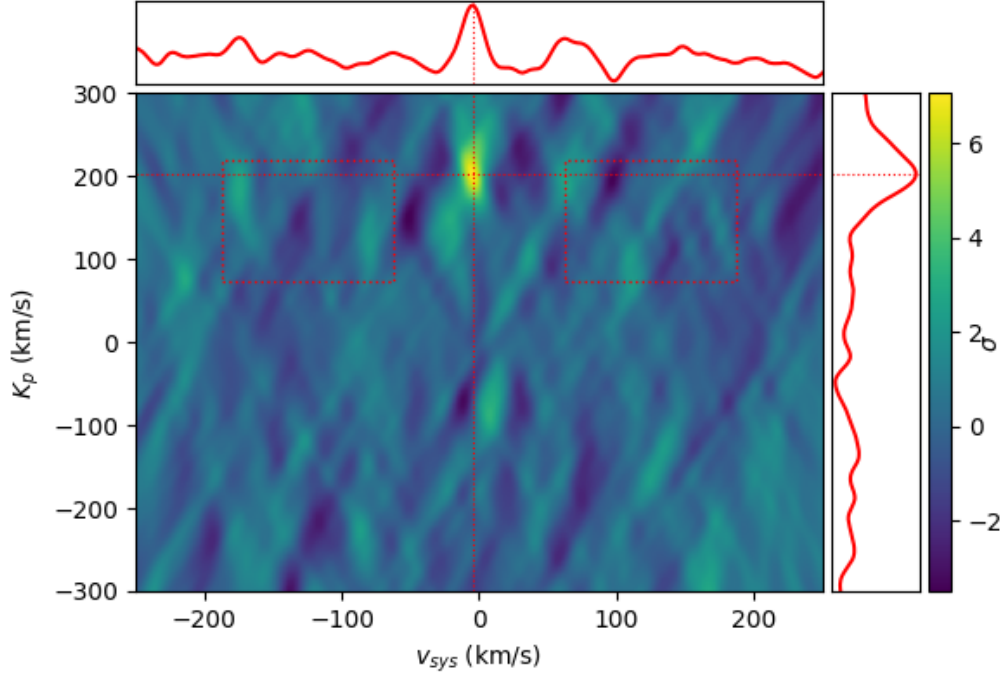


Figure 2.7: A velocity summation map with a $> 7\sigma$ detection peak of neutral iron Fe I.

Parameter	Description	Prior	Posterior
α	Model scaling factor	$\mathcal{U}(0.1, 6)$	0.92 ± 0.83
β	Noise scaling parameter	$\mathcal{U}(0.1, 2)$	0.7899 ± 0.0002
K_p	Planet RV semi-amplitude ($\text{km}\cdot\text{s}^{-1}$)	$\mathcal{U}(170, 250)$	204.2 ± 7.2
v_{sys}	Systemic velocity ($\text{km}\cdot\text{s}^{-1}$)	$\mathcal{U}(-10, 10)$	-4.54 ± 1.24
δf	Flux offset	fixed	0
W_{conv}	Convolution width	$\mathcal{U}(1, 50)$	1.47 ± 0.47
$\log_{10}(\kappa_{\text{IR}})$	Mean infrared opacity	$\mathcal{U}(-2, 6)$	-0.40 ± 1.43
$\log_{10}(\gamma)$	Visible-to-infrared opacity ratio	$\mathcal{U}(-2, 20)$	0.52 ± 0.74
T_{irr}	Irradiation temperature (K)	$\mathcal{U}(1200, 4000)$	2153 ± 511
T_{int}	Internal temperature (K)	fixed	20
$\log_{10}(P_0)$	Reference pressure (bar)	$\mathcal{U}(-11.9, 1.9)$	-7.72 ± 3.91
$\log_{10}(P_{\text{cloud}})$	Grey cloud-top pressure (bar)	$\mathcal{U}(-2, 10)$	9.43 ± 3.46
$\log_{10}(\chi_{\text{Ray}})$	Rayleigh scattering scaling	fixed	1
$\log_{10}(\chi_{\text{Fe}})$	Fe mixing ratio	$\mathcal{U}(-10, -1.5)$	-1.71 ± 1.71

Table 2.4: Parameter vector with prior and posterior distribution for high-resolution retrieval of neutral iron in the WASP-121b spectrum.

2.3 Joint Retrievals

2.3.1 Framework for Joint Retrievals

In the previous sections, we described how both low- and high-resolution retrievals were performed. The key point of these tests is the use of the same forward atmospheric model (with the same parametric model for T–P profiles) for both retrievals. The only difference lies in the wavelength grid, which is defined according to the studied datasets. The prior spaces are based on the same uniform distributions, with identical physically motivated bounds for the T–P profile, and we adopt the same likelihood function.

To combine the constraints from both datasets, we are currently developing a joint retrieval framework by defining a combined posterior distribution. We assume the datasets are statistically independent. Under this assumption, the framework combines the information content of the datasets by summing their log-likelihoods while sharing a common parameter vector. The joint log-posterior is formulated as the sum of the individual log-posteriors from the low- and high-resolution retrievals, and is expected to enable both datasets to simultaneously constrain a single atmospheric model.

The framework is currently under development and results are not yet finalised.

An important aspect of combining high- and low-resolution spectroscopy is the selection of atmospheric species to be included in the retrieval. For initial tests, we focus on such species, which are expected to produce a detectable signal across both datasets. This can be challenging for a combination of the UVES and JWST/NIRSpec, as they span a wide wavelength range. In the optical, high-resolution spectra are primarily sensitive to atomic species such as Fe and other metals (Gibson et al. 2020 [42], Hoeijmakers et al. 2019 [54]), while infrared parts of the spectrum are dominated by molecular absorption species (Madhusudhan 2012 [35], Molliere et al. 2019 [49]).

As for the first test, we are considering neutral iron Fe I, which has been robustly detected in high-resolution observations of ultra-hot Jupiters [42, 54]. While its signatures are weaker in low-resolution spectra, it provides a useful benchmark for testing the joint retrieval framework.

2.3.2 Scientific Potential and Future Prospects

The previous studies on joint retrievals conducted on high- and low-resolution spectra proved the potential of this method (Smith et al. 2024 [38], Ghandi et al. 2024 [55]). Low-resolution spectroscopy, usually conducted in the near-infrared to infrared parts of the spectrum, covers an area strong with molecules, especially H₂O, CO, and CO₂. It provides a broad spectral coverage, allowing us to better constrain the continuum and

cloud properties. High-resolution spectroscopy resolves individual lines, which provides an opportunity to study atmospheric dynamics such as winds, jet streams, and rotation. Retrievals on the combined high- and low-resolution datasets help to constrain currently studied atmospheric characteristics and break degeneracies, which occur when conducting retrievals on individual datasets. Combining high- and low-resolution data helped to better constrain the T-P profile of WASP-77Ab [38]

The joint retrievals have the power to enable a new approach to the study of the atmospheric physics of exoplanets. By combining information from resolved line profiles and broadband molecular features, it may become possible to investigate vertical abundance gradients, disequilibrium chemistry, and the relationship between atmospheric composition and circulation [55]. This may ultimately enable retrieval frameworks based on more realistic 3D atmospheric models, which could significantly improve our understanding of the atmospheric physics of hot and ultra-hot Jupiters.

As mentioned in subsection 1.2.6, ultra-hot Jupiters are the best targets for testing and implementing the joint retrieval method. This is for several reasons. First of all, they are orbiting very closely to their host stars (with orbital periods shorter than 10 days). This gives in combination with a favourable planet-to-star radius ratio due to their large dimensions much better chance for transit occurrence. Ultra-hot Jupiters are highly irradiated by their host stars. This

For the implementation of our framework, it is necessary to select such targets, which have been extensively observed by both high- and low-resolution spectroscopy. Especially important are data obtained by the JWST because of its wavelength range, precision, and stability. Previous studies have shown that HST spectra are generally more challenging to incorporate into joint retrievals than JWST observations due to their lower precision and the presence of additional instrumental systematics [38]. JWST is currently the best source of low-resolution data for combination with ground-based high-resolution spectroscopy. However, targets need to be bright enough to get a sufficient signal-to-noise ratio for ground-based observations. In this case, a distance from Earth is not the key parameter, as the apparent magnitude is more important¹.

Based on these criteria, promising targets for our future joint retrieval studies can be broadly divided into three categories: benchmark systems already studied with joint retrievals, well-observed hot and ultra-hot Jupiters with rich archival datasets, and targets extending the method beyond hot Jupiters.

¹On the other hand, close proximity to our Solar System is more interesting for potential study of an extraterrestrial life on exoplanets, and/or future interstellar travelling to them. However, ultra-hot Jupiters are not the life-welcoming objects. Thus, this does not play an important role in our current target selection process (but it may in the future).

For testing our joint retrieval framework, it is ideal to use targets that have already been studied using a similar approach. Ultra-hot Jupiter **WASP-76b** [55] and hot Jupiter **WASP-77Ab** [38] are such exoplanets. They both have well-characterized atmospheres observed with JWST as well as ground-based high-resolution spectrographs. WASP-76b has been studied via a joint retrieval method, but only with HST data for the low-resolution part. Since then, it has been observed with JWST/NIRSpec, MIRI, and the NIRISS instrument, offering an exciting opportunity to build on previous studies with JWST data.

Among the well-observed hot and ultra-hot Jupiters, another interesting target is the hottest known gas giant **KELT-9b**. Many species have been detected in its spectrum via high-resolution spectroscopy with HARPS-N and CARMENES, e.g., Fe I, Mg I, Ca II, and recently also Si I in emission (Ridden-Harper et al. 2023 [56]). It is scheduled to be observed with JWST in cycle 4, which is currently running. **HD 189733b** is one of the classic benchmark exoplanets. This hot Jupiter has been observed with JWST/MIRI and NIRCам, HST, and also with ground-based spectrographs such as UVES and HARPS. Various species have been detected in its atmosphere and clouds with a strong cloud scattering effect. In such a case, joint retrievals could potentially provide new insights into its atmospheric physics.

Similar exoplanets with rich archival data from high- and low-resolution spectroscopic observations are **WASP-189b**, **MASCARA-2b**, and **WASP-39b**. All of these hot/ultra-hot Jupiters have been observed with JWST and have previous detections of various atomic species. A slightly more challenging target is **WASP-33b**, due to its pulsating A-type parent star. Further application of the joint retrievals can focus on other types of exoplanets, such as hot super-Neptune **WASP-107b**.

With space missions like TESS and PLATO, designed to discover more sub-Neptune and Earth-like exoplanets, and the powerful observation capabilities of JWST, even more targets will emerge. Joint retrievals will provide a powerful framework for analyzing these future datasets, enabling increasingly detailed studies of atmospheric composition, structure, and dynamics across a broad range of exoplanet types.

3. Conclusion and Forward Plan

The aim of this work is to perform a joint retrieval of high- and low-resolution exoplanetary transmission spectra. This method can improve the atmospheric retrieval to better constrain atmospheric parameters and lead to the detection of less dominant species.

The results presented in this report show the preparation of the framework for the joint retrievals. One of the key steps was the preparation of the forward atmospheric model. We constructed and tested a numerical model based on radiative transfer using the opacity cross-sections dependent on wavelength. This model is adjustable for various datasets, as we proved by using it for both high- and low-resolution retrievals successfully.

For the low-resolution retrieval, we used the JWST/NIRSpec time-series spectra of WASP-121b. In order to perform the retrieval, we fitted the transit light curve first. We retrieved global parameters of white-light transit (Table 2.1 and Figure 2.1), followed up by fitting of the spectroscopic light curves (see Figure A.2 for examples of the transit light curves for different wavelengths). From those, we obtained the transit depths to generate a transmission spectrum (Figure 2.2). Using our forward model, we performed a retrieval on this transmission spectrum. The input parameter vector with the prior distribution and posterior distributions is presented in Table 2.3, and the Corner plot is shown in Figure A.3.

For the high-resolution retrieval, we used the UVES high-resolution spectra of WASP-121b. After the stellar and telluric line removal and model filtering, we performed the retrieval by fitting the Doppler-shifted model spectra to the data using a cross-correlation-based likelihood function. The parameters vector with initial prior space and the resulting posterior distributions are presented in Table 2.4 and the corresponding Corner plot in Figure A.5. Based on the retrieval output, we constructed a cross-correlation map (Figure 2.6), and after the velocity summation, we generated a K_p - v_{sys} map (Fig 2.7) to localize the signal in the velocity space. As the result, we present a possible detection of neutral iron Fe I with the significance 7.1σ and peak location at $v_{\text{sys}} \approx -4.5 \text{ km} \cdot \text{s}^{-1}$ and $K_p \approx 204 \text{ km} \cdot \text{s}^{-1}$.

We outlined an initial framework set-up for the joint retrieval based on the summation of individual log-posteriors from high- and low-resolution retrievals.

3.1 A Forward Plan for Future Research

Finalizing the framework and joint retrieval testing

The plan for the next couple of weeks is to finalize the framework, including the proper implementation of the log-posterior function summation. Following the successful setup of the log-posterior, the MCMC algorithm will be prepared for the retrieval. It needs to be optimized for computational efficiency, as the high-resolution model can lead to significant computational overhead. Adjustments to the prior distributions may be necessary to mitigate this issue.

Validation of joint retrieval results

When the MCMC set-up is finalized, we will proceed to the joint retrieval performed on testing datasets of WASP-121b. Neutral iron (Fe I) will be used as the initial species for the atmospheric retrieval. Subsequently, additional species will be selected and tested. UVES high-resolution and JWST/NIRSpec low-resolution spectra will be used for the initial tests, with the possibility of incorporating other archival datasets of the same target. A proper validation scheme for the framework is yet to be developed. It must ensure that the retrieval produces accurate results with sufficient precision and robustness. If validated, the results of the WASP-121b joint retrieval will be published.

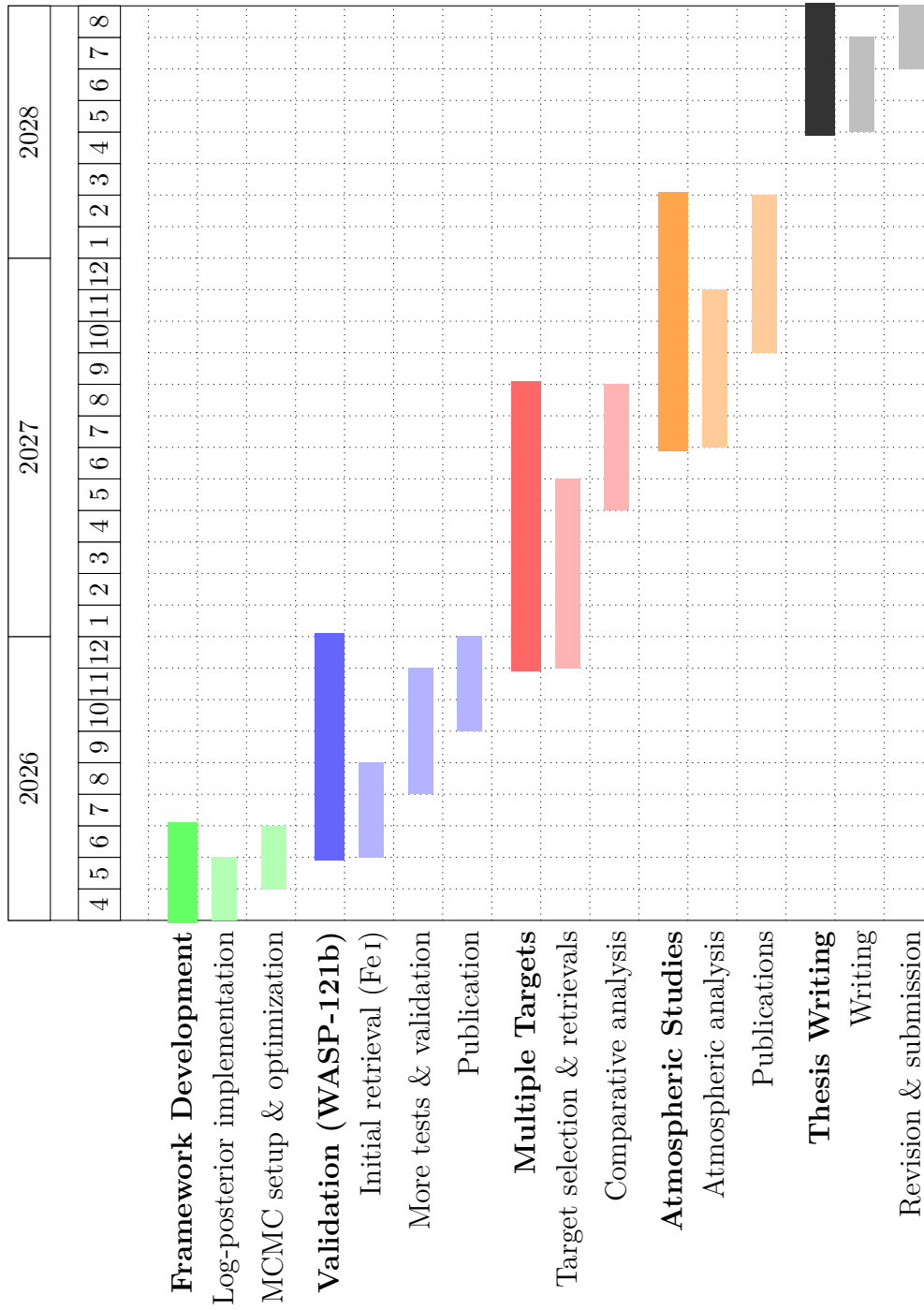
Performing joint retrievals on different targets

Following the initial tests and validation, the framework will be applied to a range of targets. We will identify well-observed exoplanets suitable for atmospheric studies, with a focus on hot and ultra-hot Jupiters. The exact criteria for target selection will be derived from the results of the test retrievals. The results will be compared across targets in order to refine the framework if necessary.

Atmospheric studies based on the joint retrieval method

The main goal of this PhD project is to utilize joint retrieval methods that combine high- and low-resolution spectroscopy. The aim is to study exoplanet atmospheres in greater detail, potentially searching for biomarkers and making other significant discoveries. Once validated, the framework will enable robust atmospheric studies of exoplanets. Specific projects will be defined based on the capabilities of the method.

3.2 A Gantt Chart



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List of Abbreviations

AJ	The Astronomical Journal
ApJ	The Astrophysical Journal
ApJL	The Astrophysical Journal Letters
AU	Astronomical unit (used as a standard distance unit)
A&A	Astronomy & Astrophysics
CCD	Charge-Coupled Device
CCF	Cross-correlation function
CoRoT	Convection, Rotation and planetary Transits
DEMC	Differential-Evolution Markov Chain
ESO	European Organisation for Astronomical Research in the Southern Hemisphere
FOV	Field Of View
HJ	Hot Jupiter
HST	Hubble Space Telescope
IAU	The International Astronomical Union
JWST	James Webb Space Telescope
LM	Levenberg–Marquardt (algorithm)
ly	Light year (a distance unit)
MCMC	Markov chain Monte Carlo (algorithm)
MNRAS	Monthly Notices of the Royal Astronomical Society
M_J	Mass of the planet Jupiter (used as a standard unit)
$M_\oplus$	Mass of the Earth (used as a standard unit)
PASP	Publications of the Astronomical Society of the Pacific
PLATO	PLANetary Transits and Oscillations of stars
PCA	Principal Component Analysis
PNAS	Proceedings of the National Academy of Sciences
RM	Rossiter-McLaughlin effect
RV	Radial Velocity
SNR	Signal to noise ratio
TESS	Transiting Exoplanet Survey Satellite
T-P profile	Temperature-pressure profile
VLT	Very Large Telescope
VMRs	Volume mixing ratios

A. Attachments

WASP-121b Datasets Overview

Facility / Instrument	Mode	λ [μm]	R	Obs.	Year(s)
HST/STIS	G230L+G430L+G750L	0.23–1.03	500–30 000	T	2015–2016
HST/WFC3	G102+G141	0.80–1.65	130–210	T,E,FP	2016–2021
Spitzer/IRAC	Ch1+Ch2	3.2–5.0	<i>Photometry</i>	E,FP	2015–2019
JWST/NIRSpec	G395H	2.73–5.17	2 700	T,E,FP	2022
JWST/NIRISS	SOSS	0.60–2.80	700	T,FP	2023
Gemini/GMOS	R400/R600	0.50–0.95	1 000	T	2018–2019
VLT/UVES	437+860 DIC	0.33–1.10	60 000	T	2016–2017
ESO/HARPS	HAM	0.378–0.691	115 000	T	2018–2023
VLT/ESPRESSO	HR21/MR	0.38–0.79	140 000	T	2019–2021
VLT/CRIRES+	K2148	1.96–2.48	100 000	T	2022–2023
ESO/NIRPS	HE	0.95–1.80	80 000	T	2023–2024

Table A.1: Overview of the datasets covering spectroscopic observations of WASP-121b. Top part of the table lists space-based low-resolution spectroscopy observations, bottom part of the table lists high-resolution spectroscopy. Observation modes represent transit (T), eclipse (E), and full phase curve (FP) observations.

Transit fitting

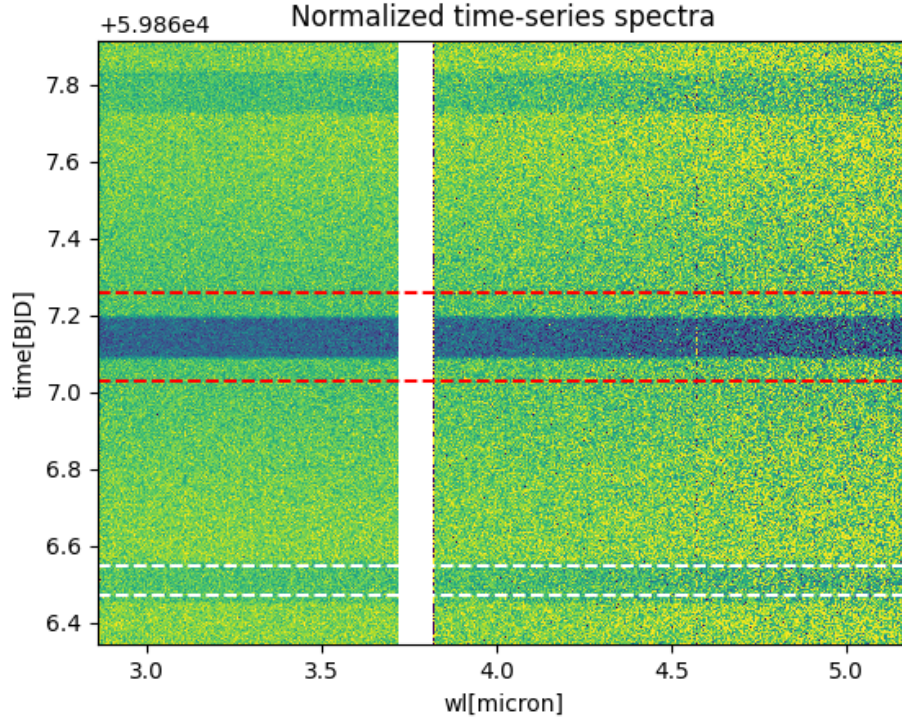


Figure A.1: Normalized time-series spectra of WASP-121b obtained by the JWST/NIR-Spec. Red dashed lines show area used for transit fitting, white dashed lines mark the part of the phase curve used for normalisation (we used the part of the phase curve, when planet was in the eclipse, as then the spectra contain only the stellar flux).

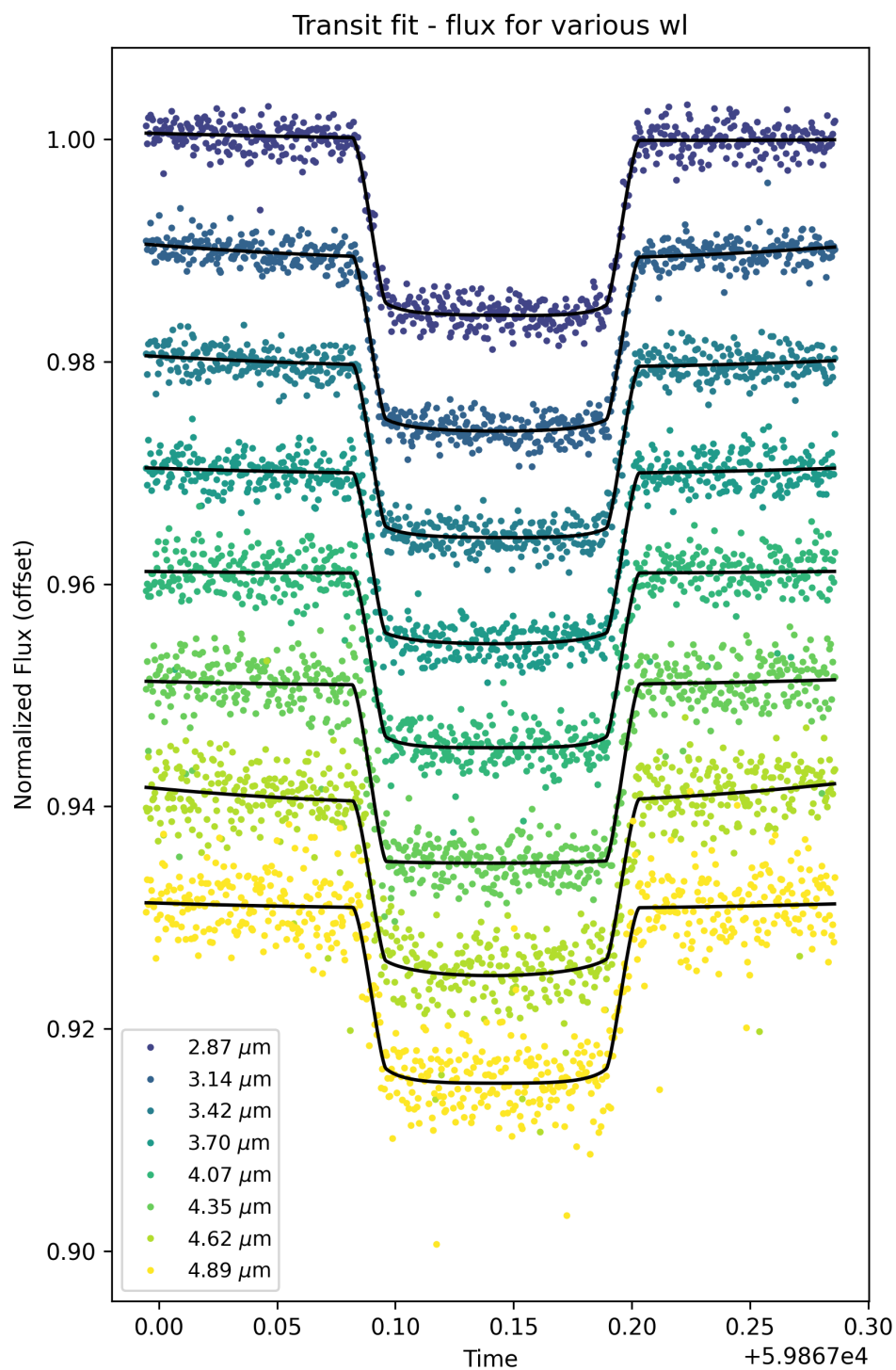


Figure A.2: Selected spectroscopic light curves of WASP-121b with fitted transit models.

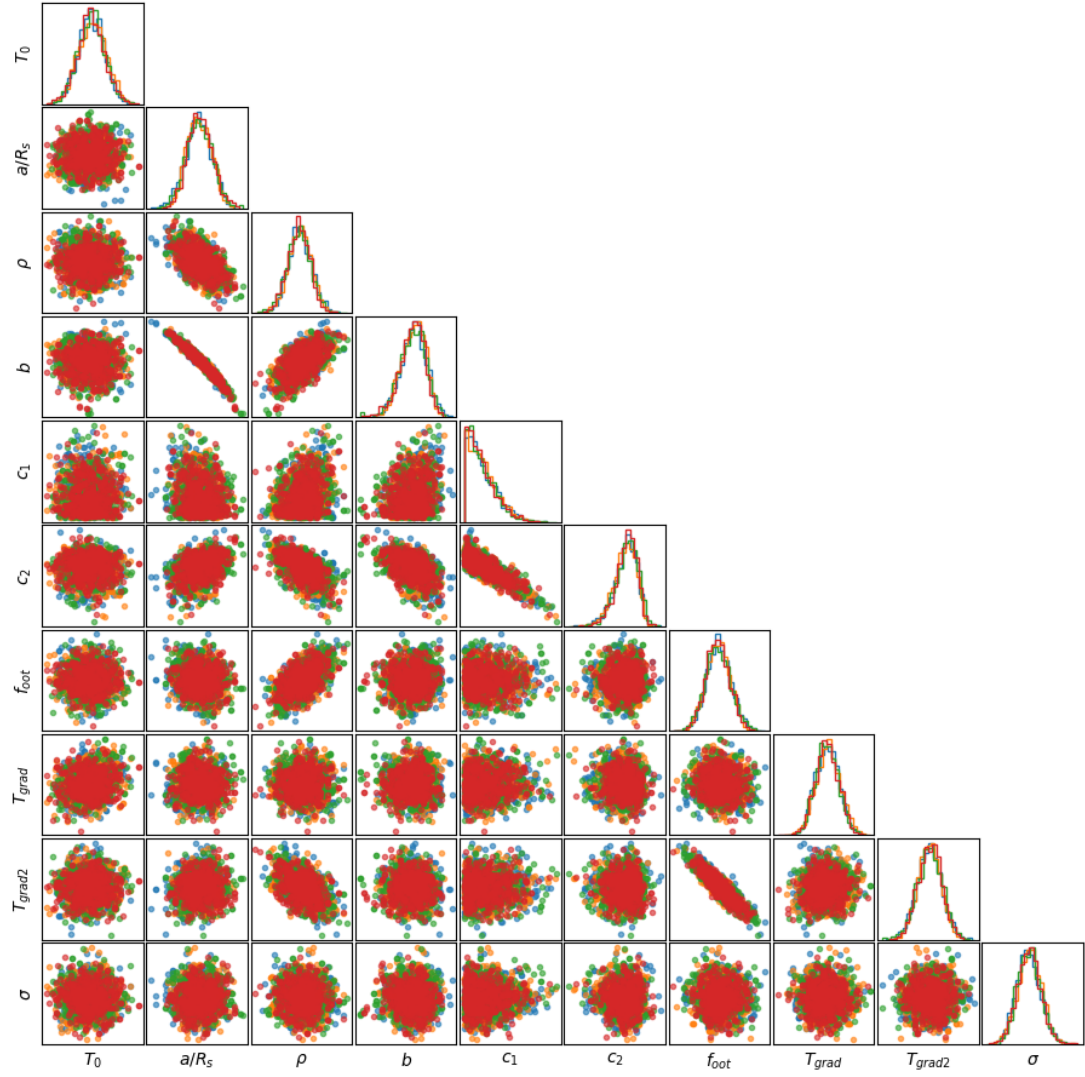


Figure A.3: Posterior distributions for the fit parameters of the white light transit curve. For a description of each parameter, see Table 2.1.

Transmission spectrum posterior distributions.

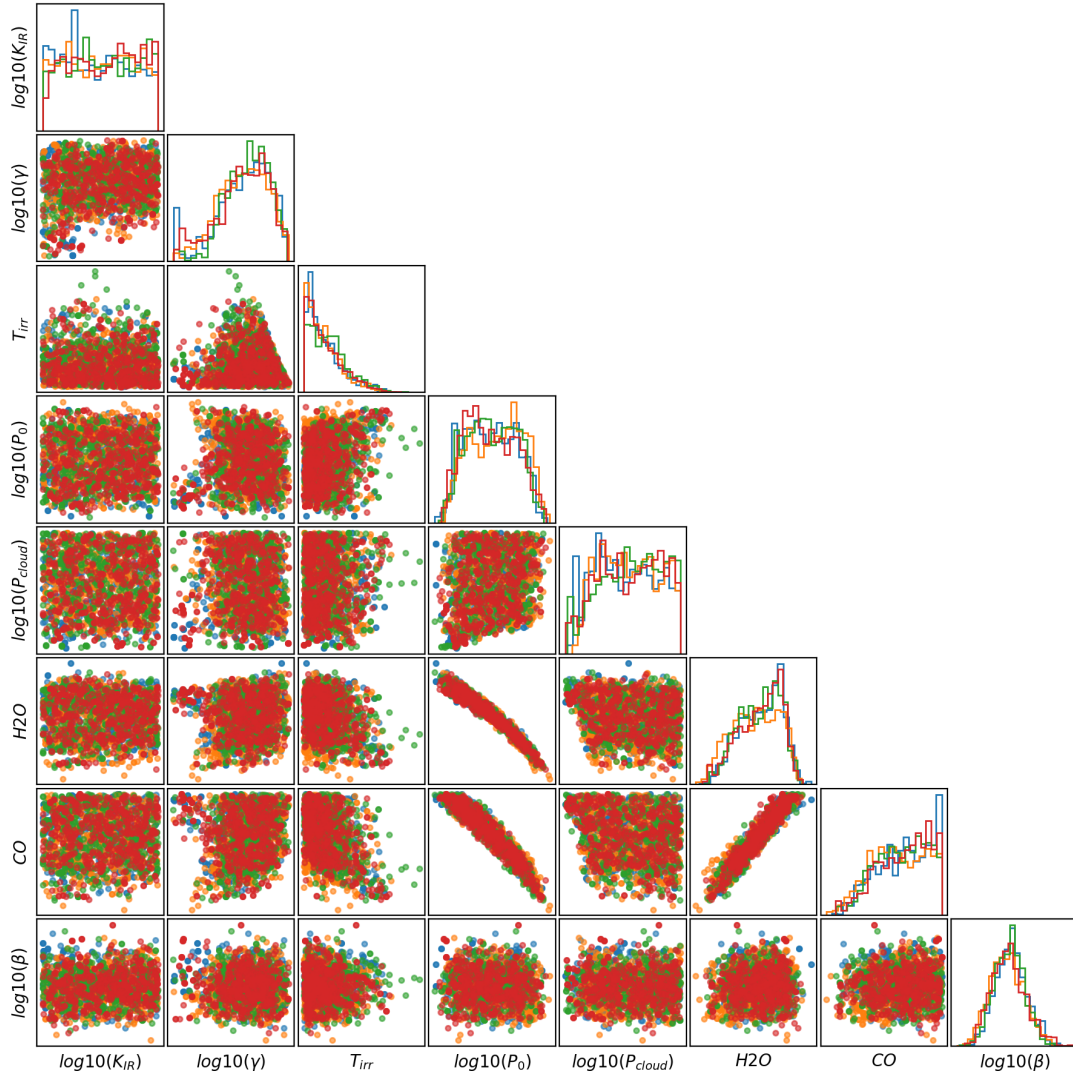


Figure A.4: Posterior distributions for the fit parameters of WASP-121b transmission spectrum. For a description of each parameter, see Table 2.3.

Results from the high-resolution retrieval.

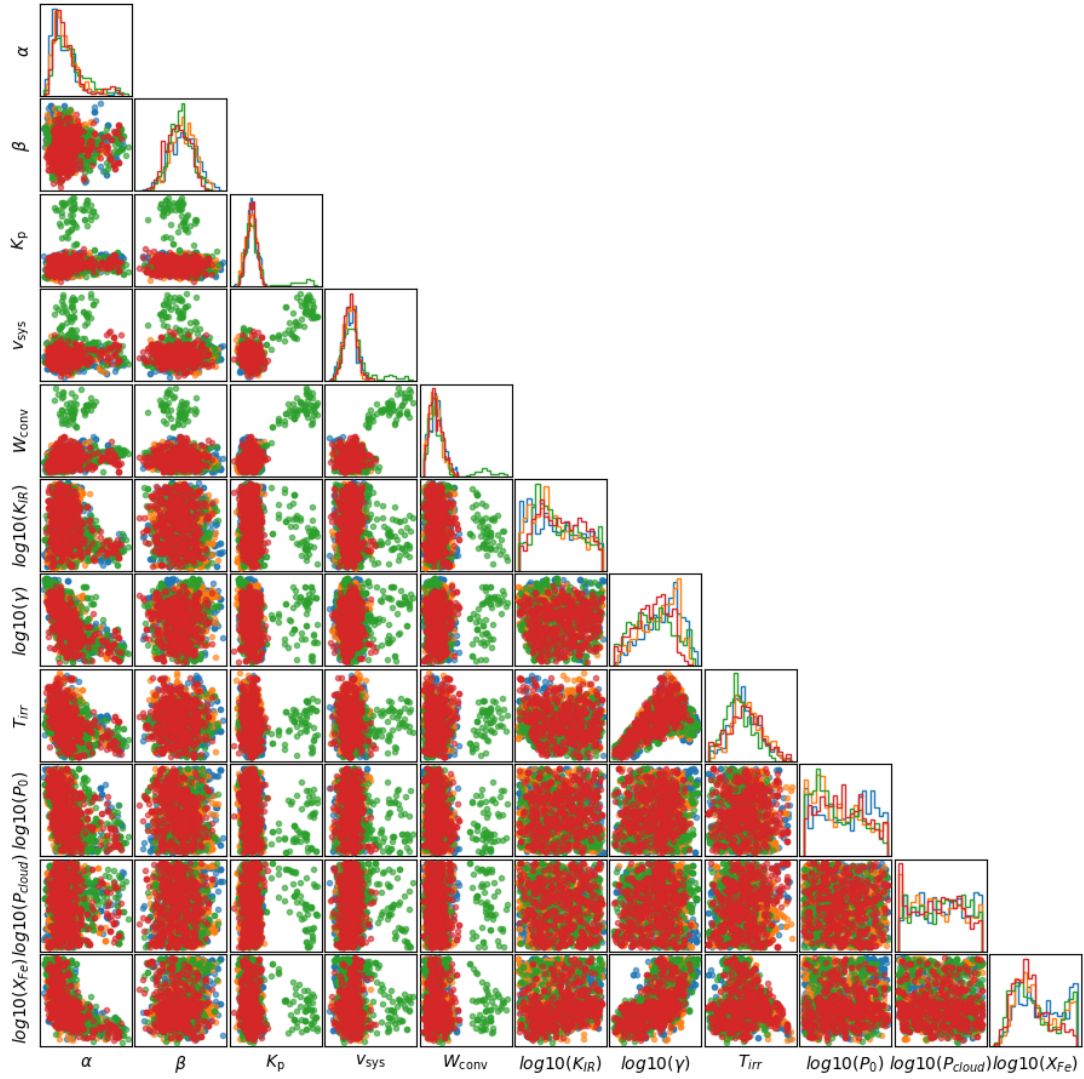


Figure A.5: Posterior distributions for the high-resolution retrieval of WASP-121b UVES data. For a description of each parameter, see Table 2.4.

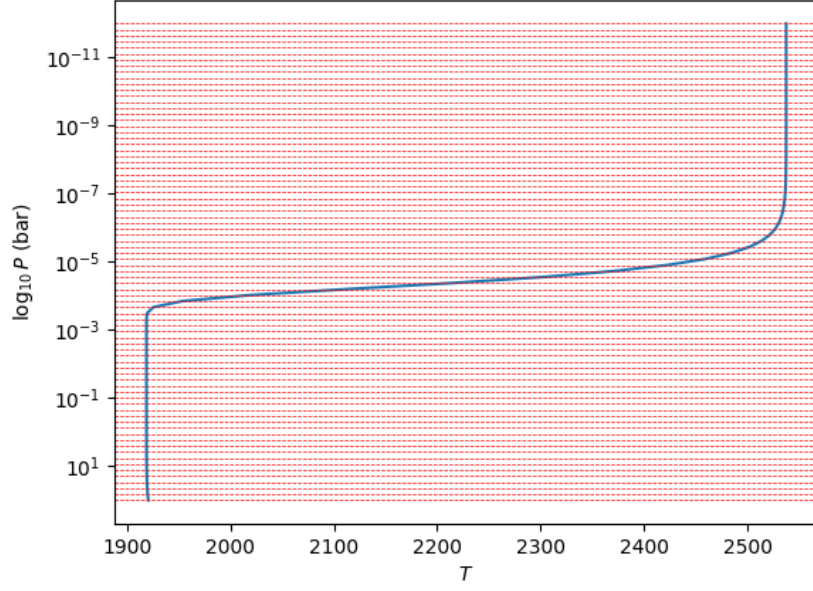


Figure A.6: T-P profile of WASP-121b atmosphere for the best-fit model parameters retrieved from high-resolution retrieval.

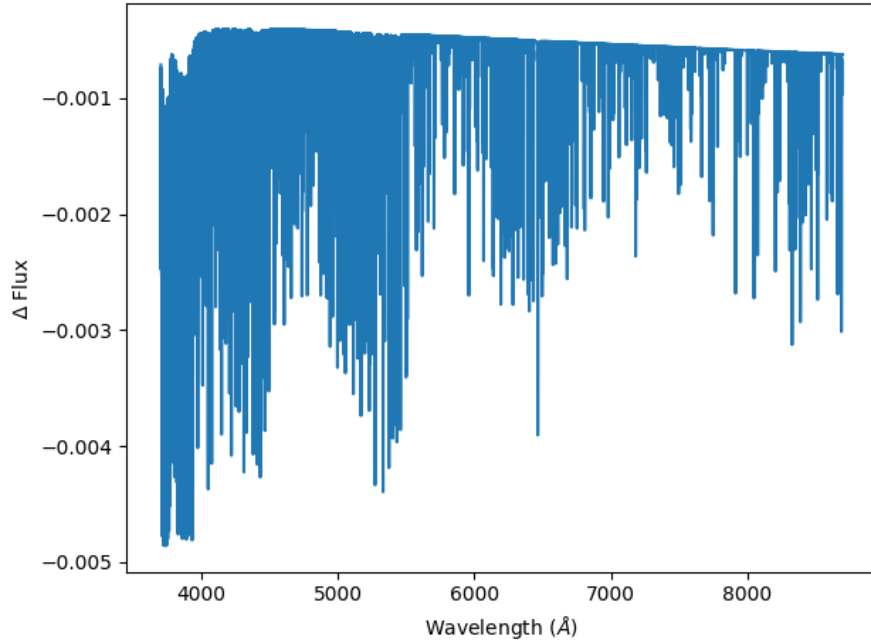


Figure A.7: Negative model template for WASP-121b for the best-fit model parameters retrieved from high-resolution retrieval.