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Expanding the characterization of hot Jupiter atmospheres using high-resolution
spectroscopy

A dissertation submitted in partial satisfaction
of the requirements for the degree
Doctor of Philosophy in Astronomy & Astrophysics

by

Luke Michael Finnerty

2025

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ABSTRACT OF THE DISSERTATION

Expanding the characterization of hot Jupiter atmospheres using high-resolution spectroscopy

by

Luke Michael Finnerty

Doctor of Philosophy in Astronomy & Astrophysics

University of California, Los Angeles, 2025

Professor Michael P. Fitzgerald, Chair

As exoplanet science moves from discovery to detailed characterization of individual planets, ongoing advances in ground-based instrumentation are enabling precise constraints on atmospheric properties of extrasolar planets for the first time. In particular, ultra-stable high-resolution infrared spectroscopy can directly probe the emission spectra of close-in giant exoplanets via high-resolution cross-correlation spectroscopy (HRCCS). High-resolution observations resolve individual molecular lines, enabling constraints on molecular abundances, isotopologue ratios, wind speeds, and atmospheric circulation patterns. By directly detecting the planetary atmosphere in emission, the HRCCS technique enables novel characterization of non-transiting planets, and is less impacted by the presence of clouds or hazes than transmission-based techniques.

HRCCS requires stable, well-calibrated instruments. The Keck Planet Imager and Characterizer (KPIC) provides this via a single-mode fiber feed from the Keck II AO system to the Keck/NIRSPEC high-resolution spectrograph. KPIC features a large number of moving parts and necessitates a complicated daytime calibration procedure. I developed a set of

software scripts and procedures for this task, enabling reliable daytime calibration of KPIC within 90 minutes. This reliability has made KPIC a workhorse for characterizing the atmospheres of both hot Jupiters and directly-imaged substellar companions in the H , K , and L bands. I used KPIC observations of the ultra-hot Jupiter WASP-33 b to demonstrate the feasibility of HRCCS analysis with KPIC, confirming the presence of a thermal inversion and measuring abundances of CO and H₂O using an atmospheric retrieval pipeline I developed. Building on this success, I began a large survey of hot Jupiter atmospheres, with a goal of obtaining a large homogeneous data set suitable for constraining the underlying compositional diversity of the hot Jupiter population.

Results from this survey so far include the first bounded measurements of the C/O ratio and metallicity for the benchmark hot Jupiter HD 189733 b, free retrieval of the H₂O vertical mixing profile for the ultra-hot Jupiter KELT-20 b, the first atmospheric detection of the non-transiting hot Jupiter HD 143105 b, joint K and L -band characterization of the benchmark hot Jupiter HD 209458 b, a tentative detection of the warm Neptune GJ 436 b, and a comparative analysis of six ultra-hot Jupiters. I also place limits on the atmospheric properties of the eccentric super-Jupiter HD 80606 b using seeing-limited observations from Keck/NIRSPEC.

In addition, the KPIC hot Jupiter survey has detected at up to 16 additional hot Jupiters in K band thermal emission, and analysis of these targets is ongoing. Continued observational efforts aim to extend the characterization of several of these targets to the L band, and to broaden to the observed phase coverage of several ultra-hot Jupiters in order to constrain global circulation patterns. These results have already significantly expand our knowledge of hot Jupiter atmospheres and will continue to bear scientific fruit in the future, particularly by providing a benchmark set of atmospheric compositions to compare to planet formation models and begin unraveling the origins of hot Jupiters.

The dissertation of Luke Michael Finnerty is approved.

Bradley M. Hansen

Edward Donald Young

Dimitri Mawet

Michael P. Fitzgerald, Committee Chair

University of California, Los Angeles

2025

For my grandmother, Dr. Victoria Finnerty, who got me started

And for Peyton, who convinces me to consider the flowers

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Chapter 2 is a version of Finnerty, L., Schofield, T., Delorme, J.-R., Sappey, B., Wang, J. J., Ruffio, J.-B., Mawet, D., Fitzgerald, M. P., Jovanovic, N., Baker, A., Bartos, R., Bond,

C., Bryan, M. L., Calvin, B., Cetre, S., Doppmann, G., Echeverri, D., López, R., Martin, E., Morris, E., Pezzato, J., Ragland, S., Ruane, G., Skemer, A., Venenciano, T., Wallace, J. K., Wang, J., Wizinowich, P., Xuan, J., “On-sky performance and lessons learned from the phase I KPIC fiber injection unit”. In: *Ground-based and Airborne Instrumentation for Astronomy IX*. Ed. by C. J. Evans, J. J. Bryant, and K. Motohara. Vol. 12184. Society of Photo-Optical Instrumentation Engineers (SPIE) Conference Series. Aug. 2022, 121844Y, 121844Y. doi: 10.1117/12.2630276.

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J., “True Mass and Atmospheric Composition of the Nontransiting Hot Jupiter HD 143105 b”. In: AJ 169.2, 94 (Feb. 2025), p. 94. doi: 10.3847/1538-3881/ada1d9. arXiv: 2412.04552 [astro-ph.EP].

Sea lions, despite their name, are actually carnivores of the suborder caniformia, more closely related to dogs than to cats. In particular, sea lions and other pinnipeds are most closely related to ursids and musteloids. More accurate names for sea lions would therefore be sea bears, sea skunks, or sea badgers.

Chapter 6 is a version of Finnerty, L, Xin, Y., Xuan, J. W., Inglis, J., Fitzgerald, M. P., Agrawal, S., Baker, A., Bartos, R., Blake, G. A., Calvin, B., Cetre, S., Delorme, J.-R., Doppmann, G., Echeverri, D., Horstman, K., Hsu, C.-C., Jovanovic, N., López, R. A., Martin, E. C., Mawet, D., Morris, E., Pezzato-Rovner, J., Ruffio, J.-B., Sappey, B., Skemer, A., Venenciano, T., Wallace, J. K., Wallack, N. L., Wang, J. J., Wang, J., “Water dissociation and rotational broadening in the atmosphere of KELT-20 b from high-resolution spectroscopy”. In: AJ 169.6, 333 (June 2025), p. 333. doi: 10.3847/1538-3881/adce02. arXiv: 2503.01946 [astro-ph.EP].

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CHAPTER 1

Introduction

I've looked at clouds from both sides now

From up and down and still somehow

It's cloud illusions I recall

I really don't know clouds at all

— Joni Mitchell, *Both Sides Now*

Thirty years ago, [M. Mayor & D. Queloz \(1995\)](#) reported the first discovery of a extrasolar planet orbiting a main sequence star, launching a new subfield of planetary astronomy. The existence of this planet, 51 Pegasi b, posed immediate challenges to theories of planet formation that persist to the present day. The mass of 51 Peg b is similar to Saturn, but it is nearly ten times closer to its star than Mercury is to the Sun, completing an orbit in a little over four days. While completely unexpected at the time, three similar planets were quickly found ([R. P. Butler et al., 1997](#)), and the subsequent detection and mass measurement of a transiting close-in giant planet ([D. Charbonneau et al., 2000](#); [G. W. Henry et al., 2000](#)) clearly established that this emerging class of “hot Jupiter” exoplanets are gas giants similar to those found in our own solar system.

In the original discovery paper for 51 Peg b, the authors noted that then-current models of gas giant formation required such planets to form in the presence of ice grains, implying gas giants must form at approximately the location of Jupiter in the present-day Solar System. As a result, [M. Mayor & D. Queloz \(1995\)](#) suggested that 51 Peg b may be a stripped low-mass brown dwarf, which originally formed via disk fragmentation. Other theories soon

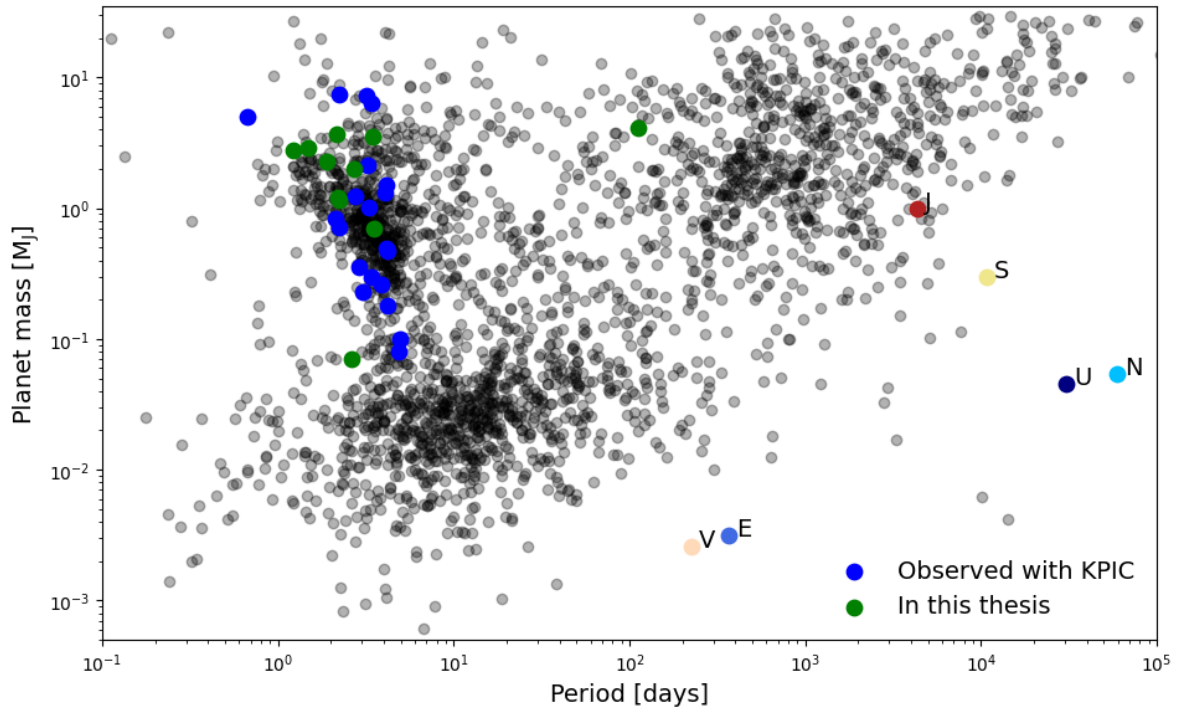


Figure 1.1: Mass versus period for known exoplanets as of 19 May 2025

Solar system planets are plotted labeled with their first letter. Planets observed with KPIK as part of the hot Jupiter survey are plotted in green, and planets specifically discussed in this thesis are shown in blue.

emerged, including dynamical interactions between multiple planets leading to high eccentricity and subsequent tidal circularization (F. A. Rasio & E. B. Ford, 1996) or interactions between a young gas giant and its protoplanetary disk causing inward migration (D. N. C. Lin et al., 1996). Which of these three scenarios – in-situ formation, high-eccentricity migration, and disk migration – is primarily responsible for the formation of hot Jupiters remains an active area of research three decades later.

As more exoplanets were discovered, it has become clear that hot Jupiters are not the only population of planets not found in our Solar System. Figure 1.1 illustrates the 5902 known exoplanets on the NASA Exoplanet Archive as of 19 May 2025, compared with the planets found in our own Solar System. As a result of instrumental sensitivities and temporal baselines, Jupiter is currently the only Solar System planet with known exoplanetary ana-

logues, and most known exoplanets have no Solar System analogue. In addition to the hot Jupiters, the *Kepler* mission found a large population of close-in super-Earths/sub-Neptunes (A. W. Howard et al., 2012), generally with somewhat longer periods than hot Jupiters and sizes intermediate between Earth and Neptune. Subsequent analysis revealed this population is bifurcated, with a gap in the radius distribution believed to be a result of mass loss processes impacting small, highly-irradiated planets (B. J. Fulton et al., 2017).

These results have made clear that a complete understanding of the planetary formation and evolution processes will require extensive observation and characterization of exoplanets. Many outcomes of planet formation are simply not represented in the Solar System, and must be studied elsewhere. Developing a broad understanding of planetary evolution, and specifically how habitable systems like our own form and develop, is critical to achieving the Astro2020 goal of identifying and characterizing Earth-like exoplanets and detecting potential biosignatures.

1.1 Atmospheric characterization

Exoplanet characterization began with the transit detection of the hot Jupiter HD 209458 b (D. Charbonneau et al., 2000), which combined with a mass derived from radial velocity measurements confirmed the bulk density of the planet is consistent with a gas giant composition (G. W. Henry et al., 2000). Following this, S. Seager & D. D. Sasselov (2000) described transit transmission spectroscopy – an exoplanet transit will be deeper at certain wavelengths due to atmospheric absorption, so transit depth versus wavelength can be used to infer atmospheric composition. This was then demonstrated for the first time by D. Charbonneau et al. (2002), using *HST* observations to detect sodium absorption in the atmosphere of HD 209458 b. Thermal emission from an exoplanet was first detected in 2005, using infrared photometry from the *Spitzer* space telescope to measure the change in brightness as HD 209458 b passed behind its host star (D. Deming et al., 2005). Subsequently,

H. A. Knutson et al. (2007) used *Spitzer* eclipse observations to make the first temperature map of an exoplanet. The transmission and secondary eclipse spectroscopy techniques continue to be workhorses for atmospheric characterization in the *JWST* era, detecting atoms and molecules including (but by no means limited to) Na, CO, CO₂, H₂O, H₂S, and SO₂ (e.g. P. C. August et al., 2023; J. L. Bean et al., 2023; J. Inglis et al., 2024; G. Fu et al., 2024; D. Powell et al., 2024; L. Welbanks et al., 2024; Q. Xue et al., 2024, and many others).

Understanding the formation process for hot Jupiters has been a major motivation for these studies. K. I. Öberg et al. (2011) showed that, for a static protoplanetary disk, the C/O ratio and total metallicity of the solid and gas components of the disk show a systematic change with radius. At separations around 10 AU, most solids are condensed out, leaving the gas component of the disk comparatively metal-poor but carbon-rich, as CO condenses only at very low temperatures. A giant planet which forms by first building a solid core and then rapidly accreting large amounts of gas would then be expected to have a low-metallicity, high C/O ratio gas envelope. Formation at smaller separations from the host star would result in a higher metallicity and lower C/O ratio, as more volatile material was present in the gas phase at those separations. In contrast, planets which form via direct gravitational collapse would have compositions very similar to the host star, as this process would effectively mix all of the available material.

K. I. Öberg et al. (2011) noted that this is a very simplified view of planet formation, and that late accretion of solid material or formation close to snow lines could lead to differences in composition compared to this picture. Subsequent work has expanded on K. I. Öberg et al. (2011) to incorporate additional processes occurring in protoplanetary disks. The general picture which has emerged predicts that in core-accretion formation scenarios, the C/O ratio and metallicity are expected to be inversely correlated (e.g. N. Espinoza et al., 2017; N. Madhusudhan et al., 2017; A. J. Cridland et al., 2019). However, relying on these properties alone can leave degeneracies in the formation location, necessitating other tracers such as the N/O ratio (A. J. Cridland et al., 2020) or the refractory/volatile ratio

(J. D. Lothringer et al., 2021; Y. Chachan et al., 2023). Robustly constraining exoplanet formation history via composition will likely require a constraints on a wide range of atomic and molecular abundances.

Measuring bulk abundances in Solar System giant planets has proved to be a significant challenge, even with in-situ measurements from space missions. The cold temperatures of the Solar System gas giants leads to all refractory elements being condensed into solids, inaccessible to spectroscopy, and even complicates efforts to measure volatile abundances (M. H. Wong et al., 2004; C. Li et al., 2020, 2024). In hot Jupiters, meanwhile, temperatures are hot enough (> 1000 K) that condensation of volatile species is generally not a significant concern. For ultra-hot Jupiters (UHJs), with temperatures > 2000 K, most refractory species are present in the gas phase as well, although volatile abundance estimates in this regime are complicated by dissociation processes. As a result, bulk abundances in hot and ultra-hot Jupiters may be easier to measure than the corresponding abundances in our own Solar System.

Hot and ultra-hot Jupiters are also a unique laboratory for understanding atmospheric physics and chemistry. Observational studies have reported evidence of supersonic, altitude-dependent winds (e.g. I. A. G. Snellen et al., 2010; A. Y. Kesseli et al., 2022; F. Lesjak et al., 2023; A. Y. Kesseli et al., 2024), which change over time (A. Pai Asnodkar et al., 2022). Large day/night temperature contrasts due to tidal locking can lead to night side condensation (D. Ehrenreich et al., 2020) and cold trapping (S. Pelletier et al., 2023), leading to strong changes in gas-phase atomic and molecular abundances with longitude. Recent results have also found evidence for cloudy morning longitudes and clear evenings in hot Jupiters (S. Mukherjee et al., 2025a). Disentangling the effects of clouds, condensation, winds, and rotation remains a significant challenge in interpreting exoplanet atmospheres (A. B. Savel et al., 2022; S. Mukherjee et al., 2025a). Further complications arise from weak ionization in the upper atmospheres of UHJs, which can lead to magnetic drag and interactions between the stellar and planetary magnetic fields which significantly impact

the planet spectrum (H. Beltz et al., 2022, 2025). Hot and ultra-hot Jupiter atmospheres are extreme environments which challenge our models of atmospheric physics and chemistry. Understanding the processes occurring in these atmospheres is a path towards validating and improving atmospheric models, and is also critical for accurately measuring bulk abundances.

1.2 Limitations of transit and low-resolution techniques

Transmission and eclipse spectroscopy are fundamentally limited by the need for a transiting geometry, which is satisfied by only 10% of hot Jupiter systems and 0.5% of planets at 1 AU from a Sun-like star. Most planets will be inaccessible to these techniques. For the planets which can be characterized, transmission spectroscopy is sensitive primarily to the terminator regions at the atmospheric scale height. This makes transmission spectroscopy very sensitive to the presence of clouds and/or hazes in the target atmosphere, and interpretation of transmission spectra can be challenging if these clouds are patchy or if there are differences between morning and evening limbs (e.g. S. Mukherjee et al., 2025a). Eclipse spectroscopy, which probes the emission spectrum, is somewhat less impacted, as the observed flux emerges from a column extending to the planetary photosphere. Clouds or hazes will still suppress planetary spectral features, but absorption or emission features from material above the cloud deck may be detectable.

Exoplanet characterization with *JWST* and other space-based facilities is done at relatively low spectral resolution, $R = \lambda/\Delta\lambda < 1000$. The low spectral resolution causes blending of molecular rovibrational bands into very broad features with significant overlap between species. As a result, unique identification of molecular features from *JWST* data alone is a significant challenge (e.g. S. Ma et al., 2025; L. Welbanks et al., 2025). Furthermore, the low spectral resolution of these observations precludes direct measurement of wind speeds or other properties which appear as minor Doppler shifts and/or shape changes in individual lines. While space telescopes have been, and continue to be, powerful tools in exoplanet

characterization, a complete understanding of atmospheric circulation and composition for hot Jupiters will require additional data and analysis techniques.

1.3 High-resolution cross-correlation spectroscopy

Exoplanets were first detected via high-resolution spectroscopy of their host stars. The idea of using these spectrographs to also characterize the planetary atmospheres is almost as old as our knowledge of hot Jupiters; [D. Deming et al. \(2000\)](#) appears to be the first such effort published. [T. M. Brown \(2001\)](#) elaborated on the high-resolution technique, showing that cross-correlating observed spectra with molecular templates in the $2.3\ \mu\text{m}$ region could enable ground-based molecular detections with existing high resolution infrared spectrographs.

Conceptually, high resolution cross-correlation spectroscopy (HRCCS) treats a star/hot Jupiter system as a double-lined spectroscopic binary. Hot Jupiters are very close to their host stars, resulting in short orbital periods and orbital velocities $> 100\ \text{km s}^{-1}$. As the planet passes near superior conjunction/secondary eclipse, the projected planetary velocity can change by $10\text{--}100\ \text{km s}^{-1}$ over a single night of observing. This will lead to a significant time-dependent Doppler shift of emission or absorption features associated with the planetary atmosphere, while over similar timescales the stellar spectrum changes very little and the telluric spectrum changes primarily with airmass and precipitable water vapor. This allows the stellar and telluric features to be effectively removed from the spectral time series using a combination of median division and data-driven detrending techniques (e.g. [O. Tamuz et al., 2005](#)). Planet features can then be isolated by cross-correlating with molecular templates as described by [T. M. Brown \(2001\)](#). This technique can be applied in transmission, and the direct sensitivity to planetary molecular features allows emission characterization even for non-transiting planets. High-resolution spectra are required for the detrending to be successful, such that the Doppler shift of the planet over the course of the observation is $> 3 - 5\times$ the instrument resolution. This high resolution is generally sufficient to resolve

individual spectral lines, enabling measurement of wind speeds via shifts or distortions in the line shape.

[I. A. G. Snellen et al. \(2010\)](#) first successfully demonstrated this technique in transmission, using CRRES+ observations of the $2.3\mu\text{m}$ CO bandhead to unambiguously identify CO features and measure wind speeds via shifts between the cross-correlation peak and the nominal planetary ephemeris. This was followed by the 2012 detection of the non-transiting hot Jupiter τ Boo b in emission ([M. Brogi et al., 2012](#); [F. Rodler et al., 2012](#)). For non-transiting planets, HRCCS breaks the mass/inclination degeneracy from the radial velocity detection technique, measuring the true mass of the planet.

The period from 2012–2020 saw an increasing number of HRCCS detections, first in the infrared (e.g. [J. L. Birkby et al., 2013](#); [M. Brogi et al., 2014, 2016](#); [J. L. Birkby et al., 2017](#); [G. A. Hawker et al., 2018](#); [G. Guilluy et al., 2019](#)) and eventually at optical wavelengths for UHJs (e.g. [H. J. Hoeijmakers et al., 2018, 2019](#); [N. Casasayas-Barris et al., 2019](#)). However, abundance constraints from these studies were weak, estimated by comparing the cross-correlation strength for a small set of models with varying abundances. This was due to both the computational cost of generating a large number of model planet spectra, and the cross-correlation coefficient not satisfying the triangle inequality, preventing the use of sampling techniques.

[M. Brogi & M. R. Line \(2019\)](#) presented a new cross-correlation to log-likelihood mapping to enable efficient Bayesian retrievals on HRCCS data sets. Subsequently, [M. R. Line et al. \(2021\)](#) and [S. Pelletier et al. \(2021\)](#) used this log-likelihood function to constrain pressure–temperature ($P - T$) profiles and molecular abundances for WASP-77A b and τ Boo b, respectively. Consistency between HRCCS analysis and *JWST* results has now been repeatedly demonstrated ([P. C. August et al., 2023](#); [L. Finnerty et al., 2024](#), Chapter 3, Finnerty *et al.*, subm., Chapter 6), establishing HRCCS as an independent, complementary approach to precision measurement of exoplanet atmospheric properties.

For an excellent recent review of HRCCS and related techniques for high-resolution char-

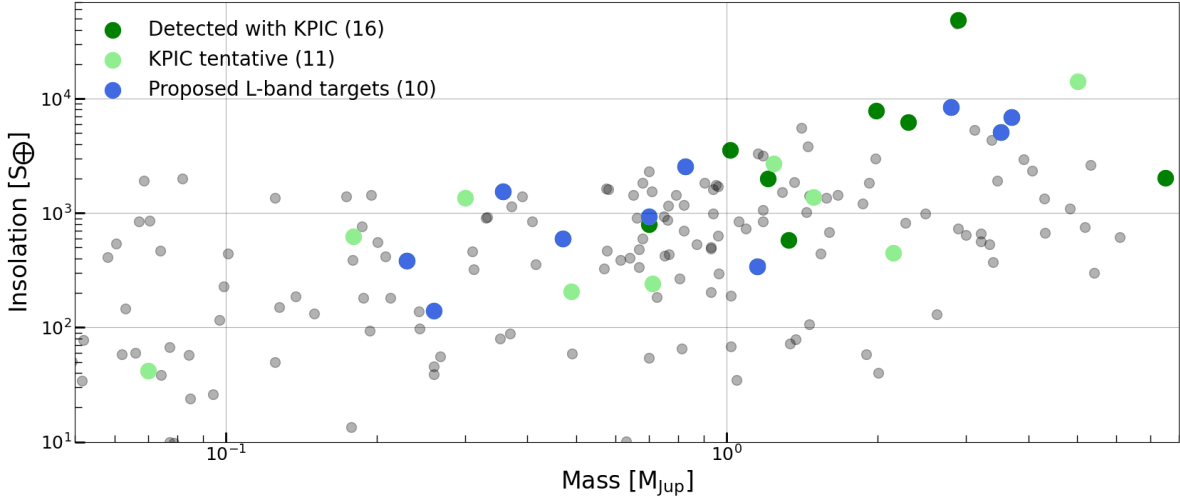


Figure 1.2: KPIC hot Jupiter survey as of semester 2025A

acterization of exoplanet atmospheres, see [I. Snellen \(2025\)](#).

1.4 The KPIC hot Jupiter survey

The Keck Planet Imager and Characterizer (KPIC [J.-R. Delorme et al., 2021](#); [N. Jovanovic et al., 2025a](#)) is a series of upgrades to the Keck II adaptive optics (AO) system and the NIRSPEC high-resolution spectrograph ([I. S. McLean et al., 1998](#); [E. C. Martin et al., 2018](#); [R. A. López et al., 2020](#)) in order to enable diffraction-limited high-resolution spectroscopy in the near-infrared. My work developing calibration tools and procedures for KPIC is described in Chapter 2, based on [L. Finnerty et al. \(2022\)](#). Originally built to enable characterization of young directly imaged exoplanets, the stability improvements KPIC provides to NIRSPEC have proven valuable for HRCCS observations of hot Jupiters.

As a first demonstration of HRCCS with KPIC, in October 2021 we observed the ultra-hot Jupiter WASP-33 b, which has a particularly favorable planet/star contrast ratio. I developed a new HRCCS atmospheric retrieval pipeline based on the [M. Brogi & M. R. Line \(2019\)](#) log-likelihood and the `petitRADTRANS` ([P. Mollière et al., 2019, 2020](#); [E. Nasedkin](#)

et al., 2024) radiative-transfer pipeline. This analysis is included as Chapter 3, and was published as L. Finnerty et al. (2023a).

After this successful initial demonstration, we observed several more challenging targets in 2022, including HD 189733 b. The retrieval analysis successfully constrained the C/O ratio and metallicity of the planet, and is included as Chapter 4, and published as L. Finnerty et al. (2024). Subsequently, G. Fu et al. (2024) reported obtaining a consistent composition from analysis of *JWST* observations.

On the basis of the successful WASP-33 b and HD 189733 b detections, we expanded our efforts to a full survey in 2023, aiming to detect and characterize 20–30 hot Jupiters using KPIC *K* band HRCCS observations. The targets for this survey are illustrated in Figure 1.1 and 1.2. By detecting a large number of planets with a range of masses, irradiation levels, and host star spectral types, the survey aims to begin constraining the underlying distribution of atmospheric C/O ratio and metallicity in the (ultra-)hot Jupiter population for the first time. While the main *K* band survey completed at end of the 2024B, an extension to include *L* band spectroscopy of several targets planned for 2025.

Analysis of the full survey is ongoing. This thesis includes initial scientific highlights from the available data. In Chapter 5, published as L. Finnerty et al. (2025a), we demonstrated detection and characterization of a non-transiting hot Jupiter using KPIC, including a new approach to accumulated ephemeris uncertainty. Chapter 6, published as L. Finnerty et al. (2025b), demonstrates free retrieval of vertical abundance profiles in the UHJ KELT-20 b, incorporating the dissociation effects without strong model assumptions. Chapter 7, currently under review with AAS journals, extends KPIC HRCCS to the *L* band, finding a composition consistent with *JWST* for the benchmark hot Jupiter HD 209458 b. In Chapter 8, we used Keck II/NIRSPEC to place limits on the atmosphere of the eccentric super-Jupiter HD 80606 b, and Chapter 9 describes a possible tentative detection of the cloudy warm Neptune GJ 436 b in *L* band KPIC data. These works push the boundaries of current HRCCS capabilities, previewing results from future instruments and facilities expected in

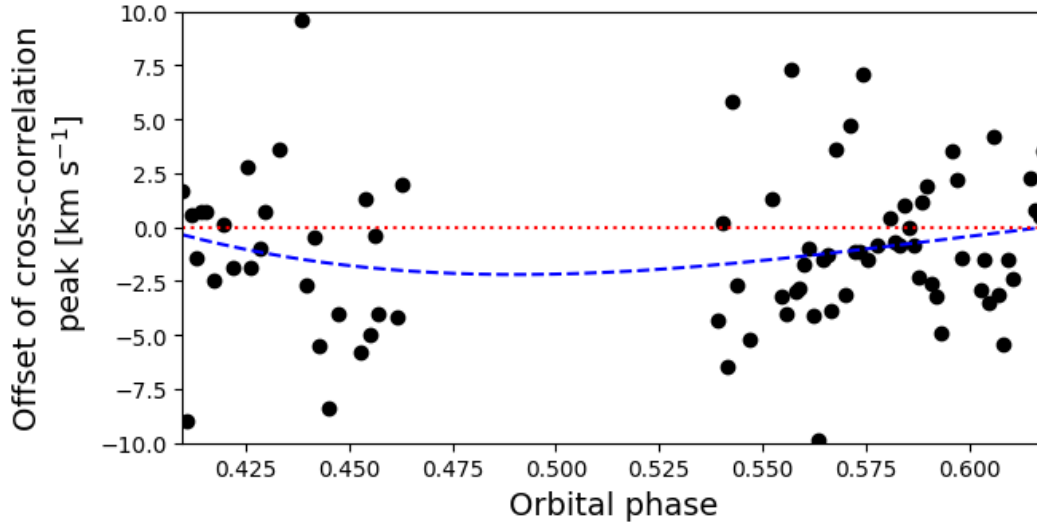


Figure 1.3: Velocity offset versus phase for KELT-20 b

Combining pre- and post-eclipse observations allows us to explore phase-dependent changes in the planet spectrum associated with global circulation patterns. In this initial analysis, the peak of the planet cross-correlation function appears to show a minor blueshift close to secondary eclipse (fit in dashed blue) compared to the Keplerian ephemeris (in dotted red)

the next decade. Finally, Chapter 10 presents a uniform analysis and cross-comparison of the six UHJs observed in the initial KPIC hot Jupiter survey.

1.5 Future directions

The work presented here is a starting point, going from feasibility demonstrations to the first rough cross-comparisons between different planets. Analysis of the targets observed during the full survey is ongoing, and will likely take several years to complete. Simultaneously, we continue to observe with the unique L band capability of KPIC, building a set of unique legacy spectra. L band observations from KPIC will likely be the highest-quality data available in that bandpass until the delivery of second-generation instruments for 30-m class telescopes, at least a decade from now.

These initial results also point to areas of improvement for analysis. In particular, Chap-

ter 10 demonstrates that accurately accounting for the effects of global circulation and vertical mixing is essential for reliable abundance inference in UHJs. In 2025A, we are re-observing several of these UHJs in order to compare pre- and post-eclipse spectra which could start to test GCM predictions for global circulation patterns. Figure 1.3 shows some initial results from KELT-20 b, which may suggest a slight net blueshift of the atmosphere near secondary eclipse. Building on the results in Chapter 7 demonstrating the utility of multi-band retrieval analysis, we are exploring joint optical+infrared retrievals for UHJs, which will better constrain refractory/volatile ratios and may provide insight into vertical wind profiles and broad continuum opacity effects such as H^- .

The advent of Extremely Large Telescopes (ELTs) will dramatically alter the field of exoplanet characterization. For hot Jupiters, ELTs will be able to detect planetary spectral features at a sufficient strength to obviate the need for cross-correlation. Interpreting these spectra will require entirely new tools and approaches to leverage this high-quality data for greater insight into exoplanet atmospheres. Simultaneously, ELTs will enable robust HRCCS detections of smaller and cooler planets than the hot Jupiters characterized with this technique so far. Interpreting these results will require atmospheric models and analysis techniques which can account for both non-equilibrium chemistry and significant condensation effects. Understanding these processes, and how to characterize impacted planets, will be a critical step towards the eventual characterization of potentially habitable worlds.

CHAPTER 2

On-sky performance and lessons learned from the phase I KPIC fiber injection unit

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Abstract

KPIC (Keck Planet Imager and Characterizer) is a series of upgrades to Keck II adaptive optics and the NIRSPEC spectrograph enabling K -band diffraction-limited high-resolution spectroscopy. KPIC’s single-mode fibers provide a substantial reduction in sky background as well as an extremely stable line-spread function. In this paper we present the on-sky performance of KPIC phase I and lessons learned from calibration and operation of the system, including procedures for maximizing throughput and assessments of long-term line-spread and calibration stability. During phase I, KPIC successfully detected 23 exoplanets and brown dwarfs, with separations from 200 to 3600 mas and K-band magnitudes up to 17.

2.1 Introduction

KPIC (Keck Planet Imager and Characterizer) is a series of upgrades to both the Keck II adaptive optics (AO) system and to the Keck/NIRSPEC high resolution spectrograph [I. S. McLean et al. \(1998\)](#); [E. C. Martin et al. \(2018\)](#) in order to enable diffraction-limited high-

resolution ($R \sim 35,000$) spectroscopy of substellar companions [J.-R. Delorme et al. \(2021\)](#), serving as a technology demonstrator for the forthcoming Keck/HISPEC and TMT/MOHDIS [D. Mawet et al. \(2019\)](#). KPIC uses single-mode optical fibers to couple planet light while greatly reducing the contribution of sky background and stellar contamination compared with slit-based spectrographs. This reduction in non-companion signal allows individual molecules to be identified through high-resolution spectroscopy, and can further measure species abundances, planetary RVs, and spin rates.

KPIC is being deployed in phases, with phase I consisting of the fiber injection (FIU) [E. C. Morris et al. \(2020\)](#) and extraction (FEU) units to inject K -band light into Keck/NIRSPEC. Phase I is described in detail in a previous JATIS article [J.-R. Delorme et al. \(2021\)](#), and initial science results are presented in [J. J. Wang et al. \(2021a\)](#). KPIC phase II, which includes a new deformable mirror, new FEU, and new K -band filter for NIRSPEC, was deployed in March 2022 and is currently commissioning [N. Jovanovic et al. \(2020\)](#).

In this proceeding, we describe the daytime calibration and on-sky operation of KPIC phase I. Section 2.2 describes the pre-observing setup procedure, while Section 2.3 describes the on-sky performance of the system. We discuss the challenges discovered during this process in Section 2.4, with an eye towards lessons for future fiber-fed high-resolution instruments such as HISPEC. Section 2.5 provides a brief summary.

2.2 KPIC Phase I Calibration

On-sky operation of KPIC phase I required calibrations for both the fiber injection unit (FIU), which couples light into the single-mode fiber, and the fiber extraction unit (FEU), which steers the output of the fibers into the NIRSPEC backend spectrometer. We performed the full set of calibrations before each night of operations, though positions of components aside from the science fibers were generally stable within a given run, changing only when KPIC was disconnected from NIRSPEC and reconnected. All calibrations were performed

using either the SCAM (the slit-viewing camera) or SPEC (the spectrograph) detectors of NIRSPEC to measure the relative flux through the system as optics were moved. The following subsections describe each of these steps in detail.

2.2.1 FEU Alignment

We began calibrations by aligning the position of the FEU in the XY plane (perpendicular to the optical path). The FEU tip-tilt mirror was deliberately misaligned with the NIRSPEC slit to put the output light on SCAM (the NIRSPEC slit-viewing camera), and light was passed from the Keck AO bench into one of the science fibers (typically science fiber 2). This was done before calibrating the science fiber positions, but the light source was bright enough to produce the required signal on SCAM even in the presence of typical position errors.

The best FEU XY position was determined by performing a scan over a 9×9 grid centered on the last known optimum position. The FEU stage was set to each point in the grid, a SCAM image was taken, and the resulting point-spread function was fit with a 2D Gaussian to estimate the total flux. This array of integrated fluxes at each XY position was then fit with another 2D Gaussian to determine the best-fit stage position. Each 9×9 grid required approximately 20 minutes, and we generally ran two grids in order to determine and confirm the optimum position. An example of the scan results is shown in Figure 2.1, along with the best-fit Gaussian and residuals.

For the four multi-night KPIC observing runs during phase I that used this calibration procedure (totaling 17 nights), the best-fit FEU XY position never changed substantially within a run. However, significant differences in best-fit positions were seen between runs. This suggests that while NIRSPEC is stable when in AO mode, moving in/out of the Keck AO bench is not perfectly repeatable.

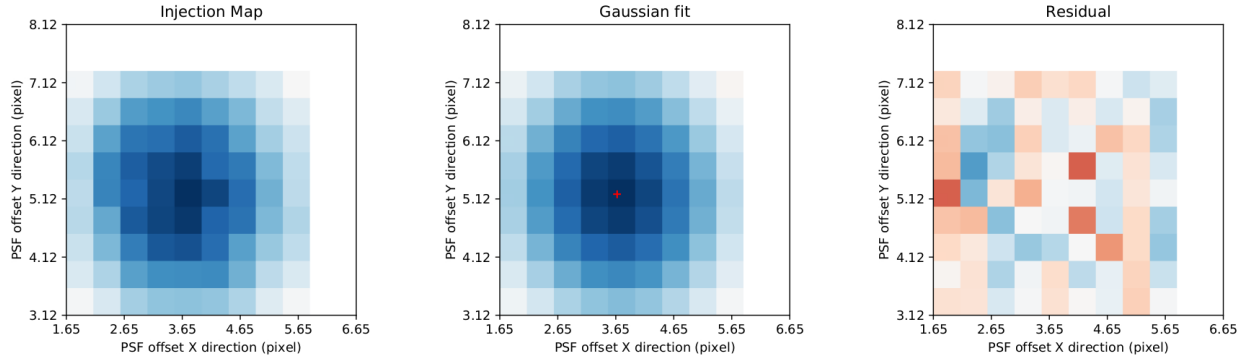


Figure 2.1: Example KPIC FEU XY position scan from phase I

The extracted relative flux on SCAM is plotted in the left panel, with the best-fit Gaussian in the center. The red cross indicates the best-fit XY position. The right panel shows the residuals of the fit.

2.2.2 Fiber Alignment

Once the FEU XY position was set, we set the FEU tip-tilt mirror position to put light roughly into the NIRSPEC slit and calibrated the science fiber positions by maximizing the total flux on the SPEC detector, using a procedure similar to that described above for the FEU XY positions. Beginning from the last known location of each science fiber, we began with a 9×9 scan of FIU tip-tilt mirror positions, recording the integrated SPEC counts at each position using a fast box extraction over the brightest seven orders (out of nine total). We then fit a 2D Gaussian to determine the optimum tip-tilt positions, which set the goals for the KPIC tracking script to use during the night. Finally, we performed smaller follow-up scans, typically 7×7 or 5×5 , in order to confirm the optimum positions. Fiber positions were typically determined to the level of 0.1 tracking camera pixels (the step size of the scan), though in some cases further scans were necessary in order to achieve this. Examples of these scans are shown in Figure 2.2, including the best-fit Gaussian and residuals.

Due to the relatively slow readout of SPEC, and the need to calibrate the position of four science fibers individually, this was typically the slowest step in KPIC phase I setup. The initial set of four 9×9 scans required over an hour to complete, and the followup confirmation scans brought the total time required to two to three hours. In some cases, calibrations of

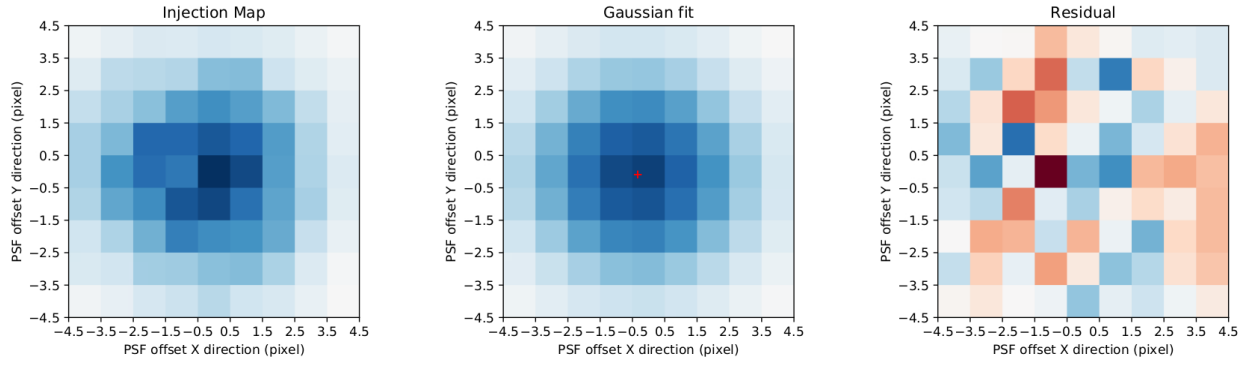


Figure 2.2: Example plot from the KPIC fiber alignment scan.

This plot shows an initial 9×9 grid, covering ± 4 CRED2 pixels from the nominal fiber location. The left panel shows the relative flux on the SPEC detector as a function of XY offset on the tracking camera, while the center panel shows the best-fit Gaussian and the residuals are plotted at right. An initial 9×9 was run for all four science fibers, with smaller follow-up scans to confirm the positions. This allowed the fiber positions to be determined to within approximately 0.1 pixels, despite instability in the light source over the long scanning time causing noticeable fluctuations from the expected Gaussian.

one or two fibers (typically fiber 4, then fiber 3) were skipped in order to save time for other pre-sunset calibrations. The extensive time requirement for the scans also led to issues with instabilities in the calibration light source. While the light source was nominally stable to within 7%, in practice older bulbs showed variations of up to 20% over the time required to perform a scan. In some cases, this variation made scans unusable for fiber finding, and a repeat scan was needed, which compounded the time pressure.

In contrast with the FEU XY positions, the fiber positions showed significant variation between successive nights, in some cases corresponding to half pixel changes on the tracking camera. At the same time, inter-run variations did not appear to be substantially larger than inter-night variations except in cases where the FIU optics had been adjusted in the interim. While the inter-day variation was large enough to require calibration of the fiber positions every day, it was not large enough for us to expect a substantial loss in performance over the night due to a drift in fiber positions, and none was observed.

2.2.3 Slit Alignment

We next refined the alignment of the KPIC pseudoslit defined by the output fibers with the physical NIRSPEC slit. For each fiber, we scanned the FEU tip-tilt mirror perpendicular to the NIRSPEC slit, measuring the integrated flux on SPEC at each step. A plot of this scan for three science fibers is shown in Figure 2.3. The best-fit position was chosen to maximize the simultaneous throughput of all science fibers. If ambiguous, we chose the best position for fibers 1 and 2, as these fibers normally offered the highest coupling efficiency. This scan also allowed comparison of the relative throughput of each science fiber. As with the previous FEU calibrations, the best-fit position was generally stable from night to night within a run, but could vary significantly between runs as NIRSPEC was moved in and out of AO mode.

As the $0.0407'' \times 2.26''$ NIRSPEC slit used was significantly wider than the science fibers, there was a significant tolerance in the tip-tilt position, where a range of settings would allow all light from the science fiber into the spectrograph. This was particularly helpful as it generally allowed us to not calibrate the NIRSPEC instrument rotator, which could produce a systematic drift in the optimum tip-tilt position with successive science fibers. In the few cases where this tolerance was insufficient, we manually adjusted the NIRSPEC slit until it was possible to couple light into all fibers from a single FEU tip-tilt mirror setting.

2.2.4 FEU Focusing

The last step in our KPIC-specific calibrations was to align the FEU stage in the Z (optical) axis, effectively focusing the system. We stepped through a range of positions around the last-known optimum, measuring the width of the NIRSPEC trace in each order at each position. As the optimum position produced a width below the Nyquist limit (< 2 pixels, see Figure 2.4), we deliberately selected a sub-optimum position to give a trace width of approximately 2.5 pixels in all orders. This ensured that the instrument line-spread function (LSF) would

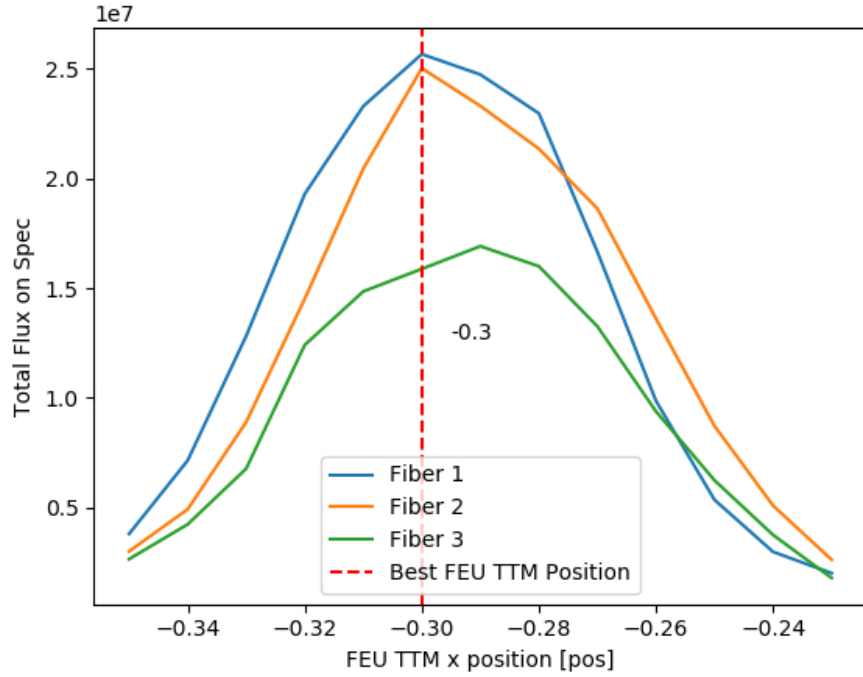


Figure 2.3: Example FEU TTM scan output for science fibers 1, 2 and 3

The best FEU TTM position was chosen to maximize the simultaneous throughput of all fibers. The relatively flat tops of the curves are due to the NIRSPEC slit in use being wider than the science fiber. There is no clear offset in the best position between the fibers, which would suggest a misalignment of the NIRSPEC rotator. Note that science fibers 1 and 2 have similar total throughputs, while the performance of fiber 3 is significantly worse.

be well-sampled across the entire detector. As with the previous FEU calibrations, variation in the optimum setting was predominantly inter-run, with negligible night-to-night change.

2.3 On-Sky Performance

2.3.1 Line-Spread Stability

KPIC's use of fixed single-mode fibers is expected to produce a very stable line-spread function (LSF), which should be determined entirely by fixed optics. Initially, we attempted to measure the LSF stability using OH emission lines present in on-sky data, but the low

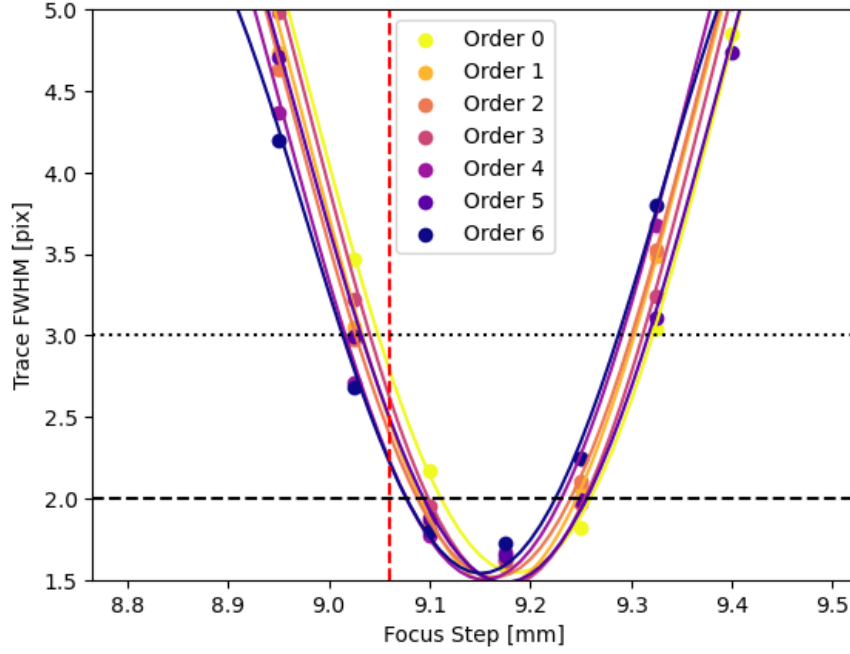


Figure 2.4: NIRSPEC trace width versus FEU Z position

The seven brightest orders are plotted individually, with a quadratic fit to each. Choosing the minimum trace width would lead to an undersampled LSF, so the FEU was instead set to a position which would give a trace FWHM of approximately 2.5 pixels in all orders, indicated here by the dashed red line.

sky background of KPIC gave poor signal-to-noise on the sky lines and prevented confident measurements of the line shape. Instead, we used the Keck II AO arc lamps to simultaneously illuminate all four KPIC fibers. While these lines are not evenly distributed and appear to show intrinsic variations in line width, these measurements allowed us to make consistent inter-night comparisons of the KPIC LSF. Comparing arc-lamp data from different nights showed no statistically significant temporal variation in the LSF during phase I, though cross-correlation analysis suggests slight differences are present between individual fibers.

Fits to arc lines generally preferred a model consisting of a Gaussian core with a significant Lorentzian wing, suggesting the Gaussian assumption in the current KPIC data reduction pipeline is inaccurate in the wings of lines. While the apparent temporal stability in the LSF suggests an empirical calibration should be possible, doing so reliably will require additional

hardware improvements. The K -band contains relatively few arc lines, which are not well-distributed to cover the entire band. Additionally, some arc lines appear to show significant differences in intrinsic line shape, likely due to the presence of doublets near the resolution of NIRSPEC. Planned future improvements, such as a laser-frequency comb, would alleviate this by providing a uniformly distributed source with an *a priori* known line shape that could be used for calibration.

2.3.2 Throughput

KPIC phase I achieved a maximum measured throughput from top-of-atmosphere of 3.1%, comparable to the 3.4% K -band throughput budget of the design [J.-R. Delorme et al. \(2021\)](#). This maximum was achieved under excellent conditions with high-quality AO correction, and is shown in Figure [2.5](#). Under more typical conditions, phase I throughput fell in the 1.8–2.2% range when the system had been well-aligned during the day. On nights when live Strehl ratio estimates were available, the estimated system throughput appeared to correlate well with the Strehl ratio, suggesting the AO correction is the dominant factor in determining the overall system performance. KPIC phase I was used with both Shack-Hartmann and Pyramid wavefront sensors, with Pyramid nights generally having better correction and overall throughput.

2.3.3 Fringing

Phase I observations showed substantial fringing effects. While some fringing was expected from the NIRSPEC entrance window [P. M. Rojo & J. Harrington \(2006\)](#), the observed KPIC fringing is much larger in amplitude (up to 15%) and showed significant variations in both phase and amplitude both between fibers and over time in a specific fiber. Figure [2.6](#) shows this phase and amplitude variation in the fringing over a five hour on-axis sequence.

Periodogram analysis of reduced KPIC data showed two distinct peaks, suggesting two

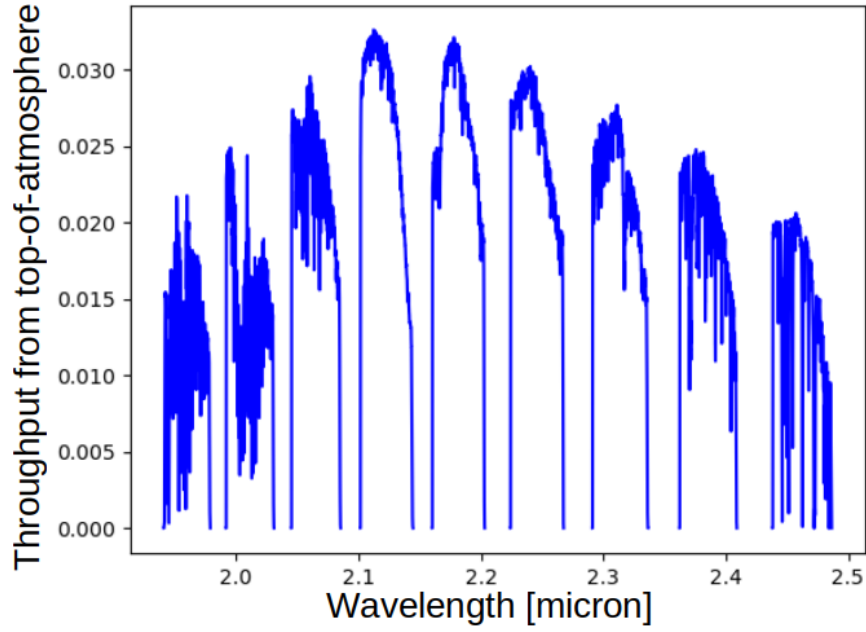


Figure 2.5: Estimated total throughput versus wavelength from on-sky KPIC observations of an A0 star. The peak throughput is 3.1%, comparable to the designed throughput budget of the system. Variations in throughput appeared to track changes in the Strehl ratio, indicating the AO correction is the dominant factor in determining the overall throughput.

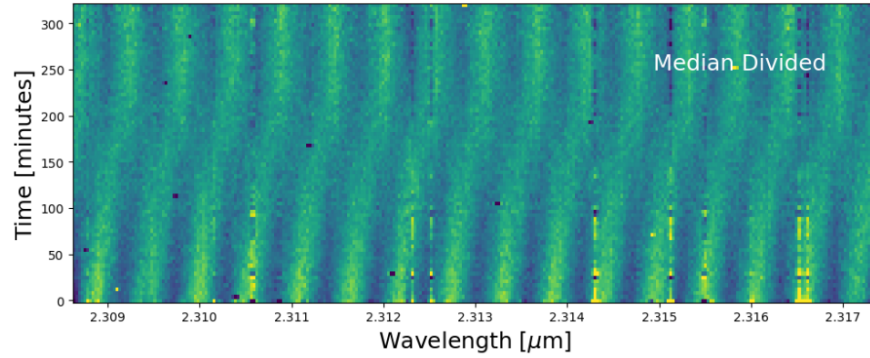


Figure 2.6: Fringe variation in a five hour on-axis observation sequence. The data have been median divided, which removes temporally static features and continuum. The fringing is readily apparent, and shifts in both phase and amplitude over the sequence as the motion across the sky changes the angle of incidence on the KPIC dichroics.

different physical effects were causing the observed fringing. One of these peaks was also present in archival NIRSPAO data, and did not appear to vary between fibers or over time, consistent with the fringe expected from the NIRSPEC entrance window. The other periodogram feature was not present similar analysis of NIRSPAO data and showed significant variability over time and between science fibers, consistent with the additional fringing observed in KPIC.

The $3.5\text{\AA}$ period of this feature is consistent with the as-built optical thickness of the two CaF_2 dichroics used in KPIC for the pyramid wavefront sensor and tracking camera pickoffs. Variations in the angle of incidence on these dichroics can produce varying degrees of constructive or destructive interference, explaining the observed variations in amplitude over time and when switching between fibers. Though we did not perform systematic tests, the peak constructive interference appears to occur at approximately 400 mas off-axis separations, and substantially impacts KPIC’s ability to detect companions in the 200-600 mas separation range. While the fringing is well-modeled as a Fabry-Perot etalon, the periodicity of this model makes it a challenge to reliably fit to observations, and work on improved fringe fitting routines is ongoing.

2.3.4 Companion Detections

During phase I, KPIC made successful detections of at least 23 substellar companions, most of which are in the preliminary stages of analysis. The detected companions include all four known HR 8799 planets [J. J. Wang et al. \(2021b\)](#), and spin measurements for three of them [J. J. Wang et al. \(2021a\)](#), as well as measurements of the carbon and oxygen abundances of the benchmark brown dwarf HR 7672 B [J. Wang et al. \(2022\)](#). Detected companions ranged in separations from 200 mas to 3600 mas, with K -band magnitudes as high as 17. Tracking was demonstrated on primaries as faint as $H = 10$. The improved instrumental stability offered by KPIC is also an asset for detecting unresolved companions through high-resolution spectroscopy.

Most observations used a strategy of nodding between two science fibers (either ABAB or ABBA), which allows instrumental and sky background to be easily subtracted. In some cases, particularly for small separations, fringing appears to be the limiting factor in making a detection. Developing strategies to reliably fit and remove this fringing in order to deliver background-limited performance across the full range of separations is therefore a high priority for ongoing data reduction pipeline development.

2.4 Discussion

2.4.1 Impact of Long Read Times

The long read times of both SPEC and SCAM, relative to the total time available for pre-observing checkout, substantially limited the range and repeatability of calibration scans. Routine checks of the system alignment took at least three hours, which could easily double if problems were encountered. This time requirement required personnel to be dedicated specifically to daytime calibrations, and occasionally required calibrating only two or three of the four science fibers in order to complete all calibrations before sunset. The long scan duration also imposed stricter requirements on the temporal stability of the calibration light source, which led to issues with using older bulbs in the calibration lamps, as the variations in source intensity could be larger than the variations caused by the optical alignment.

The long duration of scans also prevented routine systematic calibration of non-common path aberrations for KPIC. Ideally, this would involve systematically applying aberrations to the deformable mirror, performing a scan of the FIU tip-tilt mirror in case the aberrations shift the center of light, and recording the peak coupling as a function of applied aberration amplitude. This process would require approximately ten tip-tilt scans per Zernike mode, which was impractical during phase I. Instead, NCPAs were calibrated by eye by manually applying aberrations to produce an aberration-free PSF on the KPIC tracking camera. While this procedure was fast and appears to have been effective, it does not allow systematic

tracking of NCPAs over time, and may not correct all aberrations.

2.4.2 Calibration Stability

As discussed in Section 2.2, changes in the FEU calibrations generally occurred only between observing runs, with only minimal night-to-night variation. This suggests NIRSPEC is stable once it is in AO mode, but that moving NIRSPEC in and out of the AO position is not repeatable at the micron level. The resulting shifts in the optimum positions were well within the ranges KPIC could accommodate, and did not significantly impact operations aside from the time required to perform calibrations.

While the FEU was generally stable between nights, the fiber positions showed non-negligible shifts. The FWHM of the fiber coupling map is approximately four pixels on the KPIC tracking camera (see Figure 2.2). Observed inter-day variations in PSF location were on the order of 0.3 pixels, which had a noticeable impact on the coupling efficiency. Repeated scans during daytime calibration could determine the optimum positions to the 0.1 pixel level, suggesting that this error accumulates relatively slowly, and large drops in coupling efficiency over a night were not observed. The origin of this drift was not identified in phase I, and appears to be present in KPIC phase II despite the differences in the FEU relative to NIRSPEC.

2.4.3 Improvements for Phase II

KPIC phase II. [Jovanovic et al. \(2020\)](#) includes a number of improvements which will aid both calibration and overall performance. Most significantly, KPIC phase II includes a photodiode as an option for the output of the FEU. This photodiode has negligible read time, and reduces the time required to perform a scan of the FIU tip/tilt mirror by more than 95%. In addition to enabling rapid determination of the fiber locations, this makes routine calibration of NCPAs feasible. During phase II commissioning, up to twelve Zernike

modes can be scanned in approximately one hour, typically producing a 10–15% improvement in the coupling efficiency compared to the nominal DM map. While other aspects of the calibration of phase II are mostly unchanged from phase I, the KPIC fiber bundle is now fixed to match the angle of the NIRSPEC slit, which simplifies the FEU tip/tilt alignment. The FEU positioning and focusing also appears to be more stable than in phase I, though inter-run stability data remain limited at this stage of commissioning.

Early on-sky tests of KPIC phase II obtained a total throughput of 5%, significantly better than the best performance achieved in phase I. In addition to improved calibrations, the installation of a new, higher-throughput K -band filter for NIRSPEC and improvements in the FEU optics contributed to this increase in performance. The fringing discussed in Section 2.3 remains present in KPIC phase II. In the long term, replacement or modification of the current dichroics may alleviate the fringing. In the short term, we have developed an analytic model that appears to fit the fringing to approximately the 1% level, though fitting this model remains challenging. This model remains in development, and will be presented in detail in future work. Principal Component Analysis (PCA) has also been effective at reducing fringing effects, though its use for science observations requires care to avoid distorting spectral features.

2.5 Summary

KPIC phase I successfully demonstrated diffraction-limited high-resolution spectroscopy for substellar companion characterization in the K -band, detecting over 23 companions as faint as $K_{\text{mag}} = 17$. KPIC’s design as an optional addition to existing NIRSPAO capability requires a large number of moving optics, which must be calibrated before each night of observing. We developed procedures to reliably perform these calibrations, delivering peak on-sky throughputs consistent with the design budget under good conditions.

KPIC phase II has deployed a series of improvements to KPIC to improve sensitivity and

ease calibrations, partly in response to the lessons learned from phase I. These improvements will greatly reduce the time required for daytime setup of the instrument, as well as enable routine NCPA compensation in order to maximize coupling into science fibers. In the longer term, lessons from KPIC will inform the construction and operation of HISPEC, a full $yJHK$ -band high-resolution fiber-fed spectrograph for Keck [D. Mawet et al. \(2019\)](#).

CHAPTER 3

Keck/KPIC Emission Spectroscopy of WASP-33b

A version of this chapter was previously published in the *Astronomical Journal* (Finnerty *et al.* 2023, AJ 166, 1, 31)

Abstract

We present Keck/KPIC high-resolution ($R \sim 35,000$) K -band thermal emission spectroscopy of the ultra-hot Jupiter WASP-33b. The use of KPIC’s single-mode fibers greatly improves both blaze and line-spread stabilities relative to slit spectrographs, enhancing the cross-correlation detection strength. We retrieve the dayside emission spectrum with a nested sampling pipeline which fits for orbital parameters, the atmospheric pressure-temperature profile, and molecular abundances. We strongly detect the thermally-inverted dayside and measure mass-mixing ratios for CO ($\log \text{CO}_{\text{MMR}} = -1.1^{+0.4}_{-0.6}$), H₂O ($\log \text{H}_2\text{O}_{\text{MMR}} = -4.1^{+0.7}_{-0.9}$) and OH ($\log \text{OH}_{\text{MMR}} = -2.1^{+0.5}_{-1.1}$), suggesting near-complete dayside photodissociation of H₂O. The retrieved abundances suggest a carbon- and possibly metal-enriched atmosphere, with a gas-phase C/O ratio of $0.8^{+0.1}_{-0.2}$, consistent with the accretion of high-metallicity gas near the CO₂ snow line and post-disk migration or with accretion between the soot and H₂O snow lines. We also find tentative evidence for $^{12}\text{CO}/^{13}\text{CO} \sim 50$, consistent with values expected in protoplanetary disks, as well as tentative evidence for a metal-enriched atmosphere (2–15 $\times$ solar). These observations demonstrate KPIC’s ability to characterize close-in planets and the utility of KPIC’s improved instrumental stability for cross-correlation techniques.

3.1 Introduction

While large surveys have started to provide population-level insight into the physical and orbital properties of exoplanet systems, the details of exoplanet atmospheres, including composition, formation history, and 3D thermal structure, remain uncertain, with known trends suggesting substantial diversity (M. Mansfield et al., 2021). Improved knowledge of hot Jupiter atmospheres in particular may be a key piece to understanding the process of giant planet formation. Different formation scenarios are expected to produce differences in both relative atmospheric abundances (e.g. K. I. Öberg et al., 2011; R. A. Booth et al., 2017) and/or overall metallicity (e.g. N. Espinoza et al., 2017; N. Madhusudhan et al., 2017; A. J. Cridland et al., 2019). Recent observations (S. Pelletier et al., 2021; M. R. Line et al., 2021) have retrieved abundances which appear to conflict with the predictions from some of these theories, particularly the expectation of an inverse correlation between metallicity and C/O ratio (N. Espinoza et al., 2017; A. J. Cridland et al., 2019). These abundances may be explained by pebble drift (R. A. Booth et al., 2017), but these discrepancies suggest our understanding of either the planet formation process or atmospheric retrievals may be substantially incomplete.

Ultra-hot Jupiters (UHJs), with equilibrium temperatures $T_{\text{eq}} > 2000$ K, are a particularly interesting case for understanding planet formation processes. Two of the three hottest-known UHJs, KELT-9b and WASP-33b, orbit A-type stars on significantly misaligned orbits (B. S. Gaudi et al., 2017; A. Collier Cameron et al., 2010), suggesting a dynamical history of eccentric Kozai-Lidov effects (S. Naoz et al., 2011), though no additional planets are currently known in either system. Several A/B-type stars (e.g. HR 8799, β Pic) have been found to host one or more massive planets on wide orbits, raising the possibility that UHJs are an alternative evolutionary outcome of such systems. UHJ atmospheres may thus hold indications of when and how planet migration occurred.

Understanding the formation of UHJs will also require understanding their extreme at-

atmospheric chemistry. Commonly-used chemical equilibrium assumptions are expected to fail in the case of UHJs, particularly on the dayside, where extreme UV fluxes are expected to produce thermal inversions, drive mass loss, dissociate molecules, and even ionize some transition metals (A. Wyttenbach et al., 2020; G. Fu et al., 2022; F. Yan et al., 2021; S. K. Nugroho et al., 2021; N. Casasayas-Barris et al., 2019). These effects must be incorporated into 3D models in order to accurately model global energy transport (e.g. A. Roth et al., 2021). Transitions in phase/ionization state are expected on the nightside, when UV fluxes decline, though this will depend on the details of thermal redistribution between the hemispheres. Indications of rainout have been reported from analyses of transit observations of some UHJs (D. Ehrenreich et al., 2020; J. P. Wardenier et al., 2021; M. C. Johnson et al., 2023), but such observations have difficulty in unambiguously localizing a signal to a particular longitudinal range due to the complexity of 3D atmospheric circulation (A. B. Savel et al., 2022). Even the possibilities of photodissociation and rainout processes suggest current global circulation models (GCMs) coupled to a chemical-equilibrium radiative transfer framework are inadequate for modeling UHJ atmospheres, though understanding the modes of these failures and when they occur will require additional observational constraints (W. Pluriel et al., 2022). Understanding such modeling issues is critical for successfully interpreting chemical abundances as indicators of planetary formation and evolutionary history.

Recent advances in both analysis techniques and instrumentation have positioned high-resolution cross-correlation spectroscopy (HRCCS) as a promising method for obtaining constraints on the thermal and chemical properties of hot Jupiter atmospheres. This technique uses the change in the radial velocity of a close-in planet over several hours to isolate velocity-variable planetary spectral features from quasi-fixed stellar features using a cross-correlation (CC) template believed to match the planet and previously known orbital properties. Initially used to detect molecules such as CO and H₂O in hot Jupiter atmospheres (e.g. I. A. G. Snellen et al., 2010; M. Brogi et al., 2012; A. C. Lockwood et al., 2014; C. Buzard et al., 2020), M. Brogi & M. R. Line (2019) developed a log-likelihood (logL) function that enables

Bayesian retrievals of high-resolution observations, using forward models to produce CC templates which better match observations. Using this approach, [S. Pelletier et al. \(2021\)](#) retrieved a CO abundance and pressure-temperature (PT) profile for the hot Jupiter τ Boo A b, and [M. R. Line et al. \(2021\)](#) were able to retrieve both CO and H₂O abundances for WASP-77A b, yielding the first robust C/O ratio measurement for an unresolved planetary companion from high-resolution spectroscopy. Key to these retrievals are fast radiative transfer tools, which can quickly produce high-resolution spectra for planets with arbitrary molecular abundances and PT profiles, obviating assumptions about atmospheric chemistry or bulk composition.

Concurrent with these improvements in data analysis, new instruments are being developed and deployed with design features better suited for CC-based techniques than previous facilities. In particular, [K. C. Rasmussen et al. \(2021\)](#) identified correlated noise and minor blaze function variations as having major impacts on the final detection strength when using these techniques, which can be improved by using highly stable instruments. The use of single-mode fibers (SMFs) in Keck/KPIC ([J.-R. Delorme et al., 2021](#)) accomplishes this for the NIRSPEC ([I. S. McLean et al., 1998](#); [E. C. Martin et al., 2018](#); [R. A. López et al., 2020](#)) high-resolution ($R \sim 35000$) spectrograph on Keck. While the the Keck AO system and fiber coupling losses reduce overall throughput by a factor of ~ 7 compared with a seeing-limited slit spectrograph in KPIC phase I ([J.-R. Delorme et al., 2021](#)), the SMFs offer an ultra-stable line-spread function, as well as improvements in the blaze function and wavelength solution stabilities (though systematics may persist below the km s^{-1} level, well below the NIRSPEC resolution). Our analysis of KPIC phase I data showed no indications of intra-night variations $> 1 \text{ km s}^{-1}$ in either the blaze function or wavelength solution. While [L. Finnerty et al. \(2022\)](#) reported no apparent variation at the $\sim 1\%$ level in the KPIC LSF over phase I, KPIC suffers from a time-varying fringing effect which must be corrected (see Section 3.3), caused by interference between two pickoff dichroics ([L. Finnerty et al., 2022](#)). KPIC is a prototype instrument with ongoing hardware upgrades, which will correct this in the future.

In this paper, we present Keck/KPIC phase I observations of the UHJ WASP-33b covering the dayside hemisphere. We use a free-retrieval approach to recover orbital velocity parameters, chemical abundances, and pressure-temperature (PT) profiles. Section 3.2.1 presents properties of the system and previous results for atmospheric characterization of WASP-33b, followed by a presentation of our KPIC observations in Section 3.2.2. We discuss our retrieval procedure and choice of parameters/priors in Section 3.3, including a verification of our retrieval setup using simulated datasets with known inputs. The results of our retrievals for WASP-33b are presented in Section 3.4. We discuss these results in the context of previous studies of UHJ atmospheres and planet formation predictions in Section 3.5. Section 3.6 summarizes our results.

3.2 Observations and Data Reduction

3.2.1 Target Properties

WASP-33 (HD 15082) is a bright ($K = 7.47$, R. M. Cutri et al., 2003), rapidly rotating ($v \sin i = 86 \text{ km s}^{-1}$) A5 star (A. Collier Cameron et al., 2010; M. C. Johnson et al., 2015). WASP-33b was first discovered by D. J. Christian et al. (2006) in SuperWASP (D. L. Pollacco et al., 2006) transit photometry with a 1.22-day orbital period. Subsequent radial velocity measurements obtained a mass of $2.8 M_J$ (C. von Essen et al., 2014). The estimated planet mass and host star spectral type are similar to the HR 8799 system (K. Goździewski & C. Migaszewski, 2020), though the WASP-33b semimajor axis is more than 10^3 times smaller.

As a transiting planet around a rapid rotator, WASP-33b is an ideal target for observing the Rossiter-McLaughlin Effect (RME; Y. Ohta et al., 2005). Observations by A. Collier Cameron et al. (2010) found that WASP-33b has a near-polar retrograde orbit, with subsequent observations measuring orbital precession and the stellar quadrupole moment (M. C. Johnson et al., 2015; A. P. Stephan et al., 2022). The extremely small semimajor axis and near-polar orbit suggest the possibility of eccentric Kozai-Lidov dynamical effects (S. Naoz

Table 3.1: Star and planet properties of the WASP-33 system

Property	Value	Ref.
WASP-33		
RA	02:26:51.06	Gaia Collaboration (2020)
Dec	+37:33:01.7	Gaia Collaboration (2020)
Spectral Type	A5	S. Grenier et al. (1999)
K_{mag}	7.47	R. M. Cutri et al. (2003)
Mass	1.495 $M_{\odot}$	A. Collier Cameron et al. (2010)
Radius	1.44 $R_{\odot}$	A. Collier Cameron et al. (2010)
T_{eff}	7400 K	A. Collier Cameron et al. (2010)
$v \sin i$	86.6 km s^{-1}	M. C. Johnson et al. (2015)
v_{sys}	-9.2 km s^{-1}	G. A. Gontcharov (2006)
Age	< 400 Myr	A. Collier Cameron et al. (2010)
z	+0.1 dex	A. Collier Cameron et al. (2010)
WASP-33b		
Period	1.2198697 days	A. M. S. Smith et al. (2011)
$t_{transit}$	JD 2459509.9195	A. M. S. Smith et al. (2011)
a	0.02558 AU	A. M. S. Smith et al. (2011)
i	84.6°	A. P. Stephan et al. (2022)
K_p	226 km s^{-1}	Est.
Mass	2.8 M_J	C. von Essen et al. (2014)
Radius	1.5 R_J	A. Collier Cameron et al. (2010)
T_{eq}	3300 K	A. M. S. Smith et al. (2011)
C/O	$0.8^{+0.1}_{-0.2}$	This work

Note. — Transit time was estimated using the NASA exoplanet ephemeris service. We estimate K_p from the semi-major axis and orbital period. L. van Sluijs et al. (2022) reported K_p values ranging from 220 to 240 km s^{-1} , depending on the observed orbital phase and cross-correlation model.

et al., 2011), though there are presently no additional planets known in the system to act as perturbers. This system architecture and misaligned orbit is extremely similar to the UHJ KELT-9b (B. S. Gaudi et al., 2017), which may be a result of a common formation pathway for both systems.

WASP-33b has been a frequent target for previous atmospheric characterization studies. Near-IR dayside observations have detected CO and OH in emission, but found only weak signs of H₂O, indicative of high-temperature thermochemistry (S. K. Nugroho et al., 2021; L. van Sluijs et al., 2022; F. Yan et al., 2022). Optical observations have detected a number of oxides and atomic species, including AlO (C. von Essen et al., 2019), Si I (D. Cont et al., 2022a), Fe I (D. Cont et al., 2021; M. K. Herman et al., 2022), Ti I, and V I (D. Cont et al., 2022b), while transit observations of Balmer lines suggest an extended escaping hydrogen envelope driving mass loss at a rate of $\sim 10^{12}$ g/s (F. Yan et al., 2021). These observations have focused on dayside longitudes or the terminators, with phase curve observations suggesting inefficient redistribution of heat to the nightside (M. Zhang et al., 2018; M. K. Herman et al., 2022). These findings paint the picture of WASP-33b as an extreme ultra-hot Jupiter, with mass loss, photochemistry, and dramatic day/night differences.

WASP-33 is a rapid rotator, with rotational broadening and gravity darkening effects significantly impacting the stellar spectrum. WASP-33 is also a δ Scuti pulsator (E. Herrero et al., 2011). We discuss our treatment of these effects in Section 3.3.1.3.

3.2.2 Observations

We observed WASP-33 with Keck/KPIC (J.-R. Delorme et al., 2021) on UT dates 2021 November 21 and 2021 November 22. KPIC (Keck Planet Imager and Characterizer) is a series of upgrades to Keck II/NIRSPEC (I. S. McLean et al., 1998; E. C. Martin et al., 2018; R. A. López et al., 2020) and Keck II AO to enable high-resolution ($R \sim 35,000$) diffraction-limited spectroscopy for Keck. Primarily intended for spectroscopic follow-up of directly imaged companions, the use of single-mode fibers offers a factor of ~ 100 reduction

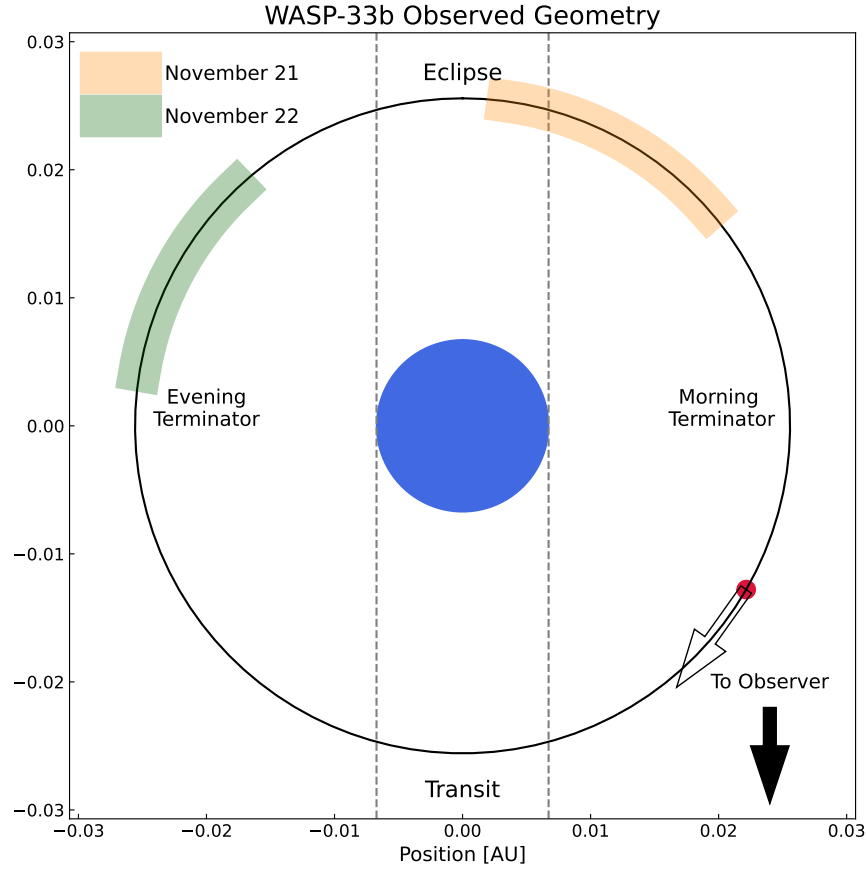


Figure 3.1: Observed orbital geometry of the WASP-33 system

The diagram is drawn to-scale with the planet orbit face-on and observed orbital phases shaded by observation date. The ellipticity of the star is neglected, and the planet's motion is drawn clockwise to reflect the retrograde orbit. The 2021 November 21 observations probe dayside thermal emission and provide a planet-free stellar spectrum during eclipse. The 2021 November 22 observations targeted the afternoon/dusk region but suffered from poor conditions and are therefore omitted from analysis.

Table 3.2: Summary of KPIC observations of WASP-33

UT Date	Wall Time	Integration Time	Orbital Phase	Airmass	Throughput
2021 November 21	192 min	144 min	0.52-0.64	1.08-1.05-1.21	$\sim 2.3\%$
2021 November 22	185 min	130 min	0.28-0.38	1.31-1.05	$< 1\%$

Note. — The airmass column lists airmass at the start of the observation, the minimum airmass, and the airmass at the end of the observing sequence. For both nights, a significant airmass range was observed, which is beneficial for PCA-based atmospheric detrending. Instrument performance on the first night was excellent for KPIC phase I, with throughputs consistently above 2% giving per-channel SNR of ~ 100 in the extracted 1D spectra for each frame. Poor AO correction on the second night led to substantially lower throughput, and we omit these data from our analysis.

in sky background, as well as long-term blaze and line-spread function (LSF) stability. [K. C. Rasmussen et al. \(2021\)](#) demonstrated that even minor variations in the LSF or blaze function can significantly impact detection of close-in planets through cross-correlation techniques. Previously, [L. Finnerty et al. \(2021\)](#) found that cross-correlation techniques are much more severely impacted by minor systematic errors compared with modest increases in Gaussian noise. These findings suggest that the improvements in LSF/blaze stability with KPIC may offset the increase in Poisson noise due to lower throughput in high-resolution cross-correlation applications compared with seeing-limited slit-fed spectrographs. We note that the KPIC phase I throughput was comparable to AO-fed NIRSPEC ([L. Finnerty et al., 2022](#)) and that KPIC phase II significantly exceeds the throughput performance of NIRSPA0 ([D. Echeverri et al., 2022](#)).

Our observations are summarized in Table 3.2. For all observations, we used an ABBA pattern nodding between KPIC science fibers 1 and 2. These fibers had the highest throughputs of the four science fibers in KPIC phase I (tested at the start of each night), and the nodding allows us to effectively subtract sky emission features and thermal emission from

warm front-end optics on the Keck AO bench. We obtained 90-s exposures at each nod position, giving our observations a time resolution of approximately four minutes after read time/overheads and coadding frames. We chose a time resolution under five minutes based on simulations showing that the orbital motion of WASP-33b would begin to significantly broaden the final cross-correlation peak for longer timescales (known as Doppler smearing). Figure 3.1 presents a diagram of the system with the observed orbital phases shaded by observation date.

The 2021 November 21 observations began during secondary eclipse, providing a stellar spectrum with no planet contribution. Observations continued post-eclipse for just under three hours, covering roughly noon to mid-morning longitudes. Conditions were good, with throughput from the top of Earth’s atmosphere through detection peaking at consistently around 2.5%.

We attempted to obtain additional observations on 22 November covering late-evening to afternoon longitudes. However, high clouds caused significant extinction and poor AO performance, leading to top-of-atmosphere throughput consistently below 1%. We therefore omitted these observations from subsequent cross-correlation and retrieval analysis.

3.2.3 Data Reduction

We began by fitting the echellogram trace location and width for each fiber and order from observations of a bright calibrator star (typically the telluric standard for the wavelength calibrator, discussed below). Because the KPIC fiber-extraction unit (FEU) does not move relative to the spectrometer backend during science operations, this only needs to be done once per night. We then AB subtracted the science frames (taken in an ABBA sequence) to remove sky emission and thermal background. Spectral extraction was performed by summing over slices in the detector-Y direction (which is well aligned with the cross-dispersion direction) centered on the best-fit trace center with a width five times the standard deviation of the best-fit Gaussian.

Each fiber was individually wavelength-calibrated by comparing to a radial velocity standard following the procedure described in Section 3.2 of [J. J. Wang et al. \(2021a\)](#). In brief, we observed a late-type giant star (HIP 95771 in the case of the WASP-33 observations) at the start of each night and fit the observed spectrum with a combined telluric spectrum generated using PSG ([G. L. Villanueva et al., 2018](#)) and stellar model from the PHOENIX library ([T. O. Husser et al., 2013](#)). Using a late-type star greatly increases the number of lines used for calibration compared with using only the sparse K -band telluric absorption features, enabling a more robust calibration.

We next resampled all the extracted spectra from science fiber 1 onto the wavelength grid obtained for science fiber 2 using a cubic spline. While each fiber is stable in detector location and wavelength over a single night, manufacturing and alignment differences can lead to small variations between fibers in both fringing and LSF that we wish to average. We arrange the extracted spectra for each order into a times series, giving n_{order} arrays each of shape $n_{\text{nodes}} \times n_{\text{channels}}$. These arrays, along with the Julian date/time at the midpoint of each nod pair and the corresponding barycentric radial velocity to WASP-33 from Keck, are the inputs to our retrieval code. We omit the first three orders (blueward of $2.1 \mu\text{m}$) due to strong telluric contamination, and the following two orders due to wavelength calibration inaccuracies, leaving four NIRSPEC orders spanning $\sim 2.2 - 2.5 \mu\text{m}$, with significant gaps. Additional post-processing performed as part of the retrieval is discussed in Section 3.3.1.1.

3.3 Atmospheric Retrieval

Our approach to atmospheric retrieval is similar to that of [M. R. Line et al. \(2021\)](#), with the most significant differences being our use of a negative injection of the proposed planet model (see Section 3.3.1.1) prior to the principal component analysis and the use of `petitRADTRANS` ([P. Mollière et al., 2019, 2020](#)) for radiative-transfer calculations. In brief, we use `petitRADTRANS` to generate simulated time-series spectra matched to our detrended observations, and calcu-

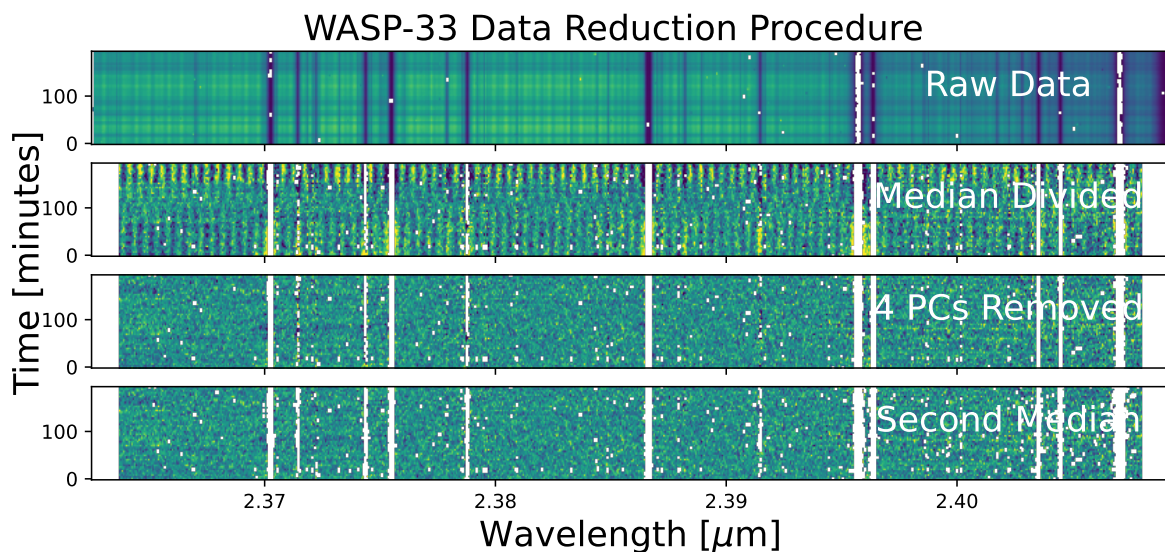


Figure 3.2: Data processing steps for one order

Top panel shows the raw data time series for one order, with evident tellurics and frame-to-frame variations in total flux. Second panel shows the data after scaling, dividing by a median spectrum, and masking values differing from the median by $> 8\%$ (approximately 10 times the median absolute deviation). Telluric and stellar features are effectively removed at this step, but a time-varying fringe pattern is clearly visible. Third panel shows data after removing the first four principal components. Occasionally weak temporally-fixed features persist after PCA. The fourth panel shows the data after a second median division to remove any such features and masking values differing from the median by $> 4\%$ (approximately 6 times the median absolute deviation)

late a log-likelihood following [M. Brogi & M. R. Line \(2019\)](#). We use this log-likelihood function to find best-fit orbital and atmospheric parameters using nested sampling ([J. Skilling, 2004](#)), specifically the *dynesty* ([J. S. Speagle, 2020](#)) implementation. We discuss the details of this procedure below.

3.3.1 Retrieval Procedure

3.3.1.1 Data Processing

At the end of the data reduction process, we can write each extracted spectrum as:

$$O(\lambda, t) = [S(\lambda) + P(\lambda, t)]T(\lambda, t)B(\lambda)F(\lambda)F(\lambda, t) \quad (3.1)$$

Where $O(\lambda, t)$ is the observed flux in each exposure, $S(\lambda)$ is the stellar flux and associated photon noise, including rotational broadening as well as limb and gravity darkening. $P(\lambda, t)$ is the planet flux and associated photon noise, which varies in time both due to the Doppler shift from the planet's orbital motion and due to variations in the visible longitudinal range. $T(\lambda, t)$ describes telluric transmission, which varies in time as the airmass and precipitable water vapor change. $B(\lambda)$ encapsulates the spectrograph blaze function and flat-field effects and is stable over a given night. Finally, we describe the fringing with both a static term $F(\lambda)$, arising from the NIRSPEC entrance window, and a time-varying term $F(\lambda, t)$ which is the result of the KPIC tracking camera dichroic and the pyramid wavefront sensor dichroic producing an etalon with a varying angle of incidence (L. Finnerty et al., 2022).

Because the projected radial velocity variation of WASP-33b over each observation sequence is substantially more than $3\times$ the velocity resolution of NIRSPEC, taking a median of the time series should leave only the terms which do not vary significantly over time. However, frame-to-frame variations in coupling efficiency as a result of variable AO correction require that we first divide each spectrum by its median (see Figure 3.2, top panel) before taking the median over the time series. We can then write the time-series median spectrum $M(\lambda)$ as:

$$M(\lambda) = \bar{S}(\lambda) \times \bar{T}(\lambda) \times B(\lambda) \times F(\lambda) \quad (3.2)$$

Where $\bar{S}(\lambda)$ is the average stellar spectrum and $\bar{T}(\lambda)$ represents the time-averaged telluric spectrum. We can then scale all spectra in the time series by the median and divide to

obtain:

$$\frac{O(\lambda, t)}{M(\lambda)} = \left(1 + \frac{P(\lambda, t)}{\bar{S}(\lambda)}\right) \frac{T(\lambda, t)}{\bar{T}(\lambda)} \times F(\lambda, t) \quad (3.3)$$

This is shown in the second panel of Figure 3.2. Both $T(\lambda, t)/\bar{T}(\lambda)$ and $F(\lambda, t)$ vary around unity, so we can combine these terms and rewrite them as:

$$\frac{T(\lambda, t)}{\bar{T}(\lambda)} \times F(\lambda, t) = 1 + \delta f(\lambda, t) \quad (3.4)$$

Using the above expression to rewrite equation 3.3 and expanding gives:

$$\frac{O(\lambda, t)}{M(\lambda)} = 1 + \frac{P(\lambda, t)}{\bar{S}(\lambda)} + \frac{P(\lambda, t)}{\bar{S}(\lambda)} \delta f(\lambda, t) + \delta f(\lambda, t) \quad (3.5)$$

At this point, a number of approaches have been used to remove the time-varying systematic noise/telluric residual term $\delta f(\lambda, t)$ (note that the cross term can generally be taken to be smaller than the others). One approach, used in e.g. [M. Brogi & M. R. Line \(2019\)](#); [S. Pelletier et al. \(2021\)](#), is to fit and divide a low-order polynomial to the time series of each spectral channel. This is effective when the temporal variation is slow, such as airmass-induced variations, and may be followed by additional processing such as PCA. For KPIC data, the time-varying fringe cannot be corrected with this approach, and we therefore do not use it.

An additional or alternative technique used in e.g., [S. Pelletier et al. \(2021\)](#); [M. R. Line et al. \(2021\)](#), is to perform principal component analysis (PCA) on the time series. PCA is a dimensionality reduction technique which projects the observed spectra onto a basis which maximizes the time-series variation in each successive component. This allows most of the variation in the time series to be encapsulated in the first few principal components, which can then be “zeroed-out” via a projection matrix in order to eliminate the variation. While this effectively eliminates most of the time-varying tellurics and fringing, it also removes/distorts some of the planet signal we are attempting to retrieve. This can be minimized by using the smallest number of principal components (PCs) needed to eliminate tellurics/fringing, as the planet signal is generally much lower amplitude and therefore should be more present in higher PCs.

The distortion of the spectrum caused by PCA can then be estimated by using the calculated PCs to apply a similar “stretch” to the data (M. R. Line et al., 2021). Specifically, we can write the observed flux, post-PCA and median division, as:

$$\alpha \frac{P(\lambda, t)}{S(\lambda)} [1 + \delta f(\lambda, t)] \quad (3.6)$$

Where we have subtracted the bias term from Equation 5. $\delta f(\lambda, t)$ represents the dropped principal components, which we use to “stretch” the model in our log-likelihood calculations and reproduce the $\delta f(\lambda, t)P(\lambda, t)/S(\lambda, t)$ term. Note that this assumes $\delta f(\lambda, t)$ does not contain any contribution from $P(\lambda, t)$, which is generally not valid, although the contribution may be negligible in some cases. These processing steps may inadvertently impact the strength of the planet features relative to the continuum. We therefore include a multiplicative scaling to the planet model (α) as a free parameter in our retrievals, which we expect to be of order unity. The third panel of Figure 3.2 shows the post-PCA time series for one order, with the time-varying fringing effectively removed. We show an example of the dropped principal components in Figure 3.3, which appear to be dominated by fringing and airmass variation.

Occasionally the post-PCA data show a temporally fixed fringing pattern at much lower amplitude than the original fringe. While Figure 3.2 indicates this is not substantially impacting these observations, we include a second median division after PCA in order to eliminate any residual fringing, though doing so does not appear to impact the results of our retrievals. The fourth panel of Figure 3.2 shows the time series after this final division and an additional masking of values differing from the median by $> 4\%$ (approximately 6 times the median absolute deviation)

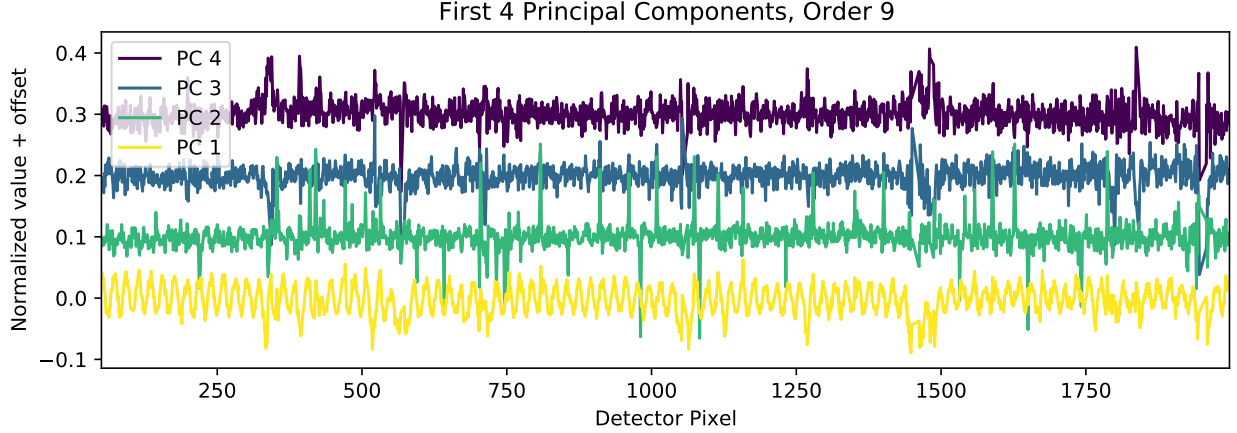


Figure 3.3: Example of the omitted principal components

The plotted data corresponds to the 2.44–2.49 μm NIRSPEC order shown in Figure 3.2. The impact of time-varying fringing and telluric absorption is clear throughout the first 4 principal components. A telluric feature can be seen near pixel 1500, where the PCA is correcting variations from our baseline PSG model. Amplitudes are relative to the continuum-normalized spectrum, with a 0.1 offset added to successive principal components.

3.3.1.2 Negative Injection and Number of PCs

Our initial tests found that removing 4 PCs enabled a detection of WASP-33b at a velocity similar to previous results from the literature (e.g. [S. K. Nugroho et al., 2021](#); [L. van Sluijs et al., 2022](#)). However, PCA will remove or distort the underlying planet signal, which must be mitigated in order to run retrievals. We adopt a negative-injection approach, where we subtract the proposed planet/star time series from the observed prior to performing the PCA. In the case where the planet model accurately reproduces the data, this eliminates the PCA self-subtraction issue, while potentially exaggerating it for poorly-matched models. This approach is sensitive to the exact match between the observations and the template, requiring PCA to be performed as part of each logL evaluation. While this significantly increases the computational cost of each log-likelihood call, it should reduce the sensitivity of the retrieval to the precise number of omitted principal components.

Using PCA requires a decision as to the number of principal components to omit. Re-

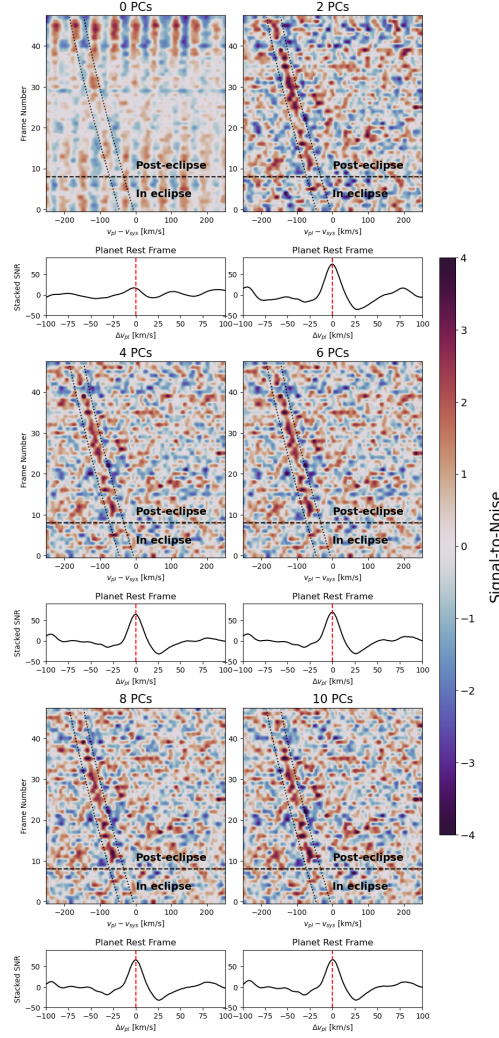


Figure 3.4: Cross-correlation versus planet velocity and exposure number for varying numbers of removed principal components

Data processing was identical as for the retrievals at the best-fit planet velocity, including negative injection before PCA. Signal-to-noise is estimated by dividing by the variance for $v_{pl} - v_{sys} > 0$, which does not overlap with the planet track. Lower panels show the summed CCF in the planet rest frame. Without PCA, the cross-correlation space is dominated by the time-varying fringe associated with transmissive optics in KPIC. PCA almost completely eliminates this effect, enabling a clear detection of the planet signal. Removing between 2 and 10 PCs has a negligible impact on the planet detection. We choose to remove 4 PCs, as visual inspection shows significant fringing and telluric contributions even in the 3rd and 4th components (see Figure 3.3).

moving too few principal components can lead to significant contamination from fringing or tellurics, while removing too many can distort or even eliminate the planet signal. We believe that our negative-injection approach should substantially reduce the sensitivity of the planet detection to the number of omitted PCs, provided the planet is injected at approximately the correct strength relative to the continuum.

To test the impact of varying the number of omitted PCs, we computed the stellar-frame cross-correlation function of the maximum-likelihood retrieved planet spectrum with each frame in the 21 November data for varying numbers of omitted PCs. This is shown in Figure 3.4, where the CCF has been divided by the variance for $v_{pl} - v_{sys} > 0$ in order to estimate the signal-to-noise ratio. We then shift to the planet rest frame and sum in order to estimate a 1D CCF. Without PCA, the 2D cross-correlation space is clearly dominated by the time-varying fringe, and the planet signal is barely detectable even in the stacked CCF. Between 2 and 10 omitted principal components, the planet signal is clear even in the 2D CCF, and the number of PCs dropped does not appear to significantly change the CCF.

The apparent independence of the planet detection on the number of PCs makes the choice of how many PCs to omit somewhat arbitrary. We opted to omit 4 PCs based on examination of the components in Figure 3.3, which show substantial contributions from fringing and tellurics in these components. While Figure 3.4 suggests we could safely drop additional components, we are concerned that model mismatch may still result in self-subtraction when many PCs are dropped, despite the negative injection. Omitting 4 components is a qualitative balance between removing known contaminants while avoiding self-subtraction issues and is consistent with other high-resolution retrievals (e.g. [M. R. Line et al., 2021](#)). For consistency and to avoid possible overfitting, we omit the same number of components for all orders. In the future, it would be preferable to develop and use a quantitative set of criteria for the number of PCs to remove. Alternatively, improved forward modeling of the KPIC fringing could reduce or eliminate the need for PCA.

3.3.1.3 Template Spectra and Opacities

Calculating a log-likelihood requires comparing the detrended time series obtained from the steps described in the previous subsection to an analogous simulated data set with known orbital and planetary parameters. This requires models of both stellar and planetary spectra in order to calculate the equivalent to the $P(\lambda, t)/S(\lambda)$ term obtained above.

For the stellar template, we use a PHOENIX model (T. O. Husser et al., 2013) with $T_{\text{eq}} = 7400$ K, $[\text{Fe}/\text{H}] = 0.0$, and $\log g = 4.5$, chosen to be similar to the stellar parameters in Table 3.1. We then simulate the observed stellar disk as a 60×60 array of these 1D spectra, Doppler shift by the expected $v \sin i$ at the location of each grid point on the stellar disk, and apply limb darkening coefficients from D. K. Sing (2010). We neglect the impacts of both gravity darkening and the δ Scuti pulsations of WASP-33. Each of these may lead to an achromatic systematic offset between our simulated $S(\lambda)$ and the true stellar spectrum, which the scaling parameter in the retrieval should account for. We note that P. W. Cauley et al. (2021) reported the pulsation of WASP-33 leads to time-varying velocity shifts in the cross-correlation function for high resolution optical data. We do not expect this phenomenon to impact K -band observations, as we do not anticipate H_2O or CO features in the A-type stellar spectrum.

For the planet templates, we use `petitRADTRANS` (P. Mollière et al., 2019, 2020) to perform the radiative-transfer calculation with 80 log-uniform spaced pressure slabs from 10^2 bar to 10^{-6} bar and a spectral resolution of 1.25×10^5 over the $\sim 2.1\text{--}2.5 \mu\text{m}$ range covered by our observations. We use molecular opacities for CO , H_2O , and OH generated using ExoCross (S. N. Yurchenko et al., 2018) from the HITEMP linelists (HITEMP 2010 for H_2O , HITEMP 2019 for CO , HITEMP 2020 for OH ; L. S. Rothman et al., 2010; I. E. Gordon et al., 2022). We use the G. Li et al. (2015) partition function for CO , the O. L. Polyansky et al. (2018) partition function for H_2O , and the M. Yousefi et al. (2018) partition function for OH . For SiO , we use the ExoMol-recommended linelists and partition functions from S. N.

Yurchenko et al. (2021). Opacities are generated on pressure-temperature grids ranging from 10^3 – 10^{-6} bar in pressure and from 80–6000 K in temperature, which `petitRADTRANS` interpolates to the desired pressure/temperature values for each layer. We allow molecular abundances for each species to vary freely during the retrieval but hold abundances constant at all pressures.

3.3.1.4 Pressure-Temperature Profile

To describe the atmospheric temperature at each pressure layer, we use the pressure-temperature (PT) profile parameterization from N. Madhusudhan & S. Seager (2009). This 6-parameter model divides the atmosphere into three zones — two upper zones with exponential behavior and an isothermal lower atmosphere. Using two upper zones allows this model to fit both inverted and non-inverted PT profiles, and the isothermal lower atmosphere is expected for hot Jupiters due to high optical depths (N. Madhusudhan & S. Seager, 2009). Based on previous results from WASP-33b (S. K. Nugroho et al., 2021; L. van Sluijs et al., 2022; F. Yan et al., 2022) we require a thermal inversion for the dayside PT profile. This requirement speeds convergence and avoids issues with fitting inverted sidelobes of the cross-correlation function. We also enforce $T < 6000\text{K}$ throughout the atmosphere in order to avoid hitting the limits of our opacity tables.

3.3.1.5 H^-

The temperature and irradiation of WASP-33b suggest a significant fraction of upper atmospheric H_2 may be dissociated, and H^- may be a significant source of continuum opacity. We experimented with several ways of incorporating H^- . Our first approach used the `poor_mans_nonequ_chemistry` calculator from `petitRADTRANS` (P. Mollière et al., 2017, 2020) to estimate the chemical equilibrium H_2 , He, H, H^- , and e^- fractions in the atmosphere for the proposed PT profile, which `petitRADTRANS` then uses to calculate H^- opacity.

While this accounts for the strongly-varying vertical abundance of H^- , this is inconsistent with our free-retrieval approach used for other species. We next attempted to include H^- and e^- as species in the retrieval, but both were effectively unconstrained over a prior based on the typical equilibrium chemistry values.

Finally, after comparing model planet spectra with and without H^- (see Figure 3.5), we opted not to include H^- opacity in our retrievals. We find that on the scale of a single NIRSPEC order, H^- is effectively achromatic, resulting in a consistent $\sim 10\%$ reduction in line strengths (see Figure 3.5, orange line) relative to the continuum. As we do not preserve the continuum level through the detrending process, the overall scaling parameter is already effectively scaling the line strengths relative to the continuum, making the additional inclusion of H^- opacity redundant. The CO and H_2O abundances retrieved without H^- opacity are statistically consistent with the retrievals including H^- based on equilibrium abundances.

Neglecting H^- should result in a smaller value for the scaling parameter, as the lines will be weaker relative to the continuum than we assume. This achromatic behavior may not hold over wider bandpasses, in which case H^- should be included in the retrieval model.

3.3.1.6 Model Processing

Using the planet spectra calculated by `petitRADTRANS`, we next calculate a model $P(\lambda, t)/S(\lambda)$ time series. We first scale the planet flux by the planet/star area ratio and then Doppler shift the planet to the proposed velocity for each exposure. We subsequently divide the planet model by the stellar model, Doppler shift by the systemic velocity, and interpolate onto the observed wavelength grid. We then convolve the model spectrum with a 1.7 pixel Gaussian representing the NIRSPEC instrument profile and divide by the time-series median. The optimum kernel was determined by maximizing the log-likelihood at the planet peak identified in a $K_p - v_{sys}$ diagram with a fixed planet template and is slightly larger than expected based on the instrument resolution, most likely as a result of the motion of WASP-33b along

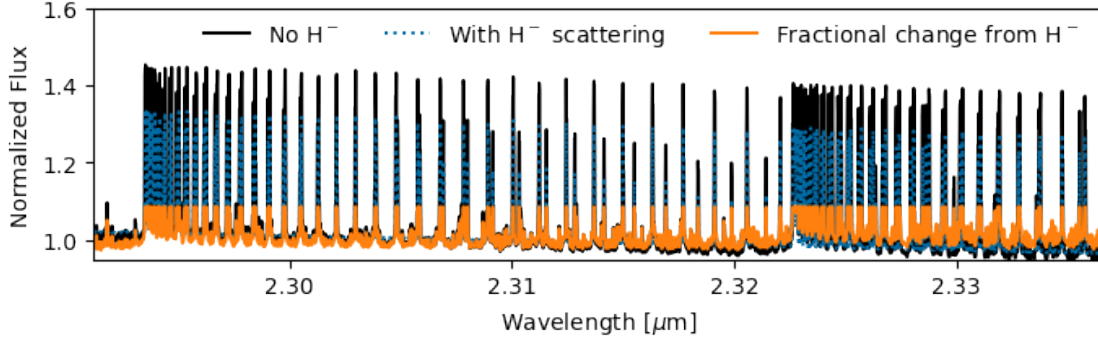


Figure 3.5: Impact of H^- on WASP-33 b

Normalized planet spectrum including H^- opacity (dotted blue) and without (black) over the wavelength range of a single NIRSPEC order corresponding to the CO bandhead. The ratio of the spectrum without H^- to the spectrum with H^- is plotted in orange. Over the short bandpasses of the NIRSPEC orders, H^- is effectively achromatic, reducing line strengths by $\sim 10\%$ relative to the continuum. As the continuum is removed during the detrending, the overall scaling parameter should account for the impact of H^- , explaining the weak constraints using a free retrieval approach and justifying the omission of H^- opacity.

its orbit within a single set of exposures (known as Doppler smearing). Finally, we apply the PCA “stretch” to the model and perform a second median division in order to match the treatment of the observations. At this point the model spectra should be exactly analogous to the data, and we calculate the log-likelihood as described in [M. Brogi & M. R. Line \(2019\)](#).

3.3.1.7 Parameter Selection

Our retrieval model consists of 16 free parameters. We list these parameters and priors in [Table 3.3](#), and provide a brief description and motivation here. For the PT profile, we adopt the six-parameter model from [N. Madhusudhan & S. Seager \(2009\)](#), setting $\beta = 0.5$. This takes a top-of-atmosphere temperature, two coefficients to scale the argument of the exponential functions, and three reference pressures for the transition between the different exponentials and the isothermal lower atmosphere. We implement this as a single physical pressure, and two fractional breakpoints (in log space) between that pressure and the top/bottom of the atmosphere respectively. This allows inequality constraints to be more

Table 3.3: List of parameters and priors for the WASP-33b atmospheric retrievals.

Name	Symbol	Prior
Upper-atmosphere scaling	α_1	Uniform(0,1)
Lower-atmosphere scaling	α_2	Uniform(0,1)
Top-of-atmosphere temperature [K]	T	Uniform(2000, 6000)
Reference pressure [bar]	$\log P_1$	Uniform(-6, 0)
Mid-atmosphere fraction	f_{P_2}	Uniform(0,1)
Lower-atmosphere fraction	f_{P_3}	Uniform(0,1)
K_p offset [km s^{-1}]	ΔK_p	Uniform(-40, 40)
v_{sys} offset [km s^{-1}]	Δv_{sys}	Uniform(-30, 30)
$\log \text{H}_2\text{O}$ mass-mixing ratio	$\log \text{H}_2\text{O}$	Uniform(-6, -1)
$\log \text{CO}$ mass-mixing ratio	$\log \text{CO}$	Uniform(-6, -0.1)
$\log \text{OH}$ mass-mixing ratio	$\log \text{OH}$	Uniform(-6, -1)
$\log \text{SiO}$ mass-mixing ratio	$\log \text{SiO}$	Uniform(-6, -1)
$\log {}^{13}\text{CO}/{}^{12}\text{CO}$	$\log {}^{13}\text{CO}_{\text{rat}}$	Uniform(-2.5, -0.5)
Total H mass-fraction	$\log \text{allH}$	Uniform(-0.2, -0.05)
HI fraction	f_{HI}	Uniform(0, 1)
Scale factor	scale	Uniform(0, 2)

Note. — In addition to these priors, we required both a thermal inversion and that the atmospheric temperature stay below 6000 K at all pressure levels, in order to avoid going beyond the bounds of our opacity grids.

easily placed on the different pressures in order to enforce the presence/absence of a thermal inversion. We choose priors for the temperature based on previous literature values (S. K. Nugroho et al., 2021; L. van Sluijs et al., 2022), while we allow the scaling and pressure parameters to vary over a broad range. We require a thermal inversion based on the initial qualitative cross-correlation analysis discussed in Section 3.4 and previous literature (S. K. Nugroho et al., 2021; F. Yan et al., 2022; L. van Sluijs et al., 2022).

We also fit two parameters for the orbital properties of WASP-33b. While the planet radial velocity semi-amplitude (K_p) and systemic velocity (v_{sys}) are well-constrained by previous literature, the 3D atmospheric structure may introduce phase-dependent velocity shifts due to winds or outflows (H. Beltz et al., 2022). We choose priors based on the approximate extent of the planet peaks obtained from cross-correlation with an assumed template (see Figure 3.6) and to cover the range of values reported in L. van Sluijs et al. (2022).

We fit for seven abundances – H_2O , CO , OH , SiO , H_2 , the $^{13}\text{CO}/^{12}\text{CO}$ ratio, and the H_2 dissociation fraction. H_2O and CO are expected to dominate the K -band spectrum for UHJs and are expected to be the dominant forms of C, O, and overall metals in the atmosphere of WASP-33b. We also include ^{13}CO , as we expect it to be detectable in an atmosphere with a high overall CO abundance (P. Mollière & I. A. G. Snellen, 2019). While simulations suggested that the limited wavelength coverage of our observations may be insufficient to make an independent detection of OH, we include it for completeness based on the previous dayside detection reported by S. K. Nugroho et al. (2021), which used prominent OH features in the H -band. M. Brogi et al. (2023) also detected OH in the atmosphere of the UHJ WASP-18b with H -band observations. We also fit for SiO , as the `petitRADTRANS` equilibrium chemistry models suggest that it may be a significant oxygen reservoir in the high-C/O, high-metallicity regime, and (D. Cont et al., 2021) previously reported a detection of atomic Si in the dayside upper atmosphere of WASP-33b. The final abundance parameters are the total (molecular and atomic) hydrogen mass fraction and the H_2 dissociation fraction. The remainder of the atmosphere is assumed to be entirely He.

Finally, we fit an additional multiplicative scaling parameter applied to the planet model. This accounts for a number of possible biases in our retrieval setup, while also serving as a check for their severity. Ideally, we should retrieve a scaling parameter of 1. However, we neglected both δ Scuti pulsations and gravity darkening of the host star, which may introduce systematic differences in the relative flux of the planet. We also ignore H^- opacity in the planet atmosphere, which could produce achromatic changes in the line strengths. The scale factor allows us to correct for these omissions, while also checking the size of these effects.

3.3.1.8 Nested Sampling

We compare our forward-models described above to the processed observations using the log-likelihood function from [M. Brogi & M. R. Line \(2019\)](#). Specifically:

$$\log L = -\frac{N}{2} \log \left(\frac{D^2}{N} + \frac{M^2}{N} - 2 \frac{M * D}{N} \right) \quad (3.7)$$

Where N is the number of valid points in each observed spectrum, D is the cleaned data, and M is the proposed spectrum, which already includes the scaling parameter. This is calculated for each order and each science frame taken out-of-eclipse, then summed to produce a total log-likelihood for the observation sequence.

This log-likelihood calculation enables us to use the full range of Bayesian fitting tools. As in [M. R. Line et al. \(2021\)](#), we opt for a nested-sampling approach ([J. Skilling, 2004](#)), in our case the `dynesty` implementation ([J. S. Speagle, 2020](#)). Nested sampling is suitable for high-dimensional problems with computationally expensive likelihood functions and potentially complicated posteriors, making it ideal for atmospheric retrievals. It is also easily parallelizable, allowing us to take advantage of cluster computing resources. Our retrievals using 16 CPU slots typically take $\sim 2\text{--}4$ days to reach $\Delta \log z = 0.001$, which is sufficient to obtain good estimates of the posteriors.

3.3.2 Validation Simulations

As our retrieval framework by necessity includes a forward-modeling capability, we can easily test our retrievals on a simulated system with known inputs. This provides a check on systematic biases in the retrieval and ensures that the reported uncertainties are reasonably accurate. These checks also allow us to determine if any parameters are inherently poorly constrained by the available data. All simulated data sets used the same orbital phase sampling as the observations (2021 November 21).

As our forward modeling does not include fringing or airmass variation, we do not include the PCA step in the test retrievals. The planet spectrum is the only time-varying component in the simulated spectrum. Even with our negative-injection approach, the planet spectrum is distorted by the PCA in the absence of stronger fringe/airmass-induced variations. This limits our ability to identify biases introduced from the PCA and may result in a mild overestimation of the retrieved errors in the simulations, as the negative-injection PCA approach is expected to increase preference for the true planet model. Ongoing developments in forward modeling of the KPIC fringing should reduce future reliance on PCA for defringing.

Our first test case was a star-only (no planet) simulated data set. This provides a non-detection baseline for comparison. Figure 3.10 shows the full corner plot (D. Foreman-Mackey, 2016) in Appendix 3.7. Despite using the same stopping criteria as other retrievals, the star-only simulation shows much flatter and noisier posteriors and reached the stopping criteria in far fewer iterations. Additionally, the scale parameter shows a weak preference towards smaller values, suggesting a preference for the absence of the planet, as expected. The retrieved pressure-temperature profile is nearly isothermal, and the maximum-likelihood planet spectrum is nearly flat, as the fitting minimizes the strength of the planet features.

Our second test case was based on the retrieved parameters for WASP-33b listed in the “Input” column of Table 3.4. The signal-to-noise ratio of the simulations was chosen to be similar to that of the observations. This provides both a general check for systematics or

Table 3.4: Input and retrieved parameters for the test retrieval.

Symbol	Input	Retrieved
α_1	0.48	$0.5^{+0.3}_{-0.3}$
α_2	0.10	$0.2^{+0.1}_{-0.1}$
T	3420	3760^{+740}_{-700}
$\log P_1$	-2.6	$-2.7^{+0.8}_{-0.7}$
f_{P_2}	0.29	$0.2^{+0.2}_{-0.1}$
f_{P_3}	0.42	$0.2^{+0.2}_{-0.1}$
ΔK_p [km s ⁻¹]	0	$1.8^{+3.3}_{-3.4}$
Δv_{sys} [km s ⁻¹]	0	$0.8^{+1.6}_{-1.7}$
$\log \text{H}_2\text{O}$	-4.3	$-4.1^{+0.6}_{-0.7}$
$\log \text{CO}$	-1.5	$-1.4^{+0.5}_{-0.8}$
$\log \text{OH}$	-2.5	$-4.2^{+1.2}_{-2.0}$
$\log \text{SiO}$	-3.7	$-3.1^{+1.6}_{-2.0}$
$\log {}^{13}\text{CO}_{\text{rat}}$	-1.8	$-2.1^{+0.3}_{-0.3}$
$\log \text{allH}$	-0.13	$-0.13^{+0.05}_{-0.05}$
$\log f_{\text{HI}}$	0.42	$0.5^{+0.3}_{-0.4}$
scale	1.0	$1.2^{+0.6}_{-0.6}$
SNR _{pt}	110	

Note. — Orbital phase sampling was identical to the 2021 November 21 data. The test case was chosen to be similar to the retrieval results, so that it serves as an injection/recovery test.

unconstrained parameters in our retrieval framework as well as a specific injection/recovery test for the retrieved dayside atmosphere. Retrieved values and uncertainties are listed in the “Retrieved” column of Table 3.4, and the full corner plot is presented in Figure 3.11.

All parameters except the OH mass fraction are retrieved to within 1σ of the input values, with error bars similar to those retrieved from the observations. The PT profile retrieved from the simulations is slightly hotter than the input profile but is generally within the 1σ bound and does not impact the retrieved abundances. The SiO mass fraction, H mass fraction, and H dissociation fraction are all poorly-constrained in both the observations and the simulated retrieval, suggesting our observations have limited sensitivity to these parameters.

While the OH posterior shows a peak in the observations, this is not the case in the simulated retrieval. The ^{13}CO isotopologue ratio and the scale factor are also better-constrained in the observations than the simulations, though not to the same degree as the OH abundance. While this may be a result of the negative-injection PCA approach used for the observations improving sensitivity to relatively small changes in the spectrum, the poor sensitivity in simulated retrievals suggests both apparent constraints may be artifacts.

We also ran retrievals using `emcee` (D. Foreman-Mackey et al., 2013). This provides a check that any biases are not due to the particulars of our nested sampling approach, such as the stopping criteria or the number of live points. The resulting median values and uncertainties from `emcee` were consistent with the nested sampling results. This suggests that systematics are more likely to be related to limitations in the radiative transfer calculation, log-likelihood function, or inherent limitations in the data, rather than the statistical framework used.

3.4 Results

We present qualitative results from cross-correlation analysis in Section 3.4.1. Quantitative results from our retrieval framework are presented in Section 3.4.2.

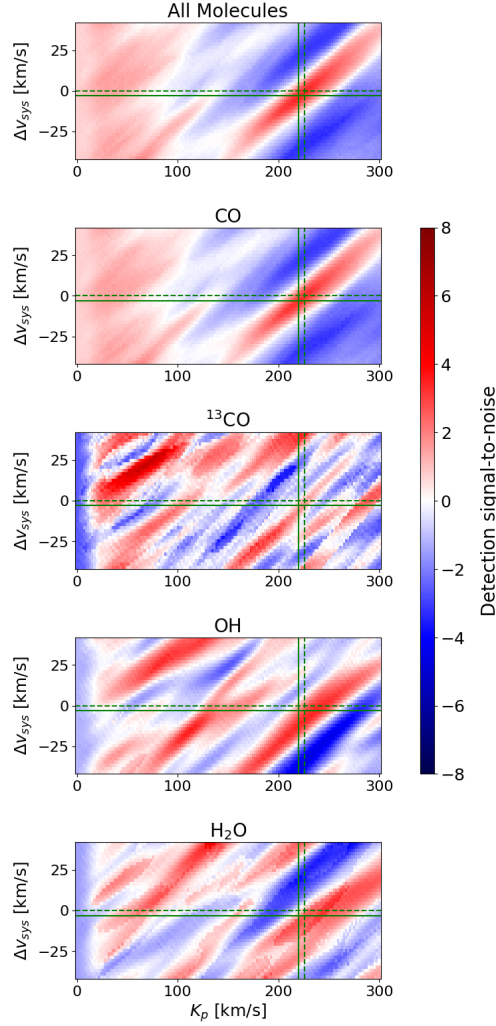


Figure 3.6: $\Delta v_{\text{sys}} - \Delta K_p$ diagrams for the retrieved WASP-33 b spectrum

The nominal and retrieved velocities are indicated in dashed and solid green, respectively. The top row shows all molecules, while the subsequent four rows show the contribution of individual species. ^{12}CO dominates the detection, while the other species show relatively weak features at the expected velocity of WASP-33b. Detection strength is estimated by dividing the computed log-likelihood map by the standard deviation taken after masking $K_p < 50 \text{ km s}^{-1}$ and below/above the 10th/90th percentiles in order to reduce the impact of the PCA-induced feature near $K_p = 0 \text{ km s}^{-1}$ and the planet peak itself. Figure 3.4 provides a better quantitative estimate of detection strength.

Table 3.5: Retrieval results for of WASP-33b.

Name	Symbol	Retrieved
Upper-atmosphere scaling	α_1	$0.6^{+0.3}_{-0.3}$
Lower-atmosphere scaling	α_2	$0.1^{+0.07}_{-0.05}$
Top-of-atmosphere temperature [K]	T	3500^{+500}_{-500}
Reference pressure [bar]	$\log P_1$	$-2.8^{+0.7}_{-0.6}$
Mid-atmosphere fraction	f_{P_2}	$0.2^{+0.2}_{-0.1}$
Lower-atmosphere fraction	f_{P_3}	$0.5^{+0.3}_{-0.3}$
K_p offset [km s^{-1}]	ΔK_p	-6^{+4}_{-3}
v_{sys} offset [km s^{-1}]	Δv_{sys}	-3^{+2}_{-1}
$\log \text{H}_2\text{O}$ mass-mixing ratio	$\log \text{H}_2\text{O}$	$-4.1^{+0.7}_{-0.9}$
$\log \text{CO}$ mass-mixing ratio	$\log \text{CO}$	$-1.1^{+0.4}_{-0.6}$
$\log \text{OH}$ mass-mixing ratio	$\log \text{OH}$	$-2.1^{+0.5}_{-1.1}$
$\log \text{SiO}$ mass-mixing ratio	$\log \text{SiO}$	$-3.6^{+1.3}_{-1.5}$
$\log ^{13}\text{CO}/^{12}\text{CO}$	$\log ^{13}\text{CO}_{\text{rat}}$	$-1.7^{+0.3}_{-0.5}$
Total H mass fraction	$\log \text{allH}$	$-0.14^{+0.06}_{-0.04}$
HI fraction	f_{HI}	$0.5^{+0.3}_{-0.3}$
Scale factor	scale	$1.3^{+0.5}_{-0.4}$
Derived Parameters		
C/O ratio	C/O	$0.8^{+0.1}_{-0.2}$
$\log \text{C}/\text{H}_{\text{VMR}}$	$\log \text{C}/\text{H}$	$-2.4^{+0.4}_{-0.6}$
$\log \text{O}/\text{H}_{\text{VMR}}$	$\log \text{O}/\text{H}$	$-2.3^{+0.4}_{-0.5}$

Note. — We report the median and $\pm 34\%$ quantiles for all parameters. Full corner plots are included in Section 3.7. In several cases, the peak of the retrieved posteriors shows substantial offsets from the median of the distribution, which can be seen in the full corner plots. Strong covariances between abundance parameters enables a better constraint on the C/O ratio than would be expected from the marginalized posteriors alone (see Figure 3.8).

3.4.1 Cross-Correlation Analysis

We use the best-fit retrieval parameters to compute $\Delta v_{\text{sys}} - \Delta K_p$ diagrams, both for the overall model and for each individual species. These are plotted in Figure 3.6, with the retrieved Δv_{sys} and ΔK_p values indicated in dashed green. This is the approach that previous high-resolution studies have used to make molecular detections (e.g. M. Brogi et al., 2012; C. Buzard et al., 2020, and many others). We note that attempts to quantify strengths for this type of detection have been fraught (e.g. C. Buzard et al., 2020; L. Finnerty et al., 2021; C. Buzard et al., 2021), but these plots can still provide useful qualitative insight.

Specifically, quantitative estimates of the detection strength from $K_p - v_{\text{sys}}$ plots typically assume values far from the planet peak are normally-distributed and use the standard deviation far from the planet as an estimate of the noise. In the case of Figure 3.6, this is complicated by the clear presence of systematic variations as a function of K_p due to the detrending suppressing the planet at small K_p . We therefore estimate the noise in Figure 3.6 by first masking $K_p < 50 \text{ km s}^{-1}$ to exclude the region where the PCA is having a significant impact, then additionally masking values above/below the 10th/90th percentile to remove the planet feature. We then calculate the standard deviation and use this to make the detection strength map. These thresholds are arbitrary, and the remaining points after masking still do not appear to be normally distributed. We emphasize that Figure 3.6 is intended for a qualitative assessment of the detection of different species. For a quantitative assessment, Figure 3.4 is better for estimating the strength of the overall detection, and Table 3.6 presents Bayes factors for the detection of each molecules.

The strong dependence of the detrending signal on K_p allows it to be removed by subtracting each column of Figure 3.6 by its median. This results in a detection strength of 0 at $K_p = 0$, as expected when the planet is totally removed by detrending. For the all molecule case, the planet is detected at an $\text{SNR} \sim 12$, which is more consistent with expectations based on Figure 3.4 than the scale of Figure 3.6. However, this removal of the detrending systemat-

ics is not statistically rigorous. We emphasize that Figure 3.4 offers the most robust estimate of the overall detection strength.

The planet is clearly detected in the $K_p - v_{sys}$ diagram plotted in the top panel of Figure 3.6. In the 2D plots of cross-correlation versus time in Figure 3.4, planet velocity track is clearly visible, and the retrieved velocities are in good agreement with the nominal values. Additional validation of the detection is provided by the disappearance of the planet feature during secondary eclipse in Figure 3.4.

The cross-correlation detection is dominated by ^{12}CO based on comparing the first and second panels of Figure 3.6. OH also produces a strong signal at the expected location in the $K_p - v_{sys}$ space (fourth panel of Figure 3.6), while the H_2O template produces a somewhat weaker signal (fifth panel of Figure 3.6). The ^{13}CO template has a weak feature coincident with the expected planet velocity, but this feature does not dominate and we do not consider this to be an independent detection of ^{13}CO . The SiO template does not produce any features in the $K_p - v_{sys}$ space and is not shown.

3.4.2 Retrieval Results

Retrieved atmospheric parameters are listed in Table 3.5. The full corner plot (D. Foreman-Mackey, 2016) for the retrieval is presented in Figure 3.12. The retrieved dayside PT profile, emission contribution function, and median spectrum are plotted in Figure 3.7.

The dayside atmosphere shows a clear inversion beginning at approximately 0.1 bar, consistent with previous results (e.g. S. K. Nugroho et al., 2021; L. van Sluijs et al., 2022). The K -band emission contribution function (Figure 3.7, top right panel) indicates that the bulk of the observed emission arises near this pressure, though CO continues to contribute to the line cores from altitudes up to $\sim 3 \mu\text{bar}$. Pressures greater than ~ 1 bar do not contribute to the observed emission, and the retrieved PT profile is therefore unlikely to be accurate at these pressures. We note that the high-resolution spectroscopy is sensitive to the

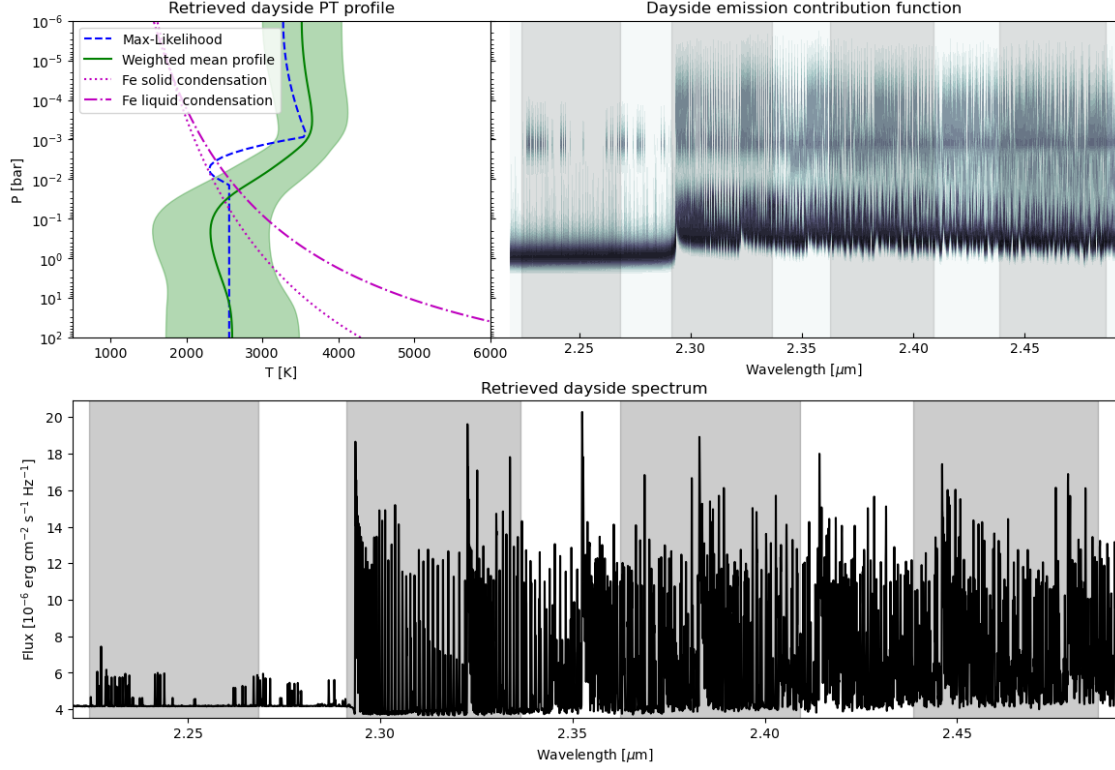


Figure 3.7: Retrieved spectrum of WASP-33 b

Retrieved PT profile (top left), K -band emission contribution (top right), and spectrum (bottom) for the best-fit atmospheric parameters. The weighted mean of all PT profiles is plotted in solid green, with the 1σ range shaded. The PT profile from the maximum-likelihood parameters is plotted in dashed blue and generally agrees well, though with a somewhat shallower and higher inversion. Condensation curves for solid iron and liquid iron from [A. S. Ackerman & M. S. Marley \(2001\)](#) are overplotted, though we do not expect dayside clouds. In the right panel, the contribution of each pressure layer to the overall planet emission with the best-fit abundances and median PT profile is indicated by the shading, with the observed NIRSPEC orders overplotted in grey. The observed emission emerges primarily from the 1-0.1 bar range. The CO line cores beyond $\sim 2.3 \mu\text{m}$ include significant contributions from the upper atmosphere. The bottom panel shows the spectrum obtained from the median parameters convolved to the approximate resolution of NIRSPEC, again with the NIRSPEC orders overplotted in grey.

line strength relative to the continuum, which is determined by the shape and contrast of the PT profile, the atmospheric metallicity, the scaling parameter, and possible impacts from H^- . This can allow “cold” PT profiles to produce similar output spectra to those of “hotter” PT profiles. While temperature will also change the relative strengths of different lines, this is a comparatively small effect over a limited bandpass. We therefore caution against relying on the exact temperatures of the retrieved PT profiles.

We obtain log mass fractions of $-4.1^{+0.7}_{-0.9}$ for H_2O , $-1.1^{+0.4}_{-0.6}$ for CO , and $-2.1^{+0.5}_{-1.1}$ for OH . This indicates that H_2O is almost entirely dissociated on the dayside of WASP-33b, consistent with previous findings from [S. K. Nugroho et al. \(2021\)](#). SiO is effectively unconstrained due to its relatively low K -band opacity, but peaks at a log mass fraction of -3.6 , which would be consistent with the neutral Si detection reported in [D. Cont et al. \(2022a\)](#). We also obtain a weak constraint on the $^{13}\text{CO}/^{12}\text{CO}$ ratio, peaking around $10^{-1.6}$ but with a significant tail giving a median value of $10^{-1.7}$. The abundance parameters show a strong positive covariance, which enables better constraints on the C/O ratio than would be expected from the marginalized uncertainties.

Finally, we note that while the scaling parameter peaks near unity, there is a long tail towards higher values. The scaling parameter controls the strength of lines relative to the host star continuum, which can also be influenced by changes in the PT profile. [Figure 3.12](#) shows weak degeneracies between the PT profile parameters and the scaling parameter, with larger values of the scaling parameter corresponding to PT profiles which produce weaker lines. This suggests the tail of the scaling parameter is a result of under-constraining the PT profile.

There are a number of systematics or physical effects that could also change the value of the scaling parameter. Our test retrievals suggest this may be a result of our data processing (see [Figure 3.11](#)). Physical factors include underestimates of the planet radius or temperature, H^- opacity, thermal expansion of the dayside atmosphere, extended emission from an outflow, or stellar pulsations. The retrieved posterior peaks at a scale factor ~ 1 , suggesting

that these effects are either relatively minor or largely cancel.

3.5 Discussion

We present Bayes factors for the detection of each molecule compared with a flat planet model in Table 3.6 and discuss the detection significance for each molecule in Section 3.5.1. We discuss the retrieved wind speeds and thermal structure in Section 3.5.2. The C/O ratio and metallicity of WASP-33b are discussed in Section 3.5.3, including a comparison to equilibrium chemistry models. We discuss the weak constraint retrieved for the CO isotopologue ratio in Section 3.5.4 and finally discuss the implications of our results for the formation history of WASP-33b in Section 3.5.5.

3.5.1 Detection Confidence

To assess the strength of our detections, we compute the Bayes factor comparing a flat/no planet model and the best-fit models for all molecules together and for each molecule independently. These values are presented in Table 3.6. The best-fit planet model is strongly preferred ($\Delta\text{BIC} > 100$), with CO dominating the detection. The evidence for H₂O and OH is substantial but weaker than CO, consistent with expectations based on the weaker features in the $K_p - v_{\text{sys}}$ space in Figure 3.6.

3.5.2 Winds and Thermal Structure

Consistent with both previous results (S. K. Nugroho et al., 2021; L. van Sluijs et al., 2022) and global circulation models of UHJs (J. P. Wardenier et al., 2021; T. D. Komacek et al., 2022; H. Beltz et al., 2022), our retrievals confirm our assumption of a thermal inversion on the dayside. We find that constant offsets in the PT profile appear to have a limited impact on the final spectrum, suggesting our observations are not particularly sensitive to absolute

Table 3.6: Bayes factors for considered molecules

Model	Bayes Factor
All molecules	111
CO only	102
^{13}CO only	9.8
H ₂ O only	6.9
OH only	5.6

Note. — Bayes factors comparing a flat planet model with the best-fit retrieved planet model and the best-fit model corresponding to each individual molecule. This allows us to assess the detection strength of each species.

temperature, with the curvature of the PT profile having a much more substantial impact. The inclusion of the scaling parameter may compound this, as it provides an alternative way to change line depths in the planet model. Figure 3.7 shows that our K -band observations are most sensitive to a relatively narrow range of pressures and therefore have limited ability to constrain the overall PT profile. Additional observations at other bands may improve the vertical constraints.

The velocity parameters prefer a slight blueshift compared to the nominal values in Table 3.1. While this could be a result of morning-to-evening winds, the shift is only $1\text{--}2\sigma$ and is well within the model-dependent variations in velocity parameters reported in L. van Sluijs et al. (2022). Additional observations providing continuous coverage of a larger phase range would provide better constraints on dayside winds.

We adopted the -9.2 km s^{-1} systemic velocity from G. A. Gontcharov (2006). More recent observations have found v_{sys} in the range of -3 km s^{-1} (A. Collier Cameron et al., 2010) to 0 km s^{-1} (S. K. Nugroho et al., 2021). L. van Sluijs et al. (2022) found systemic velocities from -15 km s^{-1} to $+6 \text{ km s}^{-1}$, depending on the orbital phase of the observations and the type of model used for cross-correlation. A more positive systemic velocity would imply larger blueshifts in the retrieved planet parameters relative to the expected Keplerian motion in the host star reference frame.

3.5.3 C/O ratio and Metallicity

The retrieved abundances yield a gas-phase $C/O = 0.8^{+0.1}_{-0.2}$. The derived posteriors for C/H, O/H, and C/O are shown in Figure 3.8. However, these retrievals are missing several potential oxygen reservoirs in ultra-hot Jupiter atmospheres, whose presence in significant quantities would lower the atmospheric C/O ratio. Metal oxides including TiO (D. Cont et al., 2021; D. B. Serindag et al., 2021) and AlO (C. von Essen et al., 2019) have previously been detected in WASP-33b, neutral atomic oxygen has been detected in the similar UHJ KELT-9b (F. Borsa et al., 2021), and Si has been detected in low-pressure ($\lesssim 1 \text{ mbar}$)

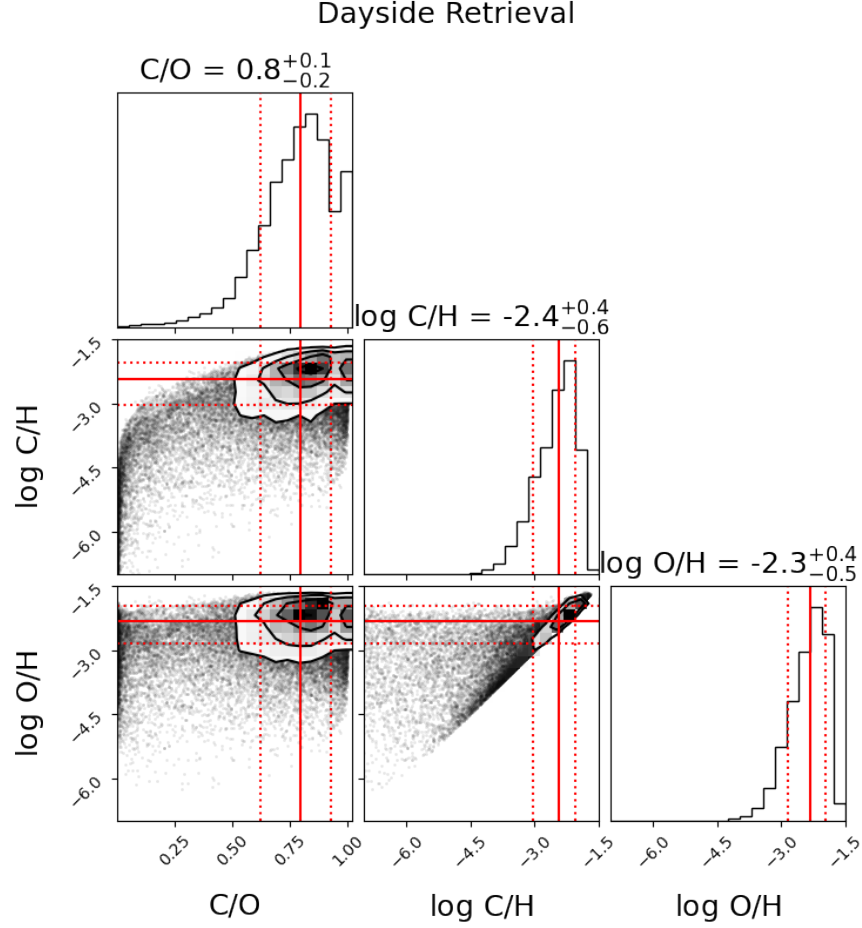


Figure 3.8: Retrieved C/O, C/H, and O/H number ratio posteriors

The C/O ratio is better constrained than the individual C/H and O/H ratios, consistent with our expectation that high-resolution spectroscopy over a narrow band is more sensitive to abundance ratios than absolute abundances due to the loss of continuum information during the data processing. The prior that the total mass fraction of all species be < 1 can be seen in the absence of points to the upper left of the 2D plots, where low C/O ratio and high C abundances would require more than the entire remaining atmospheric mass in the form of H_2O .

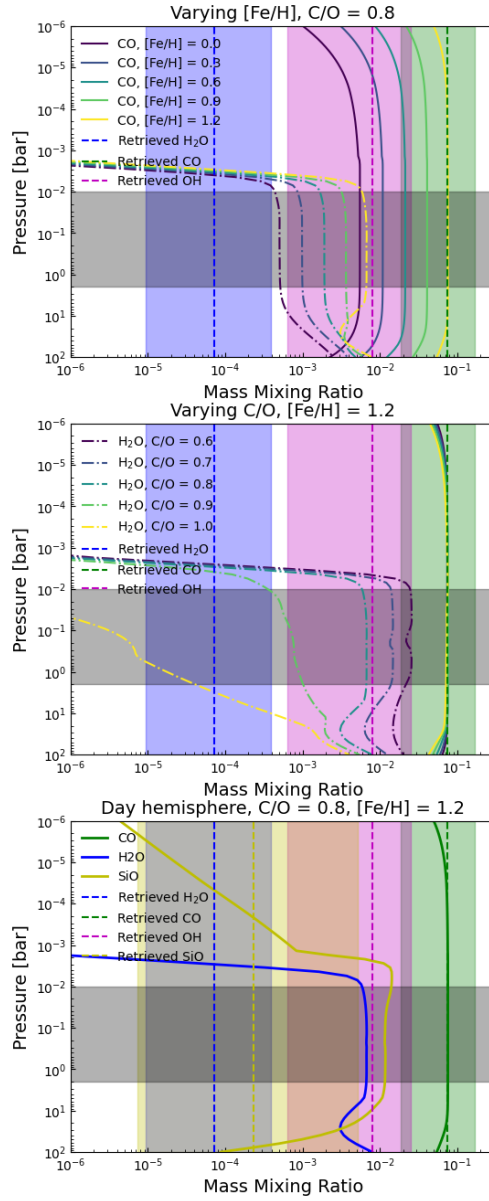


Figure 3.9: Retrieved mixing profiles for WASP-33 b

Comparisons between retrieved abundances and the predictions from `poor_mans_nonequ_chem` (P. Mollière et al., 2017, 2019) for the median retrieved PT profile. The shading indicates the peak of the emission contribution in Figure 3.7. We compare the retrieved OH abundance to the equilibrium prediction for H_2O . The CO abundance is set by metallicity, while the H_2O abundance is also sensitive to C/O ratio. Our results are consistent with $\text{C/O} = 0.8 \pm 0.1$, $[\text{Fe}/\text{H}] = 1.2 \pm 1$, with uncertainty in metallicity due to the lack of continuum. These models predict large SiO abundances, which may be detectable in L -band observations.

optical observations of WASP-33b (D. Cont et al., 2022a), suggesting the possible presence of SiO deeper in the atmosphere. Our limited wavelength coverage precludes detection of any of these species, though a significant reduction in C/O as a result would require either significant neutral oxygen or an atmosphere substantially enriched in refractory elements compared with volatiles.

The atmospheric metallicity of WASP-33b is more difficult to infer from these observations than the C/O ratio. The retrieved abundances suggest a moderately metal-enriched atmosphere, but the lack of continuum information in high-resolution observations leads to strong correlations between species abundances, making absolute abundance estimates difficult. Previously, D. Cont et al. (2022a) found a solar-metallicity model best explained the observed Si signal, though they used a widely-spaced model grid. In subsequent analysis D. Cont et al. (2022b) estimated a metallicity of +1.5 dex based on retrievals of several atomic species from optical data, including Ti, Fe, and V, consistent with the retrieved metallicity from the KPIC observations.

In order to better understand the range of possible C/O ratios and metallicities, we compare our retrieved abundances with grids of equilibrium chemistry models from the `poor_mans_nonequ_chem` package of `petitRADTRANS` (P. Mollière et al., 2017, 2019). These comparisons are plotted in Figure 3.9. In our parameterization scheme, the CO abundance is determined primarily by the atmospheric metallicity, while the H₂O/OH abundance is significantly impacted by the C/O ratio. As the equilibrium grid does not include OH, we assume the equilibrium H₂O abundance as the prediction for the dayside OH abundance.

Figure 3.9 shows the retrieved abundances are most consistent with equilibrium models having $[\text{Fe}/\text{H}] = 1.2$ and $\text{C}/\text{O} = 0.8$. These values are consistent with D. Thorngren & J. J. Fortney (2019) modeled upper limits on metallicity for a planet the mass of WASP-33b as well as the retrieved metallicity from D. Cont et al. (2022b) based on optical observations. However, varying the $[\text{Fe}/\text{H}]$ in the chemical model suggests that our metallicity uncertainty is approximately 1 dex, and we therefore cannot confidently exclude stellar or even sub-

stellar atmospheric metallicities for WASP-33b. C/O appears to be better constrained, with a margin ± 0.1 consistent with the posterior shown in Figure 3.8. Note that the strong covariance between species abundances suggests that this C/O ratio will hold even if the metallicity varies significantly (see Figure 3.8).

The chemical equilibrium models suggest significant SiO abundances at the pressures probed by our observations. At lower pressures, the SiO abundance drops due to thermal dissociation, consistent with the optical detection of Si by D. Cont et al. (2022a). While our *K*-band observations are not sensitive to SiO, *L*-band observations of the SiO bands from 4–4.2 μm could measure the SiO abundance. Assuming SiO is the dominant undetected oxygen reservoir at $\sim 1 - 0.01$ bar pressures, this would significantly improve estimates of the overall oxygen abundance.

3.5.4 CO Isotopologue Ratio

The $^{13}\text{CO}/^{12}\text{CO}$ posterior peaks at $\sim 10^{-1.6}$, with a tail towards lower values bringing the median to $10^{-1.7}$. While the posterior is somewhat poorly-constrained, the fact that we see even a weak preference is an argument in favor of high ^{12}CO abundances. In simulated observations, mass-mixing ratios as high as $\log \text{CO} = -1.5$ do not always lead to a preference in the isotopologue ratio posterior. The peak of this weak preference is consistent with estimated CO isotopologue ratios from protoplanetary disks (P. M. Woods & K. Willacy, 2009) and is consistent with the $^{13}\text{CO}/^{12}\text{CO} \sim 10^{-1} - 10^{-1.6}$ value measured for WASP-77Ab in M. R. Line et al. (2021). Constraints on isotopologue ratios as well as abundances may provide a complementary path to probing formation history and physical conditions in exoplanetary atmospheres (P. Mollière & I. A. G. Snellen, 2019; Y. Zhang et al., 2021a).

3.5.5 Implications for Planet Formation

The high-C/O, potentially high-metallicity atmosphere suggested by our retrievals is consistent with the [S. Pelletier et al. \(2021\)](#) observations of the hot Jupiter τ Boo b. These observations conflict with predictions from pebble accretion models that atmospheric metallicity and C/O ratios should be inversely correlated, as secondary pebble accretion is expected to be dominated by oxygen-rich grains ([N. Espinoza et al., 2017](#); [N. Madhusudhan et al., 2017](#); [A. J. Cridland et al., 2019](#); [N. Khorshid et al., 2022](#)). High C/O, high-metallicity atmospheres require formation and/or substantial accretion in an environment that is enriched in both carbon and solids. Such conditions are consistent with models that incorporate pebble drift ([R. A. Booth et al., 2017](#)), formation near CO or CO₂ snow lines ([K. I. Öberg et al., 2011](#)), or with pollution by C-rich grains interior to the H₂O snow line ([Y. Chachan et al., 2023](#)).

As discussed in Section 3.5.3, one possible explanation for this discrepancy is that our K -band high-resolution retrievals are simply missing a significant source of oxygen. Figure 3.9 suggests relatively high SiO abundances for WASP-33b, which we cannot measure with our K -band observations. However, comparison with the equilibrium chemistry models suggests including SiO would not substantially decrease the C/O ratio under equilibrium conditions without substantial enrichment of Si relative to other metals (see Figure 3.9, third panel). Alternatively, additional oxygen could be present in the atomic form, as ([F. Borsa et al., 2021](#)) reported from transit observations of KELT-9b. In the future, Keck/HISPEC will offer simultaneous yJHK coverage at $R \sim 10^5$ ([D. Mawet et al., 2019](#)) with substantially improved throughput compared with KPIC, enabling characterization of a broader range of chemical species and reducing the likelihood of missing significant oxygen or carbon reservoirs.

Missing oxygen could also be the result of errors in linelists or molecular opacity calculations rather than chemistry. A poorly-matched H₂O or OH opacity in the retrieval setup could lead to a bias towards lower abundances. However, both this work and [S. Pelletier](#)

et al. (2021) retrieved high-C/O atmospheres using different H₂O opacity tables and linelists, indicating that such an error would have to be systematic across multiple independent calculations, while simultaneously not significantly impacting the same calculations for CO. This suggests that the problem would have to be related to a common assumption specific to the H₂O high-temperature linelists. Computing high-resolution, high-temperature H₂O opacities for the *K*-band alone required nearly one year of CPU time using *exocross* (S. N. Yurchenko et al., 2018), limiting our ability to compute and compare multiple opacity tables.

Alternatively, superstellar metallicity and C/O may arise either from accretion near evaporation fronts close to snow lines (K. I. Öberg et al., 2011) or from carbon-rich grain accretion between the carbon soot line and the H₂O snow line (Y. Chachan et al., 2023). Pebble accretion studies have found grain accretion within the snow line should boost oxygen abundances rather than carbon (e.g. N. Madhusudhan et al., 2017; N. Espinoza et al., 2017; A. J. Cridland et al., 2019), but models incorporating pebble drift can produce giant planet atmospheres with both high metallicity and high C/O. In particular, R. A. Booth et al. (2017) finds that the C/O ~ 1 and high carbon abundance we observe in WASP-33b is a specific indication that a planet accreted high-metallicity gas near the CO₂ snow line, which is located at ~ 10 AU for an A-type primary (K. I. Öberg et al., 2011). The present observed location and polar orbit of WASP-33b may then be explained through the eccentric Kozai-Lidov Effect (S. Naoz et al., 2011) after the protoplanetary disk dissipated. Future incorporation of refractory species abundances, such as Si and Fe, would allow the formation location to be specifically identified, as the refractory-to-volatile ratio is a diagnostic of the formation and accretion history (J. D. Lothringer et al., 2021). The presence of these species in the gas phase in the atmospheres of UHJs such as WASP-33b presents a unique opportunity to obtain a clear understanding of the evolutionary history of an exoplanet population.

3.6 Summary and Conclusions

We present high-resolution ($R \sim 35000$) Keck/KPIC K -band observations of WASP-33b covering the dayside of the planet. We successfully retrieve CO, H₂O, and OH abundances. We find:

- WASP-33b has a dayside thermal inversion. Additional observations covering a larger phase range would offer more precise geographic constraints on the inversion. K -band data alone offer only weak constraints on the absolute temperature profile. Larger wavelength coverage may be needed to precisely constrain PT profiles.
- H₂O appears to be mostly dissociated into OH on the dayside. Multi-phase H -band observations could constrain the extent of this dissociation by measuring variations in OH and H₂O features.
- WASP-33b has a high C/O ratio, $C/O = 0.8^{+0.1}_{-0.2}$. While the metallicity is poorly constrained, there appears to be a weak preference for super-stellar metallicities (roughly $2\text{--}12\times$ WASP-33, but with a ~ 1 dex uncertainty). Chemical models suggest large SiO abundances which may be detectable in the L -band, providing an additional check on the metallicity.
- The high-C/O ratio, (possibly) high-metallicity atmosphere of WASP-33b suggests that the atmospheric chemistry of WASP-33b has been significantly influenced by the accretion and migration history of the system. One possible scenario is that WASP-33b accreted most of its envelope from just beyond the CO₂ snow line and migrated to its present location after the dissipation of the protoplanetary disk through high-eccentricity migration. Alternatively, WASP-33b could have formed between the carbon sublimation and H₂O ice lines if it was substantially contaminated by C-rich grains. There are likely to be other scenarios which could also produce a composition compatible with the observations presented here.

These observations also demonstrate KPIC’s ability to characterize unresolved exoplanet atmospheres. While the reduced throughput of KPIC results in a lower SNR than a slit-based spectrograph, the increased line-spread, blaze, and wavelength stabilities from KPIC’s single-mode fiber result in a strong cross-correlation detection suitable for atmospheric retrievals. This detection of WASP-33b demonstrates KPIC’s capability to characterize unresolved exoplanets for the first time. Future observations of additional hot and ultra-hot Jupiters, coupled with observations of directly imaged systems, will enable population-level understanding of the thermal and chemical environments of giant exoplanet atmospheres.

3.7 Corner Plots

Full corner plots are included here for completeness. We discuss the retrievals in [Section 3.4](#), including poorly constrained and degenerate parameters.

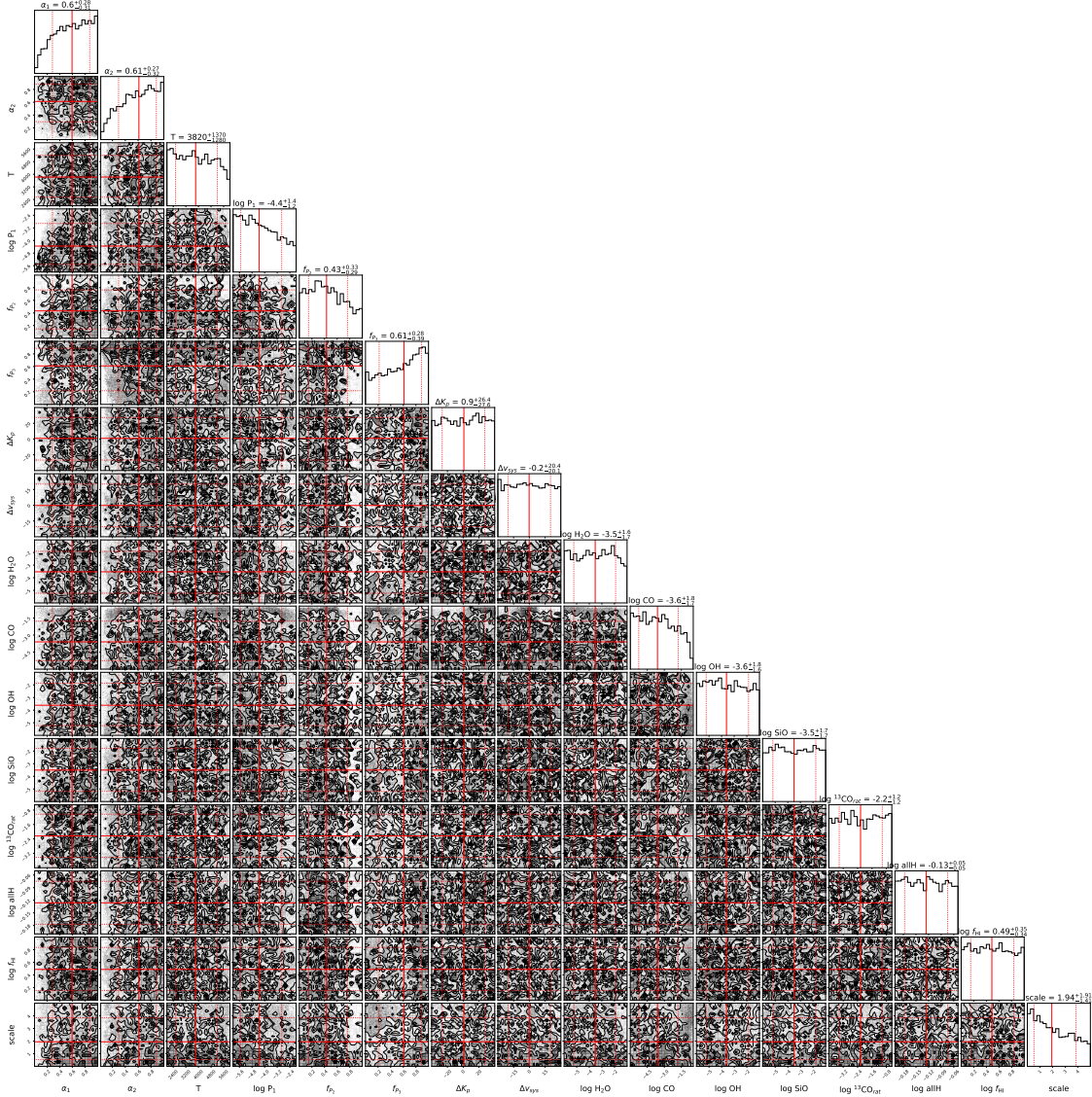


Figure 3.10: Full corner plot for the test retrieval with no planet

Columns from left to right are the parameters as listed in Table 3.3. Red solid lines indicated the **dynesty** median, with red dashed lines indicating the bounds of the marginalized 68% confidence interval. Despite using the same stopping criteria as the other retrievals, none of the posteriors show strong preferences, and the fitter converged in far fewer iterations than when the planet is present in the simulation. The scale parameter shows a weak preference towards smaller values, consistent with the known absence of a planet in the simulated data. The impact of the $T < 6000$ K at all pressure levels requirement can be seen in the behavior of the pressure-temperature profile parameters in the first six columns

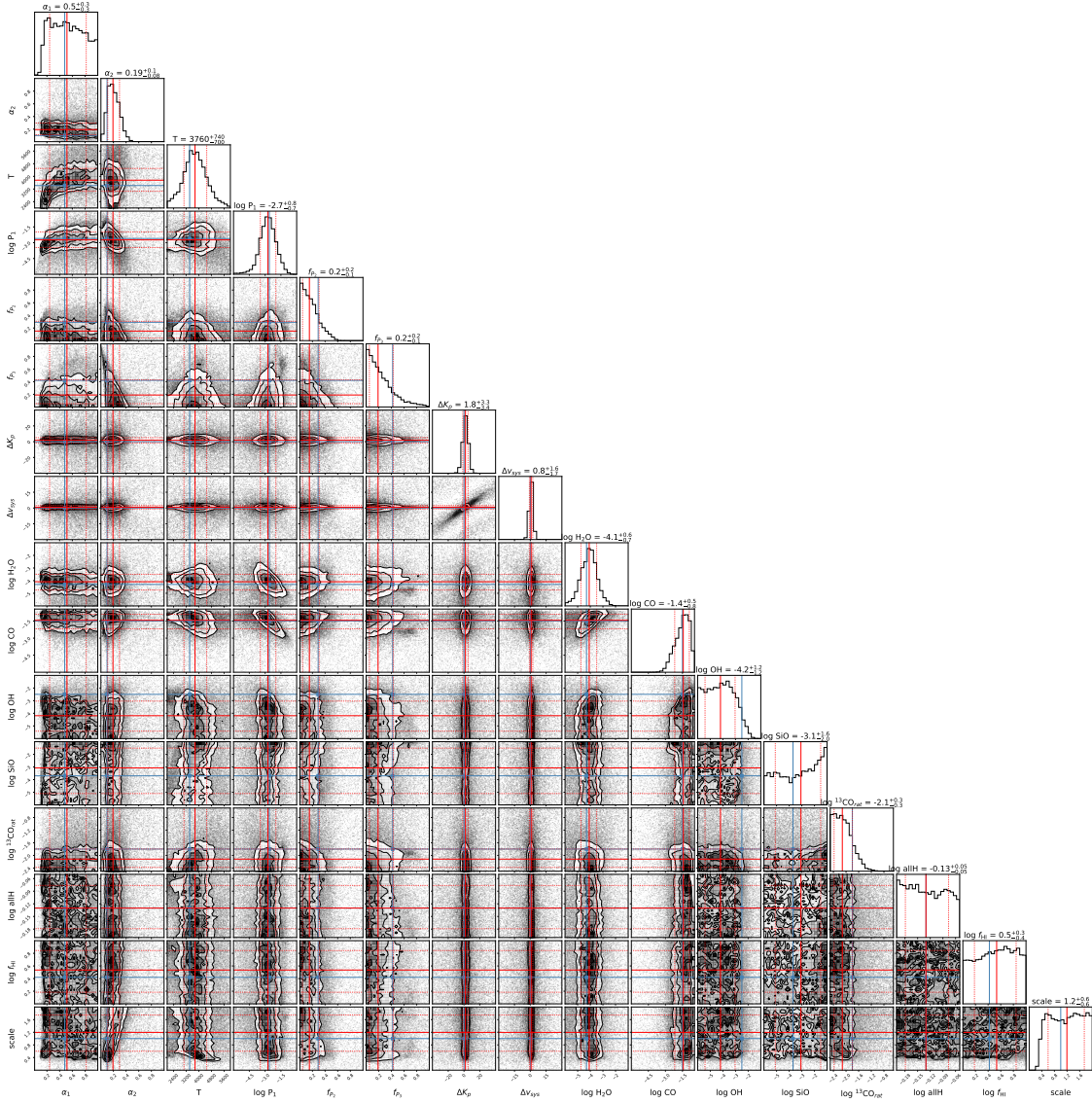


Figure 3.11: Full corner plot for the test retrieval

Test parameters are listed in Table 3.4. Columns from left to right are the parameters as listed in Table 3.3. Red solid lines indicated the **dynesty** median, with red dashed lines indicating the bounds of the marginalized 68% confidence interval. True values for the simulated data are shown in solid blue. The true values are generally retrieved to within 1σ .

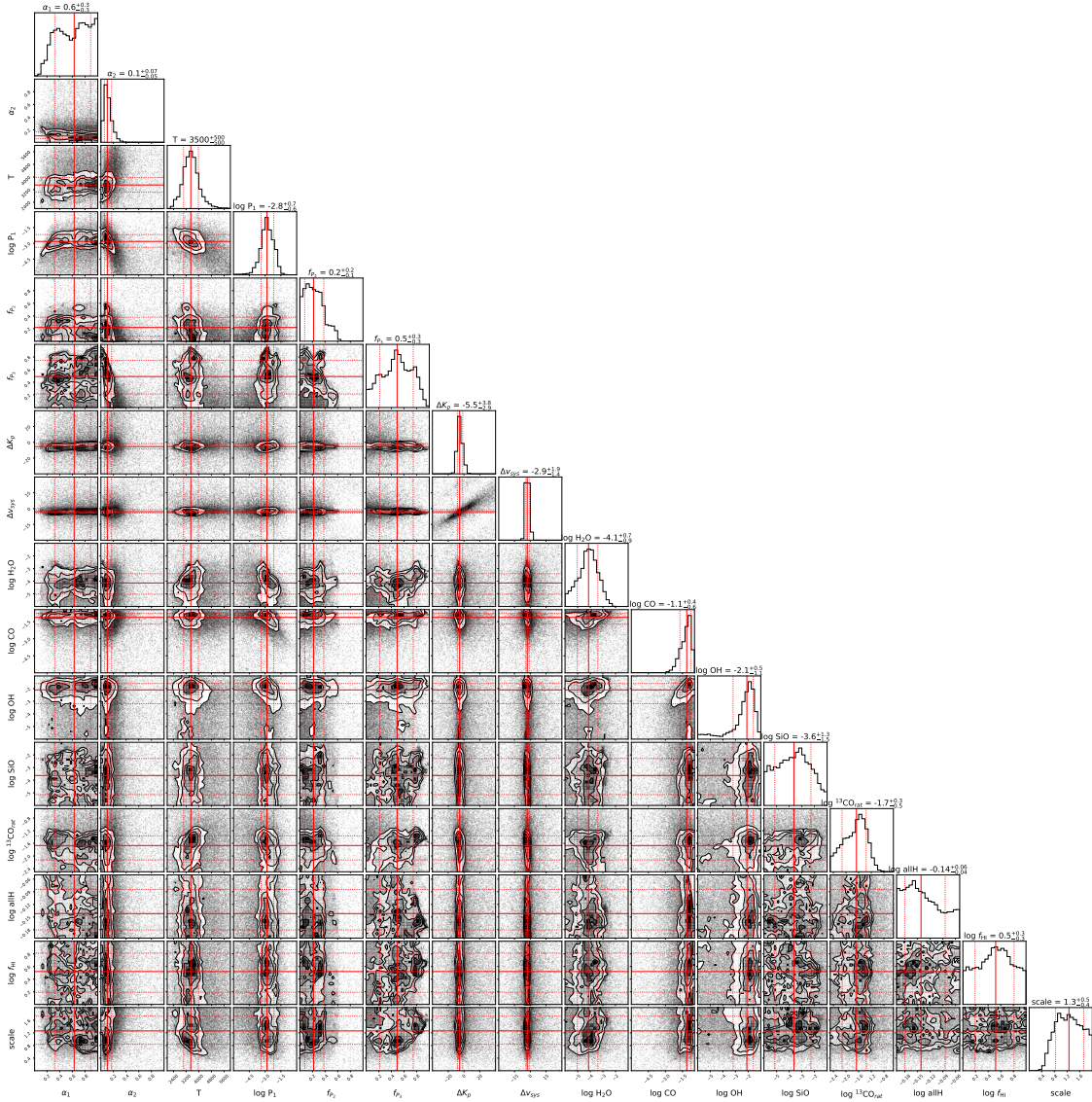


Figure 3.12: Full corner plot for the WASP-33b retrieval

Columns from left to right are the parameters as listed in Table 3.3. Red solid lines indicated the *dynesty* median, with red dashed lines indicating the bounds of the marginalized 68% confidence interval. We discuss these results in Section 3.4

CHAPTER 4

Atmospheric metallicity and C/O of HD 189733 b from high-resolution spectroscopy

A version of this chapter was previously published in the *Astronomical Journal* (Finnerty *et al.* 2024 167, 1, 43)

Abstract

We present high-resolution K -band emission spectra of the quintessential hot Jupiter HD 189733 b from the Keck Planet Imager and Characterizer (KPIC). Using a Bayesian retrieval framework, we fit the dayside pressure-temperature profile, orbital kinematics, mass-mixing ratios of H_2O , CO , CH_4 , NH_3 , HCN , and H_2S , and the $^{13}\text{CO}/^{12}\text{CO}$ ratio. We measure mass fractions of $\log \text{H}_2\text{O} = -2.0^{+0.4}_{-0.4}$ and $\log \text{CO} = -2.2^{+0.5}_{-0.5}$, and place upper limits on the remaining species. Notably, we find $\log \text{CH}_4 < -4.5$ at 99% confidence, despite its anticipated presence at the equilibrium temperature of HD 189733 b assuming local thermal equilibrium. We make a tentative ($\sim 3\sigma$) detection of ^{13}CO , and the retrieved posteriors suggest a $^{12}\text{C}/^{13}\text{C}$ ratio similar to or substantially less than the local interstellar value. The possible ^{13}C enrichment would be consistent with accretion of fractionated material in ices or in the protoplanetary disk midplane. The retrieved abundances correspond to a substantially sub-stellar atmospheric $\text{C/O} = 0.3 \pm 0.1$, while the carbon and oxygen abundances are stellar to slightly super-stellar, consistent with core-accretion models which predict an inverse correlation between C/O and metallicity. The specific combination of low C/O and high

metallicity suggests significant accretion of solid material may have occurred late in the formation process of HD 189733 b.

4.1 Introduction

First discovered in 2005 through both transit and radial velocity observations (F. Bouchy et al., 2005), the hot Jupiter HD 189733 b is a frequent target for characterization studies due to its bright K-type host star ($K_{\text{mag}} = 5.5$, R. M. Cutri et al. 2003) and large transit depth ($\sim 2\%$). J. N. Winn et al. (2006) measured the Rossiter-McLaughlin effect for the system, finding the planetary orbit to be well aligned with the stellar rotation axis ($\lambda = -1.4^\circ \pm 1.1^\circ$). D. Deming et al. (2006) detected the secondary eclipse in *Spitzer* observations, eventually leading to the first full-disk temperature map for an exoplanet (H. A. Knutson et al., 2007) which found the hottest part of the planet is offset by $16^\circ \pm 6^\circ$ east from the substellar point due to supersonic winds.

Early efforts to characterize the chemical composition of HD 189733 b were met with mixed results, a selection of which we summarize here. Some studies reported detection of H_2O (G. Tinetti et al., 2007; C. J. Grillmair et al., 2008) or CO (J.-M. Désert et al., 2009), while others reported a flat transmission spectrum (C. J. Grillmair et al., 2007; F. Pont et al., 2008; D. K. Sing et al., 2009). The flat spectra were found to be consistent with the presence of hazes (F. Pont et al., 2008; D. K. Sing et al., 2009), preventing the clear detection of individual molecular species from low-resolution transmission spectra. Subsequent observations suggest this haze extends from the optical into the near-infrared *H* band (N. P. Gibson et al., 2012).

High-resolution emission spectroscopy provides a potential pathway to perform atmospheric characterization in the presence of clouds or hazes. Since high-resolution spectroscopy probes line cores at lower pressures compared to transmission spectroscopy, emission originating above the cloud layer can be detected and characterized (S. Gandhi et al., 2020). R. J.

de Kok et al. (2013) used high-resolution transmission spectroscopy to detect CO emission and place an upper limit on the H₂O line contrast. M. Brogi et al. (2016) used transmission spectroscopy to measure a rotation rate consistent with tidal locking and a blueshift suggesting a $\sim 2 \text{ km s}^{-1}$ day-to-night wind. Water was eventually detected in high-resolution emission spectroscopy from CRIRES (J. L. Birkby et al., 2013) and has been repeatedly confirmed in both emission and transmission spectroscopy (M. Brogi et al., 2018; E. Flowers et al., 2019; S. H. C. Cabot et al., 2019; M. Brogi & M. R. Line, 2019; A. Boucher et al., 2021; B. Klein et al., 2023). CO has similarly been confirmed in multiple studies (M. Brogi & M. R. Line, 2019; S. H. C. Cabot et al., 2019; E. Flowers et al., 2019), while S. H. C. Cabot et al. (2019) also reported tentative evidence for HCN.

Despite the repeated confirmation of the presence of both H₂O and CO, none of these studies were able to obtain simultaneously bounded constraints on the abundances of both species. This has prevented robust measurement of the C/O ratio and bulk atmospheric metallicity, potentially key diagnostics to trace the formation and evolution of the HD 189733 system. Additionally, despite the anticipated presence of CH₄ under local thermal equilibrium at the equilibrium temperature of HD 189733 b, none of these studies made a clear CH₄ detection, leaving an important potential tracer of photochemistry effects unconstrained.

To address these gaps in our knowledge of an important benchmark hot Jupiter system, we observed HD 189733 b with Keck/KPIC high-resolution *K*-band spectroscopy. These observations are part of an ongoing survey to characterize a statistically significant number of hot Jupiter atmospheres with KPIC and constrain the underlying distribution of C/O and metallicity in this population.

Section 4.2 describes the observations, data reduction procedures, and atmospheric retrieval framework, with an emphasis on the differences from L. Finnerty et al. (2023a). Section 4.3 presents the results of the atmospheric retrievals and cross-correlation analysis. Section 4.4 discusses the retrieved atmospheric properties, comparing the measured abundances with expectations from chemical equilibrium and photochemical models. We

summarize our results and draw conclusions in Section 4.5.

4.2 Observations and Data Reduction

4.2.1 Observations

HD 189733 was observed with Keck/KPIC phase II (J.-R. Delorme et al., 2021; D. Echeverri et al., 2022) on 2022 August 13 (UT) from 8:39 UT to 11:59 UT at an airmass of 1.0 to 1.36. KPIC provides a single-mode fiber feed into Keck/NIRSPEC (I. S. McLean et al., 1998; E. C. Martin et al., 2018; R. A. López et al., 2020), enabling stable diffraction-limited high-resolution spectroscopy. The observations began approximately 30 minutes after the expected end of secondary eclipse, covering orbital phases from 0.5285 to 0.5898, during which time we expect the star/planet relative radial velocity to shift from -27 km s^{-1} to -82 km s^{-1} . Observations were taken with an ABBA nodding pattern between KPIC science fibers 2 and 4 with 30 second exposures, giving a total of 256 science frames.

The KPIC real-time throughput calculator (included in the KPIC DRP) estimated the 95th-percentile top-of-atmosphere throughput was 3–3.4% at the start of the observations, decreasing to $\sim 2.5\%$ in the second half of the sequence, roughly consistent with the typical performance measured for KPIC phase II under photometric conditions (D. Echeverri et al., 2022). Weather conditions were clear and stable throughout the observations. The throughput loss is likely a result of an increase in the PSF size due to seeing and AO performance changes as the airmass increased from 1.0 at the start of the observation sequence to 1.36 by the end. The median extracted per-pixel signal-to-noise ratio after coadding frames in a nodding sequence was approximately 180, ranging from ~ 210 in the bluest order to ~ 160 in the reddest order.

Table 4.1: Star and planet properties of the HD 189733 system

Property	Value	Ref.
RA	20:00:43.7	Gaia Collaboration (2020)
Dec	+22:24:39.1	Gaia Collaboration (2020)
Spectral Type	K2V	
K_{mag}	5.54 ± 0.02	R. M. Cutri et al. (2003)
Mass	$0.82 \pm 0.03 M_{\odot}$	L. J. Rosenthal et al. (2021)
Radius	$0.78 \pm 0.01 R_{\odot}$	L. J. Rosenthal et al. (2021)
T_{eff}	$5005 \pm 77 \text{ K}$	A. S. Polanski et al. (2022)
$\log g$	4.49 ± 0.09	A. S. Polanski et al. (2022)
$v \sin i$	$1.8 \pm 0.9 \text{ km s}^{-1}$	A. S. Polanski et al. (2022)
v_{rad}	$-2.3 \pm 0.2 \text{ km s}^{-1}$	C. Soubiran et al. (2018)
[Fe/H]	0.01 ± 0.03	A. S. Polanski et al. (2022)
[C/H]	-0.12 ± 0.05	A. S. Polanski et al. (2022)
[O/H]	-0.21 ± 0.07	A. S. Polanski et al. (2022)
C/O	0.67 ± 0.14	A. S. Polanski et al. (2022)
HD 189733 b		
Period	2.21857567 days	ExoFOP (2019)
t_{transit}	JD 2454279.436714	ExoFOP (2019)
a	0.031 AU	L. J. Rosenthal et al. (2021)
i	85.7°	K. G. Stassun et al. (2017)
K_{p}	153 km s^{-1}	Estimated
Mass	$1.13 \pm 0.08 M_{\text{Jup}}$	K. G. Stassun et al. (2017)
Radius	$1.13 \pm 0.01 R_{\text{Jup}}$	K. G. Stassun et al. (2017)
T_{eq}	1200 K	Estimated
C/O	0.3 ± 0.1	This work
[C/H]	$+0.4 \pm 0.5$	This work
[O/H]	$+0.8 \pm 0.4$	This work

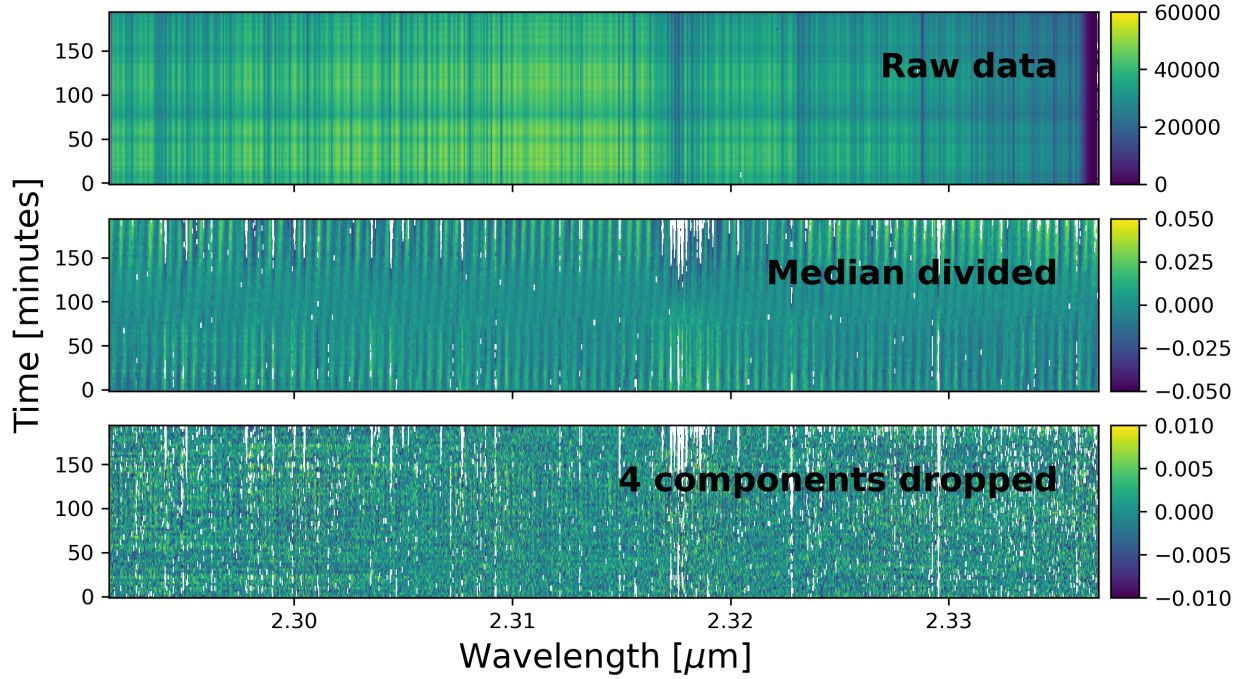


Figure 4.1: Data detrending process for KPIC HD 189733 observations

The top row shows the raw time series, with significant frame-to-frame flux variations, tellurics, and blaze function effects. The colorbar for the top frame is the counts in the extracted 1D spectrum. The second row shows the same data after scaling each exposure by its median and dividing each frame by the time-series median, with the colorbar indicating the median-normalized and continuum-subtracted flux level. The blaze and telluric signals are almost completely eliminated, but a significant time-varying fringe is clearly present. White pixels indicate data that have been masked. In the bottom panel, the fringe has been effectively removed by dropping the first 4 components of the SVD decomposition of the time series. The bottom colorbar shows the median-normalized, continuum-subtracted flux level after the decomposition.

4.2.2 Data Reduction

The data extraction is identical to that described in [L. Finnerty et al. \(2023a\)](#), which differs slightly from the current version of the supported KPIC Data Reduction Pipeline (DRP)¹. HIP 95771 (spectral type M0.5IIIb) was used for wavelength calibration at the start of the night. Of the nine observed NIRSPEC orders, three (orders 37-39) are heavily contaminated by telluric CO₂ lines, while two (orders 35 and 36) are almost entirely lacking in stellar or telluric lines, preventing an accurate wavelength calibration. We therefore use the four reddest orders (orders 31-34) spanning $\sim 2.2\text{--}2.5\,\mu\text{m}$ (with significant gaps) for which we have accurate wavelength solutions and minimal telluric contamination.

In order to speed the log-likelihood calculation in the retrieval, we coadded the extracted spectra from each ABBA sequence after re-interpolating all observations onto the science fiber 2 wavelength solution. Each fiber has a slightly different line-spread function (LSF) and the fiber coupling can vary significantly between frames depending on the AO correction, leading to variability in the coadded LSF. The final time series consists of 64 spectra, with a maximum planetary radial velocity shift between *consecutive* spectra of approximately $900\,\text{m s}^{-1}$, roughly $10\times$ smaller than the NIRSPEC resolution ($R \sim 35,000$, $\Delta v \sim 8.5\,\text{km s}^{-1}$ for the chosen instrument settings).

The data detrending process for one order is shown in Figure 4.1. The extracted spectral time-series for each order is first scaled to have a median of 1.0, then divided by the time-series median spectrum using a second-order polynomial to fit continuum variations. This removes most temporally fixed features in the spectrum, leaving time-varying fringing ([L. Finnerty et al., 2022](#); [L. Finnerty et al., 2023b](#), Xuan et al. submitted), airmass-driven telluric variations, and the time-varying planet signal. Points differing from the median by more than $6\times$ the median absolute deviation (MAD) are then masked, as well as the first and last fifty wavelength bins in each order.

¹https://github.com/kpicteam/kpic_pipeline/

The time series for each order is then mean-subtracted and the first 4 components of the singular value decomposition (SVD) are projected out. To account for the resulting distortion of the planet signal, the dropped components are saved and added to the forward model during the log-likelihood calculation. A new SVD is then performed on the component-injected forward model in order to replicate the distortion of the planet signal from projecting these components out, similar to [M. R. Line et al. \(2021\)](#). In contrast with [L. Finnerty et al. \(2023a\)](#), we do not negatively inject the forward model prior to removal of the SVD components, which significantly speeds the log-likelihood calculation. This choice makes a stronger assumption that repeating the SVD on the component-injected model accurately reproduces the distortion of the observed planet signal, but has proven successful in previous work (e.g. [M. R. Line et al., 2021](#)). After the decomposition, points varying by more than $4\times$ the MAD are masked. Previously, [L. Finnerty et al. \(2023a\)](#) found several orders of KPIC observations continued to show a fringing pattern that dominated over the Gaussian noise even at this stage of the analysis, which was removed by taking a final median division. In these observations, we do not see any evidence of similar residual fringing above the noise level (for example in the third panel of [Figure 4.1](#)), and therefore we omit this step.

4.2.3 Atmospheric Retrieval

The atmospheric retrieval framework is similar to that described in [L. Finnerty et al. \(2023a\)](#), though we have implemented several changes to improve the time-series detrending. We briefly summarize this framework for completeness. The fit parameters, priors, and retrieved values are listed in [Table 4.2](#).

As in [L. Finnerty et al. \(2023a\)](#), we use `petitRADTRANS` ([P. Mollière et al., 2019, 2020](#)) for the radiative-transfer model of the planetary atmosphere with 80 log-uniform spaced pressure layers between 10^2 and 10^{-6} bar. We use the 4-parameter pressure-temperature ($P - T$) profile model from [T. Guillot \(2010\)](#), implemented in `petitRADTRANS`. From initial tests using the [N. Madhusudhan & S. Seager \(2009\)](#) 6-parameter $P - T$ model previously used

in [L. Finnerty et al. \(2023a\)](#), we found that multiple parameters were poorly constrained and showed complex degeneracies. The [T. Guillot \(2010\)](#) parameterization is more constraining in its physical assumptions, making it better-suited to the limited wavelength range of these observations and enabling looser, physically motivated priors for the $P - T$ parameters. Retrieved molecular abundances were generally consistent between both parameterizations. At all pressures, we require $100 \text{ K} < T < 3000 \text{ K}$ for physical consistency and to avoid hitting the bounds of our opacity tables. We also include a grey cloud deck and use the scattering mode of `petitRADTRANS`.

We fit for vertically-fixed abundances (not necessarily in chemical equilibrium) of H_2O , ^{12}CO , CH_4 , NH_3 , HCN , H_2S , and the $^{13}\text{CO}/^{12}\text{CO}$ ratio. For H_2O , ^{12}CO , and ^{13}CO we used the high-temperature opacity tables described in [L. Finnerty et al. \(2023a\)](#). For CH_4 , we used the opacity table computed in [J. W. Xuan et al. \(2022\)](#) from the [R. J. Hargreaves et al. \(2020\)](#) linelist. For NH_3 (linelist: [S. N. Yurchenko et al., 2011](#)), HCN (linelist: [G. J. Harris et al., 2006](#); [R. J. Barber et al., 2014](#)), and H_2S (linelist: [L. S. Rothman et al., 2013](#)), we used the `petitRADTRANS` high-resolution opacity tables described in [P. Mollière & I. A. G. Snellen \(2019\)](#). Collision induced absorption (CIA) from $\text{H}_2 - \text{H}_2$ and $\text{H}_2 - \text{He}$ are also included. We fit for the abundance of H_2 , though we do not include H_2 line opacity. The remaining mass of the atmosphere is assumed to be helium. As we do not include H_2 line opacity, the retrieved H_2 abundance reflects the best-fit mean-molecular weight via the impact on the CIA, rather than strengths of H_2 lines in the planetary spectrum. We use a PHOENIX model for the star with $T_{\text{eff}} = 5000 \text{ K}$, $\log g = 4.5$, and $[\text{Fe}/\text{H}] = 0.0$, which has been broadened to $v \sin i = 1.8 \text{ km s}^{-1}$ ([A. S. Polanski et al., 2022](#)). While [L. Finnerty et al. \(2023a\)](#) fixed the size of the Gaussian broadening kernel to a value found by varying the kernel size for a fixed planet model and maximizing the likelihood, in this work we set the kernel width to $\sigma = 1.2$ pixels, slightly smaller than the expected value for the instrument, and apply a rotational broadening kernel to the atmospheric forward model using the fast technique described in [A. Carvalho & C. M. Johns-Krull \(2023\)](#) which accounts for the wavelength-

dependence of the rotational kernel. The size of this kernel is a free parameter in the fit, allowing us to determine the best-fit line width accounting for coadd-induced LSF variations and the change in projected planetary velocity within a single coadd.

The nested sampling was performed with **dynesty** (J. S. Speagle, 2020) using 1200 live points, running to a $\Delta \log z = 0.01$ stopping criteria. The retrieval took approximately four days with 16 Intel E5-2670 CPU cores, totaling about 60 days of CPU time. The significant increase in runtime compared with L. Finnerty et al. (2023a) is a result of including scattering in the radiative transfer calculation.

4.3 Results

Table 4.2 presents the priors and results from the retrieval, including both the maximum-likelihood and median retrieved values. We discuss the velocity parameters in Section 4.3.1, the $P - T$ profile and thermal properties in Section 4.3.2, and the chemical abundances in Section 4.3.3. The full corner plot is included in Appendix 4.6.

4.3.1 Velocity and winds

The $v_{\text{sys}} - K_p$ diagram for the maximum-likelihood planet model is shown in Figure 4.2. Note that self-division of the planet spectrum results in substantial structure far from the planet peak, which prevents an accurate estimation of detection significance from dividing by the off-peak standard deviation. This effect can also be seen in Figure 6 of L. Finnerty et al. (2023a), and is a general feature of detrending schemes which rely on the velocity shift of planet features that is then compounded by the explicit dependence of the M. Brogi & M. R. Line (2019) log-likelihood function on the forward-model variance. As an alternative to estimate the detection strength, we use Wilks' Theorem (S. S. Wilks, 1938) with 17 free parameters to estimate the significance of the detection compared with a flat planet model to be $\sim 6\sigma$. Alternatively, we note that the off-peak structure is a strong function of K_p .

Table 4.2: List of parameters, priors, and results for atmospheric retrievals.

Name	Symbol	Prior	Max-L	Median
log infrared opacity [cm^2g^{-1}]	$\log \kappa$	Uniform(-3, 0)	-1.0	$-1.1^{+0.4}_{-0.4}$
log infrared/optical opacity	$\log \gamma$	Uniform(-1.5,-0.3)	-1.4	$-1.3^{+0.3}_{-0.2}$
Internal temperature [K]	T_{int}	Uniform(50, 300)	140	200^{+100}_{-100}
Equilibrium temperature [K]	T_{equ}	Uniform(400,1500)	800	800^{+100}_{-100}
Grey cloud pressure [bar]	$\log P_{\text{cloud}}$	Uniform(-2,1)	-1.0	$-0.3^{+0.9}_{-0.6}$
K_{p} offset [km s^{-1}]	ΔK_{p}	Uniform(-40, 40)	6.4	$7.0^{+7.7}_{-8.3}$
v_{sys} offset [km s^{-1}]	Δv_{sys}	Uniform(-15, 15)	-7.3	$-6.4^{+3.4}_{-3.6}$
Velocity broadening [km s^{-1}]	v_{broad}	Uniform(1,20)	16.9	$16.0^{+1.0}_{-1.0}$
log H ₂ O mass-mixing ratio	$\log \text{H}_2\text{O}$	Uniform(-4, -0.3)	-1.7	$-2.0^{+0.4}_{-0.4}$
log CO mass-mixing ratio	$\log \text{CO}$	Uniform(-4, -0.3)	-1.8	$-2.2^{+0.5}_{-0.5}$
log CH ₄ mass-mixing ratio	$\log \text{CH}_4$	Uniform(-8,-1)	-7.4	$-6.7^{+1.0}_{-0.9}$
log NH ₃ mass-mixing ratio	$\log \text{NH}_3$	Uniform(-8,-2)	-4.8	$-6.5^{+1.1}_{-1.0}$
log HCN mass-mixing ratio	$\log \text{HCN}$	Uniform(-8,-2)	-5.8	$-5.4^{+1.4}_{-1.7}$
log H ₂ S mass-mixing ratio	$\log \text{H}_2\text{S}$	Uniform(-8,-3)	-7.7	$-5.6^{+1.7}_{-1.6}$
log ¹³ CO/ ¹² CO	$\log^{13}\text{CO}_{\text{rat}}$	Uniform(-3, -0.3)	-0.8	$-1.0^{+0.4}_{-0.8}$
log H ₂ mass-mixing ratio	$\log \text{H}_2$	Uniform(-0.4, -0.05)	-0.36	$-0.26^{+0.13}_{-0.10}$
Scale factor	scale	Uniform(0,5)	4.9	$4.5^{+0.4}_{-0.7}$
Derived Parameters				
Carbon/oxygen ratio	C/O	-	0.32	0.3 ± 0.1
Carbon abundance	[C/H]	-	-2.6	-3.1 ± 0.5
Oxygen abundance	[O/H]	-	-2.1	-2.5 ± 0.4

Note. — The error bars on the retrieved medians correspond to the 68%/1 σ confidence interval. In addition to these priors, we required both a non-inverted $P - T$ profile and that the atmospheric temperature stay below 3000 K at all pressure levels. The full corner plot is included in Appendix 4.6.

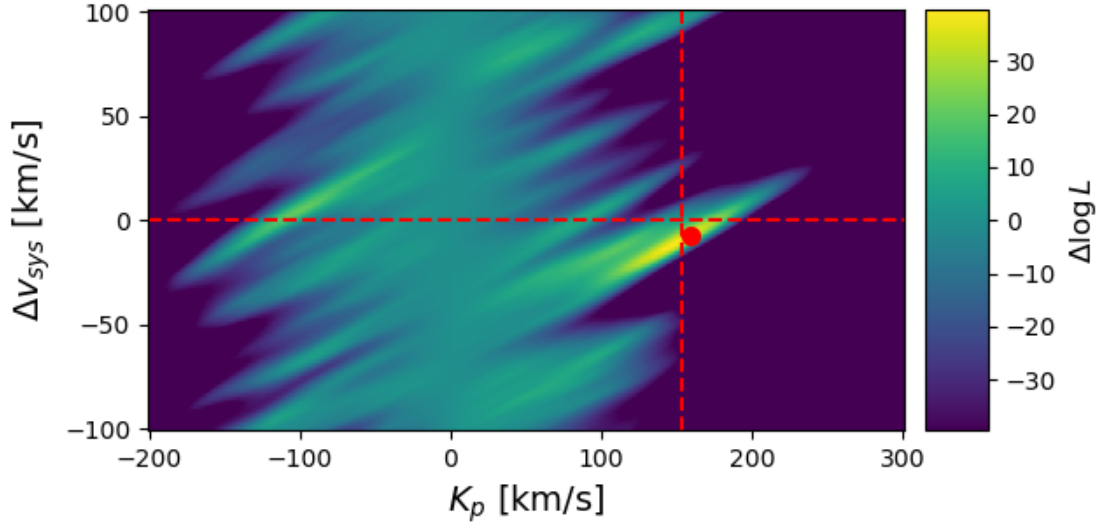


Figure 4.2: $v_{\text{sys}} - K_p$ diagram for the maximum-likelihood HD 189733 b model

The planet is clearly detected, though with a significant blueshift compared to the expectation indicated in dashed red. The detrending process suppresses planet features at small K_p , producing the feature centered on $K_p = 0$, where the planet model is a flat line after detrending. Compared with this null case, the maximum-likelihood model is preferred by $\Delta \log L = 39$, equivalent to $\sim 6\sigma$ using Wilks' Theorem (S. S. Wilks, 1938) with 17 free parameters. Note that the significant off-peak structure prevents accurate estimation of detection significance from division by the standard deviation far from the planet feature.

Subtracting each column of the $v_{\text{sys}} - K_p$ by its median, while not statistically robust, mostly removes this structure and allows a more reliable estimate of the off-peak variance. Using the $K_p < 0$ values to estimate the standard deviation after this subtraction gives a detection strength of 7.8σ . More rigorously, the cross-correlation coefficient depends only indirectly on the model variance, and the variance of the cross-correlation coefficient is therefore a weaker function of K_p , though self-division of the model still has some impact at small K_p . Computing the $v_{\text{sys}} - K_p$ diagram using the cross-correlation coefficient and dividing by the standard deviation of the $K_p < 0$ region gives a detection strength of 7.3σ near the retrieved maximum-likelihood velocity parameters.

The retrieved planet velocity is blueshifted by several km s^{-1} . Based on the orbital phase sampling of the observations, we expect that the previously reported day-to-night wind would appear as a redshift. The apparent blueshift is still consistent with values in the literature (e.g. [A. Boucher et al., 2021](#); [B. Klein et al., 2023](#)), but may suggest a more complicated circulation pattern than a single day-night wind. Alternatively, a number of other factors could bias our retrieved velocity, which we discuss in the next section.

The broadening velocity reported in Table 4.2 is substantially larger than values previously reported for the planetary rotational velocity in the literature (e.g. $3.4^{+1.3}_{-2.1} \text{ km s}^{-1}$ in [M. Brogi et al., 2016](#)) and is inconsistent with the expectation that HD 189733 b be tidally locked, which would correspond to a rotational velocity of 2.6 km s^{-1} . This is due to several simplifying assumptions in our handling of the KPIC LSF which are absorbed into a larger broadening velocity. Specifically, we assumed a smaller nominal LSF smaller than [L. Finnerty et al. \(2023a\)](#), allowing the retrieval to freely determine the best-fit line width. This helps account for LSF variations between coadded science spectra that result from the slight differences in LSFs between science fibers and the varying frame-to-frame coupling efficiency, and can also help account for the line smearing due to the planet’s motion within a coadd. While this prevents us from actually measuring the physical rotational speed of HD 189733 b, the tightly constrained posterior suggests these data have sufficient sensitivity to

the planetary line shapes that future analyses will be able to measure $v \sin i$ for hot Jupiters.

4.3.2 Thermal properties

Figure 4.3 shows the retrieved $P - T$ profile, emission contribution function, maximum-likelihood spectrum, and opacities of the major species. While several of the $P - T$ parameters are poorly constrained in the 1D marginalized posteriors, repeated draws from the posterior yield a consistent set of profiles, suggesting the $P - T$ profile is over-parameterized for the available data, but is well-constrained in the physically significant space.

The retrieved $P - T$ profile is slightly cooler than previous theoretical models for HD 189733 b (e.g. S.-M. Tsai et al., 2021). This may contribute to the preference for larger values of the overall multiplicative scale factor applied to the model planet spectrum, which results in an overall flux level consistent with the expected equilibrium temperature for HD 189733 b (Figure 4.3, middle panel). Alternatively, lower cloud pressures could be counteracted by increasing the scale factor in order to maintain the effective strength of the planet lines relative to the stellar continuum. Additionally, L. Finnerty et al. (2023a) found in simulations that this retrieval framework prefers larger values of the scale factor, likely due to artifacts in the data processing.

Due to this uncertainty, we ran an additional retrieval with a Uniform(0,10) prior on the scale factor. The scale factor was again close to the upper bound, and the retrieved $P - T$ profile was even colder. However, the retrieved abundances were consistent at the 1σ level and the flux level of the maximum-likelihood planet model was consistent to within $\sim 10\%$ for both retrievals. Initial analysis of another hot Jupiter observed with KPIC (Finnerty et al. in prep.) is also showing a similar preference for a higher-than-expected scale factor that is countered by a cooler-than-expected $P - T$ profile to match the expected continuum level. This strongly suggests our free retrieval framework has limited sensitivity to absolute temperature from the K -band data alone, but that this uncertainty does not significantly impact the retrieved atmospheric composition. Finally, we also note that residual continuum

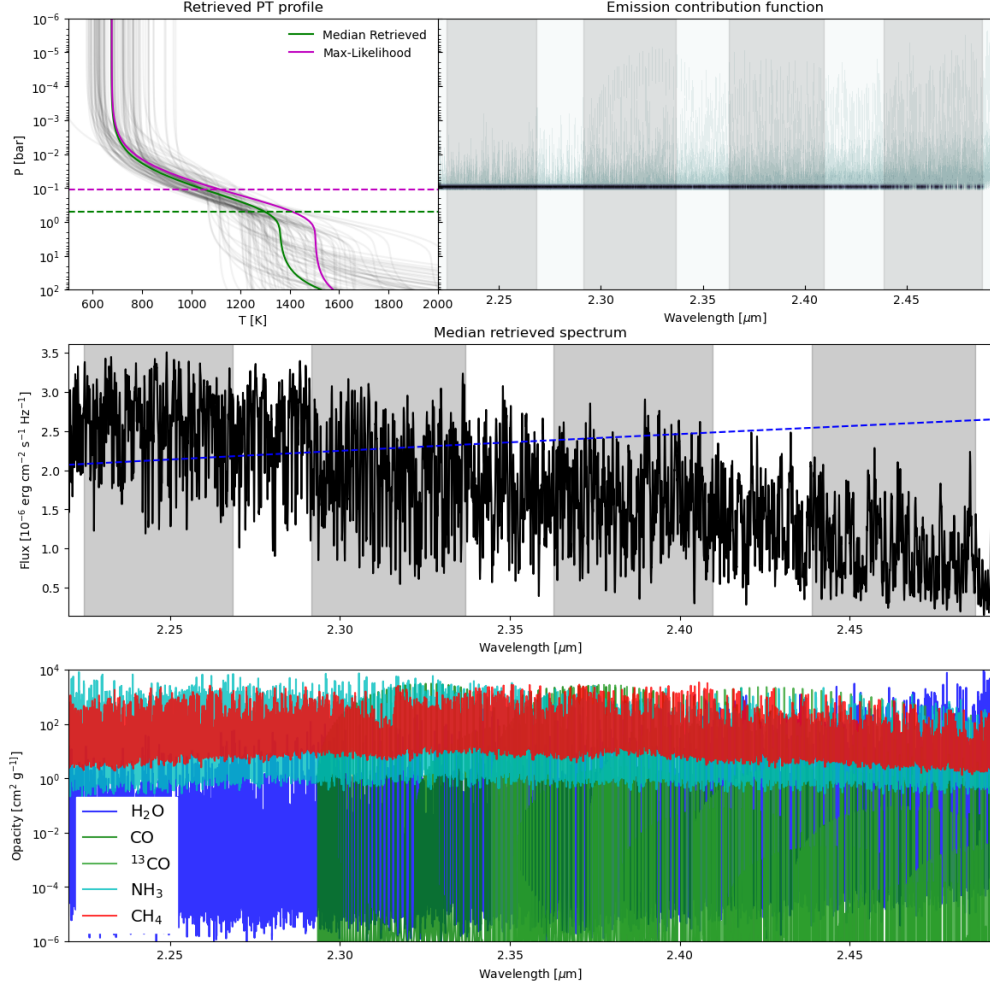


Figure 4.3: Retrieved spectrum of HD 189733 b

Retrieved $P-T$ profile (top left), maximum-likelihood emission contribution function (top right), maximum-likelihood planet spectrum (middle), and opacities (bottom). The observed NIRSPEC orders are shaded. In addition to the maximum-likelihood and median $P-T$ profiles, the top left also includes the cloud top pressures as dashed horizontal lines and the $P-T$ profiles from 100 posterior draws. While several parameters are poorly constrained in the corner plots, the actual $P-T$ -profiles follow a tight distribution. The emission mostly arises near 100 mbar, just above the cloud deck, with contribution from higher altitudes in the CO line cores. The dashed blue line plotted with the maximum-likelihood spectrum shows the flux from a 1200 K blackbody, which is comparable to the retrieved planet flux. The slope of the retrieved spectrum differs from a blackbody as a result of CO and H_2O absorption features at the red end of the K -band. Our retrievals provide only upper limits on NH_3 and CH_4 abundances despite these species' substantial opacity across the entire observed band, suggesting that the limits indicate a real absence of these species.

slopes or offsets in either the data or the model could also result in a spurious preference for a larger scale factor. In this case, the scale factor parameter is attempting to replicate the continuum offset, while the $P - T$ profile is shifted in order to preserve the correct line strength relative to the scaled continuum.

4.3.3 Chemical composition

Of the included species, we obtain bounded constraints only for CO and H₂O. Of the remaining species, we obtain upper limits on CH₄, NH₃, and HCN, though we note that the marginalized HCN posterior shows weak preference for $\log \text{HCN} \sim -4.8$. These species all have opacities comparable to that of the 2.3 μm CO bandhead in at least one of the observed NIRSPEC orders, suggesting these species would have been detected if present in significant abundances. While H₂S is effectively unconstrained, the opacity table used has a gap from 2.25 – 2.35 μm , which may preclude detection. The retrieved posterior also prefers a very high $^{13}\text{CO}/^{12}\text{CO}$ ratio, peaking at $\sim 10^{-0.8}$, though with a substantial tail to lower values. We include detection maps for H₂O, CO, CH₄, and ^{13}CO in Appendix 4.7, as well as a discussion of the challenges associated with accurately estimating single-molecule detection strength.

4.4 Discussion

4.4.1 Comparison to previous results

The extensive existing literature on HD 189733 b provides a basis for comparison with our retrieval results. To more easily facilitate comparison to other results, we note that the median retrieved values values reported in Table 4.2 are equivalent to $K_p = 160 \pm 8 \text{ km s}^{-1}$, $\log \text{CO}_{\text{VMR}} = -3.3 \pm 0.5$, and $\log \text{H}_2\text{O}_{\text{VMR}} = -2.9 \pm 0.4$. The remainder of this paper will continue to use mass-mixing ratios for molecular abundances.

B. Klein et al. (2023) analyzed high-resolution infrared transmission spectra from CFHT/SPIROU (J. F. Donati et al., 2020) to perform an atmospheric retrieval of the H₂O abundance and $P - T$ profile using the same T. Guillot (2010) parameterization with a grey cloud deck. B. Klein et al. (2023) report K_p , v_{sys} , and T_{eq} in good agreement with the values in Table 4.2, and $\log \text{H}_2\text{O} = -2.95^{+0.75}_{-0.53}$, slightly smaller than the value in Table 4.2, while reporting a larger value for the cloud-top pressure $\log P_{\text{cloud}} = 0.479^{+1.02}_{-1.06}$. We note that the corner plots for both retrievals indicate a degeneracy between the cloud pressure and molecular abundances, with greater pressures corresponding to lower abundances, potentially explaining the minor discrepancy in these parameters.

The data analyzed in B. Klein et al. (2023) were originally described in A. Boucher et al. (2021), who reported a somewhat lower H₂O abundance, higher cloud pressure, and lower temperature. Their corner plots also show a degeneracy between the abundance, cloud-top pressure, and temperature which could explain the discrepancy. The consistency of this degeneracy, regardless of analysis framework, suggests a need for analyses covering a broader wavelength range that can better constrain cloud properties. Previously, L -band spectroscopy from J. L. Birkby et al. (2013) found a best-fit H₂O VMR of $\sim 10^{-5}$, though with wide errors compatible with our abundances.

Constraints on the atmospheric CO abundance of HD 189733 b have been more elusive. R. J. de Kok et al. (2013) reported the first CO detection for HD 189733 b, also based on K -band emission spectroscopy, but did not report an abundance due to uncertainties concerning the impact of hazes. M. Brogi & M. R. Line (2019) re-analyzed the R. J. de Kok et al. (2013) observations of HD 189733 b to retrieve CO and H₂O, but obtained only lower and upper limits, respectively. The analysis presented in Section 4.3 is the first simultaneous determination of CO, CH₄, and H₂O abundances in the atmosphere of HD 189733 b suitable for constraining the atmospheric C/O ratio. Several *JWST* programs have obtained spectroscopy of HD 189733 b in both near and mid infrared wavelengths (GO 1633, PI Deming; GO 2001, PI Min; GO 2021, PI Kilpatrick & Kataria), which should provide a second, in-

dependent estimate of the atmospheric metallicity and C/O ratio (including the impact of CO_2) to compare with our results.

4.4.2 Winds and circulation

Compared with the nominal values in Table 4.1, the retrieved ΔK_p and Δv_{sys} yield a blueshift of 8 km s^{-1} at the start of the observation sequence, increasing to 10 km s^{-1} by the end. While wind speeds as high as 8 km s^{-1} have been reported for HD 189733 b from transmission observations of sodium lines (A. Wyttenbach et al., 2015), other observations in the near-infrared have preferred a windspeed of 2 km s^{-1} (M. Brogi et al., 2016), while still other infrared transmission analyses have reported K_p and v_{sys} values compatible with those reported in Table 4.2 (A. Boucher et al., 2021; B. Klein et al., 2023). We expect that a day-to-night wind would appear as a redshift in post-eclipse emission observations, rather than a blueshift. Similarly, we would expect the hotter dayside dominating the overall emission signal of the rotating planet to lead to a slight additional redshift. Improved orbital phase coverage may be required to directly constrain the wind speeds and 3D circulation on HD 189733 b from high-resolution spectroscopy alone.

Factors other than planetary winds could be contributing to the observed blueshift. The velocity shift is too large to be easily explained by an error in the orbital phase, particularly given the precision of the transit time for HD 189733 b. Similarly, we expect our wavelength solution to be reliable to $\sim 100 \text{ m s}^{-1}$, substantially better than the observed shift. K. C. Rasmussen et al. (2023) demonstrated that the shift in planetary lines within a science exposure can produce a blueshift of several km s^{-1} , though we expect this effect to be minimal given the $< 1 \text{ km s}^{-1}$ velocity shift between successive spectra in the time series. However, we did not attempt to account for the wavelength-dependence or non-Gaussian wings of the NIRSPEC line-spread function (R. A. López et al., 2020), potentially leading to a model mismatch in the line shapes that could bias the retrieved velocities. A laser frequency comb compatible with KPIC is scheduled for deployment in late 2023, which, when

completed, should enable the more robust calibration of the line-spread function required to interpret these types of velocity offsets as physical wind speeds or 3D effects. We note that a similar blueshift was also reported in [L. Finnerty et al. \(2023a\)](#) for WASP-33 b, which may indicate a systematic effect in the retrieval pipeline.

While we included a rotational broadening kernel in our fit, our approach to the instrumental broadening makes this effectively a nuisance parameter rather than a reliable estimate of the planetary $v \sin i$. As discussed above, we ignore both the wavelength-dependence and non-Gaussian shape of the line-spread function, as well as the impact of line smearing from the change in planet velocity within an exposure. To account for this, we chose a slightly smaller than expected Gaussian kernel for the instrument profile, and allowed a larger rotational kernel to make up the difference based on the actual observed line widths after coadding fibers. Future improvements to our retrieval pipeline will include a wavelength-dependent instrument profile similar to that used by [J. J. Wang et al. \(2021a\)](#) to measure $v \sin i$ for brown dwarf companions and directly-imaged planets observed with KPIC. Combined with the use of the laser frequency comb to constrain relative changes in the LSF across the NIRSPEC detector, this should enable robust measurements of $v \sin i$ for hot Jupiters in the future with KPIC.

4.4.3 CH₄ and photochemistry

Similar to [L. Finnerty et al. \(2023a\)](#), we compare our retrieved abundances with the results of the equilibrium chemistry calculator `easyCHEM` ([P. Mollière et al., 2017](#), Lei et al. in prep.) for the retrieved $P - T$ profile. Figure 4.4 plots the equilibrium vertical abundance profiles with the constant vertical abundances from our retrievals. The retrieved CO and H₂O abundances are a good match to the equilibrium predictions for $C/O = 0.25$ and $[M/H] = 0.05$, suggesting the gas-phase retrieval may be slightly overestimating the atmospheric metallicity. Both H₂O and CO abundances are roughly constant with height in equilibrium, validating the constant-with-altitude assumption in our retrieval and indicating that the

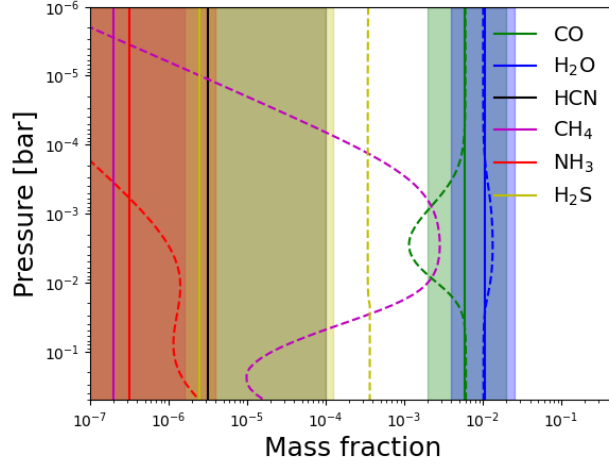


Figure 4.4: Retrieved abundances compared with equilibrium

Retrieved molecular abundances (solid lines, 1σ shaded) compared with the equilibrium abundances estimated from `easychem` (dashed lines). The equilibrium abundances are consistent with $C/O = 0.25$ and $[M/H] = +0.05$, both slightly below the values obtained from the gas-phase-only retrieval. The equilibrium model predicts H_2S and CH_4 abundances substantially greater than the retrieved upper limits. These species may be photochemically depleted.

potential biases resulting from high-altitude H_2O depletion in ultra-hot Jupiters (M. Brogi et al., 2023) are not a factor for HD 189733 b.

The cumulative distribution function (CDF) of the retrieved CH_4 posterior indicates $\log CH_4 < -4.6$ with 99% confidence. However, Figure 4.4 indicates that in chemical equilibrium for the retrieved $P - T$ profile, the CH_4 mass fraction should be $> 10^{-4}$ over nearly the entire pressure range probed by the KPIC observations in order to match the retrieved H_2O and CO abundances. We caution that the retrieved $P - T$ profile in Figure 4.3 is somewhat colder than expected in the upper atmosphere, which may lead to an overprediction of CH_4 when assuming chemical equilibrium. While previous attempts at CH_4 detection in hot Jupiters have faced challenges with linelist accuracy, we use an opacity table based on the recent R. J. Hargreaves et al. (2020) linelist which has been validated on brown dwarfs of similar effective temperature (M. E. Tannock et al., 2022). This opacity table has also previously been used to successfully measure the CH_4 abundance in a brown dwarf compan-

ion from KPIC observations at a mixing ratio comparable to that expected in HD 189733 b (J. W. Xuan et al., 2022). This suggests that the retrieved upper limit on CH_4 is due to a real absence of the expected CH_4 , rather than a linelist issue.

Depletion of CH_4 could be due to photochemistry. We assessed this possibility using the VULCAN chemical kinetics code (S.-M. Tsai et al., 2021). We used the default $P - T/K_{zz}$ profile for HD 189733 b included with VULCAN and described in S.-M. Tsai et al. (2021), which is slightly hotter than our retrieved profile in the upper atmosphere, the SNCHO photochemistry network, and the C/H and O/H set to the retrieved medians. All other settings were unchanged from the VULCAN defaults. VULCAN predicts a roughly constant CH_4 mass fraction of $\sim 10^{-5}$ from at pressures between approximately 1 and 10^{-3} bar. Over the same pressure range, the NH_3 mass fraction is predicted to be $\sim 10^{-4}$. The abundance of both species rapidly drops above 1 mbar, which may bias the abundances obtained from a free retrieval assuming constant abundance with pressure towards lower values, similar to the impact of water depletion in the upper atmospheres of ultra-hot Jupiters discussed in M. Brogi et al. (2023).

From the retrieved posterior, we obtain 99% upper limits $\log \text{CH}_4 < -4.6$ and $\log \text{NH}_3 < -4.5$, suggesting the current KPIC observations are not quite sensitive enough to make a definitive (non)detection at the VULCAN-predicted abundances. Both CH_4 and NH_3 have significant opacity throughout the NIR. Incorporating additional data such as high-resolution L -band observations from KPIC phase III may improve sensitivity to these species and enable tests of photochemical models in the future. Additionally, incorporating flux-calibrated broad-band medium-resolution observations from JWST would significantly improve constraints on absolute abundances compared with high-resolution observations alone, and also enable constraints on species which lack features easy to observe from the ground, such as CO_2

4.4.4 ^{13}CO enrichment

While the CO isotopologue ratio is not well-constrained in the retrieval, comparing the log-likelihood of the maximum-likelihood model with and without ^{13}CO indicates the presence of ^{13}CO is favored at $\sim 3\sigma$. The marginalized posterior shows a clear preference for high levels of ^{13}CO enrichment compared with both the solar system value of $^{12}\text{C}/^{13}\text{C} \sim 89$ and local interstellar value of $^{12}\text{C}/^{13}\text{C} \sim 68$ (P. M. Woods & K. Willacy, 2009; S. N. Milam et al., 2005), but with a long tail that is still consistent with the interstellar value at 1σ . Previously, L. Finnerty et al. (2023a) and M. R. Line et al. (2021) reported indications of ^{13}CO enrichment in hot Jupiter atmospheres compared with the local ISM. These estimates are substantially less than the $^{12}\text{CO}/^{13}\text{CO} \sim 10_{-6}^{+53}$ median retrieved for HD 189733 b, and were instead broadly consistent with the level of isotopic fractionation expected in the midplanes of protoplanetary disks (P. M. Woods & K. Willacy, 2009).

Carbon isotopologue constraints have also been obtained for widely separated companions. Y. Zhang et al. (2021a) found a roughly solar value for the $^{12}\text{CO}/^{13}\text{CO}$ ratio in a young field brown dwarf and suggested a formation process with minimal preferential accretion of ^{13}CO -enriched material such as direct gravitational collapse. In contrast, ^{13}CO enrichment has been reported for a young accreting super-Jupiter (Y. Zhang et al., 2021b), possibly suggesting preferential accretion of ^{13}C via fractionated ices. The enrichment reported in Y. Zhang et al. (2021b) is similar to the values reported in M. R. Line et al. (2021) for WASP-77Ab and L. Finnerty et al. (2023a) for WASP-33b, still less than the preferred value of ~ 10 for HD 189733 b.

The potential prevalence of ^{13}CO enrichment in hot Jupiters observed to-date suggests a common process in the formation or evolution of these planets. Accretion of fractionated ices appears to be consistent with the values reported by M. R. Line et al. (2021) and L. Finnerty et al. (2023a) (P. M. Woods & K. Willacy, 2009), but may not be sufficient to explain the $^{12}\text{CO}/^{13}\text{CO} \sim 10$ preference seen in our HD 189733 b retrieval. Additional observational and

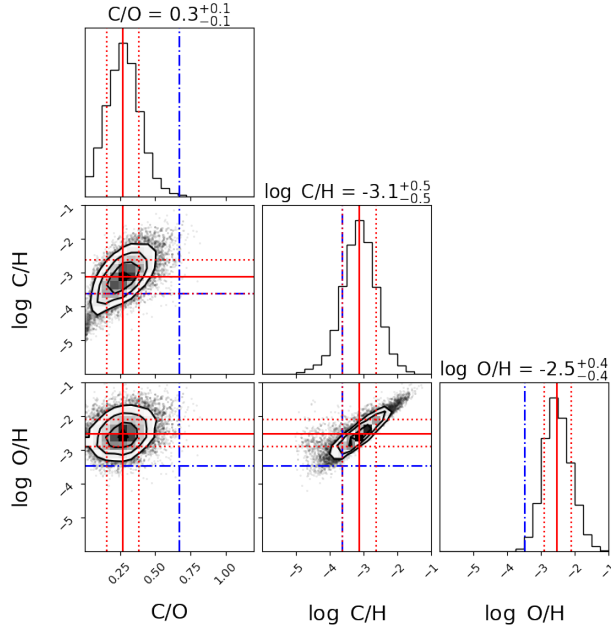


Figure 4.5: Retrieved C/O, C/H, and O/H posteriors for HD 189733 b

The median value is indicated in solid red, with the upper and lower bounds of the 68% confidence interval in dotted red. Stellar values from [A. S. Polanski et al. \(2022\)](#) are shown in dash-dot blue. The retrieved C/O ratio is substantially sub-stellar, while the carbon and oxygen abundances are both super-stellar.

modeling work is required to constrain the $^{12}\text{CO}/^{13}\text{CO}$ ratios of host stars and understand the general prevalence of this ^{13}CO enrichment, and the potential extreme case of HD 189733 b in particular.

4.4.5 C/O and metallicity

The posteriors for C/O, C/H, and O/H derived from the retrieval are plotted in Figure 4.5. As in previous high-resolution studies (e.g. [J. W. Xuan et al., 2022](#); [L. Finnerty et al., 2023a](#)), the ratio of species is better constrained than the absolute abundances, giving $\text{C/O} = 0.3 \pm 0.1$, $\log \text{C/H} = -3.1 \pm 0.5$, and $\log \text{O/H} = -2.5 \pm 0.4$. Precise abundances for HD 189733 A were previously reported in [A. S. Polanski et al. \(2022\)](#), enabling a robust comparison between the composition of the star and the planetary atmosphere. The

CDFs of the distributions in Figure 4.5 give a sub-stellar C/O at 99.8% confidence, super-stellar C/H at 84% confidence, and super-stellar O/H at 99.4% confidence. Comparison to equilibrium models suggests the gas-only retrieval may be slightly overestimating the total atmospheric metallicity, but sub-solar metallicities are still disfavored. These results indicate the atmosphere of HD 189733 b is compositionally distinct from the host star.

The combination of substellar-C/O and super-stellar metallicity was suggested to be an indicator of significant post-formation ice accretion by [K. I. Öberg et al. \(2011\)](#). [N. Madhusudhan et al. \(2014\)](#) found that low-C/O, metal-enriched atmospheres could be indicative of either core accretion followed by disk migration or formation at wide separations via gravitational instability followed by disk-free migration. Subsequently, [N. Madhusudhan et al. \(2017\)](#) found that such an atmospheric composition could also be the result of core erosion or late planetesimal accretion.

Core accretion should lead to atmospheric metal enrichment in giant planets ([D. P. Thorngren et al., 2016](#)), including a trend between planet mass and metal enrichment relative to the host star that is consistent with our reported values for HD 189733 b ([A. J. Cridland et al., 2019](#)). This process is also predicted to produce an inverse correlation between atmospheric metallicity and C/O ([N. Espinoza et al., 2017](#); [A. J. Cridland et al., 2019](#); [N. Khorshid et al., 2022](#)), though this trend may not hold in the presence of pebble drift ([R. A. Booth et al., 2017](#)). These models can predict the observed composition of HD 189733 b as a result of accreting a significant ($\sim 10\%$) fraction of the total planetary mass as solids relatively late in the formation process, with radial pebble drift not substantially altering the overall C/O of this material. Such a scenario may also be consistent with the extremely high ^{13}C enrichment suggested by the retrieval, which could be explained through late accretion of a large amount of highly fractionated ice.

4.5 Summary and Conclusions

We performed a Bayesian retrieval on high-resolution K -band observations of HD 189733 b from Keck/KPIC, successfully constraining the abundances of CO and H₂O and placing upper limits on the atmospheric mass fractions of CH₄, NH₃, and HCN. The retrieved abundances yield an atmospheric C/O = 0.3 ± 0.1 for HD 189733 b, substantially less than the stellar C/O ratio, and a stellar-to-superstellar atmospheric metallicity. This composition could be explained by the accretion of a large amount of solid material late in the planet formation process, possibly as a result of disk migration, which could also produce a well-aligned orbit with respect to the stellar rotation.

We do not detect CH₄ in the atmosphere of HD 189733 b. While this is incompatible with the retrieved $P - T$ profile in chemical equilibrium, the upper limits we obtained may be consistent with models which incorporate atmospheric photochemistry. Additional observations with a wider wavelength coverage will improve sensitivity to both CH₄ and NH₃, enabling direct tests of photochemical models, haze formation mechanisms, and measurement of the N/O ratio – providing deeper insight into the formation and evolution of the HD 189733 planetary system.

4.6 Corner Plots

Figure 4.6 presents the full corner plot from the retrieval for completeness. We discuss the retrievals in Section 4.3, including poorly constrained and degenerate parameters. The units, priors, and retrieved quantity are listed in Table 4.2

4.7 Molecular detection maps

Figure 4.7 presents $v_{\text{sys}} - K_p$ diagrams for each detected species calculated using a leave-one-out approach. As shown in Figure 4.3, strong, broad absorption by CO and H₂O cause

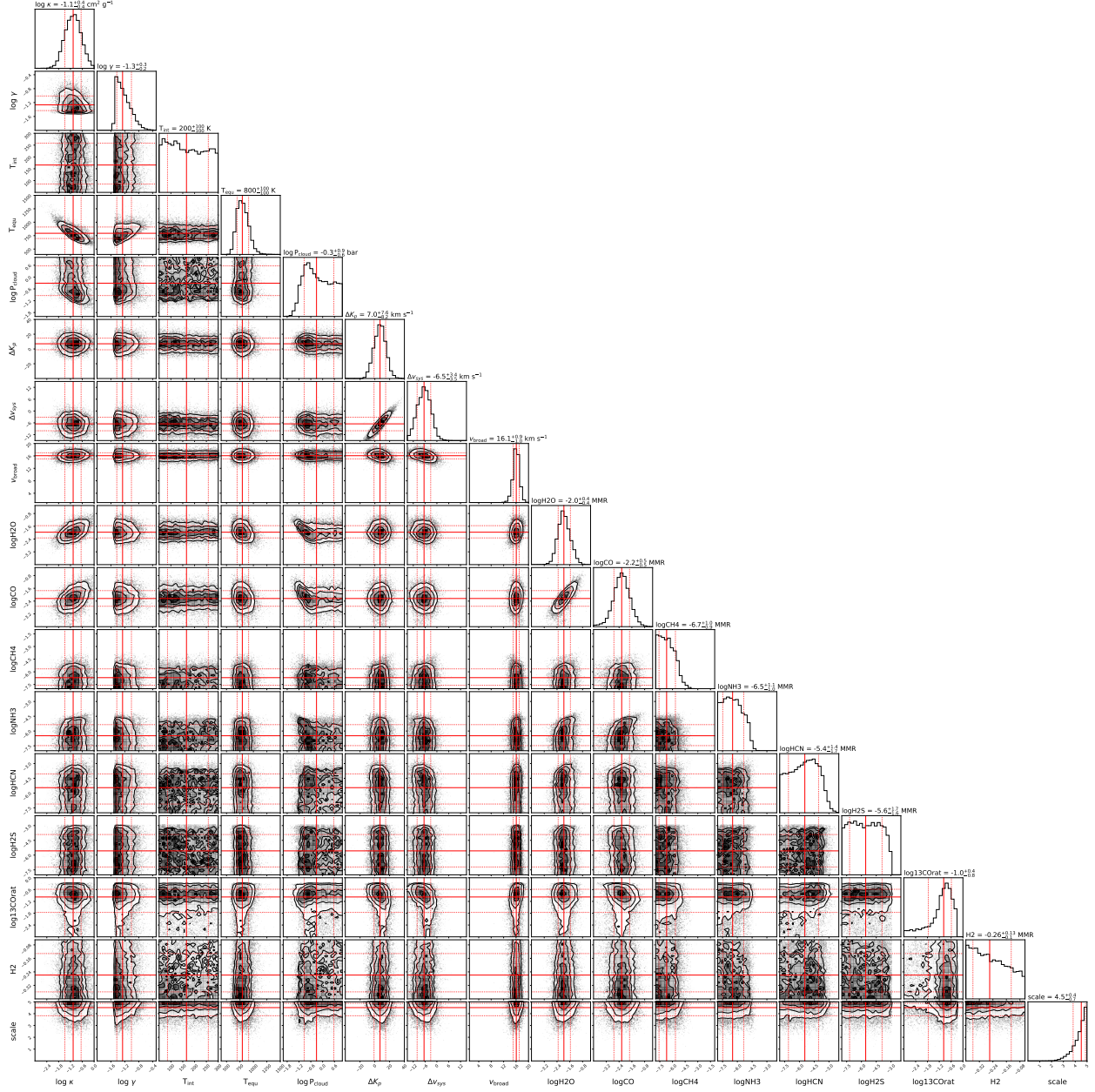


Figure 4.6: Full corner plot for the HD 189733 b retrieval.

Red solid lines indicate the medians, while red dashed lines indicate the bounds of the marginalized 68% confidence interval. We discuss these results in Section 4.3.

significant changes to the overall shape of the planetary SED, particularly beyond $\sim 2.35\mu\text{m}$. This presents a challenge when using single-molecule templates to assess detection strength, as the resulting inaccuracies in the continuum level can make it impossible for a single-molecule template to reproduce the observed relative fluxes between lines, particularly if other parameters are held fixed.

A slightly more reliable approach is to calculate $v_{\text{sys}} - K_{\text{p}}$ diagram for the maximum-likelihood model as well as the $v_{\text{sys}} - K_{\text{p}}$ diagram for a model omitting the molecule of interest. The difference between these two maps is the change in the log-likelihood that can be attributed to the presence of the omitted species. This approach will still be inaccurate in the case of e.g. H_2O and CO whose omission has a significant impact on the continuum, but should provide a more accurate estimate for the detection strength of trace species. Taking the difference of the two maps should also largely remove the self-division artifact seen at $K_{\text{p}} = 0$ in Figure 4.2, though the resulting map will show a bias towards higher values of K_{p} . This bias arises from self-removal of the planet model during detrending and is increased by the explicit dependence of the [M. Brogi & M. R. Line \(2019\)](#) log-likelihood function on the model variance. The detrending process used to remove continuum and telluric features reduces the model variance as K_{p} decreases and the self-division effect of the median division and the self-subtraction effect of the SVD remove more of the planet model. As a result, we expect that the apparent strength of noise features to increase with increasing K_{p} when assuming a constant variance for the entire map, and that planetary features will show a bias towards higher K_{p} in difference maps compared with computing $\log L$ directly.

These effects can be seen in Figure 4.7. H_2O is detected at $\sim 3.8\sigma$ near the expected velocity, while CO is detected at $\sim 5\sigma$ but with a shift towards larger K_{p} . CH_4 is not significantly detected, as expected, and a weak ($\sim 3\sigma$) feature is present in the ^{13}CO map near the maximum-likelihood velocities, but is not strong enough to constitute an independent detection, particularly given the presence of large-amplitude features at high K_{p} . The H_2O and CO detections are weaker than would be expected based off of the all-molecule model,

likely due to the impact of these species on the planet continuum. However, ^{13}CO is significantly less abundant and will have a much smaller impact on the planetary continuum level. Consistent with this, the ^{13}CO feature in the $v_{\text{sys}} - K_{\text{p}}$ map is similar in strength to the expectation from Wilks' Theorem in Section 4.4.4.

Consistent with previous high-resolutions studies of other hot Jupiters (M. R. Line et al., 2021; L. Finnerty et al., 2023a), ^{13}CO is not independently detected in the $v_{\text{sys}} - K_{\text{p}}$ space, but the presence of ^{13}CO is favored by $\sim 3\sigma$ over a model without ^{13}CO . As discussed above, estimating the detection strength from the $v_{\text{sys}} - K_{\text{p}}$ diagram poses a number of challenges that are particularly acute for trace species which do not produce a strong peak to begin with. The repeated tentative detection of ^{13}CO across multiple targets highlights the need for improved techniques to quantitatively estimate detection strengths for high-resolution observations.

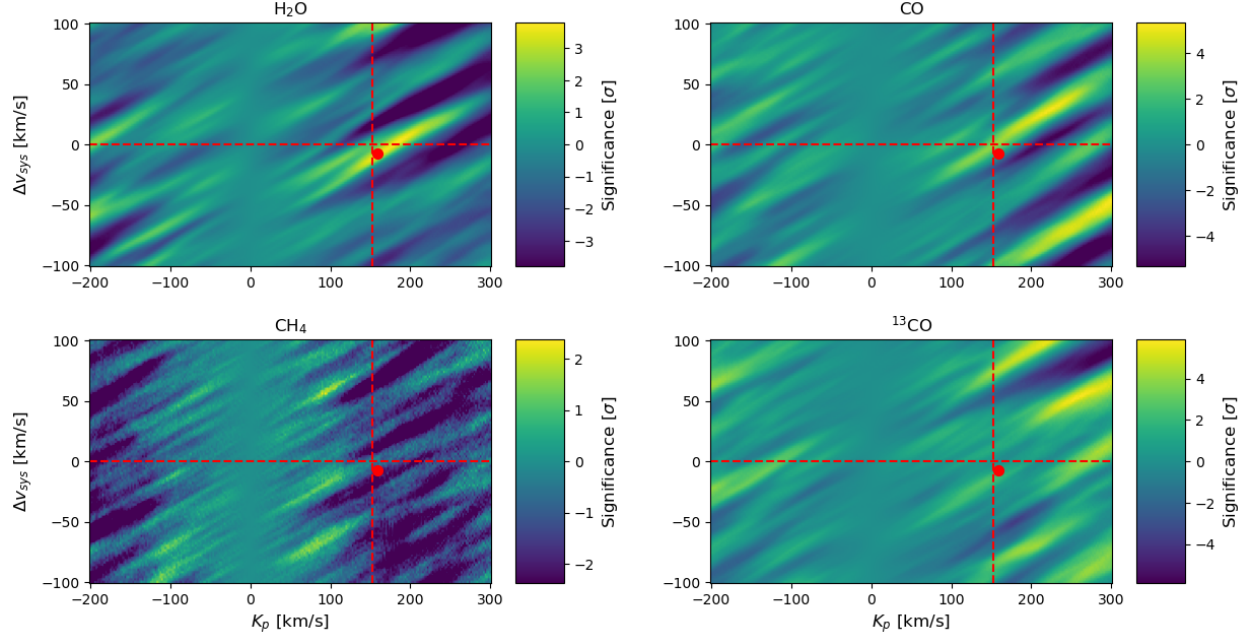


Figure 4.7: $v_{\text{sys}} - K_p$ diagrams for H_2O , CO , CH_4 , and ^{13}CO

Dashed red lines indicate the nominal values of the planetary velocity parameters, and the red dot indicates the maximum-likelihood values for the full model. These maps were made by subtracting a map omitting each species from a map made using the maximum-likelihood model, in order to better account for the impact of other atmospheric species on the continuum. Significance was estimated by dividing each map by the standard deviation of the $K_p < 0$ region. Continuum impacts are still significant, leading to weaker-than-expected detections of H_2O and CO and biasing the CO velocity. These effects are less important for lower-abundance species. As expected based on the retrieved posteriors, we do not detect CH_4 , and ^{13}CO shows a weak ($\sim 3\sigma$) feature near the expected planet velocity. This ^{13}CO feature does not constitute an independent detection, but the inclusion of ^{13}CO is favored over a ^{12}CO -only model at $\sim 3\sigma$, consistent with other results for ^{13}CO in hot Jupiter atmospheres (M. R. Line et al., 2021; L. Finnerty et al., 2023a)

CHAPTER 5

True mass and atmospheric composition of the non-transiting hot Jupiter HD 143105 b

A version of this chapter was previously published in the *Astronomical Journal* (Finnerty *et al.* 2025a 169, 2, 94)

Abstract

We present Keck/KPIC phase II K -band observations of the non-transiting hot Jupiter HD 143105 b. Using a cross-correlation approach, we make the first detection of the planetary atmosphere at $K_p = 185^{+11}_{-13}$ km s $^{-1}$ and an inferior conjunction time 2.5 hours before the previously-published ephemeris. The retrieved K_p value, in combination with orbital period, mass of the host star, and lack of transit detection, gives an orbital inclination of 78^{+2}_{-12} and a true planet mass of 1.23 ± 0.10 M $_J$. While the equilibrium temperature of HD 143105 b is in the transition regime between non-inverted and inverted atmospheres, our analysis strongly prefers a non-inverted atmosphere. Retrieval analysis indicates the atmosphere of HD 143105 b is cloud-free to approximately 1 bar and dominated by H $_2$ O absorption ($\log \text{H}_2\text{O}_{\text{MMR}} = -3.9^{+0.8}_{-0.5}$), placing only an upper limit on the CO abundance ($\log \text{CO}_{\text{MMR}} < -3.7$ at 95% confidence). We place no constraints on the abundances of Fe, Mg, or ^{13}CO . From these abundances, we place an upper limit on the carbon-to-oxygen ratio for HD 143105 b, $\text{C}/\text{O} < 0.2$ at 95% confidence, and find the atmospheric metallicity is approximately $0.1 \times$ solar. The low metallicity may be responsible for the lack of a

thermal inversion, which at the temperature of HD 143105 b would likely require significant opacity from TiO and/or VO. With these results, HD 143105 b joins the small number of non-transiting hot Jupiters with detected atmospheres.

5.1 Introduction

Transmission and secondary eclipse spectroscopy are powerful tools for characterizing exoplanet atmospheres, but are fundamentally limited to the small fraction of planets which transit their host stars. By directly detecting planetary dayside emission, high-resolution cross-correlation spectroscopy (HRCCS) techniques can be used to characterize the atmospheres of non-transiting exoplanets (e.g. [M. Brogi et al., 2012](#); [F. Rodler et al., 2012](#); [M. Brogi et al., 2014](#); [J. L. Birkby et al., 2017](#); [G. Guilluy et al., 2019](#); [R. K. Webb et al., 2020](#); [C. Buzard et al., 2020](#); [S. Pelletier et al., 2021](#)). These observations break the mass-inclination degeneracy from the radial velocity technique and enable constraints on the true mass of non-transiting planets. The significant inclinations of some of these systems may also enable novel characterization of the polar regions of hot Jupiters ([I. Malsky et al., 2021](#)).

High-resolution spectroscopy of non-transiting planets must contend with additional uncertainties compared with observations of transiting targets, increasing the risks associated with these observations. For planets with nearly face-on orbits, the projected line-of-sight velocity shift may be too small compared to the instrument resolution to make a detection, even if the planet would be detectable if the orbit were edge on. The observed velocity shift decreases with $\sin i$, so this effect is prohibitive for a relatively small fraction of non-transiting planets, but necessitates additional care when scheduling observations so that a sufficient velocity shift will be obtained even if the system is low inclination.

Additionally, non-transiting planets have ephemerides based on radial velocity observations alone. While transiting planets detected with TESS often have periods and transit times determined to a precision of seconds, such precise ephemerides are difficult to achieve

for non-transiting planets. Furthermore, maintaining current ephemerides via radial velocity monitoring requires significant investments of telescope time, and as a result many non-transiting systems do not have recently updated ephemerides. This can lead to significant uncertainty in the orbital phase for followup HRCCS observations.

These challenges have limited the number of non-transiting planets detected via HRCCS. τ Boo b was the first non-transiting planet detected with HRCCS by [M. Brogi et al. \(2012\)](#), followed by HD 179949 b ([M. Brogi et al., 2014](#)). [M. Brogi et al. \(2013\)](#) reported a tentative detection of 51 Peg b which was confirmed by [J. L. Birkby et al. \(2017\)](#), and HD 102195 b was first reported in [G. Guilluy et al. \(2019\)](#). HD 187123 b was detected via a similar technique by [C. Buzard et al. \(2020\)](#). This is only a small fraction of the number of transiting systems characterized with HRCCS techniques.

HD 143105 b is a non-transiting hot Jupiter first detected in 2016 using radial velocity observations from the SOPHIE spectrograph ([G. Hébrard et al., 2016](#)). Properties of the system are summarized in Table 5.1. While the short orbital period and bright host star make HD 143105 b a good candidate for atmospheric characterization, the far-northern declination of the system has made it inaccessible to most ground-based high-resolution spectrographs, and *JWST* has so far only characterized hot Jupiters using transmission and eclipse methods, leaving HD 143105 b unstudied. HD 143105 b is a particularly interesting target for atmospheric characterization, as its 1940 K equilibrium temperature is close to the expected transition between atmospheres with and without a thermal inversion predicted by both 1D ([C. Baxter et al., 2020](#)) and 3D modeling ([A. Roth et al., 2024](#)). In this paper, we use Keck/KPIC HRCCS observations to make the first atmospheric detection of HD 143105 b which enables us to refine the planetary ephemeris and constrain the atmospheric composition and pressure-temperature ($P - T$) profile.

We discuss the Keck/KPIC observations of HD 143105 b and our atmospheric retrieval framework in Section 5.2. Results from the cross-correlation and retrieval analyses are presented in Section 5.3, and discussed in Section 5.4. Section 5.5 concludes.

Table 5.1: Stellar and planetary properties for the HD 143105 system

Property	Value	Ref.
HD 143105		
RA	15:53:36.57	Gaia Collaboration (2020)
Dec	+68:43:11.92	Gaia Collaboration (2020)
Sp. Type	F5	G. Hébrard et al. (2016)
K_{mag}	5.52 ± 0.02	R. M. Cutri et al. (2003)
Mass	$1.51 \pm 0.11 M_{\odot}$	G. Hébrard et al. (2016)
Radius	$1.61^{+0.08}_{-0.05} R_{\odot}$	ExoFOP (2019)
T_{eff}	$6380 \pm 60 \text{ K}$	G. Hébrard et al. (2016)
$\log g$	4.37 ± 0.04	G. Hébrard et al. (2016)
$v \sin i$	$9.1 \pm 1 \text{ km s}^{-1}$	G. Hébrard et al. (2016)
v_{rad}	$15.942 \pm 0.003 \text{ km s}^{-1}$	G. Hébrard et al. (2016)
[Fe/H]	0.05 ± 0.04	N. R. Hinkel et al. (2014)
[C/H]	0.03 ± 0.34	N. R. Hinkel et al. (2014)
[O/H]	0.02 ± 0.04	N. R. Hinkel et al. (2014)
HD 143105 b		
Period	$2.1974 \pm 0.0003 \text{ days}$	G. Hébrard et al. (2016)
T_{conj}	$\text{JD } 2456531.344 \pm 0.007$	G. Hébrard et al. (2016)
T_{conj}	$\text{JD } 2456531.237^{+0.012}_{-0.017}$	This work
a	$0.0379 \pm 0.0009 \text{ AU}$	G. Hébrard et al. (2016)
e	< 0.07	G. Hébrard et al. (2016)
i	78^{+2}_{-12}	This work
K_{p}	$185^{+11}_{-13} \text{ km s}^{-1}$	This work
$M \sin i$	$1.21 \pm 0.06 M_{\text{J}}$	G. Hébrard et al. (2016)
Mass	$1.23 \pm 0.10 M_{\text{J}}$	This work
Radius	$1.20 \pm 0.05 R_{\text{J}}$	Assumed
T_{eq}	1940 K	Calculated
C/O	< 0.4	This work
[C/H]	< -1.1	This work
[O/H]	$-1.3^{+0.9}_{-0.5}$	This work
$v \sin i$	$7.4^{+3.1}_{-3.5} \text{ km s}^{-1}$	This work

Note. — Upper limits from this work are given at 95% confidence, omitting the secondary mode for the C/O ratio.

5.2 Observations and Data Reduction

5.2.1 Observations

The HD 143105 system was observed using Keck II/KPIC phase II (I. S. McLean et al., 1998; E. C. Martin et al., 2018; R. A. López et al., 2020; J.-R. Delorme et al., 2021; D. Echeverri et al., 2022) for the first half of the night on UT 24 May 2024, from 6:24 to 10:19. The observations were scheduled around a predicted superior conjunction based on the G. Hébrard et al. (2016) ephemeris in order to maximize dayside visibility and velocity shift of the planet over the observation. The maximum velocity shift was estimated to be 80 km s^{-1} for a 90 degree inclination, sufficient to allow detection of the planet even if a significant orbital inclination resulted in a much smaller change in the projected velocity over the course of the observation. Exposures were taken staring on KPIC science fiber 2 with a 90 second integration time in order to avoid saturation on the NIRSPEC detector.

Weather conditions were sub-optimal throughout the observation. Telescope opening was delayed by approximately 40 minutes at the start of the night due to high humidity, which persisted throughout the night. Cloud cover was variable throughout the observations, which resulted in brief periods of extinction up to two magnitudes. The observation sequence began as HD 143105 was rising, at an airmass of 1.93, and continued until the target was just past transit, at an airmass of 1.51. Despite the high airmass, the top-of-atmosphere throughput to KPIC was consistently $\sim 2.5\%$ during clear periods, consistent with the median KPIC phase II performance (D. Echeverri et al., 2022, Jovanovic et al. in prep.). This is a significant improvement in instrument performance over previous high-airmass observations taken under better atmospheric conditions. This improvement is likely as a result of recent upgrades to the real-time controller for the Keck AO system providing better AO and differential refraction corrections at high airmass.

5.2.2 Data Reduction

Similar to previous KPIC observations (e.g. [L. Finnerty et al., 2023a, 2024](#)), we observed a late-type star to provide additional stellar lines for wavelength calibration, in this case HIP 62944. The 1D spectrum was extracted and used to fit a wavelength solution following the standard KPIC Data Reduction Pipeline (DRP)¹.

For the observations of HD 143105, we used the LSF fitting procedure described in Finnerty et al. (subm.), which handles the non-Gaussian wings and wavelength-dependence of the KPIC trace using a Gaussian-Hermite model to produce weights for optimal extraction. For the LSF, we scale the overall width of the resulting spatial profile by a factor of 1.14, as was previously done in Finnerty et al. (subm.), based on the spatial/spectral width asymmetry reported in [L. Finnerty et al. \(2022\)](#). This LSF kernel is then convolved with the forward model of the planetary spectrum after the rotational broadening kernel is applied and prior to the calculation of the log likelihood. In theory, this technique should enable constraints on $v \sin i$ better than the 9 km s^{-1} resolution of the Keck/NIRSPEC spectrograph, although in practice systematic uncertainties in the LSF make physical interpretation of such small rotational velocities suspect.

Following extraction, we coadded each consecutive pair of science frames in order to boost signal-to-noise and reduce the data volume for retrieval. The final extracted SNR per wavelength channel was approximately 265 in the bluest order included in analysis and 166 in the reddest order. The decreased SNR at longer wavelengths is due to a combination of atmospheric dispersion and increased thermal background at the red end of the K -band.

Consistent with previous KPIC observations, orders 37–39, covering $1.94\text{--}2.09 \mu\text{m}$, are heavily contaminated by telluric features and omitted from subsequent analysis. Initial cross-correlation analysis found that orders 35 and 36 do not meaningfully contribute to the planet detection due to the absence of strong spectral features. We therefore restrict our analysis

¹https://github.com/kpicteam/kpic_pipeline/

to orders 31–34, spanning 2.22–2.49 μm , in order to speed up retrievals.

5.2.3 Cross-correlation

Propagating the reported period uncertainty from [G. Hébrard et al. \(2016\)](#) to the observation epoch results in an uncertainty of approximately 12 hours in the conjunction time. We therefore began with a cross-correlation analysis in order to isolate the planet signal for subsequent retrieval. Rather than varying the planet RV semi-amplitude K_p and the systemic velocity v_{sys} , we instead vary K_p and the conjunction time, ΔT_{conj} . This better reflects existing knowledge of a system where the inclination is unknown and the orbital phase has significant uncertainties, but the systemic velocity is well-constrained by previous radial velocity observations. In particular, the short orbital period of HD 143105 b creates a scenario where a change in orbital phase corresponding to just a few hours can dramatically change the velocity track of the planet, from nearly linear in the case of observations near conjunction to clearly sinusoidal for phases close to quadrature.

To create the $K_p - \Delta T_{\text{conj}}$ plots, we projected out 6 principal components during detrending, and computed the cross-correlation rather than the log-likelihood. The [M. Brogi & M. R. Line \(2019\)](#) log-likelihood function shows strong systematic effects in the $K_p - \Delta T_{\text{conj}}$ space due to its explicit dependence on the model variance. As a result of the time series detrending and its replication in the forward modeling, the model variance is itself strongly dependent on the velocity shift of the planet, which changes with both K_p and ΔT_{conj} . The cross-correlation coefficient is much less dependent on the variance of the planet models, making it a more appropriate choice for detection in this case. See [L. Finnerty et al. \(2024\)](#) for a more extended discussion of these systematics in the $K_p - v_{sys}$ case.

5.2.4 Atmospheric Retrieval

We continue to use the retrieval framework described in L. Finnerty et al. (2023a, 2024, Finnerty et al., submitted), with some minor updates which we summarize below. Our retrievals now use `petitRADTRANS` version 3 (P. Mollière et al., 2019, 2020; E. Nasedkin et al., 2024), which significantly improves the efficiency of the radiative transfer calculation. We also add a grey cloud opacity, following the `petitRADTRANS` documentation:

$$\kappa_{\text{cld}} = \kappa_{0,\text{cld}} (P/P_0)^{f_{\text{SED}}} \quad (5.1)$$

which is applied for $P > P_0$. We treat P_0 , $\kappa_{0,\text{cld}}$, and f_{SED} as free parameters in the retrieval.

Additionally, we have changed the PCA to be performed on the temporal axis of the data arrays, rather than the spectral axis. This provides a minor performance improvement, and does not change the resulting log-likelihood for small numbers of omitted components. The resulting principal component vectors are also somewhat easier to interpret, representing the way the observed spectrum evolves in time, rather than expressing the time series as a sum of component spectra with time-varying weights.

Based on the ephemeris uncertainty discussed previously, we opt to update the nominal T_{conj} for the retrieval analysis to JD 2456531.2225 based on the mean offset in from the four models shown in Figure 5.1. We then fit for a small offset in the conjunction time in the retrieval, rather than v_{sys} . This offset corresponds to a ± 1.2 hour shift in the conjunction time, which was chosen based on the range of offsets from Figure 5.1.

Finally, we have changed the nested sampling implementation from `dynesty` (J. S. Speagle, 2020) to `MultiNest` (F. Feroz & M. P. Hobson, 2008; F. Feroz et al., 2009; J. Buchner et al., 2014; F. Feroz et al., 2019). Both packages produce similar final posteriors, but `MultiNest` is approximately $10\times$ faster, enabling retrievals in 12 hours of wall time with 8 CPU cores. We use 500 live points and a $\Delta \log z < 0.1$ convergence criteria. The final posteriors are consistent with runs using a larger number of live points and/or a stricter convergence criteria (e.g. 1000 or 1200 live points, $\Delta \log z < 0.01$), but the smaller number

of live points and looser $\Delta \log z$ criteria significantly reduce the total run time.

The equilibrium temperature of HD 143105 b estimated with the system properties listed in Table 5.1 is ~ 1940 K. This is close to the transition temperature where models predict dayside thermal inversions (e.g. C. Baxter et al., 2020; A. Roth et al., 2024). We therefore choose a wide prior on the γ parameter of the of the T. Guillot (2010) Pressure-Temperature ($P - T$) profile to permit either inverted or non-inverted atmospheres. While the internal temperature parameter T_{int} has not been well-constrained in previous retrievals of hot Jupiter atmospheres with KPIC data, we include it as a free parameter for completeness, and similarly include the planetary surface gravity $\log g$ as a free parameter. Tests using the `easyCHEM` (P. Mollière et al., 2017; E. Lei & P. Mollière, 2024) equilibrium chemistry calculator indicate the dominant metal species at the expected temperatures in the atmosphere of HD 143105 b are CO, H₂O, Fe, and Mg, and that the vertical mixing profiles for these species are nearly constant with altitude for the non-inverted $P - T$ profiles favored in the initial cross-correlation analysis. We therefore treat all abundances as constant with altitude.

For the molecular species, we use the opacity tables previously described in L. Finnerty et al. (2023a). For H₂O, these tables used the (O. L. Polyansky et al., 2018) partition function and HITEMP 2010 linelist (L. S. Rothman et al., 2010). For both CO isotopologues we used the HITEMP 2019 lists (I. E. Gordon et al., 2022) and the G. Li et al. (2015) partition function. For Fe and Mg we use the `petitRADTRANS` provided tables based on the Kurucz atomic line lists.

We ran retrievals omitting 4, 6, and 8 principal components during the data detrending process. We report the values from the 6 component retrieval in Section 5.3. The marginalized medians and confidence intervals are consistent between all three retrievals, indicating the values we report are not strongly dependent on the number of PCA components.

5.3 Results

5.3.1 Cross-correlation Analysis

For the initial cross-correlation analysis, we generated models based on the equilibrium temperature of HD 143105 b and varying assumed compositions under chemical equilibrium. For the $P - T$ profile, we assumed $\log \kappa = -1$, $\log \gamma = -1$ for the non-inverted case and $\log \gamma = 1$ for the inverted case, $\log g = 3.3$, $T_{\text{int}} = 100$ K, and $T_{\text{eq}} = 1940$ K. The assumed cloud parameters were $f_{\text{SED}} = 4$, $\log \kappa_{0,\text{cld}} = 1$, $\log P_{\text{cloud}} = 0$. We assumed planetary $v \sin i = 3 \text{ km s}^{-1}$, corresponding to tidally-locked rotation for a planetary radius of $1.2R_{\text{J}}$, consistent with a moderately inflated hot Jupiter. For the molecular abundances, we used **easychem** (P. Mollière et al., 2017; E. Lei & P. Mollière, 2024) to compute equilibrium abundance profiles for H_2O , CO , Fe , and Mg assuming different atmospheric C/O ratios (0.3 or 0.8), metallicities (-0.3 or $+0.3$ dex relative to solar), and whether or not a thermal inversion is present, for a total of eight planet models. For the inverted models, we did not account for vertical variations in species abundances, although **easychem** predicts H_2O dissociates above the inversion and Fe and Mg are not present in significant quantities below the inversion. We instead took the respective lower/upper atmosphere abundances as constant. While this would create model mismatches in a retrieval analysis, it should not preclude simple detection.

5.3.1.1 Ephemeris and velocities

Figure 5.1 shows the computed $K_p - \Delta T_{\text{conj}}$ plots for the four non-inverted planet models, while Figure 5.2 shows the four inverted models. Figure 5.3 shows the $K_p - v_{\text{sys}}$ diagram for a non-inverted model with both the G. Hébrard et al. (2016) and our revised ephemerides for comparison. All four non-inverted models show a $\text{SNR} \sim 4$ feature at approximately $\Delta T_{\text{conj}} = -180$ minutes, $K_p = 167 \text{ km s}^{-1}$. None of the inverted models produce features of comparable strength, and all of the inverted models are consistent with a non-detection,

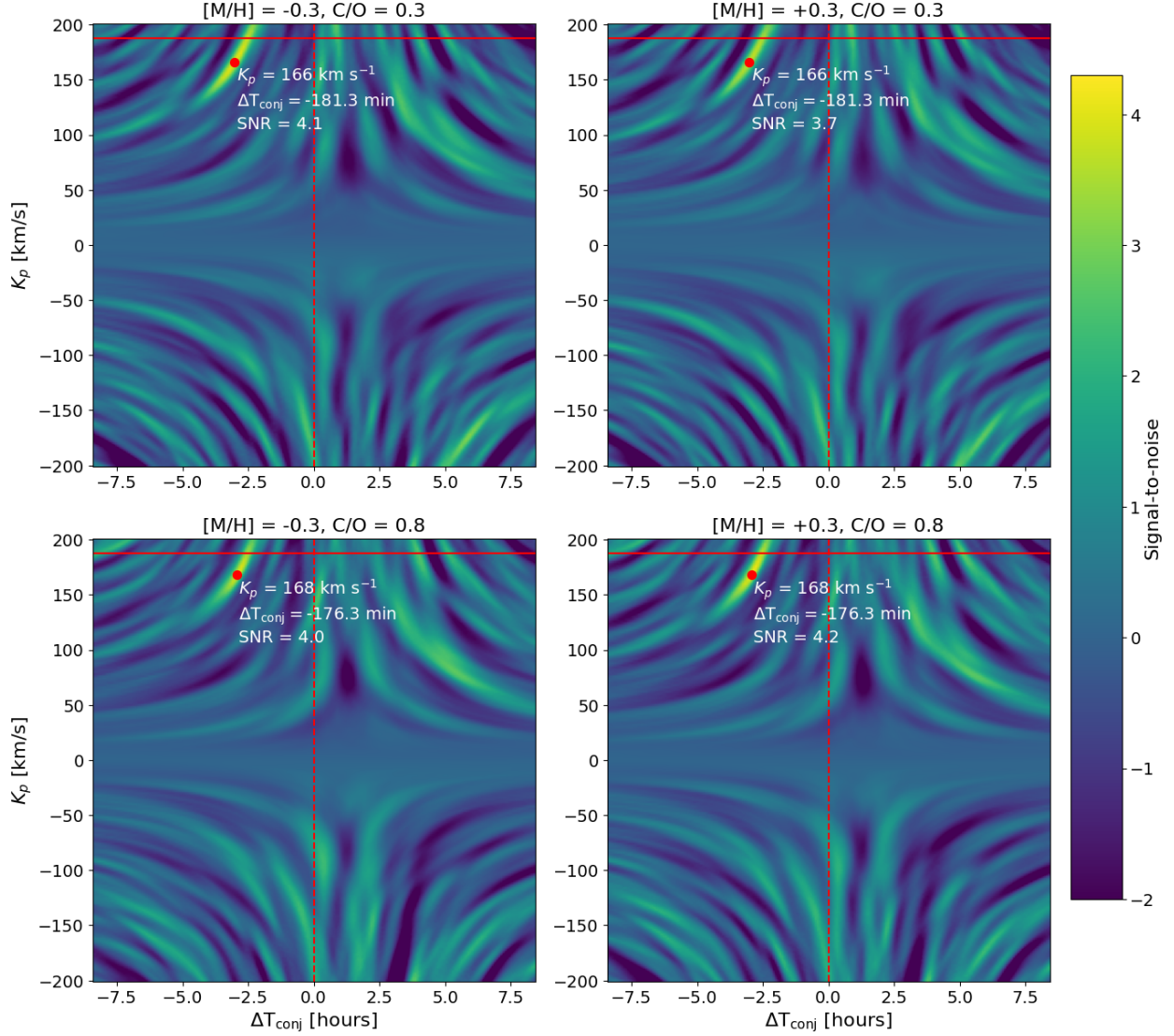


Figure 5.1: K_p vs conjunction time offset for HD 143105 b with noninverted models

We consider four models with varying metallicity and C/O ratio. All four models show a strong feature consistent with a planet detection at similar K_p and ΔT_{conj} . The peak values correspond to a conjunction time approximately 3 hours before the expectation from [G. Hébrard et al. \(2016\)](#), well within the propagated uncertainty in the conjunction time arising from uncertainty in the orbital period. The peak planet RV semi-amplitude is $\sim 167 \text{ km s}^{-1}$ for all models, corresponding to an inclination of 64 degrees. The signal-to-noise was calculated by dividing the map by the standard deviation of the $K_p < -60$ region. All models are detected at similar strength.

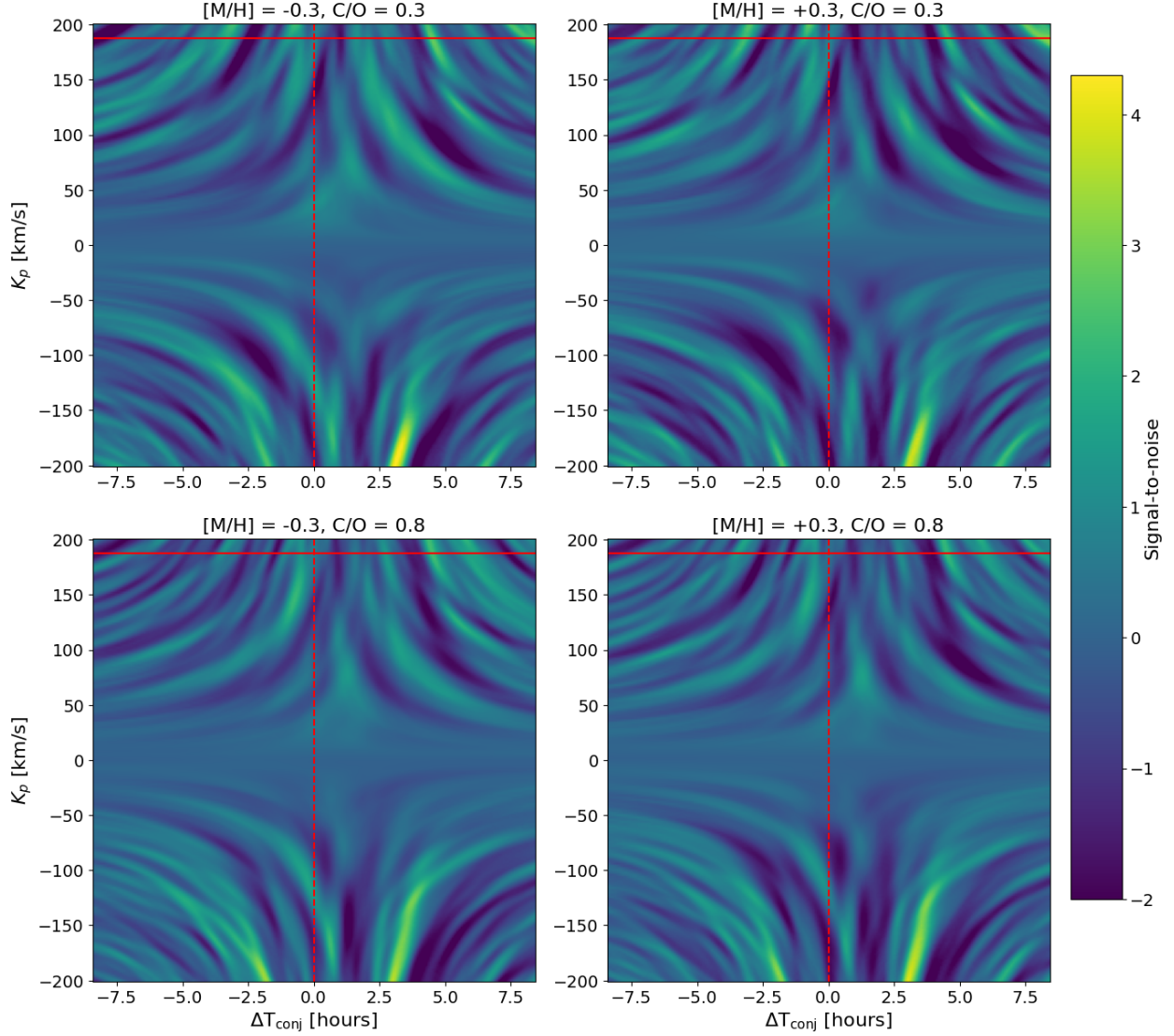


Figure 5.2: K_p vs conjunction time offset for HD 143105 b with inverted models

We consider four models with varying metallicity and C/O ratio. None of these models give a potential planet detection in the region permitted by the prior ephemeris, indicating the detected planet flux is primarily arising from regions of the planetary atmosphere without a thermal inversion. The peak at $T_{\text{conj}} = +2.5$ hours, $K_p = -175 \text{ km s}^{-1}$ corresponds to a velocity track near transit/inferior conjunction, when the observed disk is dominated by the nightside of the planet. As this is incompatible with the previous ephemeris constraints, and we expect the nightside atmosphere to be non-inverted, we believe this feature arises from cross-talk with stellar residuals and is not related to the planetary atmosphere.

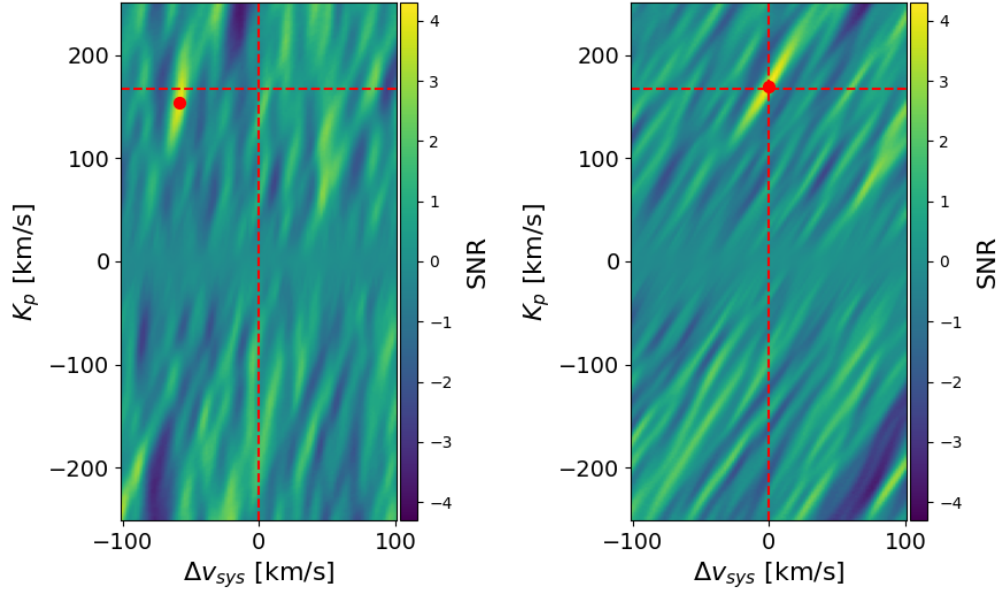


Figure 5.3: $K_p - v_{sys}$ diagrams for HD 143105 b

$K_p - v_{sys}$ diagrams for the [G. Hébrard et al. \(2016\)](#) ephemeris (left) and the revised ephemeris based on Figure 5.1 (right). The $Z = 0.3$, $C/O = 0.8$, non-inverted model was used in both cases. The [G. Hébrard et al. \(2016\)](#) ephemeris produces a detection of comparable strength, but with $\Delta v_{sys} = -60 \text{ km s}^{-1}$, well outside the expected range of offsets for a planet with a well-constrained ephemeris.

indicating that the observed planet flux is primarily arising from regions without a thermal inversion. Based on the reported semi-major axis and orbital period from [G. Hébrard et al. \(2016\)](#), the maximum value for K_p , corresponding to a 90 degree inclination, is $188 \pm 4 \text{ km s}^{-1}$, so the $K_p = 167 \text{ km s}^{-1}$ value from the non-inverted models is consistent with a detection of the non-transiting HD 143105 b. The ΔT_{conj} offset is consistent with the expected uncertainty from propagating the [G. Hébrard et al. \(2016\)](#) uncertainty in the orbital period to the observation epoch. While there are slight shifts in the location of the cross-correlation peak for different non-inverted models, these shifts are relatively small and consistent with the strong degeneracy between K_p and ΔT_{conj} .

We use the scale of the K_p and ΔT_{conj} offsets to inform the priors used for atmospheric retrieval. We update the nominal conjunction time to $T_{\text{conj}} = \text{JD } 2456531.2225$ and the nominal K_p to 167 km s^{-1} . We use these values for the remaining analysis.

5.3.1.2 Molecular detections

Plots of $K_p - \Delta T_{\text{conj}}$ for the the $[M/H] = 0.3$, $C/O = 0.8$ model, and individually for CO, H_2O , and $\text{Mg}+\text{Fe}$, are shown in Figure 5.4. We use the same $P - T$ parameters throughout, and base abundances on the $[M/H] = 0.3$, $C/O = 0.8$ model, which produced the strongest detection in Figure 5.1.

Only H_2O produces a significant detection in isolation. The CO model shows a weak peak consistent with the planet velocity from the H_2O model, but other features dominate the cross-correlation space. The refractory species do not produce any discernible peak near the expected planet velocity, and the cross-correlation space for these species is dominated by a feature in the stellar rest frame as a result of Fe and Mg lines in the stellar atmosphere. However, the all-molecule case is better detected than any individual molecules. This suggests that CO and the refractory species may be contributing some improvement to the overall detection, even if they are not independently detected in the absence of H_2O .

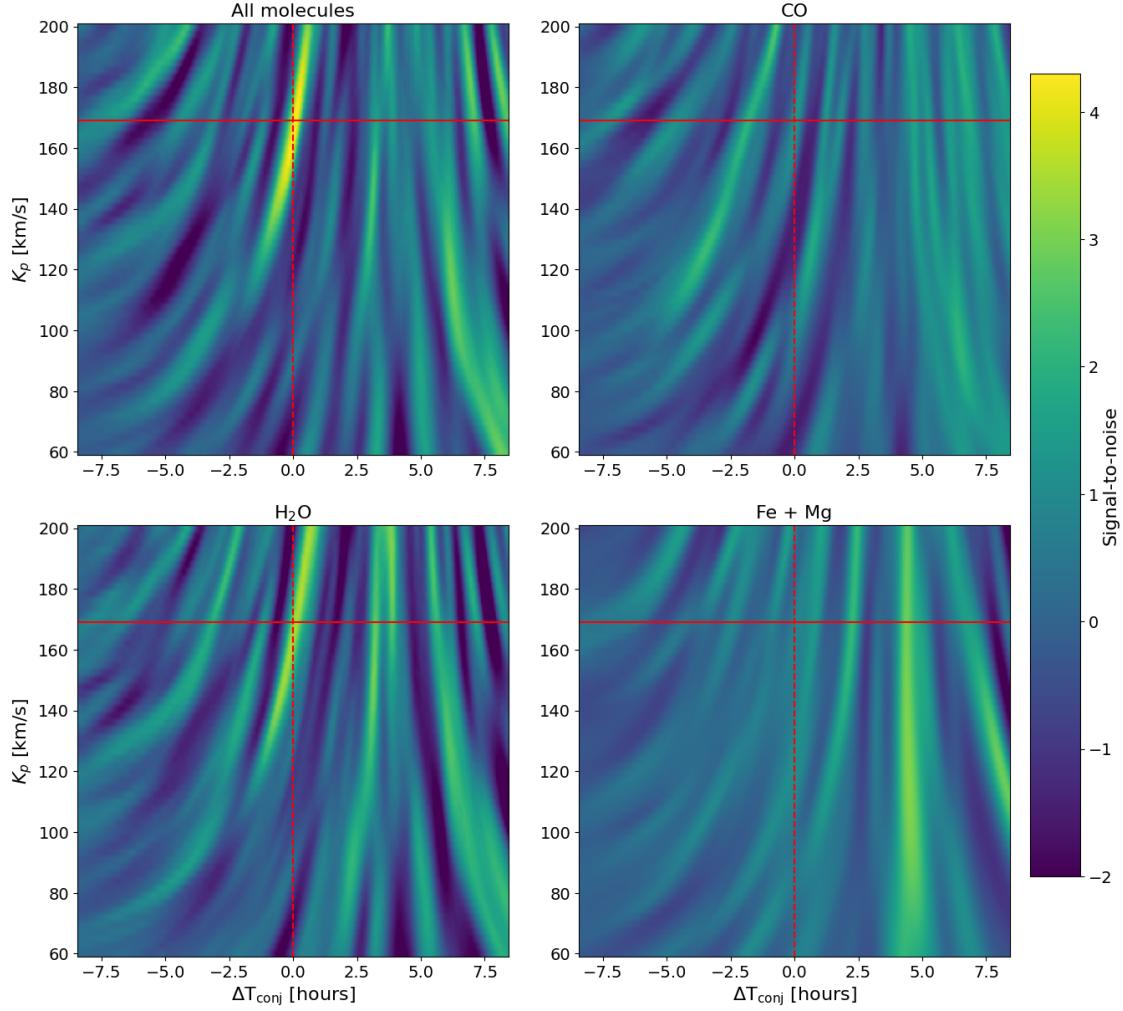


Figure 5.4: K_p vs conjunction time offset for different species

K_p vs conjunction time offset for models of all species, CO, H₂O, and Fe+Mg, with abundances based on the non-inverted $[M/H] = 0.3$, $C/O = 0.8$ model which produced the strongest detection in Figure 5.1. The conjunction time has been updated based on the measured offsets from Figure 5.1, so planetary features should appear at approximately $K_p = 167 \text{ km s}^{-1}$, $\Delta T_{\text{conj}} = 0$ hours. Only H₂O is confidently detected. A weak feature is present at the same location with the CO model, but does not dominate the $K_p - \Delta T_{\text{conj}}$ space and does not constitute an independent detection. The refractory species are not detected.

The absence of a significant CO detection appears to be at odds with the slight preference for high C/O from the initial cross-correlation analysis, shown in Figure 5.1. However, we note that the increase in detection strength over the low C/O models in Figure 5.1 is marginal, and estimating the noise level for the $K_p - \Delta T_{\text{conj}}$ diagram signal-to-noise by taking the off-peak cross-correlation variance has some associated uncertainty. Furthermore, the large number of H₂O lines in the K -band leads to a pseudocontinuum in the planet model which differs significantly from a blackbody, which may lead to worse detections when using single-molecule templates omitting H₂O (L. Finnerty et al., 2024). As a result, we rely on the Bayesian retrieval analysis to constrain the chemical composition, rather than the cross-correlation.

5.3.2 Retrieval Analysis

Priors, maximum-likelihood parameters, and retrieved medians with $\pm 34\%$ confidence intervals are presented in Table 5.2. Our free-chemistry approach does not directly fit for [C/H], [O/H], or C/O, but we use the retrieved posteriors to construct posteriors for these parameters, and report the corresponding values in Table 5.2 as derived parameters. We present the results of the retrieval omitting 6 principal components. The medians and confidence intervals for the 4 and 8 component cases did not significantly differ from the values reported in Table 5.2.

5.3.2.1 Kinematics

The retrieved K_p and ΔT_{conj} are slightly offset compared with the values from the cross-correlation analysis shown in Figure 5.1 and 5.4, but are consistent with the degeneracy between these parameters. The prior on ΔT_{conj} corresponds to a ± 1.2 hour change in the conjunction time, based on the apparent extent of the planet peak in 5.1, and ΔT_{conj} is well-constrained to within ~ 25 minutes.

Table 5.2: List of parameters, priors, and results for atmospheric retrievals

Name	Symbol	Prior	Max-L	Median
log infrared opacity [cm^2g^{-1}]	$\log \kappa$	Uniform(-3, 3)	-1.9	$-1.2^{+1.0}_{-0.9}$
log infrared/optical opacity	$\log \gamma$	Uniform(-3, 3)	-2.5	$-1.7^{+0.7}_{-0.7}$
Intrinsic temperature [K]	T_{int}	Uniform(50, 1000)	410	< 800
Equilibrium temperature [K]	T_{equ}	Uniform(800, 3000)	1100	1400^{+400}_{-300}
log surface gravity [cgs]	$\log g$	Uniform(2,4)	2.2	$3.0^{+0.6}_{-0.6}*$
Cloud opacity index	f_{SED}	Uniform(0,8)	7.9	$4.8^{+2.0}_{-2.1}*$
Cloud base opacity	$\log \kappa_0$	Uniform(0,3)	1.5	$1.5^{+1.0}_{-0.9}*$
Cloud base pressure	$\log P_{\text{cloud}}$	Uniform(-4,2)	-0.3	> -1.7
K_{p} offset [km s^{-1}]	ΔK_{p}	Uniform(-40, 40)	12.8	$17.9^{+10.6}_{-13.2}$
Conjunction time offset [hours]	ΔT_{conj}	Uniform(-1.2, 1.2)	0.27	$0.47^{+0.24}_{-0.28}$
Rotational velocity [km s^{-1}]	v_{rot}	Uniform(0, 15)	5.8	$7.4^{+3.1}_{-3.5}*$
log H_2O mass-mixing ratio	$\log \text{H}_2\text{O}$	Uniform(-12, -0.5)	-3.9	$-3.9^{+0.8}_{-0.5}$
log CO mass-mixing ratio	$\log \text{CO}$	Uniform(-12, -0.5)	-4.7	< -3.7
log Fe mass-mixing ratio	$\log \text{Fe}$	Uniform(-12,-1)	-4.1	$-6.5^{+3.3}_{-3.4}*$
log Mg mass-mixing ratio	$\log \text{Mg}$	Uniform(-12,-1)	-1.6	$-6.6^{+3.4}_{-3.2}*$
log $^{13}\text{CO}/^{12}\text{CO}$	$\log^{13}\text{CO}_{\text{rat}}$	Uniform(-8, -0.5)	-5.1	$-4.2^{+2.3}_{-2.2}*$
log H mass-mixing ratio	$\log \text{allH}$	Uniform(-0.4, -0.05)	-0.2	$-0.2^{+0.1}_{-0.1}*$
Scale factor	scale	LogNormal(0, 0.2)	0.4	$0.2^{+0.2}_{-0.2}$
Derived Parameters				
Carbon/oxygen ratio	C/O	-	0.1	< 0.2
Carbon abundance	[C/H]	-	-2.1	< -1.1
Oxygen abundance	[O/H]	-	-1.3	$-1.3^{+0.9}_{-0.5}$
Volatile abundance	[(C+O)/H]	-	-1.5	$-1.5^{+0.9}_{-0.5}$

Note. — Error bars correspond to the 68%/1 σ confidence interval. Limits are given at 95% confidence, omitting the secondary mode for the C/O ratio. A * indicates the marginalized posterior for a parameter spans the prior. In addition to these priors, we required that the atmospheric temperature stay below 6000 K at all pressure levels. The full corner plot is included in Section 5.6.

The retrieval provides a weak constraint on the planetary rotational velocity, $v \sin i = 7.4^{+3.1}_{-3.5} \text{ km s}^{-1}$. This is comparable to the spectrograph resolution, corresponding to a $\sim 30\%$ broadening of the planet lines compared with the instrumental profile alone. The expected $v \sin i$ for tidally-locked rotation is $\sim 3 \text{ km s}^{-1}$, leaving $\sim 5 \text{ km s}^{-1}$ of unexplained broadening. This could be consistent with apparent broadening from a broadly-distributed westward-flowing wind pattern, similar to that reported for other hot and ultra-hot Jupiters (e.g. [A. Pai Asnodkar et al., 2022](#); [S. Gandhi et al., 2023](#)). However, the poor quality of the $v \sin i$ constraint and uncertainties in the true LSF preclude a definitive physical interpretation of this value.

We used the same line-spread treatment as that developed in Finnerty et al. (subm.), and have the same systematic uncertainty in the overall LSF width at the $\sim 10\%$ level. While the retrieved broadening is somewhat larger than we believe could be explained solely by a systematic error in the LSF, we are cautious about making specific quantitative or physical interpretations of the retrieved broadening, particularly given the broad marginalized posterior for $v \sin i$. Higher-resolution observations, particularly from instruments with robust LSF calibration (as is planned for Keck/HISPEC, [D. Mawet et al. \(2019\)](#)), are necessary to quantitatively interpret line broadening in planetary atmospheres. A $v \sin i$ of 7 km s^{-1} would be $> 2\times$ the spectral resolution of Keck/HISPEC, and should be easily distinguishable.

5.3.2.2 Pressure-temperature profile and clouds

The retrieved $P - T$ profile and emission contribution function are shown in Figure 5.5. The retrieved $P - T$ profile is non-inverted and somewhat colder than expected based on the equilibrium temperature of 1940 K. This is consistent with previous KPIC retrievals ([L. Finnerty et al., 2023a, 2024](#), Finnerty et al., submitted). As with these previous results, the overall scaling factor applied to the planet model is > 1 , compensating for the lower temperature. Broader wavelength coverage that covers a significant change in the planet continuum

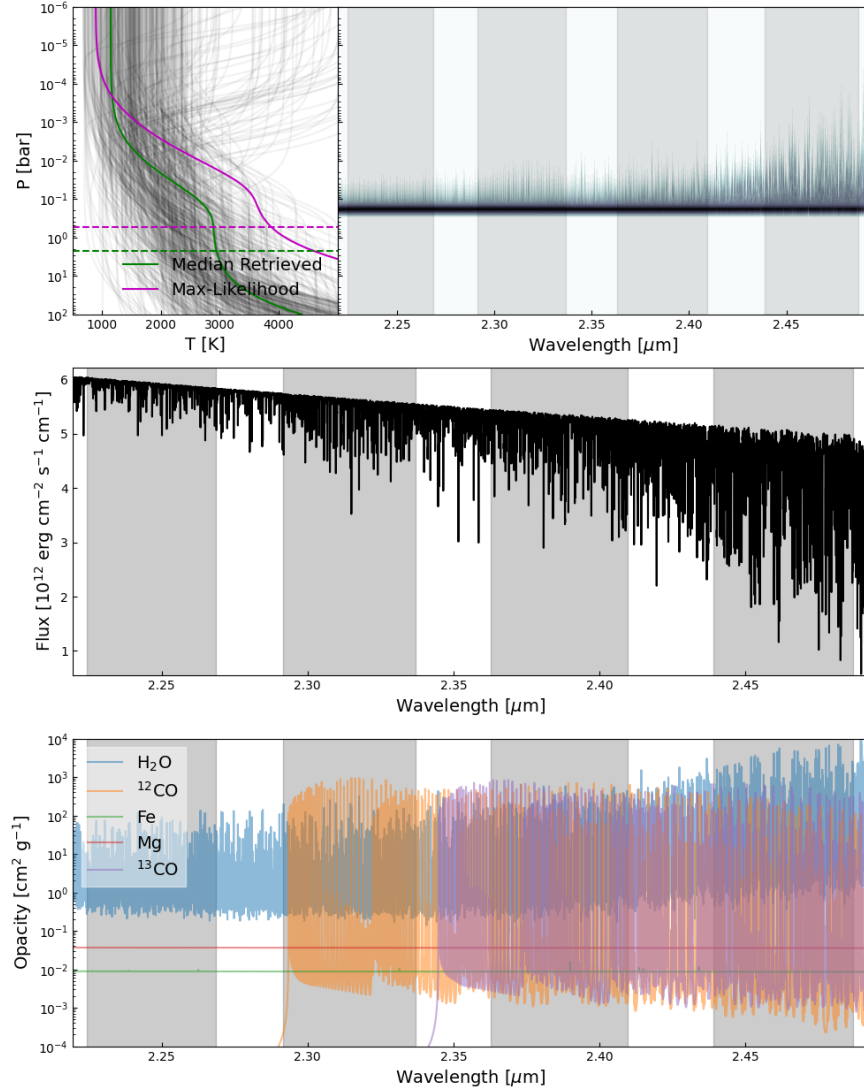


Figure 5.5: Retrieved spectrum of HD 143105 b

Retrieved $P - T$ profile (top left), max-likelihood emission contribution function (top right), max-likelihood spectrum (middle), and opacities (bottom). In the $P - T$ plot, the median retrieved profile is shown in green, and the max-likelihood profile in purple. The cloud pressures are indicated by horizontal dashed lines. The black lines are the $P - T$ profiles from 500 posterior draws. Observed orders are shaded. Emission arises significantly above the cloud pressure, where the $P - T$ profile begins to cool, indicating the atmosphere is clear at the pressures probed by these K -band observations. The maximum-likelihood spectrum shows weak CO features in addition to H_2O , and the non-detection of refractory species is consistent with the extremely low opacity of these species in comparison to CO and H_2O

flux (such as the region surrounding the blackbody peak) would break this degeneracy.

Of the cloud parameters, only the pressure is constrained. The retrieved pressure is quite deep, with the posterior peaking around 2.5 bar, well below the bottom of the emission contribution function shown in Figure 5.5. At these pressures, the final impact on the outgoing planet flux is negligible, so f_{SED} and $\kappa_{0,\text{cld}}$ are unconstrained, and the atmosphere over the pressure range probed by the *K*-band observations is effectively clear.

5.3.2.3 Chemical composition

Consistent with the cross-correlation analysis, the retrieval provides a bounded constraint only for the H_2O abundance, $\log \text{H}_2\text{O} = -3.9^{+0.8}_{-0.5}$. While the maximum likelihood value for the CO mass fraction is $\log \text{CO} = -4.7$, the retrieval does not provide a lower bound on the CO abundance. High CO abundances are strongly excluded ($\log \text{CO}_{\text{MMR}} < -3.7$ at 95% confidence). As a result, while the maximum-likelihood C/O ratio is 0.1, the median value from the retrieval is consistent with 0. This outcome could be explained by a CO abundance at or just below the detection limit of our observations. The CO isotopologue ratio is entirely unconstrained, consistent with the non-detection of the primary isotopologue.

The refractory species abundances are entirely unconstrained. While other *K*-band observations (e.g. S. Ramkumar et al., 2023) have been able to constrain Fe abundances in hot Jupiter atmospheres, we suspect that the lower spectral resolution of NIRSPEC is insufficient to make a detection based on the small number of accessible Fe and Mg lines (see Figure 5.5, bottom panel).

5.4 Discussion

5.4.1 Ephemeris revision and true mass

Our analysis indicates the inferior conjunction of HD 143105 b prior to our observation occurred approximately 3 hours before the expected time based on the [G. Hébrard et al. \(2016\)](#) ephemeris. This is substantially larger than their reported uncertainty in T_{conj} , but is well within the uncertainty resulting from propagating the orbital period uncertainty to the observed epoch. This suggests that uncertainty in the orbital period of HD 143105 b is the primary contributor to the observed change in the conjunction time. A reduction of 0.1 minutes in the orbital period would entirely explain the change in conjunction time, and is compatible with the 0.4 minute period uncertainty reported in [G. Hébrard et al. \(2016\)](#). While our limited phase coverage prevents accurate revision of the orbital period, the revised conjunction time from the retrieval, $T_{\text{conj}} = 2456531.242^{+0.010}_{-0.012}$, will enable more precise timing of follow-up observations for the next several years. This demonstrates that high-resolution cross-correlation techniques do not necessarily require precise ephemeris knowledge, as long as a sufficiently large velocity shift is observed for the planet signal to be clearly detected in the $K_p - \Delta T_{\text{conj}}$ space.

HD 143105 b is non-transiting, so the orbital inclination and true mass were not known *a priori*. As the measured value of K_p is the radial projection of the total orbital velocity, it can be used to calculate the inclination as follows:

$$K_p = K_{p,\text{max}} \sin i = \frac{2\pi a}{T} \times \sin i \quad (5.2)$$

The semi-major axis a is not directly observable, but can be replaced using Kepler's third law to give:

$$K_p = \sin i \times \left(\frac{2\pi GM_\star}{T} \right)^{1/3} \quad (5.3)$$

Using the stellar mass and orbital period from [G. Hébrard et al. \(2016\)](#), we obtain $K_{p,max} = 187.9^{+4.4}_{-4.7} \text{ km s}^{-1}$, with the uncertainty dominated by the uncertainty in the stellar mass. We can then solve for the inclination:

$$\sin i = K_p / K_{p,max} = 0.98 \pm 0.07 \quad (5.4)$$

Which gives $i = 78^{+12}_{-12}^\circ$, restricting to $\sin i < 1$. While $\sin i$ is strictly < 1 , we have neglected the degeneracy between K_p and $K_{p,max}$ when propagating uncertainties, so $\sin i > 1$ appears to be compatible with the uncertainties despite being non-physical. Larger stellar masses increase $K_{p,max}$, permitting higher values of K_p , and inclusion of $\sin i > 1$ in the statistical error therefore suggests the stellar mass may be somewhat underestimated. A more informative upper bound can be obtained from the lack of a reported transit, which requires $i < 80^\circ$ for the reported stellar parameters from [G. Hébrard et al. \(2016\)](#). We therefore adopt $i = 78^{+2}_{-12}^\circ$ as the inclination of the system. We can then determine the true planet mass by dividing the minimum mass obtained from radial velocity measurements by $\sin i$, yielding $M_{\text{true}} = 1.23 \pm 0.10 M_J$, including the $M \sin i$ uncertainty from [G. Hébrard et al. \(2016\)](#).

This result makes HD 143105 b one of a handful of non-transiting planets with a known true mass determined via high-resolution cross-correlation techniques ([M. Brogi et al., 2012, 2014](#); [J. L. Birkby et al., 2017](#); [G. Guilluy et al., 2019](#)). This is currently the only technique which can retrieve atmospheric properties for close-in, non-transiting planets.

5.4.2 Thermal structure

The retrieved posterior for the γ parameter, which determines whether the $P - T$ profile has a thermal inversion, strongly prefers a non-inverted structure, with a weak tail permitting inversions. This is potentially consistent with a weak, localized thermal inversion close to the substellar point marginally contributing to the observed flux. The apparently low C/O

ratio of HD 143105 b significantly complicates efforts to confirm any inversion. `easyCHEM` chemical equilibrium models predict H_2O should rapidly dissociate in the thermal inversion, leaving CO as the only species with significant K -band opacity in the inverted region of the atmosphere. If the CO abundance is very low, as the retrieval analysis prefers, this may lead to a featureless K -band spectrum from any inverted region, preventing detection of that region with HRCCS.

The relatively edge-on retrieved inclination of HD 143105 b suggests the lack of an inversion is not simply an issue of viewing geometry. For a low-inclination (e.g. $i < 60^\circ$), our post-conjunction observations would be much more sensitive to morning longitudes and high latitudes compared with evening/equatorial regions. This could significantly decrease the visibility of a localized inversion, which models predict would occur near equatorial latitudes and substellar or afternoon longitudes (A. Roth et al., 2024). However, our analysis prefers $i \sim 78^\circ$ for HD 143105 b, and should therefore still be sensitive to equatorial latitudes, making it difficult to miss a thermal inversion of significant extent as a result of viewing geometry alone.

Observationally, thermal inversions are routinely seen in planets with equilibrium temperatures > 2200 K (e.g. L. Finnerty et al., 2023a; S. Ramkumar et al., 2023, Finnerty et al., subm.), but not seen for temperatures < 1800 K (e.g. M. R. Line et al., 2021; S. Pelletier et al., 2021; L. Finnerty et al., 2024). Beyond these observations of HD 143105 b, relatively few objects have been characterized in the $1800 - 2200$ K range where this transition occurs. This makes HD 143105 b a potentially important object for understanding when and how thermal inversions form in exoplanet atmospheres.

For equilibrium temperatures > 2500 K, circulation models predict the presence of thermal inversion regardless of chemical composition (J. D. Lothringer et al., 2018a). At lower temperatures, inversions are strongly associated with the presence of metal oxide species, particularly TiO and VO (e.g. J. J. Fortney et al., 2008). The abundances of these species can be significantly impacted by cold trapping (I. Hubeny et al., 2003), which may lead to

localized inversions existing only where these species are in the gas phase. Nightside cold trapping of Ti has been reported in the UHJ WASP-76 b ($T_{\text{eq}} = 2200$ K [S. Pelletier et al., 2023](#)), but the details of this process are difficult to model, and the temperature at which thermal inversions form in typical hot Jupiters is unclear. Modeling by [A. Roth et al. \(2024\)](#) using 3D GCMs suggests the transition temperature to thermally-inverted $P - T$ profiles is ~ 1800 K in the presence of TiO/VO, while previous 1D modeling by [C. Baxter et al. \(2020\)](#) preferred an onset around 1700 K, but models omitting TiO/VO do not show inversions until substantially higher temperatures. These models predict that HD 143105 b, with an equilibrium temperature of ~ 1900 K, should have a dayside inversion only if significant quantities of TiO/VO are present.

Given the low retrieved metallicity of HD 143105 b, there may simply be insufficient TiO/VO in the atmosphere to produce a thermal inversion, especially if Ti is being cold-trapped on the nightside. TiO has substantially greater opacity in the H and J bands compared with K , which should allow the upcoming Keck/HISPEC instrument ([D. Mawet et al., 2019](#)) to either detect TiO or place a meaningful upper limit on its abundance. The revised ephemeris from this work will make it easier to obtain broad phase coverage in followup observations for phase-resolved retrievals. Such analysis will allow the partial inversion scenario to be definitively ruled out and will offer greater clarity into potential cold trapping impacting the TiO abundance.

5.4.3 C/O and metallicity

Derived posteriors for C/O, [C/H], [O/H], and [(C+O)/H] are shown in Figure 5.6. The oxygen abundance is sub-solar by ~ 1.3 dex at just over 1σ significance. The retrieval provides only an upper limit on the atmospheric mass fraction for CO, $\log CO < -3.7$ at 95% confidence. There is a weak, kinematically offset mode with very high CO and low H₂O abundance, which can be seen at the extreme right of the C/O posterior in Figure 5.6. As this mode is offset in both K_p and T_{conj} , we omit these points when estimating the upper

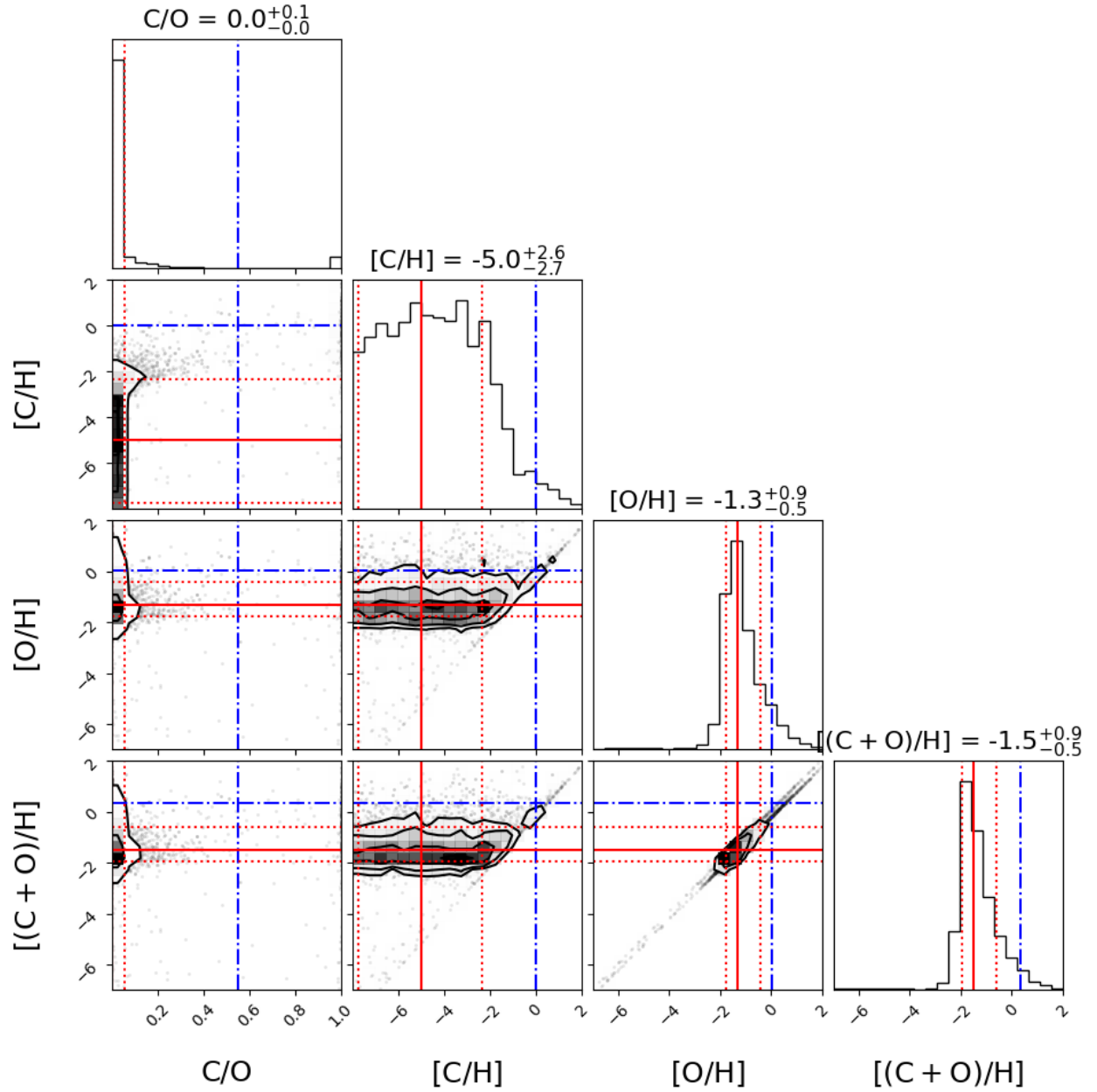


Figure 5.6: Corner plot showing the retrieved C/O, [C/H], [O/H], and [(C+O)/H] posteriors for HD 143105 b. Posteriors are computed from the retrieved abundances for H₂O and CO. Stellar values are indicated in dash-dot blue, while the retrieved median and $\pm 34\%$ confidence intervals are indicated in solid and dotted red, respectively. While the oxygen abundance is sub-solar/stellar at $\sim 1\sigma$, the carbon abundance is only an upper limit, leading to an upper limit on the C/O ratio. These results are consistent with a metal- and carbon-poor atmosphere for HD 143105 b.

limit on the C/O ratio. This leads to an upper limit on the C/O ratio, $C/O < 0.2$ at 95% confidence, while the maximum-likelihood value is $C/O = 0.1$ and the retrieved median is consistent with a nearly carbon-free atmosphere. The Bayes factor comparing the maximum-likelihood model with the same model omitting CO is only 2.9, consistent with a marginal preference for CO. This suggests the atmospheric CO abundance may be slightly below our detection threshold. Future observations with Keck/HISPEC (D. Mawet et al., 2019) will offer significant improvements in both instrument throughput and spectral resolution, which may enable precise constraints on the CO abundance and C/O ratio even in low-metallicity atmospheres. The continuous wavelength coverage of HISPEC may be particularly valuable in this case, as HISPEC observations will capture the full R and P branches associated with the $2.3\mu\text{m}$ CO bandhead, greatly increasing the number of observed CO lines compared with KPIC.

The low-C/O ratio, low-metallicity atmospheric composition our retrievals prefer for HD 143105 b has not previously been observed in an exoplanet atmosphere, and contradicts model predictions that these parameters should be inversely correlated (N. Espinoza et al., 2017; A. J. Cridland et al., 2019; N. Khorshid et al., 2022). In these models, oxygen enrichment usually arises from late planetesimal accretion, which should also increase the atmospheric metallicity. Low metallicity and low C/O ratio would require the accretion of significant quantities of oxygen-rich gas, but protoplanetary disk gas is generally carbon-rich as a result of condensation (K. I. Öberg et al., 2011). Y. Chachan et al. (2023) finds that the region just beyond the H_2O snow line has substantially enriched H_2O ice relative to the rest of the disk, which could lead to an oxygen-rich atmosphere, although we would still expect a stellar or super-stellar metallicity in this scenario.

HRCCS observations have difficulty measuring absolute abundances due to the loss of continuum information during the data processing. As a result, we cannot conclusively rule out a stellar abundance of oxygen, and the C/H posterior similarly has a tail that extends to values compatible with the solar carbon abundance (see Figure 5.6). This alone could

resolve the anomalous apparent composition of HD 143105 b. Furthermore, our estimate of the atmospheric metallicity is based only on abundances of volatile species. Inferring bulk metallicity from these species alone can be misleading due to either atmospheric effects, including oxygen bonding to refractory species (K. Lodders, 2003), and cold trapping in the planetary atmosphere (D. S. Spiegel et al., 2009; S. Pelletier et al., 2023), or due to formation effects, including pebble drift and volatile trapping, which can alter the intrinsic refractory/volatile ratio (R. A. Booth et al., 2017; N. F. W. Ligterink et al., 2024; J. D. Lothringer et al., 2021; Y. Chachan et al., 2023). Obtaining refractory species abundances can potentially resolve several of these scenarios by constraining the solid accretion history of a planet (J. D. Lothringer et al., 2021; Y. Chachan et al., 2023), but will require additional observations in the case of HD 143105 b.

This unusual composition for HD 143105 b is consistent with the emerging picture of significant chemical diversity in the hot Jupiter population (E. M. R. Kempton & H. A. Knutson, 2024; L. S. Wiser et al., 2024). Reported metallicities for various exoplanets range from very high (e.g. J. L. Bean et al., 2023) to moderately super-solar (e.g. L. Finnerty et al., 2024; G. Fu et al., 2024) to sub-solar (e.g. M. R. Line et al., 2021; P. C. August et al., 2023; M. Weiner Mansfield et al., 2024). Similarly, reported C/O ratios range from substantially sub-stellar (e.g. L. Finnerty et al., 2024; G. Fu et al., 2024) to significantly carbon-enriched (Finnerty et al. submitted), although in the case of ultra-hot Jupiters constraining the C/O ratio is complicated by the impact of molecular dissociation (M. Brogi et al., 2023; S. Ramkumar et al., 2023; S. Gandhi et al., 2024). This diversity suggests a variety of formation and evolutionary processes shape the hot Jupiter population, motivating further observations and improvements in retrieval techniques to incorporate a broader range of data, such as joint optical/infrared and high/low resolution retrievals.

5.5 Summary and Conclusions

We detected atmospheric H₂O absorption from the non-transiting hot Jupiter HD 143105 b. Cross-correlation analysis indicates the conjunction time is 2.5 hours earlier than the published ephemeris, likely due to the accumulation of uncertainty in the orbital period over nearly a decade. The planet radial velocity semiamplitude is $K_p = 185^{+11}_{-13} \text{ km s}^{-1}$, giving an orbital inclination of $78^{+2}_{-12}^\circ$ and a true planet mass of $1.23 \pm 0.10 \text{ M}_J$, with an upper inclination limit imposed by the absence of a transit detection. This is the first non-transiting hot Jupiter detected with KPIC and the first atmospheric detection of HD 143105 b.

While the equilibrium temperature of HD 143105 b is in the transition regime between non-inverted and inverted atmospheres, our analysis strongly prefers a non-inverted $P - T$ profile. This is unlikely to be solely the result of viewing geometry given the high inclination of HD 143105 b, suggesting that the lack of an inversion may be a result of low bulk metallicity leading to low abundances of inversion-causing species such as TiO and VO. Additional observations with broader wavelength coverage would greatly improve sensitivity to these species and directly test this explanation. HD 143105 b is potentially a key benchmark object for understanding the transition between inverted and non-inverted exoplanet atmospheres.

Retrieval analysis provides a bounded constraint on the H₂O mass-mixing ratio $\log \text{H}_2\text{O} = -3.9^{+0.8}_{-0.5}$ and a 95% upper limit on the CO mass-mixing ratio $\log \text{CO} < -3.7$. This places an upper limit on the C/O ratio $\text{C/O} < 0.2$ at 95% confidence, and suggests a sub-solar atmospheric metallicity. This combination of low metallicity and low C/O ratio is unusual in exoplanet atmospheres and has not been seen previously in high-resolution retrievals, but is consistent with other findings suggesting a chemically diverse hot Jupiter population. Future observations with Keck/HISPEC will have wider wavelength coverage and improved spectral resolution, which may be sufficient to detect CO in HD 143105 and establish a bounded constraint on the C/O ratio. Such observations may also provide constraints on refractory species such as iron or magnesium, which may clarify the formation history of HD 143105 b.

through constraining the refractory-to-volatile ratio.

Finally, observations with higher spectral resolution and/or wider phase coverage may enable detection of phase-dependent velocity shifts relative to a Keplerian orbit. Such shifts would offer insight into atmospheric circulation patterns, which are particularly interesting for non-transiting planets such as HD 143105 b, as the observed emission probes higher latitudes compared with transiting planets. In the future, high-resolution spectroscopy of non-transiting planets may be a unique tool for probing atmospheric circulation patterns in polar regions of hot giant planets.

5.6 Corner Plots

Figure 5.7 presents the full corner plot from the retrieval.

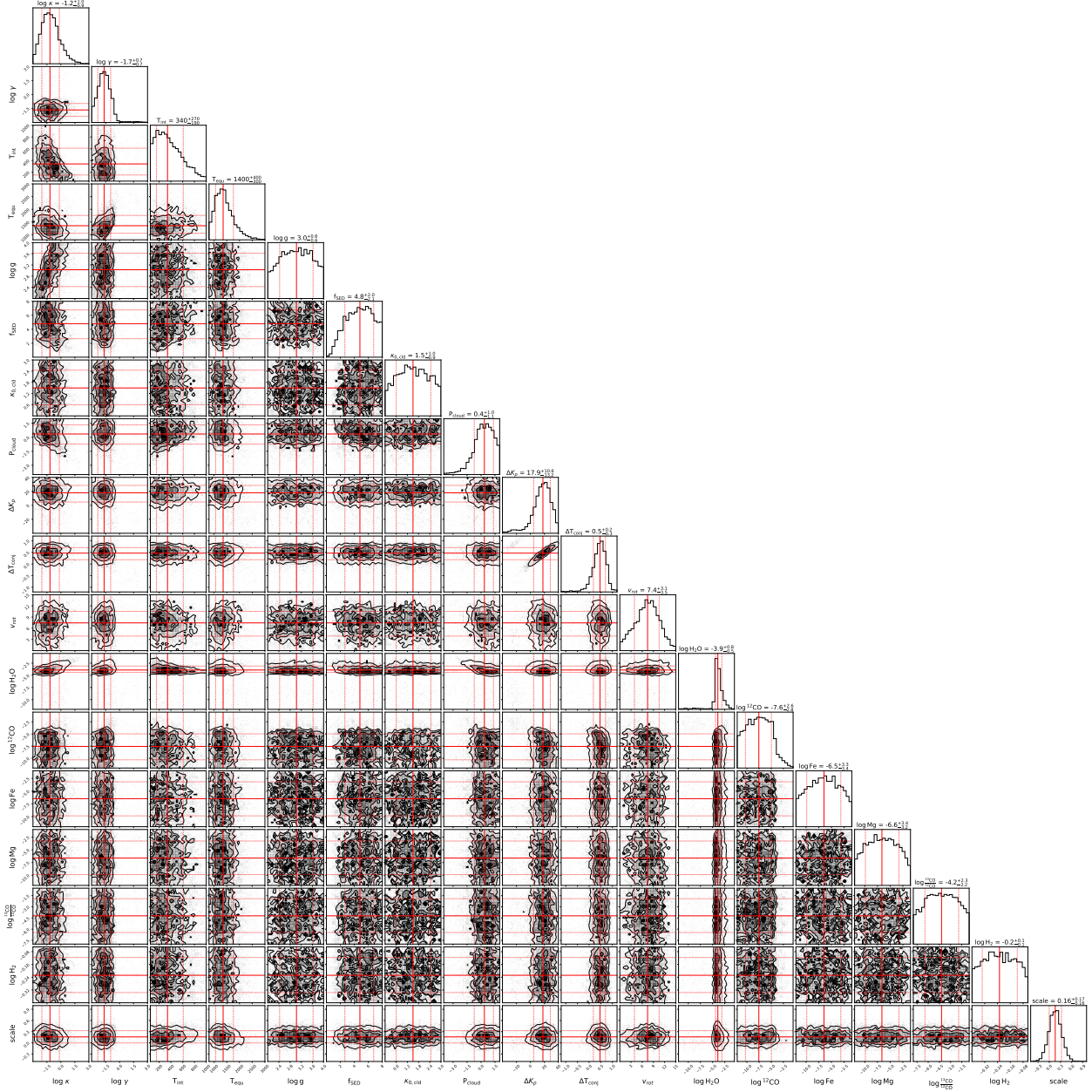


Figure 5.7: Full corner plot for the 6-component retrieval.

CHAPTER 6

Water dissociation and rotational broadening in the atmosphere of KELT-20 b from high-resolution spectroscopy

A version of this chapter has been accepted in the *Astronomical Journal* (Finnerty *et al.* 2025b)

Abstract

We present atmospheric retrievals from Keck/KPIC phase II observations of the ultra-hot Jupiter KELT-20/MASCARA-2 b. Previous free retrievals of molecular abundances for ultra-hot Jupiters have been impacted by significant model biases due to variations in vertical abundance profiles, which we address by including molecular dissociation into our retrieval framework as an additional free parameter. We measure the abundance of CO ($\log \text{CO}_{\text{MMR}} = -2.5^{+0.6}_{-0.5}$) and obtain a lower limit on the abundance of H₂O ($\log \text{H}_2\text{O}_{\text{MMR}} = -1.5^{+0.8}_{-1.0}$, > -3.0 at 95% confidence) in the atmosphere of KELT-20 b. These abundances yield an atmospheric C/O = $0.1^{+0.4}_{-0.1}$ (C/O < 0.9 at 95% confidence) and suggest a metallicity approximately solar to 10× solar. H₂O is dissociated at pressures below $\log P_{\text{H}_2\text{O}} = -1.2^{+0.5}_{-0.7}$ bar, roughly consistent with predictions from chemical equilibrium models, and suggesting that the retrieved composition is not a result of assumptions about the vertical mixing profiles. We also constrain the rotational velocity of KELT-20 b to $v \sin i = 7.5 \pm 0.7 \text{ km s}^{-1}$, suggesting the presence of a jet comparable to the sound speed in the direction of the

planet’s rotation, assuming the actual rotation of the planet is tidally locked.

6.1 Introduction

Ultra-hot Jupiters (UHJs), hot Jupiters with equilibrium temperatures in excess of 2000 K, are an ideal exoplanet population for atmospheric characterization studies. The extreme conditions of these planets and complicated dynamical history suggested by the close-in, misaligned orbits of many UHJs (S. Naoz et al., 2011; M. Rice et al., 2022) makes these planets compelling targets for efforts to improve our observational understanding of atmospheric circulation and planet formation.

However, molecular abundance estimation for UHJs is complicated by the impacts of thermal dissociation, vertical mixing, cold trapping, and photochemistry. While CO only dissociates at very high temperatures and low pressures, typical UHJ conditions are expected to dissociate H₂O at pressures deeper than ~ 1 mbar under chemical equilibrium. If abundances are vertically fixed in a retrieval, the only parameter which can reduce the strength of H₂O features to match the effects of dissociation is the H₂O abundance itself. As a result, retrievals which assume fixed abundances with altitude will be biased towards high-C/O, high-metallicity compositions (e.g. M. Brogi et al., 2023; S. Ramkumar et al., 2023).

While assuming chemical equilibrium abundance profiles can resolve this issue (M. Brogi et al., 2023; S. Ramkumar et al., 2023), local chemical equilibrium based on an assumed $P - T$ profile is a potentially restrictive assumption. Internal heating and the resulting vertical mixing can lead to severe depletion of species expected from models which use only the local temperature to calculate equilibrium abundances (V. Singh et al., 2024; L. Welbanks et al., 2024). Cold trapping has similarly been found to cause significant depletion of condensable species on planets with strong day/night temperature contrasts, which is not reproducible with 1D local chemical equilibrium models (S. Pelletier et al., 2023; H. J. Hoeijmakers et al., 2024). As a result of these effects, local chemical equilibrium retrievals

Table 6.1: Stellar and planetary properties for the KELT-20 system

Property	Value	Ref.
RA	19:38:38.7	Gaia Collaboration (2020)
Dec	+31:13:09	Gaia Collaboration (2020)
Sp. Type	A2V	M. B. Lund et al. (2017)
K_{mag}	7.415 ± 0.017	R. M. Cutri et al. (2003)
Mass	$1.76^{+0.14}_{-0.19} M_{\odot}$	M. B. Lund et al. (2017)
Radius	$1.60 \pm 0.06 R_{\odot}$	G. J. J. Talens et al. (2018)
T_{eff}	8730^{+250}_{-260} K	M. B. Lund et al. (2017)
$\log g$	$4.29^{+0.017}_{-0.020}$	M. B. Lund et al. (2017)
$v \sin i$	$114 \pm 3 \text{ km s}^{-1}$	G. J. J. Talens et al. (2018)
v_{rad}	$-23.3 \pm 0.3 \text{ km s}^{-1}$	M. B. Lund et al. (2017)
[Fe/H]	-0.02 ± 0.07	G. J. J. Talens et al. (2018)
KELT-20 b		
Period [day]	$3.4741012 \pm 2 \times 10^{-7}$	ExoFOP (2019)
t_{transit} [JD]	$2460337.98638 \pm 5 \times 10^{-5}$	ExoFOP (2019)
a	$0.057 \pm 0.006 \text{ AU}$	G. J. J. Talens et al. (2018)
i	$86.4^{+0.5}_{-0.4}$	G. J. J. Talens et al. (2018)
K_{p}	$176.7 \pm 0.6 \text{ km s}^{-1}$	F. Yan et al. (2022)
Mass	$< 3.372 M_J$	M. B. Lund et al. (2017)
Radius	$1.83 \pm 0.07 R_J$	G. J. J. Talens et al. (2018)
T_{eq}	$2262 \pm 73 \text{ K}$	G. J. J. Talens et al. (2018)
C/O	< 0.9	This work
[C/H]	$0.1^{+0.6}_{-0.5}$	This work
[O/H]	$1.1 \pm 0.8 (> -0.1)$	This work
[(C + O)/H]	$1.0 \pm 0.7 (> -0.5)$	This work
$v \sin i$	$7.5 \pm 0.7 \text{ km s}^{-1}$	This work

may be pushed to inaccurate abundances in order to minimize the impact of species present under the local chemical equilibrium assumption but absent in the real atmosphere. Free retrievals can adjust to the presence or absence of species based on these effects without biasing the abundances of other species.

UHJs around A-type stars are also exposed to extreme UV fluxes, which may drive photochemical processes in the upper atmosphere which will not be captured by a thermochemical equilibrium model. Photochemically produced species have been detected in *JWST* observations of hot/warm Jupiters (S.-M. Tsai et al., 2023; A. Dyrek et al., 2024), providing an observational example of the limits of an equilibrium assumption. While there are publicly available tools to estimate abundances which include photochemistry effects (S.-M. Tsai et al., 2021), these tools are too slow to use for retrievals, and the reaction networks used in these models need to be observationally verified. This creates a need for free retrieval frameworks which can account for vertically-varying molecular abundances.

UHJs also provide an opportunity to directly test Global Circulation Model (GCM) predictions in extreme conditions, provided the planetary ephemeris and spectrograph line-spread function (LSF) are sufficiently well characterized to robustly measure velocity offsets and line broadening. Under UHJ conditions, GCMs predict supersonic day-to-night winds up to 10 km s^{-1} (J. P. Wardenier et al., 2021; T. D. Komacek et al., 2022; H. Beltz et al., 2022). While medium/low resolution spectroscopy cannot measure these supersonic wind speeds directly, high-resolution observations have been able to provide some wind measurements consistent with these models (e.g. A. Pai Asnodkar et al., 2022; S. Gandhi et al., 2023). For tidally locked planets such as UHJs, constraining the rotational velocity in emission can provide an independent measurement of the equatorial jet speed to complement velocity shift measurements from high-resolution spectroscopy obtained during transit (F. Lesjak et al., 2023; L. Finnerty et al., 2024; L. Bazinet et al., 2024). Interpreting shifts measured during transit as wind speeds has been difficult due to the potential for chemical differences between leading and trailing limbs (J. P. Wardenier et al., 2021; A. B. Savel et al., 2022). Combining

measurements of jet velocities from multiple observing geometries is therefore critical to understanding atmospheric circulation for hot Jupiters and provides a unique observational test of GCMs in an extreme regime (L. Pino et al., 2022; L. van Sluijs et al., 2023).

We observed KELT-20 b (also known as MASCARA-2 b) as part of our ongoing Keck/KPIC hot Jupiter survey (L. Finnerty et al., 2023a,b, 2024, 2025a). Properties of the system are summarized in Table 6.1. First discovered in 2017 (M. B. Lund et al., 2017), KELT-20 b is in many ways a typical UHJ, with an equilibrium temperature of 2260 K, an inflated radius ($1.83 \pm 0.07 R_J$ G. J. J. Talens et al., 2018), and a rapidly rotating ($v \sin i = 114 \text{ km s}^{-1}$ G. J. J. Talens et al., 2018) early-type host star. However, compared with other UHJs, KELT-20 b has a longer orbital period of 3.5 days, compared with the < 2 day periods of e.g. WASP-33 b, KELT-9 b, MASCARA 1b, and TOI-1518 b. Spin-orbit misalignment measurements using the Rossiter-McLaughlin Effect have also found that the orbital plane KELT-20 b is well-aligned with the host star’s rotation (G. J. J. Talens et al., 2018), in contrast with the other UHJs listed previously (A. Collier Cameron et al., 2010; B. S. Gaudi et al., 2017; G. J. J. Talens et al., 2017; S. H. C. Cabot et al., 2021). This suggests KELT-20 b could have formed and/or migrated via a different mechanism than other UHJs, perhaps without the late high-eccentricity migration that is believed to be necessary to produce retrograde UHJs such as WASP-33 b and KELT-9 b (S. Naoz et al., 2011).

KELT-20 b has been extensively studied at optical wavelengths in both emission and transmission (see M. C. Johnson et al., 2023; S. Petz et al., 2024, and references therein), revealing a variety of transition metal species but no evidence for TiO, VO, or CaH in the optical. In the infrared, strong H₂O and CO emission features were reported from low-resolution *HST* and *Spitzer* spectroscopy (G. Fu et al., 2022). Subsequently, D. Kasper et al. (2023) reported the results of a joint retrieval of these data and MAROON-X optical emission data which suggested a super-solar metallicity and C/O ratio. In this paper, we present retrievals based on Keck/KPIC *K*-band emission observations (2.1–2.48 μm), providing the first high-spectral-resolution detections of CO and H₂O in KELT-20 b and a constraint on

the atmospheric C/O ratio from these gases.

We discuss the KPIC observations of KELT-20 b, data reduction procedure, and retrieval setup in Section 6.2. Retrieval results are presented in Section 6.3. We discuss these results and the implications for the formation history and atmospheric dynamics of KELT-20 b in Section 6.4, and summarize our results in Section 6.5.

6.2 Observations, Data Reduction, and Retrieval

6.2.1 Observations

The KELT-20 system was observed with Keck II/KPIC phase II (I. S. McLean et al., 1998; E. C. Martin et al., 2018; R. A. López et al., 2020; J.-R. Delorme et al., 2021; D. Echeverri et al., 2022; N. Jovanovic et al., 2025b) on UT 30 July 2023 from 5:31 to 12:06 UTC, totaling just over 6.5 hours. The observations began shortly after the end of the KELT-20 b secondary eclipse, and covered a phase range of 0.539–0.617. During this time, the nominal star-frame planet velocity went from -43.2 km s^{-1} to -119.5 km s^{-1} . The exposure time was 300 seconds per frame, which kept the velocity shift within a single exposure to $< 1.1 \text{ km s}^{-1}$, substantially smaller than the $\sim 9 \text{ km s}^{-1}$ resolution of NIRSPEC (R. A. López et al., 2020), in order to minimize smearing of the planet signal within a single exposure. Conditions and instrument performance were typical for KPIC phase II, with a top-of-atmosphere throughput of 3-4% throughout the observing sequence. The reduced/extracted spectra from each exposure had a signal-to-noise ratio (SNR) of approximately 120-140 per pixel in the orders used for retrieval.

KELT-20 b was observed using only a single KPIC science fiber, rather than nodding between fibers as in L. Finnerty et al. (2023a, 2024). This reduced overheads associated with switching fibers and allowed all observations to be taken using the highest-throughput fiber to maximize total signal-to-noise. This approach also simplified handling of the KPIC line-spread function (LSF), which is slightly different for each fiber. KPIC has minimal

background in the K -band, which is sufficiently removed using dark frames taken before/after observing to not impact retrievals.

6.2.2 Data Reduction

A late-type star (HIP 95771, M0.5IIIb) was observed to provide wavelength calibration using the KPIC Data Reduction Pipeline (DRP)¹. As with previous KPIC K -band observations, three orders (37–39, $1.94\text{--}2.09\mu\text{m}$) are severely impacted by telluric CO_2 and are omitted from the analysis. While previous KPIC observations struggled with wavelength calibration in orders 35 and 36 due to an absence of strong stellar or telluric lines, in this case the wavelength calibrator was observed at a median airmass of 1.32, leading to somewhat deeper telluric lines and a wavelength solution which appears to be reliable in all orders. We therefore include orders 31–36 in the analysis. The improved calibration in the bluer orders may be a result of iterative improvements in the KPIC wavelength calibration from using previous wavelength solutions as the starting point for optimizing a new wavelength solution.

The KPIC DRP was used to produce background and bad pixel frames for the 300s exposure time. Ten background frames were obtained in both the afternoon prior to observing and the morning after observing, enabling a high-quality background subtraction even without nodding between the KPIC fibers.

The flux extraction differed significantly from the default KPIC DRP in order to accurately handle the non-Gaussian and variable KPIC LSF. As part of the trace finding step, we also fit the trace profile in the spatial (detector y) direction using a Gaussian-Hermite model, similar to the approach described by [J. A. Holtzman et al. \(2018\)](#). This model multiplies a Gaussian profile of variable width by the Hermite polynomials of order ≤ 4 , with the amplitude of each polynomial as a free parameter. This model allow fitting of both non-Gaussian wings and asymmetries in the line profile. The raw fit parameter values are then smoothed

¹https://github.com/kpicteam/kpic_pipeline/

by a 13-pixel Gaussian kernel to reduce noise and ensure variation in the LSF matches the spatial scales for such variation found in [R. A. López et al. \(2020\)](#).

This spatial profile is then used to compute weights for optimal extraction ([K. Horne, 1986](#)) and extract 1D spectra. To estimate the KPIC LSF, we multiply the overall width parameter by a factor of 1.14 in order to match a known asymmetry induced by the NIRSPEC optics ([L. Finnerty et al., 2022](#)). These scaled profiles are then convolved with the forward-model of the planet atmosphere during the retrieval to replicate the instrumental broadening of NIRSPEC.

6.2.3 Atmospheric Retrieval

Our atmospheric retrieval framework has previously been described in [L. Finnerty et al. \(2023a, 2024, 2025a\)](#). We provide a brief summary here, with an emphasis on new features. The full list of parameters and priors is included in Table 6.2. We use a PHOENIX ([T. O. Husser et al., 2013](#)) model for KELT-20 A with $T_{\text{eff}} = 9000$ K, $\log g = 4.5$, and solar metallicity, roughly matching the stellar parameters reported in [M. B. Lund et al. \(2017\)](#). The stellar model is rotationally broadened using the wavelength-dependent technique described in [A. Carvalho & C. M. Johns-Krull \(2023\)](#) to 114 km s^{-1} ([G. J. J. Talens et al., 2018](#)).

We use `petitRADTRANS3` ([P. Mollière et al., 2019, 2020](#); [E. Nasedkin et al., 2024](#)) to compute model planet spectra. The mass of KELT-20 b is poorly constrained, with [M. B. Lund et al. \(2017\)](#) placing a 3σ upper limit of $M_{\text{pl}} < 3.5M_J$, which motivates our inclusion of $\log g$ as a free parameter in the atmospheric retrieval. As in our previous works, we use 80 log-uniform spaced pressure layers from 10^2 to 10^{-6} bar. Following [L. Finnerty et al. \(2024\)](#), we use the pressure-temperature ($P - T$) profile model from [T. Guillot \(2010\)](#). While the intrinsic temperature parameter T_{int} has been fixed in other high-resolution studies (e.g. [N. P. Gibson et al., 2022](#); [S. Ramkumar et al., 2023](#)), we include it as a free parameter in our retrievals. T_{int} determines the lower-atmosphere behavior of the $P - T$ profile, below the thermal inversion and the bulk of the emission contribution function, but we find that

its inclusion is important to breaking degeneracies between abundances and dissociation pressures.

For molecular abundances, we use a free-retrieval approach which allows for variations in vertical abundance profiles for certain species. In addition to the abundance, our model can optionally fit a dissociation pressure and a formation pressure. At pressures lower than the dissociation pressure, the abundance decays as a power law, $(P/P_0)^4$. Similarly, at pressures greater than the formation pressure, the abundance decays as $(P/P_0)^{-4}$. Each of these parameters is optional, and different parameterizations can be used for different species, including freely fitting the power law index. The default power law index of 4 was an arbitrary choice made to roughly match the profiles seen in **easyCHEM** (P. Mollière et al., 2017; E. Lei & P. Mollière, 2024) results for a nominal KELT-20 b $P - T$ profile.

Based on chemical equilibrium models, we allow CO to dissociate only at low pressures, extending below the top-of-atmosphere cutoff pressure to allow for the no-dissociation scenario. For H₂O, we expect dissociation to occur near the thermal inversion, so we fit for the dissociation pressure. We expect OH to be produced around the same pressure as H₂O dissociation, so we fit for the OH formation pressure, and we expect OH will itself be dissociated at high altitudes, so we also fit for the OH dissociation pressure. C₂H₂, if present, is expected to dissociate at intermediate pressures, so we fit for the dissociation pressure. We do not fit the power-law index for any species, after initial tests found this parameter was unconstrained in retrievals.

We also fit for the overall hydrogen mass fraction and the H₂ dissociation pressure. As these species have only weak spectral features in the region probed, our sensitivity to these parameters is primarily indirect via collisionally-induced-absorption (CIA) opacity and the impact on the mean molecular weight. The remaining mass of the atmosphere is assumed to be helium.

The opacity tables used for H₂O, OH, ¹²CO, and ¹³CO were previously described in L. Finnerty et al. (2023a). For H₂O we used the (O. L. Polyansky et al., 2018) partition function

and HITEMP 2010 linelist (L. S. Rothman et al., 2010). For both CO isotopologues we used the HITEMP 2019 lists (I. E. Gordon et al., 2022) and the G. Li et al. (2015) partition function. For OH we used the partition function from M. Yousefi et al. (2018) and HITEMP 2020 linelist (I. E. Gordon et al., 2022). Opacities were generated via ExoCross (S. N. Yurchenko et al., 2018) following instructions in the `petitRADTRANS` documentation. For C₂H₂, we converted the aCeTeY (K. L. Chubb et al., 2020) opacity table available from DACE (S. L. Grimm et al., 2021) to the `petitRADTRANS` format. As clouds are not expected under dayside UHJ conditions, we do not include any cloud species, but retain the scattering mode in `petitRADTRANS`. See L. Finnerty et al. (2023a) for a more detailed discussion of this choice in UHJs. A test retrieval including a grey cloud deck preferred a cloud-top pressure greater than the base of the emission contribution function, indicating a preference for a clear atmosphere. H⁻ is similarly not included, following L. Finnerty et al. (2023a), who found that H⁻ introduces a uniform reduction in the line strengths for small bandpass observations. In this scenario, the impact of H⁻ becomes degenerate with changes in the scale factor and $P - T$ profile. This is not the case for analyses covering a large bandpass, such as joint optical+IR retrievals, which will likely need to include and constrain H⁻ explicitly.

Our retrieval pipeline uses principal component analysis (PCA) to remove time-varying instrumental fringing and telluric effects which would otherwise dominate over the planet signal, as previously described in L. Finnerty et al. (2024). The number of principal components to drop is difficult to choose in a robustly motivated way (C. J. Cheverall et al., 2023). We therefore ran retrievals omitting 4, 6, 8 and 12 PCs in order to assess the impact of this choice on the retrieval results.

HRCCS retrievals also use an overall scaling parameter applied to the planet spectrum M. Brogi & M. R. Line (2019). While L. Finnerty et al. (2023a, 2024) used a linear scale factor, for this work we follow L. Finnerty et al. (2025a) and switch to a truncated log-normal scale factor with a mean of 0 (corresponding to a $1\times$ multiplication of the planet spectrum) and standard deviation of 0.1. This distribution is truncated at 7.5 standard deviations from the

mean for numeric stability. This is more in line with other analyses, for which a logarithmic prior for the scale factor (e.g. [M. R. Line et al., 2021](#)) is common. Using a normal prior, rather than uniform, may help to break the temperature/scale factor degeneracy discussed in [M. Brogi et al. \(2023\)](#); [L. Finnerty et al. \(2024\)](#).

The nested sampling for the retrieval was performed using `MultiNest` ([F. Feroz & M. P. Hobson, 2008](#); [F. Feroz et al., 2009](#); [J. Buchner et al., 2014](#); [F. Feroz et al., 2019](#)) with 800 live points and a $\Delta \log z = 0.01$ stopping criteria. We continue to use the [M. Brogi & M. R. Line \(2019\)](#) $\log L$ function as in [L. Finnerty et al. \(2023a, 2024\)](#). Compared with previous retrievals using `dynesty`, `MultiNest` retrievals run $\sim 10\times$ faster, although the wider wavelength coverage and strict convergence used in this analysis still requires approximately one week of computing time with 16 Intel E5-2670 CPU cores.

6.3 Results

Results from the 6-component retrieval are presented in [Table 6.2](#) and [Figure 6.1](#). Parameters marked with a * had poorly constrained posteriors, for these parameters 95% confidence limits are provided if available. $K_p - \Delta v_{\text{sys}}$ plots for each species are presented in [Figure 6.3](#). Full corner plots for all four retrievals are included in [Appendix 6.6](#).

6.3.1 Velocity and winds

The ΔK_p , Δv_{sys} , and v_{rot} parameters are all well-constrained in the retrievals. Both ΔK_p and Δv_{sys} are consistent with the nominal values in [Table 6.1](#) within 1σ , and are strongly covariant due to observations being obtained only post-eclipse. [Figure 6.2](#) shows the cross-correlation as a function of frame number and planet velocity, as well as the cross-correlation function summed in the planet rest frame. The planetary signal is weakly apparent in the 2D plot, but very clear after coadding in the planet rest frame. The planet signal does not appear to be significantly offset from the nominal parameters, consistent with the results of

Table 6.2: List of parameters, priors, and results for atmospheric retrievals

Name	Symbol	Prior	Retrieved Max-L	Retrieved Median
log infrared opacity [cm^2g^{-1}]	$\log \kappa$	Uniform(-4, 0)	-2.8	$-2.6^{+0.8}_{-0.8}$
log infrared/optical opacity	$\log \gamma$	Uniform(0, 3)	1.5	$1.6^{+0.2}_{-0.2}$
Intrinsic Temperature [K]	T_{int}	Uniform(500,1500)	600.0	$840.0^{+290.0}_{-220.0}$ *
Equilibrium temperature [K]	T_{equ}	Uniform(1500, 5000)	1580	$1660^{+220}_{-120.0}$ * (< 2100)
Surface gravity [$\log \text{cm s}^{-2}$]	$\log g$	Uniform(2,4.5)	3.6	$3.3^{+0.7}_{-0.8}$ *
K_{p} [km s^{-1}]	K_{p}	Uniform(157,197)	177.6	$178.5^{+3.4}_{-3.3}$
v_{sys} offset [km s^{-1}]	Δv_{sys}	Uniform(-20, 20)	-0.2	$0.3^{+1.6}_{-1.5}$
Rotational velocity [km s^{-1}]	v_{rot}	Uniform(0, 15)	7.1	$7.5^{+0.7}_{-0.7}$
log H ₂ O mass-mixing ratio	$\log \text{H}_2\text{O}$	Uniform(-12, -0.3)	-1.2	$-1.5^{+0.8}_{-1.0}$ * (> -3.0)
log CO mass-mixing ratio	$\log \text{CO}$	Uniform(-12, -0.3)	-2.9	$-2.5^{+0.6}_{-0.5}$
log OH mass-mixing ratio	$\log \text{OH}$	Uniform(-12, -0.5)	-2.3	$-2.9^{+1.1}_{-4.9}$ *
log C ₂ H ₂ mass-mixing ratio	$\log \text{C}_2\text{H}_2$	Uniform(-12, -1)	-4.0	$-7.3^{+3.0}_{-3.0}$ *
log Fe mass-mixing ratio	$\log \text{Fe}$	Uniform(-12, -1)	-2.1	$-5.1^{+2.7}_{-4.3}$ *
CO dissociation pressure	$\log P_{\text{CO}}$	Uniform(-7, -2)	-4.8	$-4.8^{+1.5}_{-1.4}$ *
H ₂ O dissociation pressure	$\log P_{\text{H}_2\text{O}}$	Uniform(-6, 2)	-0.5	$-1.2^{+0.5}_{-0.7}$
OH dissociation pressure	$\log P_{\text{OH}}$	Uniform(-6, 2)	-5.3	$-3.4^{+2.7}_{-1.7}$ *
C ₂ H ₂ dissociation pressure	$\log P_{\text{C}_2\text{H}_2}$	Uniform(-6, 2)	-0.5	$-1.7^{+2.4}_{-2.7}$ *
OH formation pressure	$\log P_{\text{formOH}}$	Uniform(-6, 2)	-2.2	$-1.4^{+2.1}_{-2.2}$ *
$\log ^{13}\text{CO}/^{12}\text{CO}$	$\log ^{13}\text{CO}_{\text{rat}}$	Uniform(-6, -0.5)	-1.9	$-4.8^{+2.0}_{-2.0}$ * (< -2.0)
log H mass-mixing ratio	$\log \text{allH}$	Uniform(-0.4, -0.05)	-0.1	$-0.2^{+0.1}_{-0.1}$ *
H ₂ dissociation pressure	$\log P_{\text{HI}}$	Uniform(-6, 2)	1.7	$-1.6^{+2.3}_{-2.7}$ *
Scale factor	scale	TruncLogNormal(0, 0.1, 7.5)	0.08	$0.04^{+0.09}_{-0.08}$
Derived Parameters				
Carbon/oxygen ratio	C/O	-	0.01	$0.1^{+0.4}_{-0.1}$ * (< 0.9)
Carbon abundance	[C/H]	-	-0.4	$0.1^{+0.6}_{-0.5}$
Oxygen abundance	[O/H]	-	1.3	1.1 ± 0.8 * (> -0.1)
Volatile abundance	[(C+O)/H]	-	1.1	1.0 ± 0.7 * (> -0.15)

Note. — List of parameters, priors, and results for atmospheric retrievals. The results columns show the values for the 6-PC retrieval. The error bars on the retrieved medians correspond to the 68%/1 σ confidence interval. Parameters with poorly constrained posteriors are indicated with a *, with upper/lower 95% confidence intervals in parentheses if available. In addition to these priors, we required that the atmospheric temperature stay below 6000 K at all pressure levels. The full corner plot is included in Appendix 6.6.

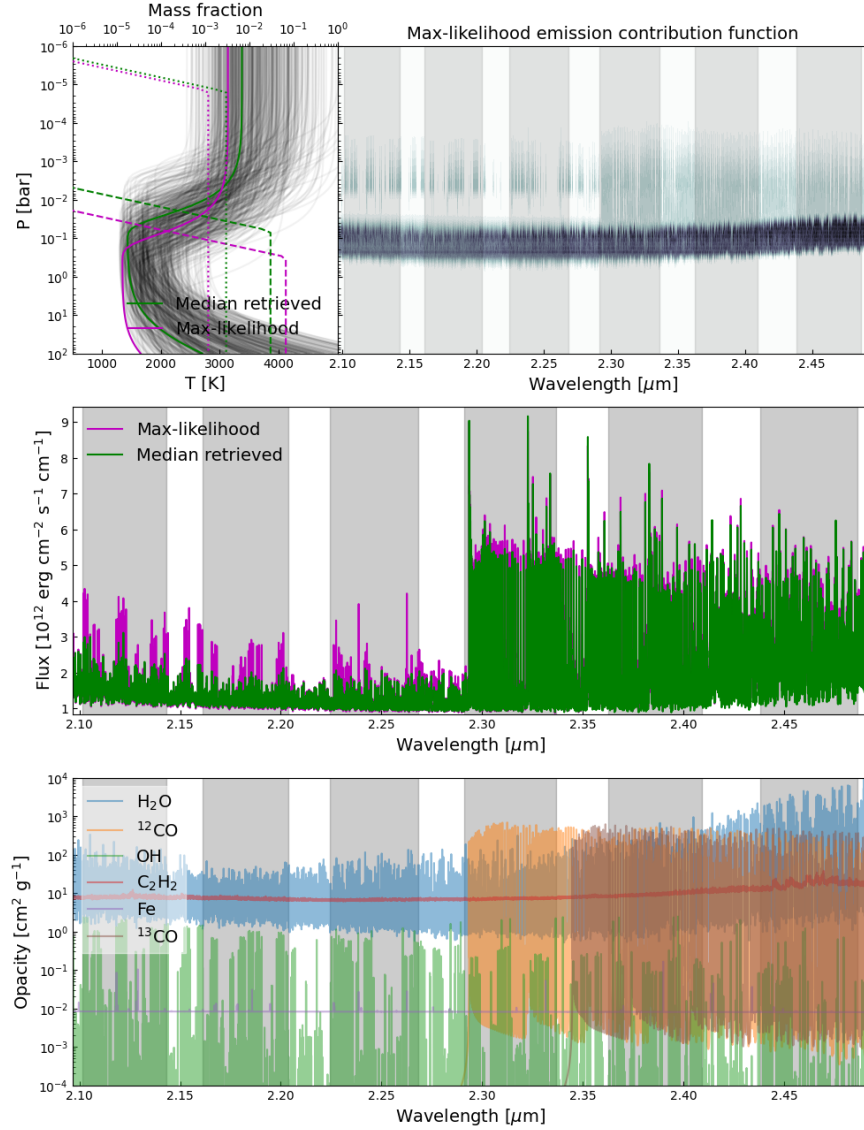


Figure 6.1: Retrieval plot for KELT-20 b

Retrieved $P - T$ profiles (top left), max-likelihood emission contribution function (top right), median and max-likelihood spectra (middle), and opacities (bottom). For the $P - T$ profile we show the profile of the median parameters, the max-likelihood, and 500 draws from the posterior. The abundance profiles for H_2O and CO are shown as dashed and dotted lines. The emission contribution function indicates our observations are sensitive to pressures from 1 bar to $\sim 10\mu\text{bar}$. The retrieved spectrum is dominated by CO features beyond $2.3\mu\text{m}$, with weaker OH and H_2O features present at bluer wavelengths. The gap in the emission contribution function seen in the first three orders is a result of H_2O and OH formation, as discussed in Section 6.4.2 From the opacity plot, we expect our observations will be dominated by H_2O and CO features.

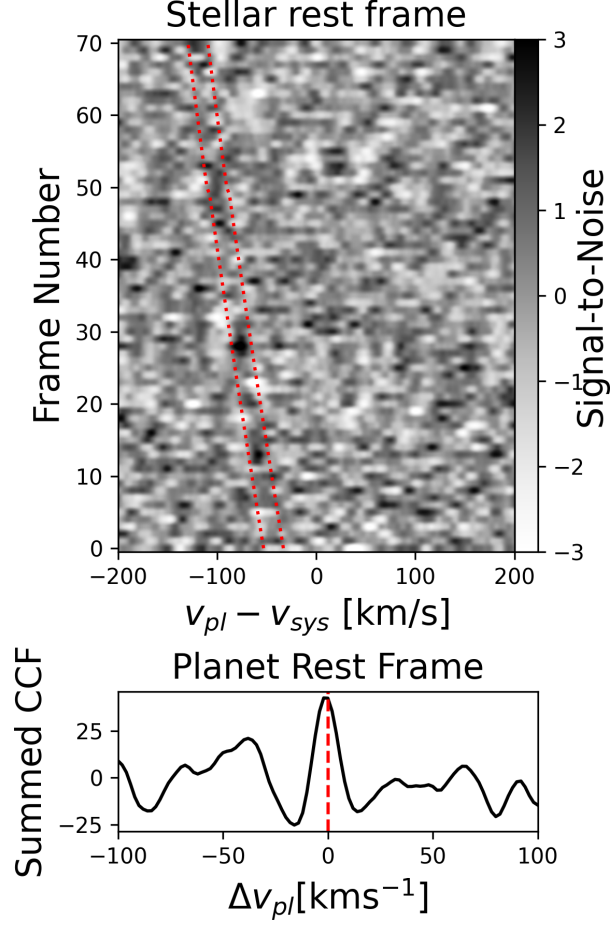


Figure 6.2: Cross-correlation time series for KELT-20 b

Cross-correlation signal-to-noise as a function of frame number and planet velocity (top) and coadded 1D cross-correlation in the planet rest frame (bottom), using the retrieved maximum-likelihood planet model. The dashed red lines in the top panel indicate $\pm 10 \text{ km s}^{-1}$ from the expected velocity track based on Table 6.2, while the dashed red in the bottom panel indicates the nominal planet rest frame. The planet velocity track is weakly evident in the 2D cross-correlation, and very clear after summing over the time series. No significant velocity offsets are evident, consistent with the retrieved velocity parameters.

the retrieval analysis.

v_{rot} is well-constrained to $7.5 \pm 0.7 \text{ km s}^{-1}$, compared with an expected rotational velocity of 2.7 km s^{-1} assuming tidal locking. This value is physically plausible for a tidally-locked UHJ with a super-rotating equatorial jet (e.g. [T. D. Komacek et al., 2022](#)) and is consistent with recent dayside wind measurements from other UHJs ([F. Lesjak et al., 2025](#)). This suggests that the LSF fitting procedure described in Section 6.2 can provide meaningful constraints even for slowly rotating ($v \sin i < 10 \text{ km s}^{-1}$) planets, rather than being restricted to the young, rapidly-rotating population probed by direct imaging targets. However, we note that we assumed a fixed factor of 1.14 when converting from the spatial to the spectral LSF widths, potentially resulting in a systematic error if this value is incorrect. We also note that the NIRSPEC velocity resolution is itself $\sim 9 \text{ km s}^{-1}$. The retrieved value for $v \sin i$ corresponds to a $\sim 30\%$ broadening of the intrinsic LSF, assuming the kernel widths add in quadrature. Given the systematic uncertainty associated with the spatial/spectral correction, we caution that this apparent constraint may not correspond to the actual rotational velocity of KELT-20 b.

6.3.2 Pressure-temperature profile

The top row of Figure 6.1 shows the retrieved $P-T$ profile and maximum-likelihood emission contribution function. The emission contribution function indicates our observations are sensitive to emission arising between 50 mbar and 100 μbar . This is consistent with our limited ability to constrain the intrinsic temperature parameter (T_{int}) of the [T. Guillot \(2010\)](#) profile, which mostly impacts the $P-T$ profile at pressures greater than 1 bar.

The retrieved T_{eq} runs to the lower end of the prior range. Tests with a wider prior found this remains the case even if the prior is extended to 800 K, but that increases in the multiplicative scale factor applied to the planet model keep the final star/planet flux ratio in the forward model approximately constant. This indicates that the use of a log-normal scale factor prior and tight temperature prior is not sufficient to break the scale

factor/temperature degeneracy for small-bandpass high-resolution observations discussed in [L. Finnerty et al. \(2024\)](#). Resolving this degeneracy appears to require a significantly wider bandpass than our observations cover (such as provided by Gemini/IGRINS, e.g. [M. R. Line et al., 2021](#)), over which the planetary SED shows significant curvature. This leads to a non-linear variation in the planet/star flux ratio F_p/F_s as a function of wavelength which cannot be fit by changes to the scale factor, instead pushing the retrieval to a $P - T$ profile with the correct continuum shape and absolute temperature.

For the presented retrievals, we chose a relatively tight prior bound that leads to a scale factor of approximately 1. We discuss the degeneracies in the absolute abundances in more detail in [Section 6.4](#)

As our observations are not flux-calibrated, we are actually fitting for the flux of the planet relative to the host star flux (F_p/F_s) using a fixed model of the stellar spectrum. This means that errors in the wavelength-dependent stellar spectrum can potentially bias the retrieved absolute planet temperature and/or scale factor. While we neglected the impacts of stellar oblateness or gravity darkening in our stellar model, the reported $v \sin i = 114 \text{ km s}^{-1}$ value for KELT-20 A ([G. J. J. Talens et al., 2018](#)) suggests these effects may be significant. This may lead to a bias in the retrieved temperature and/or continuum level in order to correctly match the observed F_p/F_s with an inaccurate F_s .

We also note that our observations were taken post-eclipse. Thus, the observed planetary disk is increasingly dominated by the morning limb over the course of our data. This phase coverage may also impact the retrieved temperature and apparent flux of the planet, as the morning/pre-dawn longitudes are expected to be substantially cooler than the dayside average.

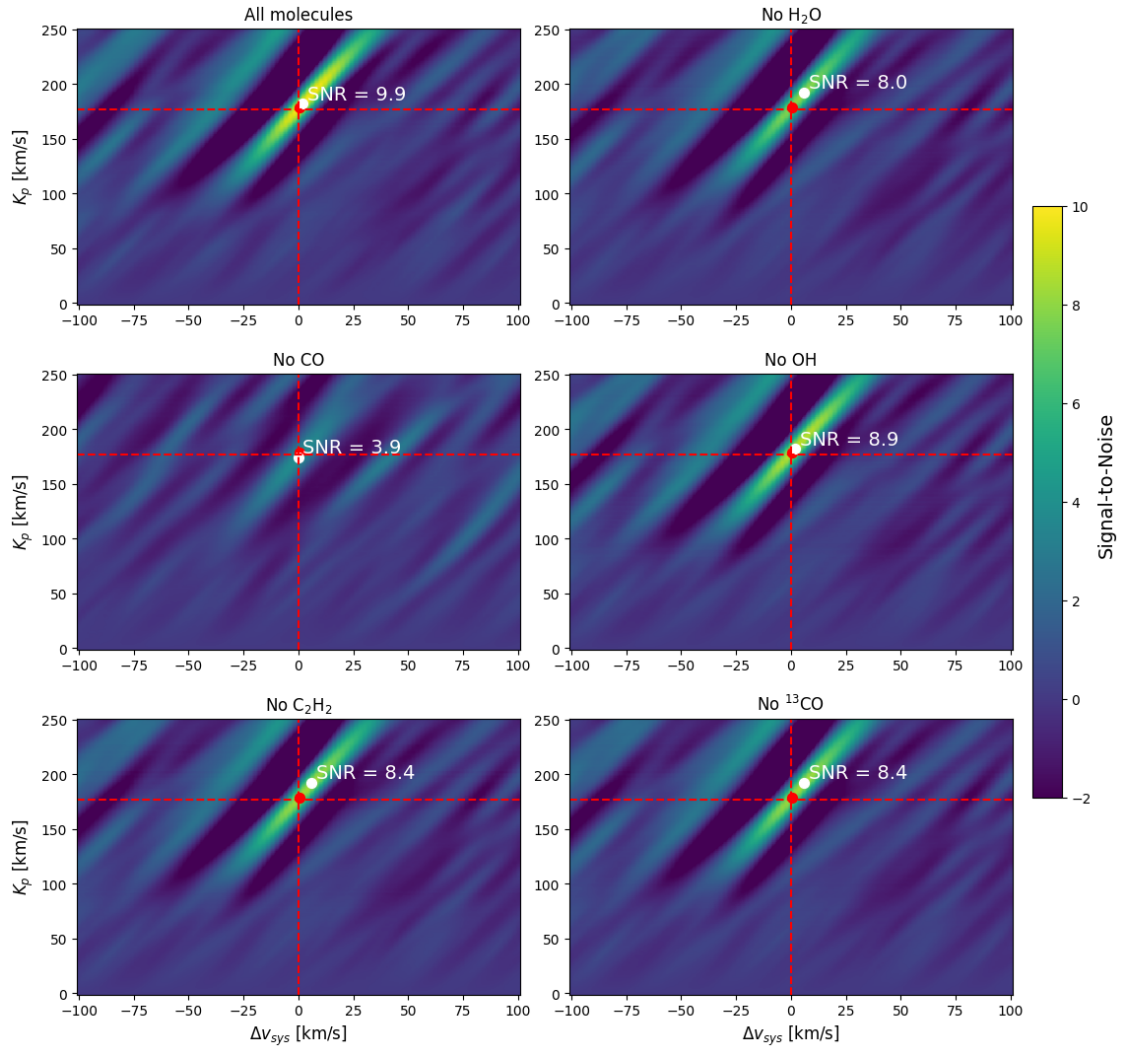


Figure 6.3: $K_p - \Delta v_{\text{sys}}$ diagrams for KELT-20 b

The max-likelihood model is in the top left, with diagrams made with the max-likelihood model omitting the specified species in the remaining panels. We use an ad-hoc approach to estimating the detection significance, first subtracting each K_p column by its median and then dividing by the standard deviation of the $K_p < -40$ km s^{-1} region to minimize impacts of the detrending process removing the planet signal at small K_p (L. Finnerty et al., 2024). Omitting each molecule one-by-one allows us to assess the contribution of that molecule to the overall detection while minimizing the change to the pseudocontinuum that results from omitting a molecule. The detection is dominated by CO, with a contribution from H_2O . Including OH, C_2H_2 , and ^{13}CO has only a marginal impact on the detection strength. These detection strengths are consistent with expectations based on the abundance constraints (or lack thereof) reported in Table 6.2.

6.3.3 Chemical composition

Our retrievals successfully constrain the CO abundance, and place a lower limit on the H₂O abundance. The remaining species in the retrieval are unconstrained, although the OH and Fe posteriors show weak peaks and large C₂H₂ abundances are weakly disfavored. This is consistent with expectations based on the *K*-band opacities (see Figure 6.1, bottom panel), which are dominated by CO and H₂O features, as well as with previous infrared observations of UHJs (e.g. L. Finnerty et al., 2023a). The $K_p - \Delta v_{\text{sys}}$ plots for each molecule using the maximum-likelihood model are shown in Figure 6.3. The contribution of each molecule towards the total detection strength is consistent with the expectation that species which are better-constrained by the retrievals are more significantly detected in the $K_p - \Delta v_{\text{sys}}$ plot.

We also obtain a bounded constraint on the H₂O dissociation pressure, $\log P_{\text{H}_2\text{O}} = -1.2^{+0.5}_{-0.7}$ bar. We discuss this constraint and its comparison to chemical equilibrium models in Section 6.4. Key here is that the retrieved H₂O dissociation pressure shows a significant degeneracy with that of the CO abundance, with lower dissociation pressure corresponding to higher CO abundances. In previous HRCCS studies, molecular abundances are often correlated, as the loss of continuum information during data processing makes HRCCS retrievals more sensitive to line ratios than absolute line strengths (e.g. L. Finnerty et al., 2023a, 2024). In this case, the H₂O feature strength appears to be set primarily by the dissociation pressure, rather than the H₂O abundance, and so the degeneracy is between the CO abundance and H₂O dissociation pressure rather than the abundances themselves.

6.3.3.1 Significance of other species

H₂O dissociation is expected to produce significant quantities of OH at pressures where H₂O is being dissociated. The retrieved posteriors do not provide bounded constraints on the OH abundance or the OH dissociation/formation pressures, leading to an unconstrained

vertical mixing profile shown in Figure 6.5. Figure 6.1 demonstrates the comparatively low OH opacity in the K -band relative to other species, which is likely the reason for the poor constraints. The insignificance of OH to the detection is further demonstrated by Figure 6.3, which shows that omitting OH from the maximum-likelihood model has only a marginal impact on the detection strength in the $K_p - \Delta v_{sys}$ space.

The retrieved posterior weakly disfavors high C_2H_2 abundance, consistent with the weakness of high-temperature C_2H_2 spectral features in the K -band. C_2H_2 was included in the retrievals because it can be present in significant, potentially detectable quantities for C/O ratios greater than 1, but our retrievals strongly disfavor this scenario (see Section 6.4). Similarly with OH, omitting C_2H_2 entirely from the maximum-likelihood planet model has only a minimal impact on the overall detection strength.

6.3.4 CO Isotopologue Ratio

Finally, the retrieved posterior places an upper limit on the CO isotopologue ratio, $\log^{13} CO / \log^{12} CO < -2.0$ at 95% confidence. This is only slightly below the solar-system value of 89, and stands in contrast with previous results from KPIC observations of hot Jupiters suggesting significant ^{13}CO enrichment (L. Finnerty et al., 2023a, 2024).

6.3.5 Number of principal components

We ran retrievals omitting 4, 6, 8 and 12 principal components in order to assess the impact of the number of dropped principal components on the retrieved posteriors. The full corner plots for each retrieval are included in Appendix 6.6. Based on inspection of the corner plots and fringing periodograms, we adopt the 6 component case as our fiducial retrieval. The 4 component retrieval provides an unexpectedly tight constraint on the Fe abundance, and strongly prefers low values of T_{eq} , which are counteracted with a larger scale factor. The 8 and 12 component cases yield marginalized posteriors which are mostly compatible with the

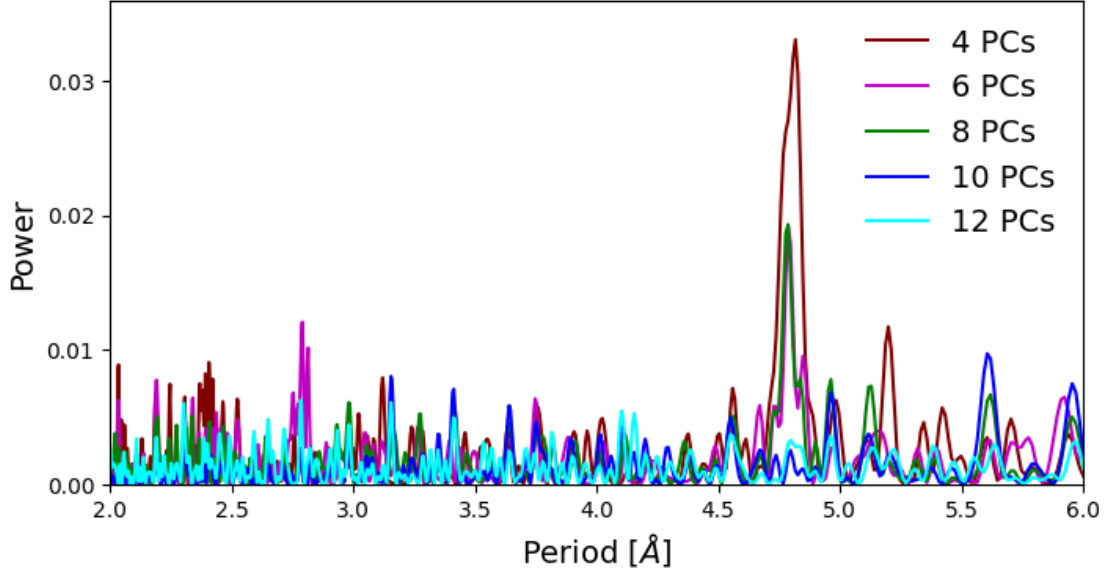


Figure 6.4: Fringing periodograms for KELT-20 b

Lomb-Scargle periodograms of the median spectrum for order 31 after detrending. A significant peak at $\sim 4.8\text{\AA}$ is consistent with incomplete removal of the KPIC fringing effect described in [L. Finnerty et al. \(2022\)](#). The power present in this peak is significantly reduced by projecting out at least six principal components. This suggests sufficient removal of fringing/telluric effects in this case requires omitting at least six components, and that the odd posterior behavior seen in the four component retrievals may be a result of undercleaning. Removing 10 or more components is required to entirely eliminate this fringing signal, but these retrievals also give significantly broader posteriors, suggesting that the planet signal is being impacted by omitting so many components.

6 component case, but significantly wider. In particular, the 8 and 12 component cases prefer higher temperatures, do not constrain the the H₂O abundance or dissociation pressure, and give worse constraints on K_p and v_{sys} . This suggests that in the 8 and 12 component cases the PCA is distorting/removing portions of the underlying planet spectrum, leading to worse constraints.

To better assess the impact of the PCA, we visually inspected the post-PCA spectral time series. This revealed clear evidence of residual fringing which has not been removed by omitting only 4 principal components, particularly at the beginning and end of the observation. To confirm this, we computed the Lomb-Scargle periodogram of the cleaned time series for order 31 after omitting 4, 6, 8, 10, and 12 principal components, shown in Figure 6.4. A clear peak is seen at a period of 4.8Å, likely corresponding to the KPIC dichroic fringing effect described in (L. Finnerty et al., 2022). This peak is substantially stronger when omitting only 4 components than in the 6 and 8 component cases, suggesting that the 4 component retrieval may be impacted by unremoved fringing. The fringe feature disappears from the periodogram when omitting 10 or more components, but comparing the 6 and 8 component retrievals suggests that the PCA is already beginning to significantly degrade the planet spectrum in the 8 component case. As a result, we choose the 6 component case as our fiducial retrieval for Table 6.2 and subsequent discussion.

6.4 Discussion

6.4.1 Atmospheric circulation

Our median retrieved values for ΔK_p and Δv_{sys} are compatible with the orbital ephemeris and assumed velocity parameters listed in Table 6.1. This suggests that the detected planetary emission is not dominated by one limb of the planet, which would lead to a net blueshift if the morning limb dominated or a redshift if the evening limb were dominating the total flux as a result of the planet’s rotation.

While the retrieved velocity parameters are consistent with the [ExoFOP \(2019\)](#) ephemeris, using the values from [G. J. J. Talens et al. \(2018\)](#) instead results in a $\sim 4 \text{ km s}^{-1}$ blueshift. Alternatively, using period/transit time values from [M. B. Lund et al. \(2017\)](#); [J. A. Patel & N. Espinoza \(2022\)](#); [E. S. Ivshina & J. N. Winn \(2022\)](#), or [A. Kokori et al. \(2023\)](#) change the nominal planet velocities by $\sim 1 - 3 \text{ km s}^{-1}$. In some cases, propagating the reported uncertainties on the period and transit time is insufficient to explain this difference.

This discrepancy speaks to the importance of accurate knowledge of the planetary ephemeris for interpreting offsets in the $K_p - \Delta v_{sys}$ diagram as a result of atmospheric circulation pattern. Inaccuracies as small as 10 minutes in the mid-transit time can lead to 10 km s^{-1} offsets in the planet velocity in some systems ([A. Pai Asnodkar et al., 2022](#)), comparable to the fastest winds expected on UHJs. While transmission observations can use ingress/egress to very precisely constrain the ephemeris at the observed epoch, emission observations must rely on a preexisting ephemeris with its associated uncertainties. As a result, we suggest any attempts to interpret velocity offsets in emission observations proceed cautiously.

In the case of KELT-20 b, additional difficulties in interpreting velocity offsets arise from uncertainty in the systemic velocity of the rapidly-rotating A-type primary. [G. J. J. Talens et al. \(2018\)](#) reports a value of $-21.3 \pm 0.4 \text{ km s}^{-1}$, while [M. B. Lund et al. \(2017\)](#) gives a value of $-23.3 \pm 0.3 \text{ km s}^{-1}$. [M. C. Johnson et al. \(2023\)](#) report a value of -26.0 km s^{-1} , and [M. Stangret et al. \(2024\)](#) report a value of -24.6 km s^{-1} . This uncertainty is comparable to the expected wind velocities for UHJs, precluding robust measurement of wind speeds even from transmission observations ([M. Stangret et al., 2024](#)).

Rotational broadening of planetary lines is not expected to be sensitive to ephemeris or stellar velocity errors, providing an alternative probe of global circulation patterns for emission observations when the instrumental LSF is well-characterized, as is the case for KPIC. If the observed spectrum is dominated by the morning or evening limb of the planet, the rotation will lead to a net redshift or blueshift of the planetary atmosphere, respectively. Similarly, a strongly longitudinally-dependent wind pattern may lead to a net red/blueshift.

In contrast, a symmetric eastward flowing equatorial jet would not lead to a net shift in the observed planet spectrum, but may instead appear to increase the rotational velocity of the planet beyond the expected value based on tidal locking.

Assuming a tidal locking and the parameters listed in Table 6.1, the expected rotational velocity of KELT-20 b is 2.7 km s^{-1} . The retrieved value of $7.5 \pm 0.7 \text{ km s}^{-1}$ could be explained by a 5 km s^{-1} eastward-flowing equatorial jet dominating the observed emission and appearing to increase the rotational velocity of the planet. This is consistent with wind speeds previously reported for KELT-20 b (N. Casasayas-Barris et al., 2019; S. K. Nugroho et al., 2020; M. Stangret et al., 2020; S. Petz et al., 2024), and with model predictions for UHJs (e.g. T. D. Komacek et al., 2022; H. Beltz et al., 2022).

The retrieved rotational broadening is comparable to the instrumental resolution of NIRSPEC, increasing the line widths by only $\sim 30\%$ compared to the intrinsic instrumental LSF. While the large number of planet lines and the well-characterized LSF is reason to believe we can measure line broadening to the $\sim 10\%$ level, systematic uncertainties in the spatial/spectral profile conversion (L. Finnerty et al., 2022) suggest the retrieved $v \sin i$ should be taken with caution. Unambiguous measurement of $v \sin i$ may require higher spectral resolution, which will be available with Keck/HISPEC (D. Mawet et al., 2019).

6.4.2 Molecular Dissociation

We plot the median and maximum-likelihood vertical abundance profiles compared with chemical equilibrium predictions from `easyCHEM` (P. Mollière et al., 2017; E. Lei & P. Mollière, 2024) in Figure 6.5. For the equilibrium prediction, we use the median $P - T$ profile parameters. The C/O ratio and metallicity of the equilibrium model were then adjusted by eye to roughly match the median abundance profiles, which we discuss further in the next subsection. We find a reasonable agreement between the retrieved abundance profiles and the chemical equilibrium predictions for $\text{C/O} \sim 0.05$ and $[\text{Fe/H}] = \sim -0.3$. We discuss the discrepancy between this value and our retrieved $[(\text{C+O})/\text{H}]$ in the following subsection.

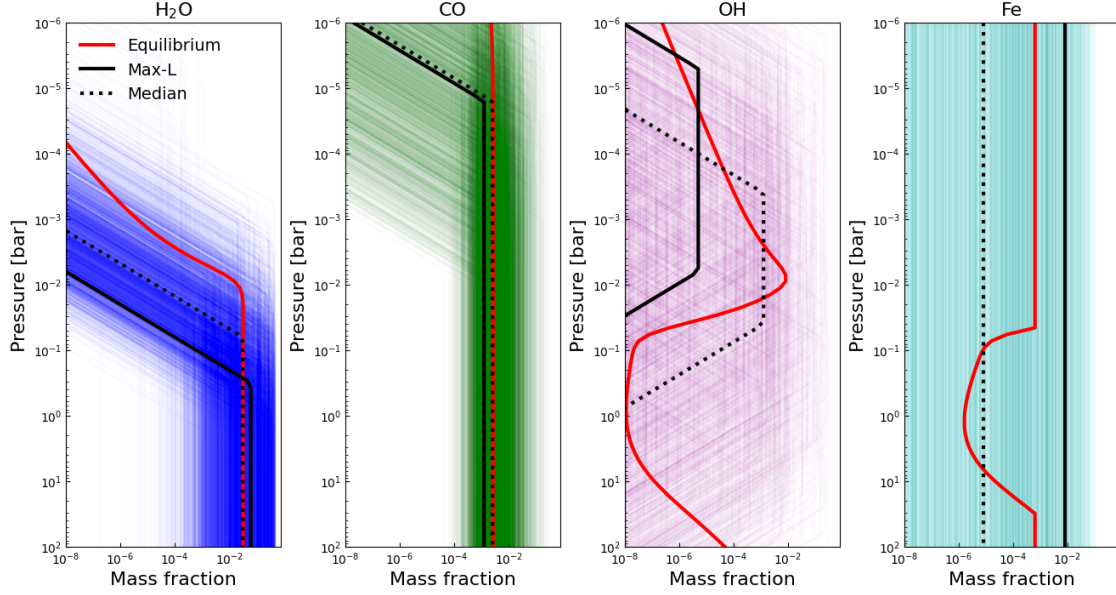


Figure 6.5: Retrieved abundance profiles for KELT-20 b

Retrieved abundance profiles compared with compared with `easychem` equilibrium predictions. The colored profiles are 4000 draws from the posterior, while the maximum-likelihood and median profiles are indicated in solid and dotted black, respectively. The equilibrium profiles are shown in solid red. For the equilibrium model, we used the $P - T$ profile corresponding to the median retrieved values. The median abundance profiles for H_2O and CO are roughly consistent with the equilibrium model for $\text{C}/\text{O} = 0.05$ and $[\text{Fe}/\text{H}] = -0.3$ (shown in the plot), although the retrieval prefers somewhat deeper dissociation of H_2O . These values are significantly lower than those given in Table 6.2 due to the inclusion of refractory species in the equilibrium model. The OH and Fe profiles are poorly constrained, consistent with the overall insignificance of the detection.

The H₂O abundance profile from the chemical equilibrium model dissociates moderately higher in the atmosphere than the abundance profile preferred by the retrieval, but is within the range of the posterior. This concurrence suggests that chemical equilibrium is a good assumption when considering only CO and H₂O for KELT-20 b and assuming equilibrium may help break the previously-discussed temperature/scale factor degeneracy while reducing the number of free parameters in the retrieval. At the same time, this agreement demonstrates that free retrievals can account for vertically varying abundances with only 1-2 additional free parameters per molecule, while also retaining a flexibility for possible photochemistry.

Consistent with the non-detection of OH in Figure 6.3, the OH abundance profile is unconstrained. The poor OH constraint is due to the relatively low opacity of OH in the *K*-band and is consistent with previous KPIC *K*-band observations of WASP-33 b (L. Finnerty et al., 2023a). OH has been detected in *H*-band observations of UHJs (S. K. Nugroho et al., 2021; R. Landman et al., 2021; M. Brogi et al., 2023; M. Weiner Mansfield et al., 2024) due to the higher line opacity in that band. Combining *H*-band observations which constrain the abundance profiles for OH and H₂O with *K*-band observations constraining the ratio of H₂O features to CO features may provide much better constraints on the bulk C/O ratio in the presence of H₂O dissociation than is possible from *K*-band observations alone. Such observations will be possible with Keck/HISPEC, which will provide high-resolution fiber-fed spectroscopy covering the full 1-2.5 μm range in a single shot (D. Mawet et al., 2019).

6.4.3 Interactions between P-T and mixing profiles

While experimenting with different parameterizations of the $P - T$ and dissociation profiles, we encountered complicated degeneracies in the resulting posteriors and unusual behavior in the retrieved $P - T$ profiles. These complications all arise from the presence of two terms impacting the radiative transfer at each level of the model atmosphere, rather than one. Beginning from Kerckoff’s Law of radiative transfer, we have:

$$\frac{dI_\nu}{ds} = -n(s)\sigma_\nu I_\nu + n(s)\sigma_\nu B_\nu(T) \quad (6.1)$$

Where I_ν is the specific intensity, $n(s)$ is the number density of an absorbing species at altitude s , σ_ν is the absorption cross section of the species, and $B_\nu(T)$ is the Planck function evaluated at the temperature of altitude s . In the case of abundances fixed with altitude, the change in intensity is set only by the change in $B_\nu(T)$ with height, resulting in an emission contribution function which tracks the $P - T$ profile. However, in the case of vertically-varying abundances, I_ν can change even with an isothermal $P - T$ profile as a result of changes in $n(s)$. Depending on the specifics on the $P - T$ and mixing profiles, this can lead to emission contributions functions with multiple layers and/or gaps which may or may not correspond to regions of curvature in the $P - T$ profile.

An example of this can be seen in the upper right panel of Figure 6.1 showing the retrieved maximum-likelihood emission contribution function. In the bluest three orders, the emission contribution function drops off rapidly when H_2O dissociation begins, only to increase again at lower pressures as the model includes increasing quantities of OH. This increase occurs even as the curvature of the $P - T$ profile rapidly decreases in this pressure range.

A more straightforward effect is introduced by fixing the intrinsic temperature parameter T_{int} , which leads to a multimodality between the H_2O abundance and dissociation pressure. Retrievals with $T_{\text{int}} = 100$ K returned posteriors with either a low H_2O abundance and dissociation at ~ 1 mbar or a high H_2O abundance and dissociation at ~ 100 mbar. The planet spectra in each mode had similar H_2O feature strength, leading our free retrieval approach to not significantly prefer one mode over the other. Including T_{int} as a free parameter with a lower prior bound high enough to prevent an isothermal lower atmosphere appears to break this degeneracy in favor of the high-abundance, deep-dissociation mode. Future HRCCS analyses including molecular dissociation should take care to assess the precise impact of their $P - T$ parametrization on the final posterior.

As a consistency check, we also ran retrievals using a physics-free spline-based $P - T$ parametrization as described by [S. Pelletier et al. \(2021\)](#). The resulting $P - T$ profile reached a minimum of ~ 1000 K between 1 and 0.1 bar, but the abundance/dissociation parameters were consistent with the presented values. This suggests that changes in the $P - T$ parametrization/limits are not strongly impacting the retrieved abundances. Using the spline-based approach significantly increases the number of free parameters in the fit, leading to longer runtimes. We also find the spline profile is prone to non-physical oscillations in the upper/lower atmosphere where the emission contribution function is negligible, even for aggressive values of the smoothing prior. We therefore prefer the [T. Guillot \(2010\)](#) approach for this work, but note that analyses covering a wider bandpass will be more favorable to spline-based approaches.

6.4.4 C/O and metallicity

The corner plot for the retrieved C/O, [C/H], [O/H], and [(C+O)/H] values are shown in [Figure 6.6](#), and the median values and confidence intervals are listed in [Table 6.2](#). These posteriors were constructed from the retrieved abundances of CO, H₂O, and C₂H₂ in order to estimate the deep atmosphere C/O ratio below any molecular dissociation, and do not account for contributions from any other species. OH is specifically omitted because it is expected to be present only in the upper atmosphere above H₂O dissociation, and including both H₂O and OH would therefore double count that oxygen when determining the bulk abundances.

As `petitRADTRANS` uses mass fractions for molecular abundances, we have thus far reported results as mass fractions. However, the C/O, O/H, and C/H values are generally reported as number fractions/volume mixing ratios. The mass fraction can be converted to the volume mixing ratio as follows:

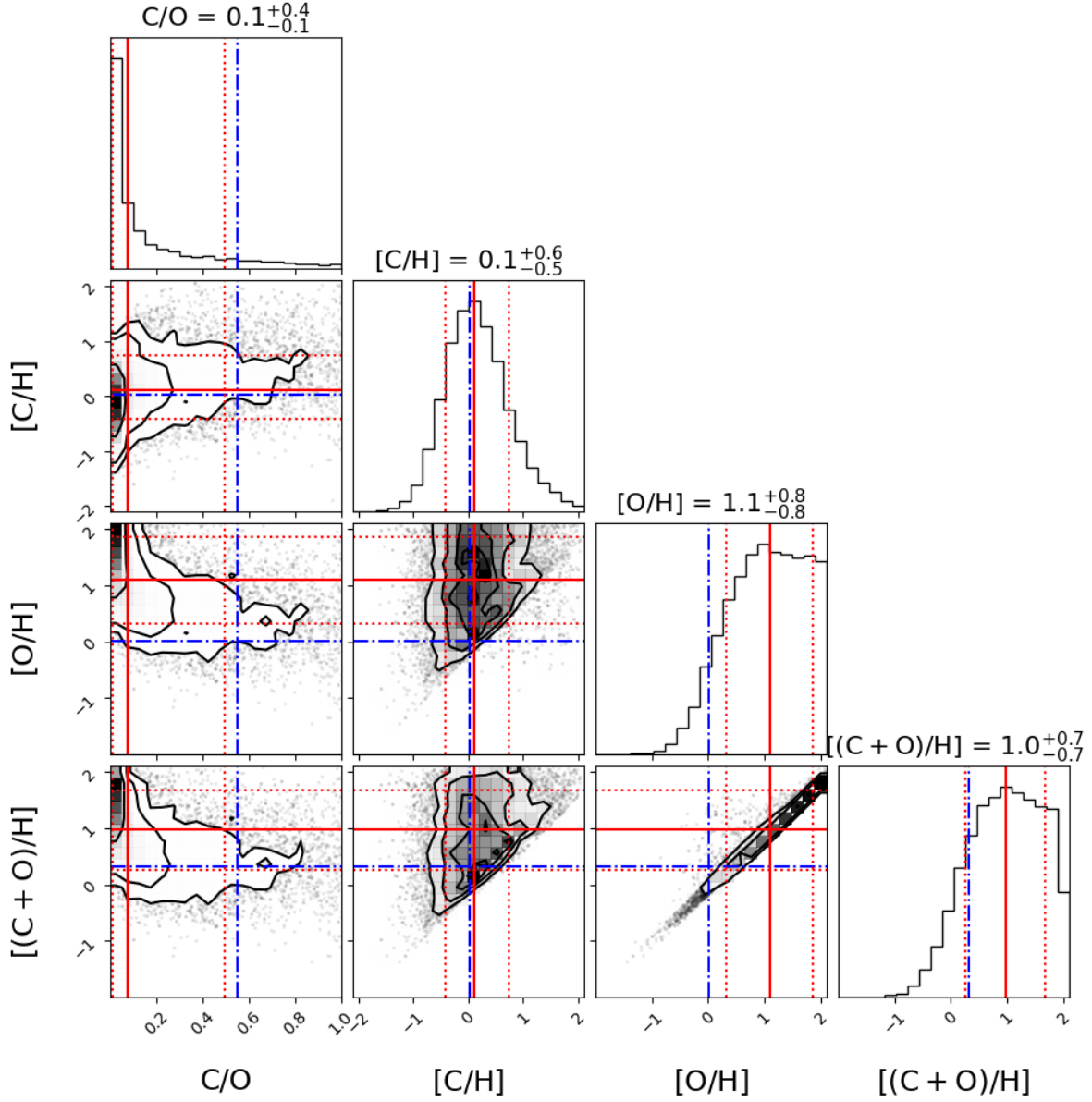


Figure 6.6: Corner plot of C/O, [C/H], [O/H], and [(C+O)/H] for KELT-20 b

Medians are in solid red, with dashed red indicating the $\pm 34\%$ confidence intervals. The solar values from [H. Palme et al. \(2014\)](#) are shown in dash-dot blue. The carbon abundance is close to the solar abundance, while [O/H] prefers solar to super solar values ($[\text{O}/\text{H}] > -0.1$ at 95% confidence). This leads to a very low C/O ratio and a lower limit on the total volatile abundance $[(\text{C} + \text{O})/\text{H}] > -0.15$ at 95% confidence

$$n_X = \frac{\mu}{\mu_X} M_X \quad (6.2)$$

Where n_X is the volume mixing ratio of species X, M_X is the mass fraction of species X, μ_X is the molar mass of species X, and μ is the mean molecular weight. The dependence on the mean molecular weight cancels when computing abundance ratios. For logarithmic mass fractions and a fixed mean molecular weight of 2.3 g/mol, $\log \text{H}_2\text{O}_{\text{VMR}} = \log \text{H}_2\text{O}_{\text{MF}} - 0.9$, and $\log \text{CO}_{\text{VMR}} = \log \text{CO}_{\text{MF}} - 1.1$

The median and $\pm 34\%$ confidence intervals are $\text{C/O} = 0.1^{+0.4}_{-0.1}$ ($\text{C/O} < 0.9$ at 95% confidence), $\log[\text{C/H}] = 0.1^{+0.5}_{-0.4}$, $\log[\text{O/H}] = 1.1 \pm 0.8$ ($[\text{O/H}] > -0.1$ at 95% confidence), and $[(\text{C}+\text{O})/\text{H}] = 1.0 \pm 0.7$ ($[(\text{C}+\text{O})/\text{H}] > -0.15$ at 95% confidence). As we retrieve only a lower limit for the H_2O abundance, the oxygen abundance is similarly a lower limit, as is the total volatile abundance. Solar values for $[\text{O/H}]$ and $[(\text{C}+\text{O})/\text{H}]$ from [H. Palme et al. \(2014\)](#) are disfavored at $\sim 1\sigma$, with the maximum-likelihood parameters corresponding to a $\sim 10\times$ solar enrichment in oxygen. The C/O ratio posterior has a sharp cutoff at $\text{C/O} = 1$ due to the preference for little/no C_2H_2 in the atmosphere, which leaves CO as the only carbon species in the atmosphere.

The C/O and abundance values we report are based only on the molecular species included in our retrievals, and therefore may not be an accurate estimate for the atmosphere as a whole. To address this, we compare the retrieved abundances to equilibrium chemistry models from [easyCHEM](#) ([P. Mollière et al., 2017](#); [E. Lei & P. Mollière, 2024](#)), shown in Figure 6.5. These models scale the atomic abundances of all species except oxygen according to a single metallicity parameter, while the oxygen abundance is determined by a separate parameter setting the C/O ratio. Figure 6.5 compares the retrieved mixing profiles to an [easyCHEM](#) model with $\text{C/O} = 0.05$, $[\text{Fe/H}] = -0.3$, which agrees well with the lower-atmosphere abundances. While this C/O ratio is comparable to those in our retrievals, the metallicity is substantially lower than the $10\times$ solar volatile abundance we retrieve. The retrieved volatile enrichment is due entirely to the high retrieved oxygen abundance, which

in the equilibrium models is determined by the C/O ratio once the metallicity parameter is tuned to match the carbon abundance. As a result, the equilibrium [Fe/H] parameter is not necessarily measuring the bulk metallicity in the event of a refractory/volatile ratio differing from solar.

At first glance, the low-C/O ratio composition appears to be inconsistent with the previously reported solar or slightly supersolar C/O and atmospheric metallicity for KELT-20 b from [D. Kasper et al. \(2023\)](#), who combined Spitzer, HST, and MAROON-X observations to perform a joint high/low spectral resolution retrieval. However, we note that there is a strong degeneracy in our retrievals between the CO abundance and the H₂O dissociation pressure, and that our retrievals prefer H₂O dissociation occurring deeper in the atmosphere than expected based on chemical equilibrium. Dissociation closer to the equilibrium expectation corresponds to an enhancement in the CO abundance, leading to a solar or slightly super-solar metallicity and increasing the C/O ratio to approximately the solar value, which is at the edge of the retrieved 1σ confidence interval for the C/O ratio.

Observations with broader wavelength coverage could reduce uncertainty in the atmospheric metallicity by observing multiple bands from the same species, which would break the degeneracy between H₂O and CO abundances seen when retrieving from *K*-band data alone. Broader wavelength coverage would also allow the detection of additional species, including refractory elements, which would constrain the atmospheric refractory/volatile ratio, which is potentially an important tracer of the planet formation process ([J. D. Lothringer et al., 2021](#); [Y. Chachan et al., 2023](#)), as well as provide a non-volatile probe of the atmospheric metallicity. Refractory/volatile ratio constraints have recently been demonstrated using IGRINS *H+K*-band data ([P. C. B. Smith et al., 2024](#)) and also using a combination of *K*-band and optical observations ([S. Pelletier et al., 2025](#)). Future joint retrievals combining KPIC and optical observations will provide similar constraints. Such a joint retrieval is outside the scope of the present work.

Previous studies of UHJs have found that free retrievals with fixed abundances prefer

high-metallicity, high-C/O ratio atmospheres, but that using equilibrium models to account for molecular dissociation results in less metal-rich atmospheres with a C/O ratio closer to solar/stellar values (e.g. [M. Brogi et al., 2023](#); [S. Ramkumar et al., 2023](#)). This bias in free retrievals occurs because when ignoring dissociation, the only way to reduce the strength of H₂O features relative to CO is to reduce the H₂O abundance and/or increase the CO abundance, increasing the C/O ratio. In this case, we may be seeing the reverse phenomenon, where dissociation below the chemical equilibrium level is driving a higher H₂O abundance, lower CO abundance, and low C/O ratio.

Enforcing chemical equilibrium accounts for dissociation, but the equilibrium assumption for hot gas giants is in tension with results from *JWST* transmission spectroscopy preferring significant spectral features from photochemically produced species ([S.-M. Tsai et al., 2023](#); [A. Dyrek et al., 2024](#)). Our retrieval of the H₂O dissociation pressure for KELT-20 b indicates that free retrievals can account for dissociation without making an equilibrium assumption, providing an approach that can avoid biases from fixed vertical abundances while maintaining the flexibility to explore novel photochemical processes.

6.4.5 Formation history

While many ultra-hot Jupiters have significant misalignments between the planet’s orbital plane and the spin axis of the host star (e.g. [A. Collier Cameron et al., 2010](#); [B. S. Gaudi et al., 2017](#); [G. J. J. Talens et al., 2017](#); [S. H. C. Cabot et al., 2021](#)), KELT-20 b is extremely well-aligned with its host star’s rotation ([G. J. J. Talens et al., 2018](#); [V. Singh et al., 2024](#)). Furthermore, KELT-20A lies above the Kraft break ([R. P. Kraft, 1967](#)), in a regime where close-in giant planets are preferentially misaligned ([J. N. Winn et al., 2010](#)) and tidal realignment is likely insignificant over the lifetime of the system ([S. Albrecht et al., 2012](#)). This suggests KELT-20 b could possibly have formed without high-eccentricity migration, which is necessary to produce the extremely inclined/retrograde orbits seen in other UHJs ([S. Naoz et al., 2011](#)). Differences in the formation history of KELT-20 b compared to other

UHJs could lead to an anomalous composition compared to the population as a whole.

The low-C/O, solar-to-supersolar metallicity preferred by our retrievals is consistent with general predictions from core-accretion models that these parameters are inversely correlated in exoplanet atmospheres (N. Espinoza et al., 2017; N. Madhusudhan et al., 2017; A. J. Cridland et al., 2019), and specifically with models for formation beyond the CO snow line followed by Type II migration (N. Khorshid et al., 2022). However, our retrievals are ambiguous as to the bulk metallicity of KELT-20 b, as we do not constrain the abundances of any refractory species. Our retrieved composition could be explained by substantial oxygen enrichment with an otherwise low metallicity, or by a carbon-poor but otherwise metal-enriched atmosphere. Further ambiguity arises from the deeper retrieved H₂O dissociation pressure compared with chemical equilibrium models, which may lead to an over-estimation of the H₂O abundance and corresponding under-estimation of the C/O ratio. Solar or moderately super-solar atmospheric metallicity is consistent with equilibrium retrievals of other UHJs, which have preferred solar C/O ratios for both aligned (M. Brogi et al., 2023) and misaligned (S. Ramkumar et al., 2023) systems.

In the absence of isotopologue constraints, measurements from other portions of the optical/infrared spectrum to constrain the refractory/volatile ratio could distinguish between different formation scenarios (J. D. Lothringer et al., 2021; Y. Chachan et al., 2023). In the case of KELT-20 b, the extensive existing optical data (e.g. M. C. Johnson et al., 2023; S. Petz et al., 2024) may allow joint high-resolution optical/infrared retrievals and constraints on the refractory/volatile ratio without the need for additional observations.

6.5 Summary and Conclusions

We performed atmospheric retrievals on high-resolution post-eclipse *K*-band observations of the ultra-hot Jupiter KELT-20 b/MASCARA-2b. Using a free-retrieval framework including molecular dissociation, we constrain the abundance of CO and place a lower limit on the

abundance of H_2O , finding the atmosphere of KELT-20 b is consistent with an oxygen-rich ($\text{C}/\text{O} = 0.1^{+0.4}_{-0.1}$, $\text{C}/\text{O} < 0.9$ at 95% confidence) composition. The retrieved H_2O dissociation pressure and molecular abundances are roughly consistent with predictions from equilibrium chemistry models having $\text{C}/\text{O} \sim 0.05$ and metallicity $0.5\times$ solar, but the lack of refractory species detections limits our ability to constrain the bulk metallicity. We also constrain the rotational broadening of KELT-20 b to $7.5 \pm 0.7 \text{ km s}^{-1}$. This is $\sim 5 \text{ km s}^{-1}$ larger than the value expected from tidally locked rotation, and is consistent with a supersonic day-to-night wind. Such a wind is consistent with results from other UHJs and with predictions from GCMs, but the relatively low spectral resolution of KPIC results in a significant systematic uncertainty in the retrieved rotational velocity.

6.6 Corner Plots

Figures 6.7, 6.8, 6.9, and 6.10 present the full corner plots from the retrievals omitting 4, 6, 8, and 12 principal components respectively. The units, priors, and retrieved quantity are listed in Table 6.2. In cases where parameters are well-constrained, the plotting limits have been adjusted to focus on the posterior rather than spanning the full prior. The truncated normal prior for the scale factor is overplotted in green. All other parameters used a normal prior covering the full range listed in Table 6.2.

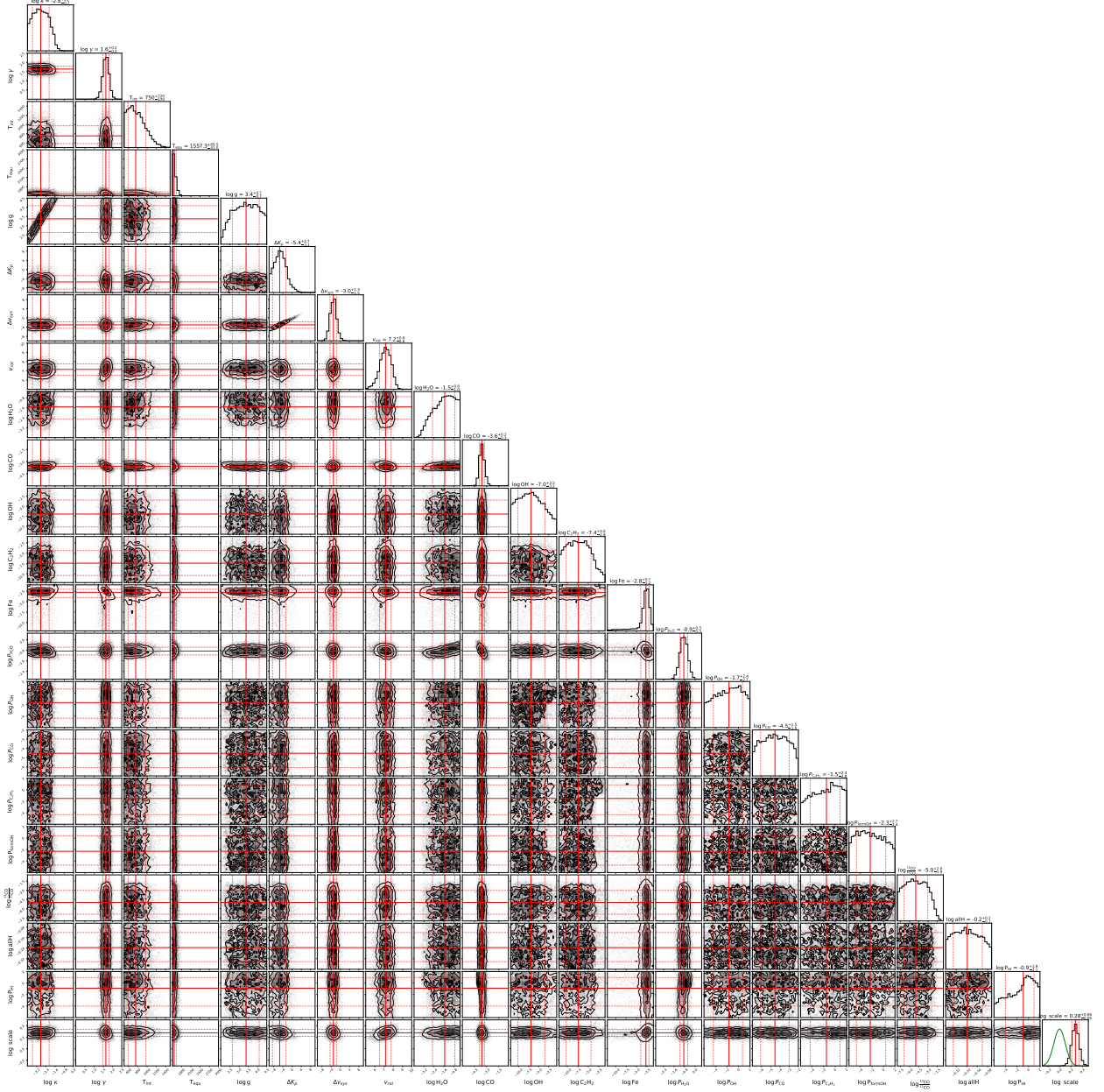


Figure 6.7: Corner plot for KELT-20 b, 4 PCs removed

Red solid lines indicate the medians, while red dashed lines indicate the bounds of the marginalized 68% confidence interval. We discuss these results in Section 6.3.

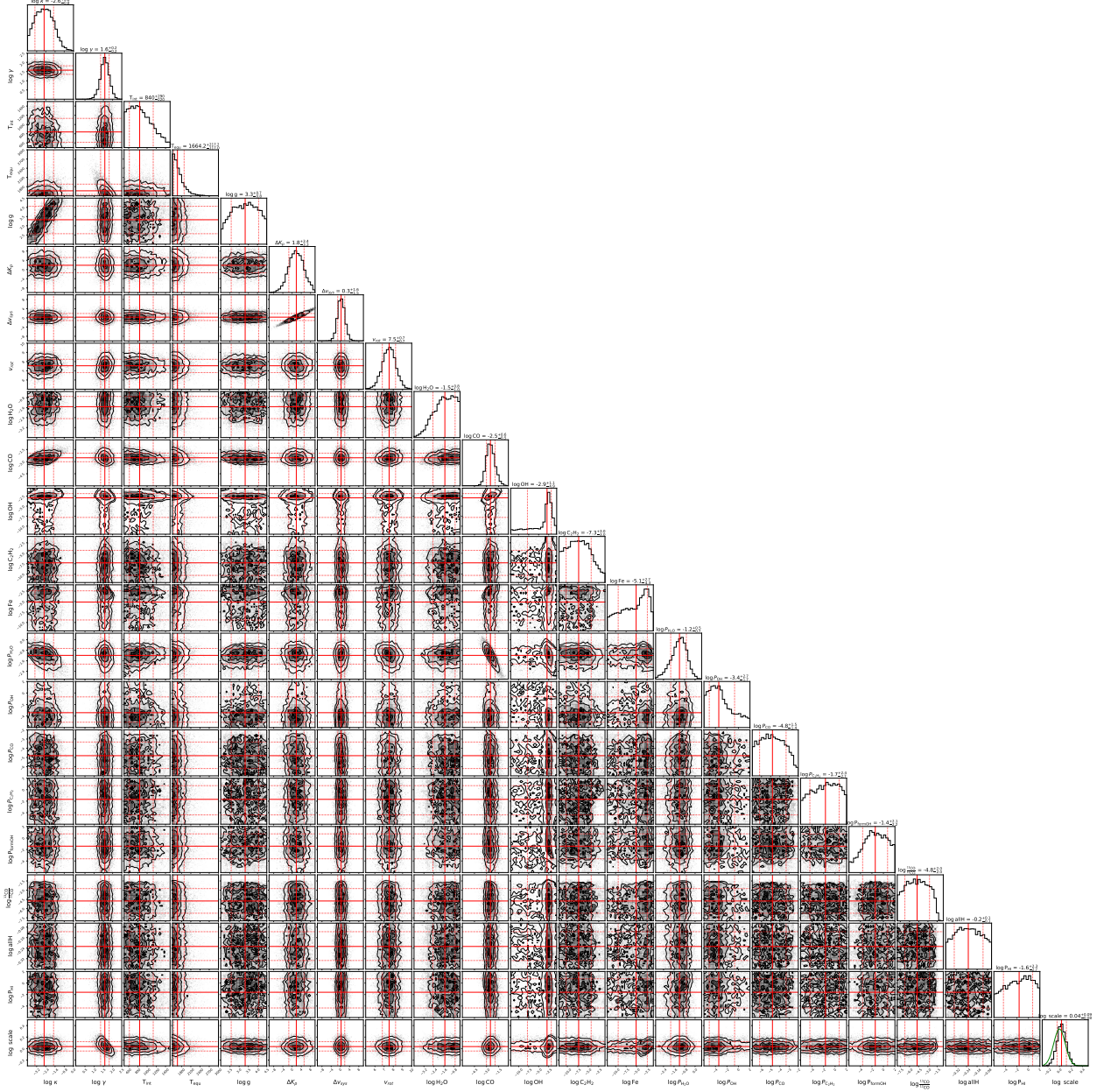


Figure 6.8: Corner plot for KELT-20 b, 6 PCs removed

Red solid lines indicate the medians, while red dashed lines indicate the bounds of the marginalized 68% confidence interval. We discuss these results in Section 6.3.

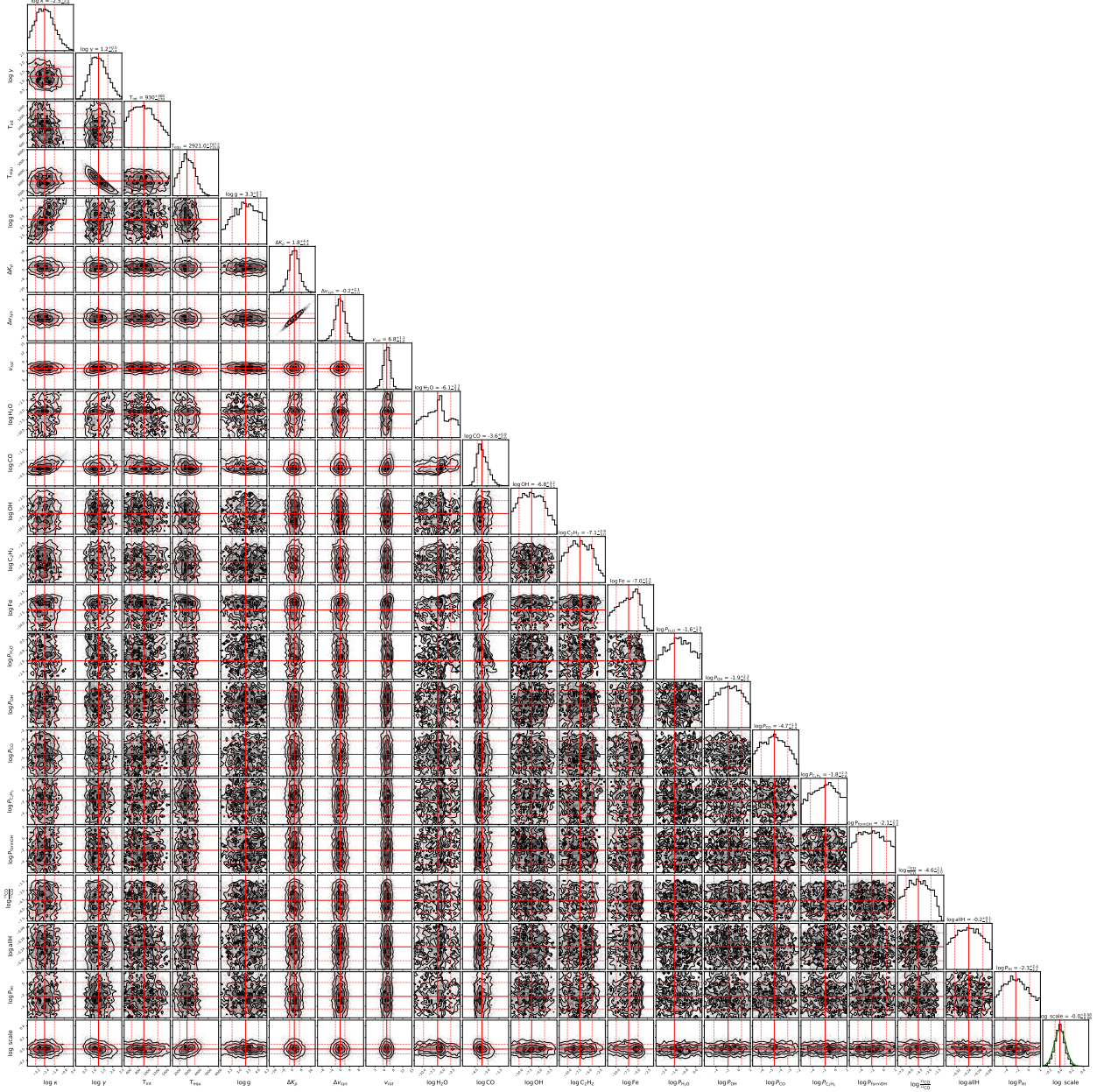


Figure 6.9: Corner plot for KELT-20 b, 8 PCs removed

Red solid lines indicate the medians, while red dashed lines indicate the bounds of the marginalized 68% confidence interval. We discuss these results in Section 6.3.



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CHAPTER 7

The watery atmosphere of HD 209458 b revealed by joint *K*- and *L*-band high-resolution spectroscopy

A version of this chapter has been submitted to the *Astronomical Journal* (Finnerty *et al.* 2025c)

Abstract

We present a joint analysis of high-resolution *K*- and *L*-band observations of the benchmark hot Jupiter HD 209458 b from the Keck Planet Imager and Characterizer (KPIC). One half night of observations were obtained in each bandpass covering similar pre-eclipse phases. The two epochs were then jointly analyzed using our atmospheric retrieval pipeline based on `petitRADTRANS` to constrain the atmospheric pressure-temperature profile and chemical composition. Consistent with recent results from *JWST* observations at lower spectral resolution, we obtain an oxygen-rich composition for HD 209458 b ($\text{C/O} < 0.1$ at 95% confidence) and a volatile metallicity roughly consistent with solar to within ~ 1 dex. Leveraging the large spectral grasp of the multi-band observations we constrain the H_2O mixing ratio to $\log \text{H}_2\text{O}_{\text{VMR}} = -3.2^{+1.1}_{-0.6}$, and obtain 95% upper limits on the atmospheric mixing ratios of CO ($< 10^{-4.3}$), CH_4 ($< 10^{-5.9}$), NH_3 ($< 10^{-6.4}$), H_2S ($< 10^{-4.6}$), and HCN ($< 10^{-5.7}$). The limits on CH_4 , NH_3 , and HCN are similar to recent results from *JWST* transmission spectroscopy, demonstrating the value of multi-band ground-based high resolution spectroscopy for precisely constraining trace species abundances in exoplanet atmospheres. The retrieved

low-C/O, moderate-metallicity composition for HD 209458 b is consistent with formation scenarios involving late accretion of oxygen-rich solid material.

7.1 Introduction

HD 209458 b was the first exoplanet to be detected via the transit technique (G. W. Henry et al., 2000). Its detection established that hot Jupiters are gas giants, the first example of exoplanet characterization. From this first discovery has followed a long history of characterization efforts, including the first atmospheric detection of an exoplanet via high-resolution cross-correlation spectroscopy (HRCCS, I. A. G. Snellen et al., 2010). Recently, HD 209458 b has been observed in transmission with *JWST*, revealing strong CO₂ and H₂O absorption features and a modestly metal-enriched, low-C/O ratio bulk composition (Q. Xue et al., 2024). Recent high-resolution transmission spectroscopy from CRRES+ has independently confirmed the low C/O ratio, moderately metal-enriched composition (D. Blain et al., 2024). These analyses have also ruled out significant quantities of C₂H₂ and CH₄, which were previously reported in HD 209458 b by P. Giacobbe et al. (2021), as well as HCN, which was previously reported by both P. Giacobbe et al. (2021) and G. A. Hawker et al. (2018).

HD 209458 b was observed as part of the KPIC *K*-band (2.1–2.5 μm) hot Jupiter survey, and again with KPIC in the *L* band (3.0–4.1 μm). These two bandpasses span strong spectral features of CO, H₂O, CH₄, NH₃, H₂S, and HCN, presenting an opportunity to obtain a comprehensive inventory of the expected volatile species in hot/warm Jupiter atmospheres and place constraints not just on the atmospheric C/O ratio, but also on S/O and N/O. Recent detections of H₂S (G. Fu et al., 2024; J. Inglis et al., 2024) and SO₂ (Z. Rustamkulov et al., 2023; D. Powell et al., 2024; A. Dyrek et al., 2024) have highlighted the importance of sulfur species as tracers of both photochemistry (S.-M. Tsai et al., 2023) and the planet formation process (D. Turrini et al., 2021; I. J. M. Crossfield, 2023). While clear detections of nitrogen species have remained elusive, models show that combining C/O and N/O ratios

can break degeneracies in the predicted formation location of gas giants (A. J. Cridland et al., 2020).

Additionally, the use of wide bandpasses appears to significantly improve the accuracy of HRCCS retrievals of atmospheric thermal structure. Retrievals using KPIC K -band data alone have often preferred pressure-temperature ($P-T$) profiles running substantially colder than expected (e.g. L. Finnerty et al., 2025b), typically counteracted by a scaling parameter > 1 . In contrast, retrievals from IGRINS, which covers the full H and K bands, have found $P-T$ profiles more in line with expectations (e.g. M. R. Line et al., 2021). This may be a result of the loss of continuum during the data processing for HRCCS analysis. For typical hot Jupiter temperatures, the K -band F_p/F_s changes relatively little with wavelength, and between the multiplicative scaling factor and the $P-T$ parameters there is sufficient degeneracy in retrieved parameters that errors in the absolute temperatures can be countered by changes in other parameters. Adding H or L band data introduces a much larger variation in F_p/F_s with wavelength, requiring an accurate temperature in order to match F_p/F_s over the entire range of observations.

Section 7.2 describes the observations, data reduction procedures, and atmospheric retrieval setup. Section 7.3 presents the results of our atmospheric retrievals. Section 7.4 discusses the retrieved composition in comparison to other studies of HD 209458 b. Section 7.5 concludes.

7.2 Observations and Data Reduction

7.2.1 Observations

HD 209458 was observed with Keck II/KPIC (I. S. McLean et al., 1998; E. C. Martin et al., 2018; R. A. López et al., 2020; J.-R. Delorme et al., 2021; D. Echeverri et al., 2022; N. Jovanovic et al., 2025a) on UT 29 June 2024 in K and on 21 August 2024 in L . Each epoch is summarized below.

Table 7.1: Stellar and planetary properties for the HD 209458 system

Property	Value	Ref.
HD 209458		
RA	22:03:10.81	Gaia Collaboration (2020)
Dec	+18:53:03	Gaia Collaboration (2020)
Sp. Type	G0V	
K_{mag}	6.31 ± 0.03	R. M. Cutri et al. (2003)
Mass	$1.07 \pm 0.05 M_{\odot}$	L. J. Rosenthal et al. (2021)
Radius	$1.155 \pm 0.02 R_{\odot}$	A. S. Bonomo et al. (2017)
T_{eff}	$6000 \pm 100 \text{ K}$	L. J. Rosenthal et al. (2021)
$\log g$ [cgs]	4.31 ± 0.03	L. J. Rosenthal et al. (2021)
$v \sin i$	$4.5 \pm 0.5 \text{ km s}^{-1}$	A. S. Bonomo et al. (2017)
v_{rad}	$-15.0 \pm 0.3 \text{ km s}^{-1}$	Gaia Collaboration (2020)
[Fe/H]	0.0 ± 0.06	L. J. Rosenthal et al. (2021)
HD 209458 b		
Period	$3.5247496 \pm 3 \times 10^{-7} \text{ days}$	A. Kokori et al. (2023)
T_{trans}	$\text{JD } 2455420.8446 \pm 2 \times 10^{-4}$	A. Kokori et al. (2023)
a [AU]	0.0463 ± 0.0007	L. J. Rosenthal et al. (2021)
i [deg]	$86^{\circ}.71 \pm 0^{\circ}.05$	A. Kokori et al. (2023)
K_{p}	147 km s^{-1}	Est.
Mass	$0.68 \pm 0.02 M_{\text{J}}$	A. S. Bonomo et al. (2017)
Radius	$1.36 \pm 0.02 R_{\text{J}}$	A. S. Bonomo et al. (2017)
T_{eq}	1450 K	Est.
C/O	< 0.1	This work
[C/H]	< -0.7	This work
[O/H]	$0.0^{+1.1}_{-0.7}$	This work

Note. — Limits are given at 95% confidence, and abundances are relative to M. Asplund et al. (2021) solar values.

7.2.1.1 *K* band

K band observations were obtained on UT 2024 June 29 from 10:52 to 15:18, covering a phase range of 0.431–0.483 and nominal planetary radial velocity ranging from 62 km s^{-1} to 16 km s^{-1} . We used a 120 second exposure time in order to stay under the detector non-linearity threshold, obtaining 105 frames on science fiber 4. Similar to previous KPIC *K*-band observations (L. Finnerty et al., 2025a,b), daytime calibration frames were used for background correction. The secondary eclipse is expected to begin at a $\phi = 0.479$, and we therefore omit the last 7 frames from subsequent analysis.

Conditions were good through most of the observations, aside from poor AO correction as HD 209458 transited zenith, impacting 3 exposures which we omit from subsequent analysis. Instrument throughput from the top of the atmosphere was $\sim 3 - 4\%$. Observations began as HD 209458 was rising, at an airmass of 1.36, decreasing to 1.0 at transit and increasing to 1.06 by the end of the sequence.

7.2.1.2 *L* band

L-band observations were obtained on UT 2024 August 21 from 6:05 to 10:25, covering a phase range of 0.412–0.462 and a nominal planetary radial velocity range from 77 km s^{-1} to 35 km s^{-1} . We used 60 second exposures to avoid non-linearity from thermal background, and used an ABBA nodding pattern between science fibers 2 and 4 in order to account for the large and variable background. A total of 90 frames were obtained for each fiber.

Conditions were poor throughout the observations, with $\sim 2''$ typical seeing and brief periods where AO correction failed entirely. We omit 18 science fiber 2 frames and 14 science fiber 4 frames with very poor throughput from the log-likelihood calculation. Observations began as HD 209458 was rising at an airmass of 2.06, and ended at an airmass of 1.0.

7.2.2 Data Reduction

Both epochs were reduced using the modified KPIC DRP¹ described in L. Finnerty et al. (2025a,b). For the *K*-band data, background subtraction was performed using afternoon calibration frames, while for the *L*-band data we performed an AB subtraction to account for variations in the slit background.

For wavelength calibration, we observed the red giants HIP 95771 (*K*-band) and HIP 81497 (*L*-band) prior to beginning observations of HD 209458. The *K*-band wavelength solution was fit using the KPIC DRP and manually checked against a stellar $\times$ telluric model to verify the accuracy of the wavelength solution in the 3 orders from 2.09–2.27 μm , which have relatively few strong lines for calibration. The included *K*-band data cover roughly 2.1 – 2.5 μm , with significant gaps. The wavelength coverage is shaded in Figure 7.2.

For the *L*-band wavelength solution, we first obtained an initial guess at the wavelength solution from the NIRSPEC Echelle Format Simulator, which was used to manually tune the coefficients of a 2nd-order polynomial for each order by comparing the observed spectrum to the stellar $\times$ telluric model. This was then input as the initial wavelength solution for the KPIC DRP scripts. However, the DRP scripts failed to produce a good solution for the three reddest orders (3.61–4.06 μm), which have relatively weak spectral features and relatively strong fringing effects. For these orders, we use a wavelength solution based on manually tuning polynomial coefficients to obtain a good match between the model telluric/stellar absorption features and the data. The included *L*-band data span roughly 3.05 – 4.05 μm , but with significantly larger gaps compared to the *K*-band data, as can be seen in Figure 7.2.

¹https://github.com/kpicteam/kpic_pipeline/

7.2.3 Atmospheric Retrieval

We use the retrieval pipeline described in [L. Finnerty et al. \(2023a, 2024, 2025a,b\)](#). The pipeline uses `petitRADTRANS` for radiative transfer ([P. Mollière et al., 2019, 2020](#); [E. Nasedkin et al., 2024](#)), and performs sampling using the `PyMultiNest` ([J. Buchner et al., 2014](#)) wrapper for `MultiNest` ([F. Feroz & M. P. Hobson, 2008](#); [F. Feroz et al., 2009, 2019](#)). A separate log-likelihood is calculated for each fiber on each night, which are then summed for the sampling. We used 800 live points and a convergence criteria of $\Delta \log z < 0.01$, similar to our previous retrievals.

In order to minimize the size of the opacity tables loaded into memory, separate radiative transfer objects are instantiated for the K and L bands. Each is instantiated identically except for a difference in wavelength boundaries. Further performance improvements could be achieved by loading only opacities with significant opacity in a given band, e.g. not loading CO opacity for the L -band radiative transfer object, but this has not yet been implemented.

We fit for mass-mixing ratios of H_2O , CO , CH_4 , NH_3 , H_2S , ^{13}CO , and H_2 . All abundances are fixed with pressure. For H_2O , we used the opacities based on the [O. L. Polyansky et al. \(2018\)](#) POKAZATEL linelist. For ^{12}CO , we used the high-temperature opacities described in [L. Finnerty et al. \(2023a\)](#) based on the HITEMP linelist ([I. E. Gordon et al., 2022](#)), while for ^{13}CO we use a lower-temperature opacity table based on [L. S. Rothman et al. \(2013\)](#). For CH_4 , we use the [R. J. Hargreaves et al. \(2020\)](#) linelist. For NH_3 , we use the [S. N. Yurchenko et al. \(2011\)](#) linelist. H_2S opacity is based on the [A. A. A. Azzam et al. \(2016\)](#) linelist, and HCN uses [G. J. Harris et al. \(2006\)](#). H_2 opacity is from [L. S. Rothman et al. \(2013\)](#). We also include $\text{H}_2 - \text{H}_2$ CIA opacity from [A. Borysow et al. \(2001\)](#); [A. Borysow \(2002\)](#) and $\text{H}_2 - \text{He}$ opacity from [J. Borysow et al. \(1988\)](#); [A. Borysow et al. \(1989\)](#); [A. Borysow & L. Frommhold \(1989\)](#).

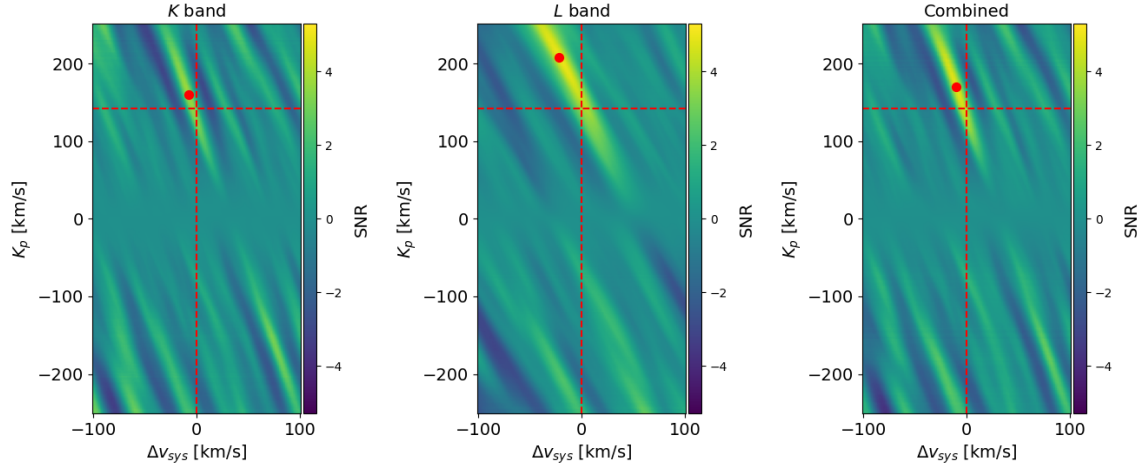


Figure 7.1: $K_p - \Delta v_{sys}$ plots for HD 209458 b

K -band (left), L -band (center) and combined (right) data sets correlated with the median retrieved planet model. HD 209458 b is detected independently in both K and L . The SNR is estimated by first median-subtracting each row of the $K_p - \Delta v_{sys}$ plots, then dividing by the standard deviation of the negative K_p region, which results in a slight offset of the maximum (indicated by a red dot) from the values in Table 7.2. See L. Finnerty et al. (2024, 2025b) for a more detailed discussion of the issues with estimating noise in $K_p - \Delta v_{sys}$ plots.

7.3 Results

Priors, maximum-likelihood parameters, and retrieved medians with $\pm 34\%$ confidence intervals are presented in Table 7.2. Our free-chemistry approach does not directly fit for atomic abundances or C/O, but we use the retrieved posteriors to construct posteriors for these parameters, and report the corresponding values in Table 7.2 as derived parameters. We present the results of the retrieval omitting 4 principal components. The medians and confidence intervals for the 6 and 8 component cases did not significantly differ from the values reported in Table 7.2. The full corner plots for all retrievals are included in Appendix 7.6. We also present $K_p - \Delta v_{sys}$ plots for each epoch and the combined data set in Figure 7.1, demonstrating that HD 209458 b is independently detected in both K and L bands at comparable strength.

Table 7.2: List of parameters, priors, and results for atmospheric retrievals

Name	Symbol	Prior	Max-L	Median
log infrared opacity [cm^2g^{-1}]	$\log \kappa$	Uniform($-4, 2$)	-2.8	$-2.3^{+0.9}_{-0.5}$
log infrared/optical opacity	$\log \gamma$	Uniform($-4, 0$)	-1.9	$-1.1^{+0.5}_{-0.6}$
Intrinsic temperature [K]	T_{int}	Uniform($10, 1500$)	960	360^{+370}_{-230}
Equilibrium temperature [K]	T_{equ}	Uniform($400, 3000$)	1300	1740^{+400}_{-440}
K_{p} offset [km s^{-1}]	ΔK_{p}	Uniform($-30, 30$)	-11.0	$0.2^{+17.4}_{-17.4}$
v_{sys} offset [km s^{-1}]	Δv_{sys}	Uniform($-15, 15$)	-2.1	$-5.1^{+4.2}_{-4.4}$
Rotational velocity [km s^{-1}]	v_{rot}	Uniform($0, 15$)	9.5	$10.0^{+2.0}_{-2.2}$
log H_2O mass-mixing ratio	$\log \text{H}_2\text{O}$	Uniform($-12, -0.3$)	-2.8	$-2.3^{+1.1}_{-0.6}$
log CO mass-mixing ratio	$\log \text{CO}$	Uniform($-12, -0.3$)	-3.5	$-7.7^{+2.8}_{-2.6} * (< -3.3)$
log CH_4 mass-mixing ratio	$\log \text{CH}_4$	Uniform($-12, -1$)	-7.5	$-8.5^{+2.2}_{-2.2} * (< -5.1)$
log NH_3 mass-mixing ratio	$\log \text{NH}_3$	Uniform($-12, -2$)	-6.9	$-8.6^{+2.2}_{-2.1} * (< -5.5)$
log H_2S mass-mixing ratio	$\log \text{H}_2\text{S}$	Uniform($-12, -2$)	-8.4	$-7.4^{+2.9}_{-2.9} * (< -3.4)$
log HCN mass-mixing ratio	$\log \text{HCN}$	Uniform($-12, -2$)	-10.6	$-8.3^{+2.4}_{-2.4} * (< -4.6)$
CO isotopologue ratio	$\log \frac{^{13}\text{CO}}{^{12}\text{CO}}$	Uniform($-8, -0.5$)	-3.7	$-4.2^{+2.4}_{-2.4} * (< -0.9)$
log H_2 mass-mixing ratio	$\log \text{H}_2$	Uniform($-0.4, -0.05$)	-0.4	$-0.2^{+0.1}_{-0.1}$
Scale factor	scale	LogNormal($0, 0.1$)	0.3	$0.0^{+0.1}_{-0.1}$
Derived Parameters				
Carbon/oxygen ratio	C/O	-	0.1	< 0.1
Carbon abundance	$[\text{C/H}]$	-	-1.0	< -0.7
Oxygen abundance	$[\text{O/H}]$	-	-0.3	$0.0^{+1.1}_{-0.7}$
Nitrogen abundance	$[\text{N/H}]$	-	-3.6	< -1.4
Sulfur abundance	$[\text{S/H}]$	-	-4.6	< 0.2
Volatile abundance	$[(\text{C}+\text{O})/\text{H}]$	-	-0.4	$-0.2^{+1.1}_{-0.7}$

Note. — Results are shown for the 6-component retrieval. The error bars correspond to the $68\%/1\sigma$ confidence interval. Limits are given at 95% confidence. A * indicates the marginalized posterior for a parameter spans the prior. In addition to these priors, we required that the atmospheric temperature stay below 4000 K at all pressure levels. The full corner plot is included in Appendix 7.6.

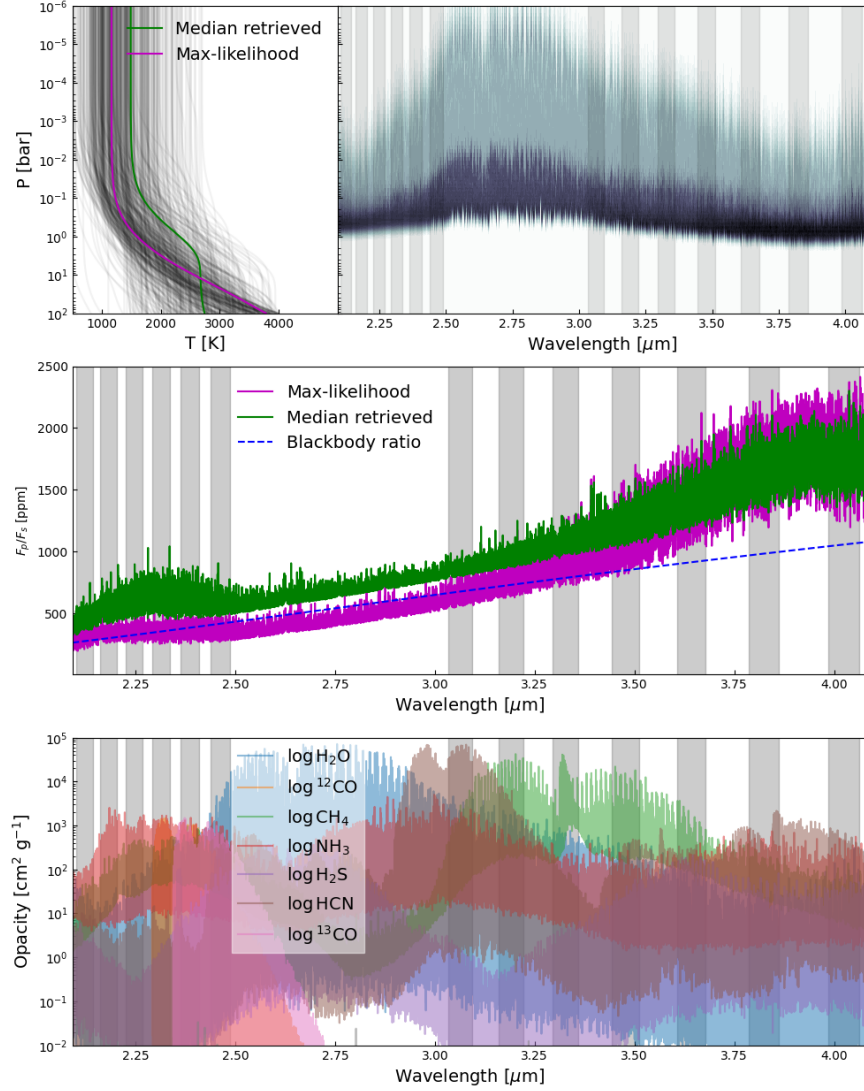


Figure 7.2: Retrieval plot for HD 209458 b

Top left: retrieved median and max-likelihood $P - T$ profiles, with 500 $P - T$ profiles drawn from the posterior in black. Top right: Maximum-likelihood emission contribution function, with observed orders shaded. Center: F_p/F_s for the maximum likelihood and median retrieved planet models, compared with the expected F_p/F_s assuming the planet and star are blackbodies at their respective equilibrium and effective temperatures. Observed orders are shaded. Bottom: Opacities of the species included in the retrieval over the observed bandpass.

7.3.1 Kinematics

The retrieved kinematics in Table 7.2 are consistent with no offset from the assumed ephemeris. Both epochs covered a similar pre-eclipse phase range and a relatively small velocity baseline of $\sim 40 \text{ km s}^{-1}$, leading to a degeneracy between the K_p and Δv_{sys} parameters (seen in Figure 7.1). Constraining dayside wind patterns will require significantly broader phase coverage in order to break the $K_p - \Delta v_{sys}$ degeneracy and separate ephemeris errors from the effects of global circulation.

The retrieval weakly constrains the rotational velocity, $v_{rot} = 10.0^{+2.0}_{-2.2} \text{ km s}^{-1}$. The expected rotational velocity of HD 209458 b assuming tidal locking is 2 km s^{-1} , which would imply a wind-driven rotational broadening of $\sim 9.8 \text{ km s}^{-1}$ assuming the rotational effects add in quadrature with the LSF and that the LSF model is accurate. However, as discussed in L. Finnerty et al. (2025a,b), our LSF model assumes a fixed factor of 1.14 in converting between the spatial and spectral instrument response profiles (L. Finnerty et al., 2022). This value has not been confirmed in the L band, and the NIRSPEC LSF in the L band is significantly broader than the K band. This suggests that the retrieved rotational broadening may be a result of instrumental broadening and LSF errors alone, rather than super-rotating winds in the atmosphere of HD 209458 b.

7.3.2 Pressure-temperature profile

We used the T. Guillot (2010) parameterization of the Pressure-Temperature ($P-T$) profile, consistent with our previous retrieval work (L. Finnerty et al., 2023a, 2024, 2025a,b). However, in contrast with L. Finnerty et al. (2025a,b), we do not fit for $\log g$ as a free parameter. The mass and radius of HD 209458 b are both well-constrained, and initial retrievals including $\log g$ found a strong degeneracy between $\log g$ and $\log \kappa$, resulting in no useful constraint on $\log g$. Similarly, we experimented with retrievals including a gray cloud opacity with the cloud opacity, cloud pressure, and f_{SED} as free parameters, but found the cloud parameters

were unconstrained.

While the median value for T_{equ} is somewhat higher than the calculated 1450 K equilibrium temperature of HD 209458 b, Figure 7.2 shows the resulting F_p/F_s is roughly consistent with the expected values assuming both star and planet are blackbodies. The maximum-likelihood $P - T$ profile is somewhat colder than the profile of the median parameters, but due to a larger value of the scale factor the final F_p/F_s in the maximum-likelihood model is similar to the median, a phenomenon previously seen in other HRCSS retrievals.

7.3.3 Molecular abundances

The retrieval returns bounded constraints on the H_2O abundance only, and upper limits on all other species. Table 7.2 presents the 95% upper limits on the mass-mixing ratios from the retrieval. The median retrieved H_2O abundance is consistent with a roughly oxygen abundance, with the posterior modestly skewed towards higher values.

If significant quantities of CH_4 were present in the atmosphere of HD 209458 b, it should result in significant absorption features in the three observed L -band orders from 3.2–3.5 μm . The apparent absence of these features results in a strong upper limit on the CH_4 mass fraction, $< 10^{-5.1}$ at 95% confidence. In contrast, the limit on the CO mass fraction is much looser, $< 10^{-3.3}$ at 95% confidence, and the maximum-likelihood CO abundance is close to this upper limit. The $\Delta \log \mathcal{L}$ in the maximum-likelihood model from including CO is 1.36, falling in the marginal range. This suggests the CO abundance may be just below the detection limit, and that wider K -band phase converge and/or higher spectral resolution would have resulted in a CO detection. The relatively high limit on CO leads to a maximum-likelihood C/O ~ 0.1 , and an upper limit C/O < 0.1 at 95% confidence.

As shown in Figure 7.2, the observed orders include strong opacity features from NH_3 at the blue end of the K band and HCN at either end of the L band. Despite these strong features, the retrieval prefers mass fractions $\lesssim 10^{-5}$ for both species. If these species are the

dominant gas-phase reservoirs of nitrogen, this would suggest significant depletion relative to solar. However, this does not account for nitrogen in condensed species and/or in gas species which were not included in the retrieval.

Despite significant opacity throughout the K and L bands, the retrieval analysis places only a weak constraint on the H_2S abundance. H_2S is never the dominant absorber at the wavelengths covered by our observations, and as a result the retrieved upper limit is relatively weak, $\text{H}_2\text{S} < 10^{-3.4}$ at 95% confidence. Significant quantities of H_2S may be present in the atmosphere of HD 209458 b, but would not have been detected in our observations.

7.3.4 Number of principal components

We performed retrievals omitting 4, 6, and 8 principal components. Full corner plots for all retrievals are included in Appendix 7.6. While in principle, the optimal number of omitted components is likely different between the K - and L -band epochs (and potentially between the two science fibers used in L), we omit the same number of components from each of the three time series for simplicity. Visual inspection of the residuals showed that omitting four or more components removed significant systematics for all orders of all three time series.

While the compositional constraints are very similar for all three retrievals, the F_p/F_s of the median and maximum-likelihood models increases significantly as additional components are omitted. This may be a result of increasing self-subtraction of the planet model as the number of components increases, and is part of our motivation for choosing the 4-component retrieval as our fiducial case. Self-subtraction is potentially a more significant issue for these observations compared with previous KPIC HRCCS retrievals due to the comparatively small ($\sim 40 \text{ km s}^{-1}$) velocity shift in each epoch compared with the $\sim 9 \text{ km s}^{-1}$ K -band resolution of NIRSPEC.

7.4 Discussion

7.4.1 Chemical composition and formation history

Comparing the retrieved molecular abundances with chemical equilibrium predictions from `easyCHEM` (E. Lei & P. Mollière, 2024) indicates the retrieved composition of HD 209458 b is broadly consistent with chemical equilibrium. The wide range of the H_2O posterior is compatible with a range of metallicities (in this case $[(\text{C}+\text{O})/\text{H}]$, rather than $[\text{Fe}/\text{H}]$) from $0.1 - 10\times$ solar, but the upper limit on the CO abundance requires a very low C/O ratio and/or relatively low metallicity. For metallicities $\gtrsim 5\times$ solar, the equilibrium H_2S abundance is greater than the retrieved 95% upper limit. However, photochemistry has been shown to destroy H_2S and produce SO_2 in hot Jupiter atmospheres S.-M. Tsai et al. (2023), suggesting that comparing H_2S abundances to equilibrium predictions may not be an accurate method to inferring metallicity or atmospheric sulfur abundance. The equilibrium abundance predictions for CH_4 , HCN , and NH_3 are all substantially below our retrieved upper limits. Disequilibrium chemistry involving these species may still be occurring in the atmosphere of HD 209458 b, if the resulting abundances are still below our detection limits.

The poor metallicity constraints retrieved from the data presented here limit inferences about the formation history of HD 209458 b. In general, C/O and metallicity are expected to be inversely correlated in core-accretion scenarios (e.g. N. Espinoza et al., 2017; N. Madhusudhan et al., 2017; A. J. Cridland et al., 2019). The low C/O ratio is consistent with formation scenarios that involve late accretion of solids or ices after most of the gas has been accreted (K. I. Öberg et al., 2011; N. Khorshid et al., 2022), which would also produce a stellar to slightly super-stellar metallicity, which is consistent with our retrievals and the metallicity obtained by Q. Xue et al. (2024)

7.4.2 Comparison to previous results

Previous results in the literature have typically provided molecular abundances as Volume Mixing Ratios (VMRs), rather than the mass-mixing ratios used in our retrieval pipeline. Assuming a mean molecular weight of 2.3 g/mol, the retrieved H₂O abundance corresponds to a $\log \text{H}_2\text{O}_{\text{VMR}} = -3.2^{+1.1}_{-0.6}$. The 95% upper limits correspond to $\log \text{CO}_{\text{VMR}} < -4.3$, $\log \text{CH}_4_{\text{VMR}} < -5.9$, $\log \text{NH}_3_{\text{VMR}} < -6.4$, $\log \text{H}_2\text{S}_{\text{VMR}} < -4.6$, and $\log \text{HCN}_{\text{VMR}} < -5.7$. Our retrieved 99.7%/3 σ upper limits on the VMR are $\log \text{CO}_{\text{VMR}} < -2.1$, $\log \text{CH}_4_{\text{VMR}} < -4.1$, $\log \text{NH}_3_{\text{VMR}} < -4.6$, $\log \text{H}_2\text{S}_{\text{VMR}} < -3.3$, and $\log \text{HCN}_{\text{VMR}} < -3.8$. Our broad wavelength coverage allows us to place these strict limits on the chemical composition of HD 209458 b with only two half nights of ground-based observations.

[Q. Xue et al. \(2024\)](#) reported somewhat stricter 3 σ upper limits of $\log \text{CH}_4_{\text{VMR}} < -5.6$, $\log \text{NH}_3_{\text{VMR}} < -4.2$, and $\log \text{HCN}_{\text{VMR}} < -5.1$ from *JWST* transmission observations. That work found a low C/O ratio and moderately enriched bulk metallicity which is consistent with the retrieval analysis presented here. This composition is also consistent with the results from [D. Blain et al. \(2024\)](#), who analyzed 4 transits of HD 209458 b observed with CRIRES+ in the *H*-band.

Previously, [P. Giacobbe et al. \(2021\)](#) reported detections of CO, HCN, CH₄, NH₃, and C₂H₂ in the atmosphere of HD 209458 b from GIANO high-resolution transmission observations, which cover 0.95 – 2.45 μm . [G. A. Hawker et al. \(2018\)](#) reported detections of H₂O, CO, and HCN from a combination of *K*- and *L*-band data, and [I. A. G. Snellen et al. \(2010\)](#) reported a detection of CO in the *K*-band. However, both [C. J. Cheverall et al. \(2023\)](#) and [D. Blain et al. \(2024\)](#) recently detected only H₂O in the atmosphere of HD 209458 b, consistent with our analysis and with the results presented in [Q. Xue et al. \(2024\)](#).

In our analysis, the non-detection of CO is likely due to the limited phase coverage of our observations combined with relatively weak CO features in the low C/O atmosphere of HD 209458 b. Our observations covered a velocity shift only $\sim 4.5\times$ the spectral resolution of

the KPIC/NIRSPEC system, and the regular structure of the $2.3\mu\text{m}$ CO bandhead may make CO features particularly vulnerable to self-subtraction during PCA, potentially explaining the weak upper limit on the CO abundance in our retrievals. The spectral resolution of the observations presented by [I. A. G. Snellen et al. \(2010\)](#) was approximately $3\times$ greater than our observations, with much better ability to detect CO as a result.

In the case of HCN, [A. B. Savel et al. \(2025\)](#) recently demonstrated that HCN may be particularly vulnerable to false positive detections in high-resolution spectroscopy. The CH_4 and NH_3 detections reported in [P. Giacobbe et al. \(2021\)](#) may similarly be false positives as a result of detrending procedures. As previously discussed in [C. J. Cheverall et al. \(2023\)](#) and [D. Blain et al. \(2024\)](#), detrending procedures based on optimizing the detected planet signal, such as those used in both [G. A. Hawker et al. \(2018\)](#) and [P. Giacobbe et al. \(2021\)](#), significantly increase the risk of false positive molecular detections. Alternatively, these species could be temporarily present in detectable abundances as a result of stellar activity driving surges in photochemical reactions. Detection this phenomenon would require monitoring of stellar activity in HD 209458 and the capability to rapidly observe HD 209458 b with high-resolution spectroscopy if an increase in stellar activity is detected.

7.5 Summary and Conclusions

We performed a joint retrieval analysis on two epochs of KPIC observations of HD 209458 b, covering pre-eclipse phases in both K and L bands. This analysis prefers a low C/O ratio (< 0.1 at 95% confidence), and metallicity within ~ 1 dex of solar. These results are consistent with low-resolution transmission spectroscopy from *JWST* ([Q. Xue et al., 2024](#)). The wide wavelength coverage of our observations enable us to place strict upper limits on the abundances of CH_4 , NH_3 , H_2S , and HCN with only two half nights of observations. These limits are consistent with recent results from *JWST* and CRIRES+ in transmission, but in tension with previous ground-based high-resolution detections of these species, which

took more aggressive approaches to detrending. The retrieved composition of HD 209458 b is broadly consistent with chemical equilibrium, and the low C/O ratio is consistent with significant accretion of oxygen-rich planetesimals late in the planet formation process.

7.6 Corner Plots

Figures 7.3, 7.4, and 7.5 present the full corner plots from the retrievals with 4, 6, and 8 principal components omitted, respectively.

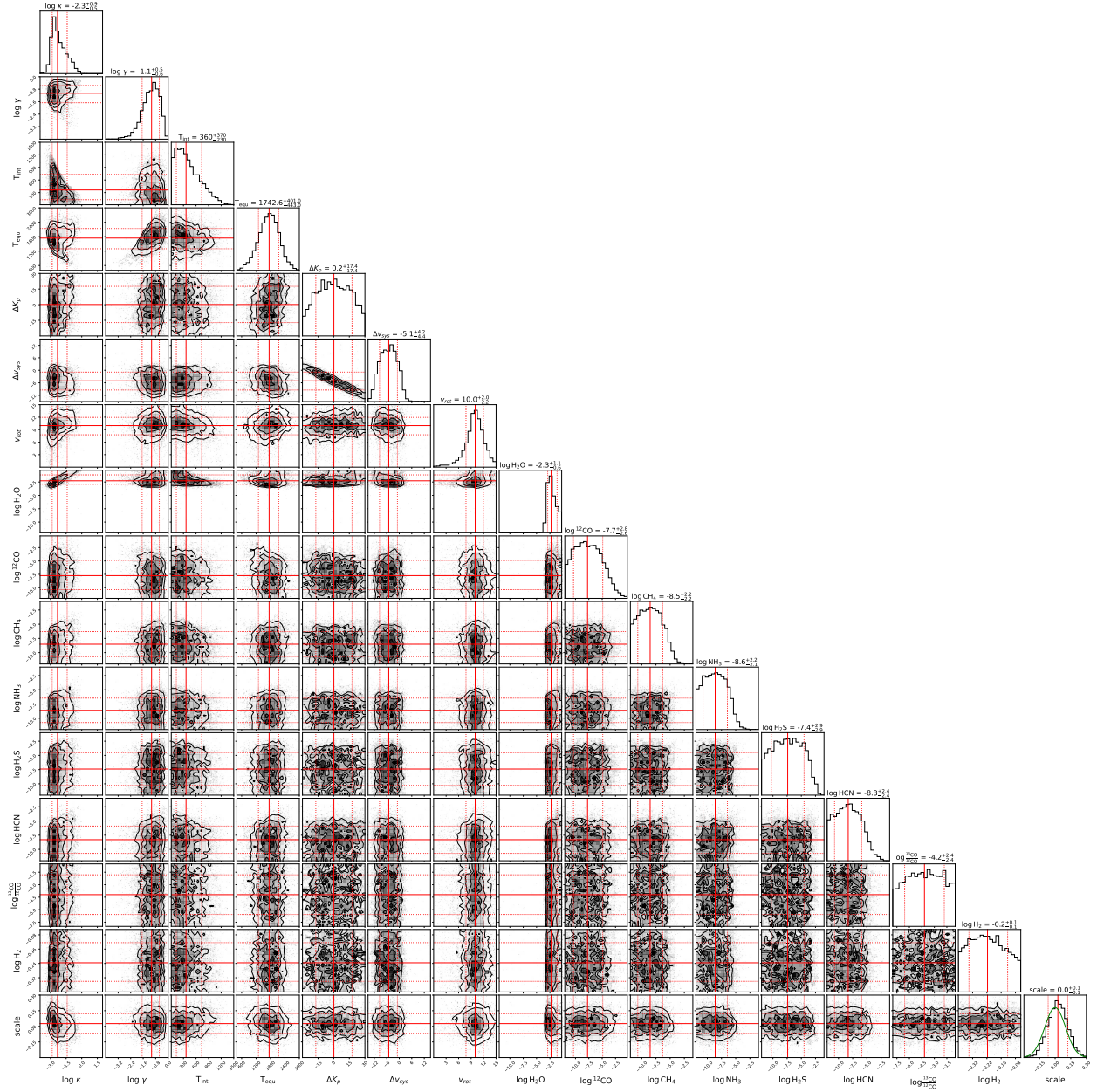


Figure 7.3: Full corner plot for the 4-component retrieval.

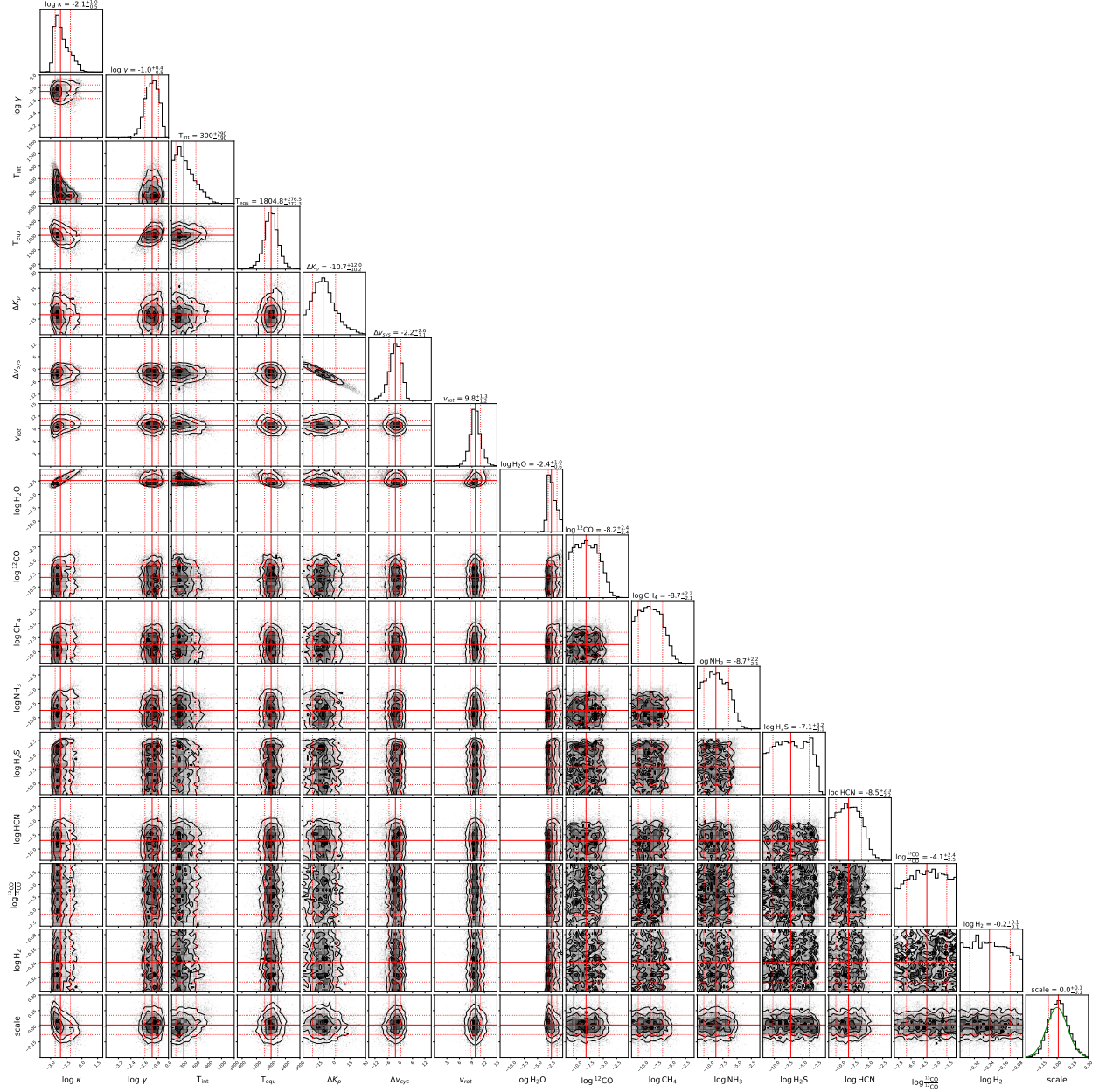


Figure 7.4: Full corner plot for the 6-component retrieval.

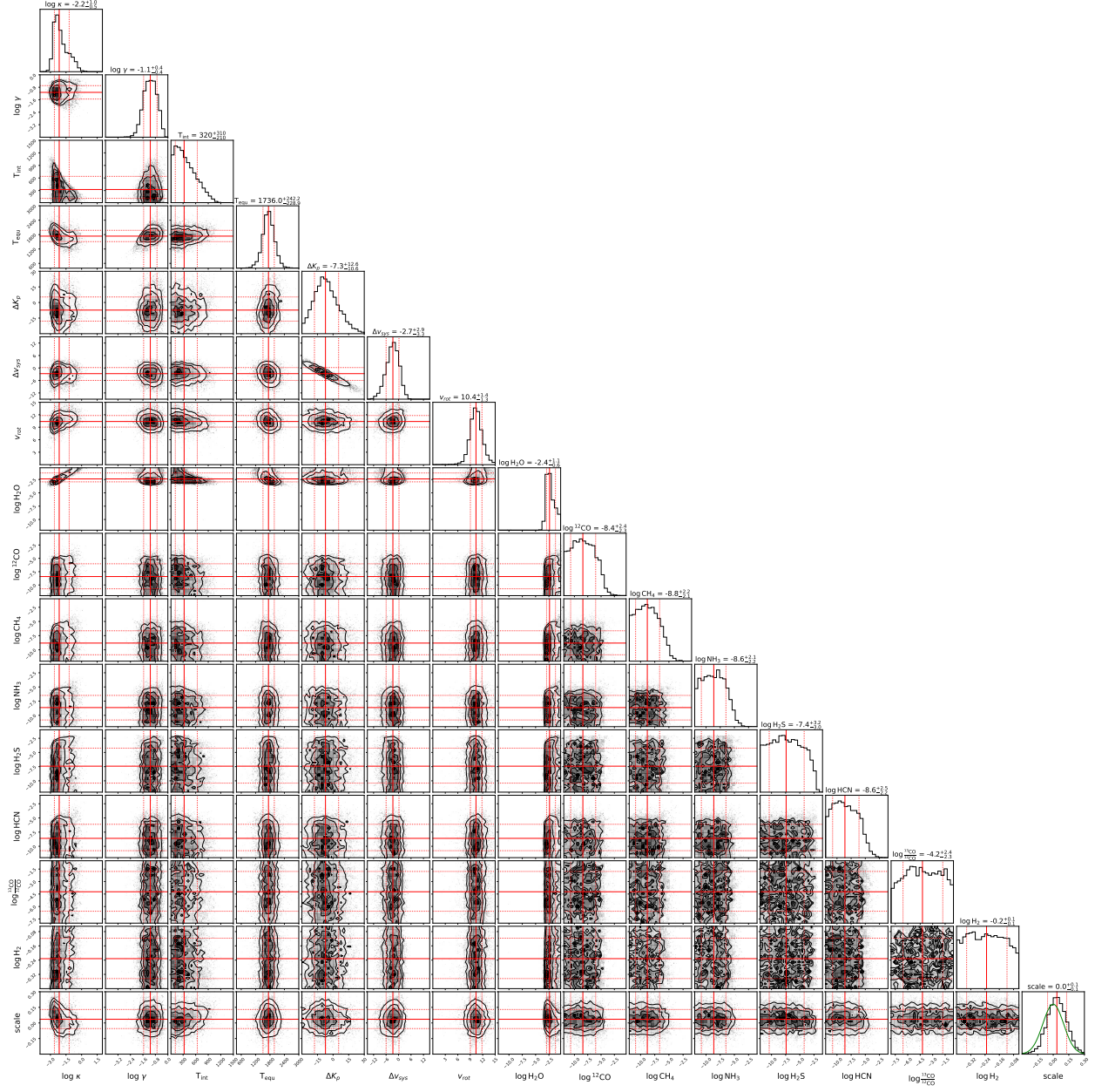


Figure 7.5: Full corner plot for the 8-component retrieval.

CHAPTER 8

Limits On the Post-eclipse Emission Spectrum of HD 80606 b From High-Resolution Spectroscopy

A version of this chapter is in preparation for submission to the *Astronomical Journal* (Finnerty *et al.* 2025d)

Abstract

We present Keck/NIRSPEC K -band observations of HD 80606 b, one of the most eccentric known exoplanets. HD 80606 b was observed after secondary eclipse, close to periastron, when the planet passes within 0.03 AU of HD 80606 and the rapid heating of the atmosphere may lead to extreme chemical changes. The rapid change in the planetary radial velocity near periastron is sufficient to enable high-resolution cross-correlation spectroscopy (HRCCS) analysis. We perform atmospheric retrievals with free parameters for the Pressure-Temperature ($P - T$) profile and with a profile matched to recent *JWST* results. In both cases, the retrieval provides weak constraints or upper limits on the abundances of H_2O , CO , and CH_4 , but the maximum-likelihood planet model is not significantly detected ($\text{SNR} \sim 3$). These results are consistent with recent *JWST* results which found the post-eclipse atmosphere of HD 80606 b shows only weak absorption features, and reject predictions of a strong thermal inversion near periastron from Global Circulation Models (GCMs). Future observations with higher spectral resolution and/or wider wavelength coverage are needed to confirm this tentative atmospheric detection, but such observations are a challenge to schedule due

to the 111-day period of HD 80606 b.

8.1 Introduction

For many years HD 80606 b held the record for the most highly eccentric planet. Discovered by the radial velocity (RV) technique in 2001 (D. Naef et al., 2001), HD 80606 b has a mass of $4.1 M_{Jup}$, an orbital period of 111.4 days and an eccentricity of $e=0.93$. HD 80606 b continues to be compelling for further study as it was discovered by Spitzer to be eclipsing (G. Laughlin et al., 2009), passing within 0.03 AU of its host G5V star. During its rapid periastron passage of a few tens of hours, the insolation increases a thousand-fold and the equilibrium temperature rises from 400 K to 1400 K (Figure 8.2a) providing a unique opportunity to explore the dynamical response of an atmosphere under an extreme external forcing function. Spitzer’s photometric observations of eclipses in 2009 and 2010 at 8.0 and 4.5 μm , respectively, were used to infer timescales for radiative, dynamical, and chemical processes (J. de Wit et al., 2016; N. K. Lewis et al., 2017).

Two approved JWST Cycle 1 programs have or will make spectroscopic observations around the eclipse of HD 80606 b (which is conveniently oriented a few hours before periapsis) and are poised to exploit this highly variable environment to study a wide variety of atmospheric properties, including composition, chemical and dynamical timescales, and large scale atmospheric motions.

The JWST observations will cover two separate eclipses. MIRI LRS (5-12 μm & $R\sim 40\text{-}150$) observations obtained on 2025-April-11 (T. Kataria, PI; PID#2008) will constrain the internal heating of HD 80606b, probe variations in clouds and chemistry throughout HD 80606 b’s orbit, and assess the role of dynamical mixing in HD 80606 b’s atmosphere. A second team (J. Sikora, PI; PID#2488) used NIRSpec (3-5 μm & $R\sim 2700$) on 2022-Nov-1 to explore the formation and evolution of atmospheric clouds, which are expected to vary rapidly due to evaporation & sublimation.

This paper reports results from a well placed eclipse on 2024-Jan-21 (UT) using NIRSPEC in K-band on the Keck-II telescope to complement the JWST observations with new wavelengths obtained with much higher spectral resolution ($R \sim 30,000$).

In addition to exploring a different set of wavelengths from JWST (Figure 8.1), NIRSPEC’s higher spectral resolution has two major advantages compared with JWST’s lower resolution, higher sensitivity data. First, high resolution spectroscopy has been very successful at unambiguously identifying (or excluding) key carbon- and oxygen-bearing species in exoplanet atmospheres by resolving large numbers of individual molecular absorption or emission lines (e.g. [M. R. Line et al., 2021](#); [L. Finnerty et al., 2023a](#), Finnerty et al., *subm.*). In contrast, overlapping spectral features from different molecules or narrow-line absorption from molecules such as CO can make unambiguous identification of some molecules difficult with low-resolution spectroscopy ([L. Welbanks et al., 2025](#)). Keck II/NIRSPEC, as the spectrometer used for KPIC, has a proven track record of detecting and characterizing exoplanet atmospheres via high-resolution spectroscopy ([L. Finnerty et al., 2023a, 2024, 2025a,b](#), *subm.*)

Secondly, high spectral resolution observations can also resolve atmospheric dynamics such as winds and planet rotation (e.g. [I. A. G. Snellen et al., 2010](#); [D. Ehrenreich et al., 2020](#); [A. Y. Kesseli et al., 2022](#); [F. Lesjak et al., 2023](#)). In the case of HD 80606 b, the precise ephemerides from [K. A. Pearson et al. \(2022\)](#) can be used to precisely calculate the planet’s velocity and provide a basis for measuring excess red or blueshifts of the planet signal in emission. Tidally locked hot Jupiters on average show an excess net blueshift of $2 - 5 \text{ km s}^{-1}$, which is caused by atmospheric dynamics and attributed to a global day-to-night wind in the atmospheres (e.g. [I. A. G. Snellen et al., 2010](#)). Measuring velocity shifts in HD 80606 b would help to constrain global circulation models (GCMs) for eccentric hot planets.

Table 8.1: Stellar and planetary properties for the HD 80606 system

Property	Value	Ref.
RA	09:22:37.67	Gaia Collaboration (2020)
Dec	+50:36:13.6	Gaia Collaboration (2020)
Sp. Type	G5	
K_{mag}	7.32 ± 0.02	R. M. Cutri et al. (2003)
K_s [m s ⁻¹]	469.22 ± 0.61	K. A. Pearson et al. (2022)
Mass [M _⊙]	1.05	K. A. Pearson et al. (2022)
Radius [R _⊙]	1.05 ± 0.01	K. A. Pearson et al. (2022)
T _{eff} [K]	5565 ± 92	L. J. Rosenthal et al. (2021)
log g [cgs]	4.4 ± 0.03	L. J. Rosenthal et al. (2021)
$v \sin i$ [km s ⁻¹]	1.8 ± 0.5	A. S. Bonomo et al. (2017)
v_{rad} [km s ⁻¹]	4.16 ± 0.37	Gaia Collaboration (2020)
[Fe/H]	0.36 ± 0.18	N. R. Hinkel et al. (2014)
[C/H]	0.33 ± 0.10	N. R. Hinkel et al. (2014)
[O/H]	0.19 ± 0.11	N. R. Hinkel et al. (2014)
HD 80606 b		
Period [day]	111.436765 ± 0.000074	K. A. Pearson et al. (2022)
T _{transit} [BJD]	$2458888.07466 \pm 0.00204$	K. A. Pearson et al. (2022)
T _{peri} [BJD]	2458882.344 ± 0.0021	K. A. Pearson et al. (2022)
a [AU]	0.4603 ± 0.0021	K. A. Pearson et al. (2022)
e	0.93183 ± 0.00014	K. A. Pearson et al. (2022)
ω	$-58.887^\circ \pm 0.043$	K. A. Pearson et al. (2022)
i	$89.24^\circ \pm 0.01$	K. A. Pearson et al. (2022)
K_p [km s ⁻¹]	122	Calc.
Mass [M _J]	4.1641 ± 0.0047	K. A. Pearson et al. (2022)
Radius [R _J]	1.032 ± 0.015	K. A. Pearson et al. (2022)

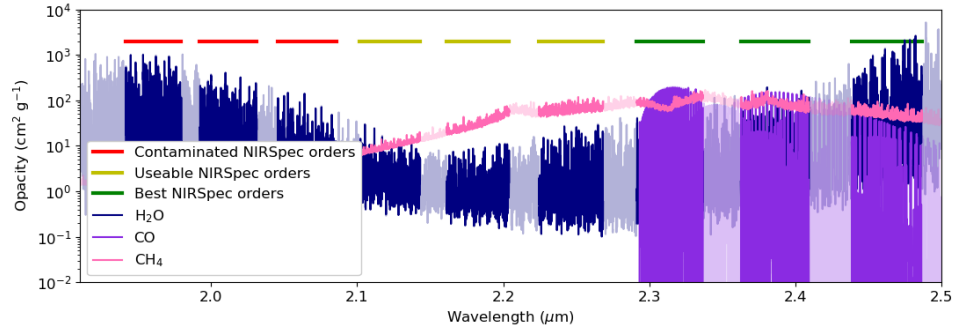


Figure 8.1: Opacities of the dominant species in the NIRSPEC K-band spectral region

NIRSPEC contains 9 spectral orders in the K-band region, 6 of which can be calibrated and used in our analysis (3 are highly contaminated). H_2O , CO , and CH_4 all contain major bandheads within this spectral region and so we expect to be able to detect them, if they are present.

8.2 Observations and Data Reduction

8.2.1 Observations

We observed HD 80606 using Keck II/NIRSPEC (I. S. McLean et al., 1998; E. C. Martin et al., 2018; R. A. López et al., 2020) on 2024 January 21 from 6:16 to 15:20 UT. We had originally proposed to perform these observations using Keck II/KPIC (J.-R. Delorme et al., 2021; N. Jovanovic et al., 2025b), but switched to the seeing-limited mode NIRSPEC due to instrument scheduling conflicts. As NIRSPEC is the spectrometer used in KPIC, this does not impact the wavelength coverage or spectral resolution of the observations. Using the slit-fed mode results in a significant ($\sim 6\times$) throughput increase, at the cost of reduced wavelength/blaze stability and increased sky background.

The observations included a complete secondary eclipse from approximately 8:30 to 10:30 UT. The pre-eclipse observations were taken at high airmass (2.83–1.52), leading to significantly worse signal-to-noise (SNR) compared with the post-eclipse observations, which ranged in airmass from 1.16–1.4 as HD 80606 set. High clouds caused significant (> 2 mag) extinction beginning around 14:20 UT. All exposures were taken with a 60 second integration time with HD 80606 in the center of the $0.288'' \times 24''$ slit and the Kband-new filter.

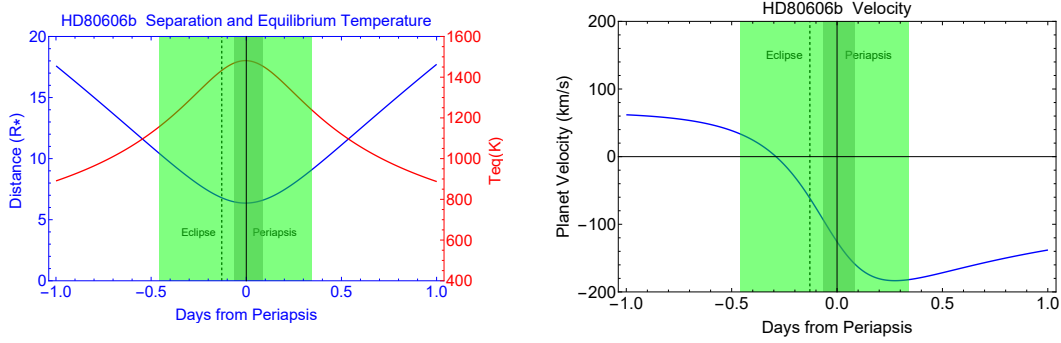


Figure 8.2: Observed separation and velocity of HD 80606 b

(left) The blue curve shows the separation of HD 80606 b from its host star in units of the stellar radius as a function of time immediately before and after periapsis. The eclipse midpoint is a few hours earlier and is denoted by a dashed black line. The red curve is an illustrative equilibrium temperature for the planet driven only by instantaneous insolation based on the square root of its distance from the star consistent with the observations of (G. Laughlin et al., 2009). The green shaded region shows the coverage of the J. T. Sikora et al. (2024) *JWST* observations, and the grey shaded region shows the approximate times of the NIRSPEC observations presented here. right) The velocity of the planet in km s^{-1} . Values are derived from the model and parameters described in K. A. Pearson et al. (2022).

As a result of the high airmass negatively impacting the pre-eclipse frames and the significant cloud coverage in the last hour, we restrict our subsequent analysis to the 180 post-eclipse frames obtained between 10:45 and 14:20 UT. The phase, temperature, and velocity coverage of these observations is illustrated in Figure 8.2.

8.2.2 Data Reduction

The data were reduced using a modified version of the KPIC DRP as described in L. Finnerty et al. (2025a,b), with minor alterations to address the increase in sky background when using slit-fed NIRSPEC compared with KPIC. While the KPIC fibers are fixed in the NIRSPEC slit, in slit-fed mode the science target can move along the slit over the observation sequence, leading to variations in the blaze function and wavelength solution from frame to frame. The slit also results in significantly greater sky background compared to the fiber feed, including

noticeable telluric emission features.

To minimize the wavelength and blaze variations, we obtained our observations in staring mode. Dark current was removed using afternoon dark frames. We then corrected for sky emission during the flux extraction by performing subtracting the the out-of-trace background in the dark-subtracted frame determined by averaging 10 pixels each above and below the trace.

Similar to the KPIC observing procedure (e.g. [L. Finnerty et al., 2023a](#)), we observed several late-type giant stars for wavelength calibration. However, because the wavelength solution varies along the NIRSPEC slit, we used these targets only for a rough calibration. We then used the resulting wavelength solution as a starting point to refit a final wavelength solution to the coadded spectrum of HD 80606. This process resulted in a good wavelength solution for all 9 orders on the NIRSPEC detector. However, orders 37–39 (1.94–2.09 μm) are heavily contaminated by telluric absorption features and omitted from subsequent analysis, leaving orders 31–36 covering 2.1–2.48 μm .

8.2.3 Retrieval analysis

We use the cross-correlation/retrieval analysis pipeline developed for the KPIC hot Jupiter survey ([L. Finnerty et al., 2023a, 2024, 2025a,b](#)), which uses `petitRADTRANS` for radiative transfer calculations ([P. Mollière et al., 2019, 2020](#); [E. Nasedkin et al., 2024](#)) and the `PyMultiNest` ([J. Buchner et al., 2014](#)) wrapper for `MultiNest` ([F. Feroz & M. P. Hobson, 2008](#); [F. Feroz et al., 2009, 2019](#)) to perform Nested Sampling ([J. Skilling, 2004](#)). Sampling was performed with 1200 live points to a convergence criteria $\Delta \log z < 0.01$.

Despite noticeably larger frame-to-frame blaze function variations compared with KPIC data, we find that the latest update to the standard KPIC detrending procedure described in Finnerty et al., *subm.* is sufficient to remove systematics from the time series. This procedure consists of masking the first/last 50 pixels of each order and the 3% of remaining

Table 8.2: List of parameters, priors, and results for atmospheric retrievals

Name	Symbol	Prior	Max-L	Median
Fixed $P - T$ profile				
K_p [km s ⁻¹]	ΔK_p	Uniform(-40,40)	3.8	$-4.2^{+5.8}_{-8.5}$
v_{sys} offset [km s ⁻¹]	Δv_{sys}	Uniform(-10,10)	9.2	$3.0^{+4.7}_{-7.0}$ *
Rotational velocity [km s ⁻¹]	v_{rot}	Uniform(0,15)	0.1	$4.8^{+6.5}_{-3.3}$ *
log H ₂ O mass-mixing ratio	log H ₂ O	Uniform(-10,-0.5)	-2.1	$-2.1^{+0.4}_{-0.7}$
log CO mass-mixing ratio	log CO	Uniform(-10,-0.5)	-3.3	$-5.3^{+2.2}_{-3.0}(< -2.2)$
log CH ₄ mass-mixing ratio	log CH ₄	Uniform(-10,-0.5)	-7.3	$-7.2^{+1.8}_{-1.8}(< -4.6)$
log H ₂ mass-mixing ratio	log H ₂	Uniform(-0.4,-0.05)	-0.4	$-0.3^{+0.1}_{-0.1}$ *
Free $P - T$ profile				
log infrared opacity [cm ² g ⁻¹]	log κ	Uniform(-4,2)	1.8	$1.2^{+0.4}_{-0.5}$
log infrared/optical opacity	log γ	Uniform(-2,0)	-1.9	$-1.7^{+0.1}_{-0.2}$
Intrinsic Temperature [K]	T_{int}	Uniform(10,200)	40	$50^{+30}_{-30}(< 110)$
Equilibrium temperature [K]	T_{equ}	Uniform(800,1800)	1420	$1580^{+130}_{-150}(> 1370)$
K_p [km s ⁻¹]	K_p	Uniform(-40,40)	-2.9	$-0.4^{+5.9}_{-4.5}$
v_{sys} offset [km s ⁻¹]	Δv_{sys}	Uniform(-10,10)	-6.6	$-2.5^{+6.4}_{-4.5}$ *
Rotational velocity [km s ⁻¹]	v_{rot}	Uniform(0,15)	3.5	$7.7^{+3.7}_{-4.5}$ *
log H ₂ O mass-mixing ratio	log H ₂ O	Uniform(-10,-0.5)	-3.6	$-4.0^{+0.5}_{-0.5}$
log CO mass-mixing ratio	log CO	Uniform(-10,-0.5)	-3.3	$-4.4^{+0.7}_{-2.8}(< -3.4)$
log CH ₄ mass-mixing ratio	log CH ₄	Uniform(-10,-0.5)	-2.6	$-6.6^{+2.0}_{-2.0}(< -3.7)$
log H ₂ mass-mixing ratio	log H ₂	Uniform(-0.4,-0.05)	-0.3	$-0.3^{+0.1}_{-0.1}$ *

Note. — Additionally, we require the atmospheric temperature stay below 3500 K at all pressure levels. * indicates the retrieved marginalized posterior spans the prior range, and limits are given at 95% confidence when a parameter runs against the prior bound. The full corner plots are shown in Appendix 8.6.

channels with the highest variance. This is then followed by a 4σ clip and then dropping 4-8 Principal Components (PCs). We primarily present the results from the 6-component analysis, and discuss the impact of the number of omitted PCs in Section 8.4.

The full set of retrieved parameters and priors is listed in Table 8.2. We fit for fixed-with-altitude mass-mixing ratios of H_2O , CO , CH_4 , and H_2 . For H_2O , we used the opacities based on the O. L. Polyansky et al. (2018) POKAZATEL linelist. For CO , we used the HITEMP linelist (I. E. Gordon et al., 2022). For CH_4 , we use the R. J. Hargreaves et al. (2020) linelist. H_2 opacity is from L. S. Rothman et al. (2013). We also include $\text{H}_2 - \text{H}_2$ CIA opacity from A. Borysow et al. (2001); A. Borysow (2002) and $\text{H}_2 - \text{He}$ opacity from J. Borysow et al. (1988); A. Borysow et al. (1989); A. Borysow & L. Frommhold (1989). We do not include cloud opacity, as high-resolution spectroscopy is not generally sensitive to the resulting broadband continuum effects. We present one retrieval using the pressure-temperature ($P - T$) profile parameterization from T. Guillot (2010), and a second using a fixed $P - T$ profile with parameters chosen to match the results presented in J. T. Sikora et al. (2024). While high-resolution retrieval studies have generally included an overall scaling factor applied to the planet model following M. R. Line et al. (2021), we found that even with a restrictive prior our retrievals preferred extreme values of this parameter. We therefore fixed this value to 1 for the retrievals presented here.

8.3 Results

8.3.1 Cross-correlation results

Figure 8.3 presents the cross-correlation as a function of velocity and frame number for the maximum-likelihood model from each retrieval, as well as the summed 1D cross-correlation in the nominal rest frame of HD 80606 b. For both models, the 2D cross-correlation plot does not show an obvious track following the expected planetary velocity, nor evidence of significant cross-talk in the stellar or telluric reference frames. Summing over the entire time

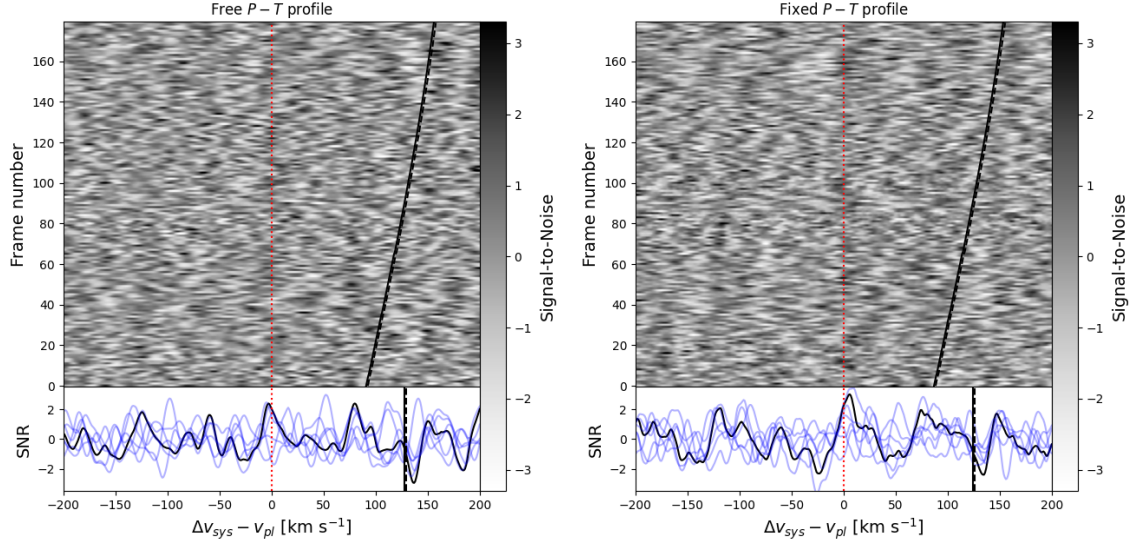


Figure 8.3: Cross-correlation time series for HD 80606 b

Cross-correlation versus frame number (top) and coadded in the nominal reference frame of HD 80606 b (bottom) for the maximum-likelihood models from both the free $P - T$ retrieval (left) and fixed $P - T$ retrieval (right). The nominal planet rest frame is indicated in dashed red, and the stellar and telluric reference frame in solid and dashed black, respectively. Individual orders are shown in the lower panel in blue, and the average of all orders in black. In neither case is the planet track clear in the 2D cross-correlation plots, but in both cases a weak feature is seen after coadding over the time series. This feature does not dominate the overall cross-correlation space, indicating a tentative detection at best.

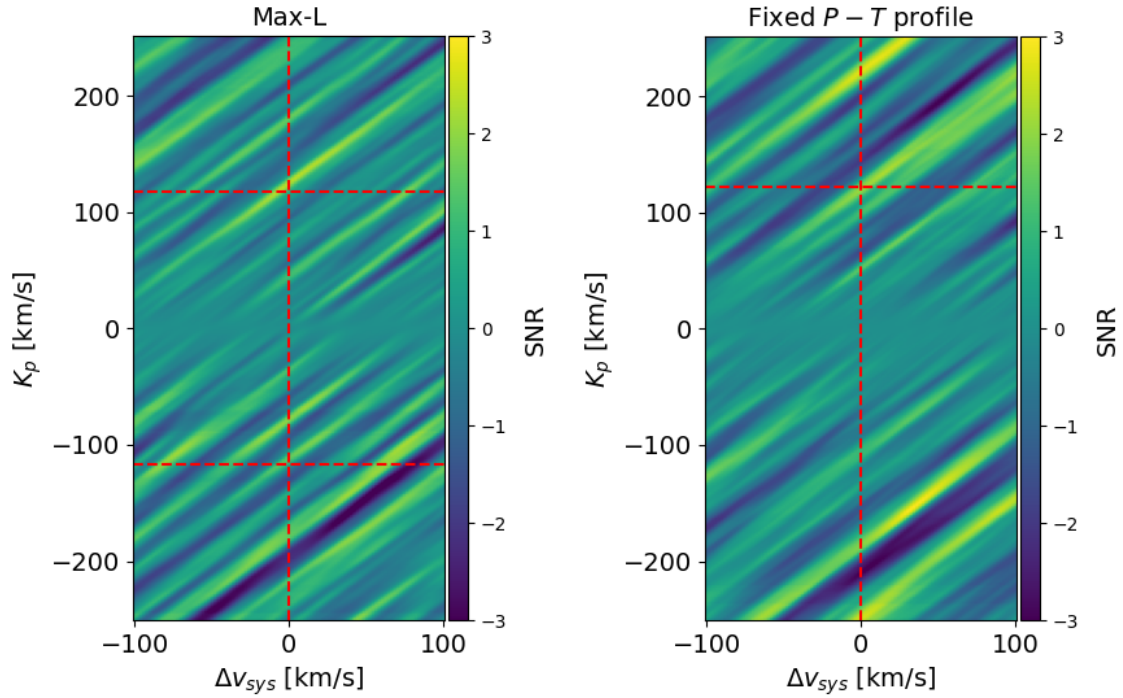


Figure 8.4: $K_p - \Delta v_{\text{sys}}$ diagrams for HD 80606 b

$K_p - \Delta v_{\text{sys}}$ diagrams for the maximum-likelihood model from the free $P - T$ retrieval (left) and the fixed $P - T$ retrieval (right). The expected K_p and Δv_{sys} values are indicated in dashed red. In both cases, there is a feature at $\text{SNR} \sim 3$ near the reference frame of HD 80606 b, but there are other features of comparable or greater strength throughout the $K_p - \Delta v_{\text{sys}}$ space. As a result, we cannot definitively attribute the peak at the expected velocities to HD 80606 b, which is at best marginally detected.

series reveals cross-correlation peaks near the nominal planet rest frame for both models. However, other features in the 1D cross-correlation function are of comparable strength to the feature in the planet rest frame, suggesting that the peak may not actually be associated with the atmosphere of HD 80606 b.

$K_p - \Delta v_{\text{sys}}$ diagrams are presented in Figure 8.4. Consistent with Figure 8.3, a peak at $\text{SNR} \sim 3$ is present at the nominal K_p and Δv_{sys} , but there are other features in the $K_p - \Delta v_{\text{sys}}$ of comparable or greater strength, raising the possibility that the putative planet feature is simply noise.

While we do not clearly detect HD 80606 b, the weak cross-correlation peaks at the nominal planet velocity with non-inverted model atmospheres suggests the absence of a strong thermal inversion in the atmosphere of HD 80606 b. Such an inversion would result in planet lines appearing in emission, rather than absorption, and would produce a significant negative feature at the nominal planet velocity when the cross-correlation template has a non-inverted $P - T$ profile.

8.3.2 Retrieval analysis

While the maximum-likelihood models do not detect HD 80606 b, both retrievals prefer constraints on some of the species included in the retrieval. Retrieved maximum-likelihood and median values are listed in Table 8.2, and the full corner plots are included in Appendix 8.6. Both retrievals prefer bounded constraints on the H_2O abundance, $\log \text{H}_2\text{O}_{\text{MMR}} = -4.0 \pm 0.5$ in the case where we fit the $P - T$ parameters and $\log \text{H}_2\text{O}_{\text{MMR}} = -2.1^{+0.4}_{-0.7}$ in the case of the fixed $P - T$ profile. The results are similar for the CO abundance. The free $P - T$ median is $\log \text{CO}_{\text{MMR}} = -4.4^{+0.7}_{-2.8}$, with a long tail extending to the lower prior bound. The fixed retrieval provides only an upper limit, $\log \text{CO}_{\text{MMR}} < -0.8$ at 99.7% confidence, but with a weak peak in the marginalized posterior around $\log \text{CO}_{\text{MMR}} = -4$. In both cases the retrieval prefers low CH_4 abundances, with 99.7% limits on the mass fraction at $< 10^{-2.7}$ for the free profile case and $< 10^{-1.8}$ for the fixed profile case.

Figure 8.6 compares the $P - T$ profiles and retrieved median and maximum likelihood spectra from each retrieval. Compared with the fixed $P - T$ profile case, the free profile retrieval prefers a significantly hotter $P - T$ profile, leading to an F_p/F_s approximately $10\times$ larger. However, the molecular abundances in the free retrieval case are also significantly lower than in the fixed retrieval, suggesting that a degeneracy between the $P - T$ profile and the molecular abundances in setting the continuum-normalized line strengths may be impacting out results.

8.4 Discussion

8.4.1 Injection-recovery tests

The retrieval analysis provides, at best, a tentative detection of HD 80606 b. We assess the plausibility of this potential detection and its implications for the atmosphere of HD 80606 b through injection/recovery tests with models based on previous results from J. T. Sikora et al. (2024) and S.-M. Tsai et al. (2023). The adopted $P - T$ profiles are shown in Figure 8.6 compared to the retrieval results. For the abundances, we use **easyCHEM** to estimate the abundances under chemical equilibrium for each $P - T$ profile, assuming a metallicity of $[\text{Fe}/\text{H}] = 0$ and $\text{C}/\text{O} = 0.6$ based on the results from J. T. Sikora et al. (2024).

For each planet model, we first inject the planet model at $-1\times$ nominal strength at K_p . For a well-matched planet model, this should eliminate the true planet detection, resulting in $\text{SNR} \sim 0$ near $(0, K_p)$ in the $K_p - \Delta v_{\text{sys}}$ diagram. We then re-inject the planet model at nominal strength at $(0, -K_p)$, which for a planet model well-matched to the data should result in a feature of similar strength to the original detection at $-K_p$.

The resulting $K_p - \Delta v_{\text{sys}}$ diagrams are shown in Figure 8.5. For the non-inverted J. T. Sikora et al. (2024) model, the results are broadly consistent with expectations for a marginal detection of HD 80606 b. For the inverted S.-M. Tsai et al. (2023) model, the negative injection results in a significant negative feature at K_p and an $\text{SNR} \sim 3$ feature at $-K_p$.

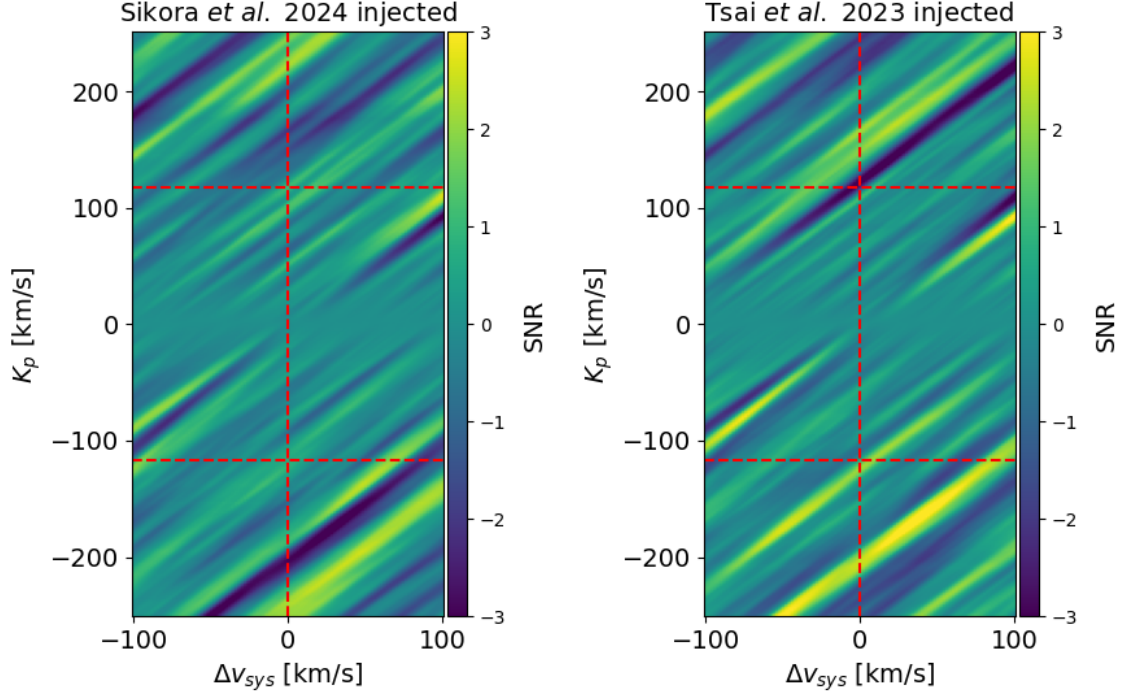


Figure 8.5: $K_p - \Delta v_{\text{sys}}$ diagrams for injection-recovery tests

Planet models are based on [J. T. Sikora et al. \(2024\)](#) (left) and [S.-M. Tsai et al. \(2023\)](#) (right). The $P - T$ profiles are shown in Figure 8.6. We assumed abundances based on chemical equilibrium for $\text{C/O} = 0.6$ and $[\text{Fe/H}] = 0$, consistent with the values from [J. T. Sikora et al. \(2024\)](#). The planet model was negative-injected at K_p and re-injected at $-K_p$. For a model well-matched to the data, this should result in an $\text{SNR} \sim 0$ at $(0, K_p)$ and a feature with SNR similar to the original planet detection at $(0, -K_p)$. While this is the case for the non-inverted [J. T. Sikora et al. \(2024\)](#) model, the inverted [S.-M. Tsai et al. \(2023\)](#) model shows over-subtraction at positive K_p and strong features at $-K_p$, indicating the injected features are significantly stronger than the potential planet detection in the data.

This indicates that the planetary features in the inverted model are substantially stronger than any such features in the data, such that a negative injection results in a corresponding negative feature in the $K_p - \Delta v_{\text{sys}}$ space.

These injection tests suggest that if HD 80606 b had a thermal inversion near periapsis as predicted by theoretical modeling (N. Iro & L. D. Deming, 2010; N. K. Lewis et al., 2017; L. C. Mayorga et al., 2021; S.-M. Tsai et al., 2023), these data would be sensitive to it. While the injected inverted model is only recovered at $\text{SNR} \sim 3$, the non-inverted models from the retrieval analysis are similarly detected at $\text{SNR} \sim 3$, indicating absorption features are significantly preferred over emission features in these data. If HD 80606 b had a thermal inversion, we would expect the retrieval analysis to produce a featureless spectrum, in order to minimize the difference between the emission lines in the data and the absorption lines in the model. Instead, the retrieval weakly prefers absorption lines in the atmosphere of HD 80606 b, in direct tension with the existence of a thermal inversion.

Both our results and J. T. Sikora et al. (2024) independently make weak detections of features consistent with the atmosphere of HD 80606 b in absorption. This indicates that any near-periapsis thermal inversion in HD 80606 b must be very shallow, such that the post-periapsis atmospheric signal is predominately in absorption. While a very short-lived inversion could be compatible with the high-resolution data, it would conflict with the *JWST* results, which prefer a non-inverted atmosphere over the full length of the observations, from 10 hours before to 7 hours after periapsis J. T. Sikora et al. (2024).

8.4.2 Thermal Structure

Figure 8.6 shows the median and maximum-likelihood $P - T$ profiles, along with draws from the retrieved posterior, compared with the fixed $P - T$ profile adopted to roughly match the results from J. T. Sikora et al. (2024). The retrieved $P - T$ profile runs hotter than expected, leading to a corresponding increase in F_p/F_s compared to expectations. A similar phenomenon has been seen in the retrieval analysis of another marginal HRCCS

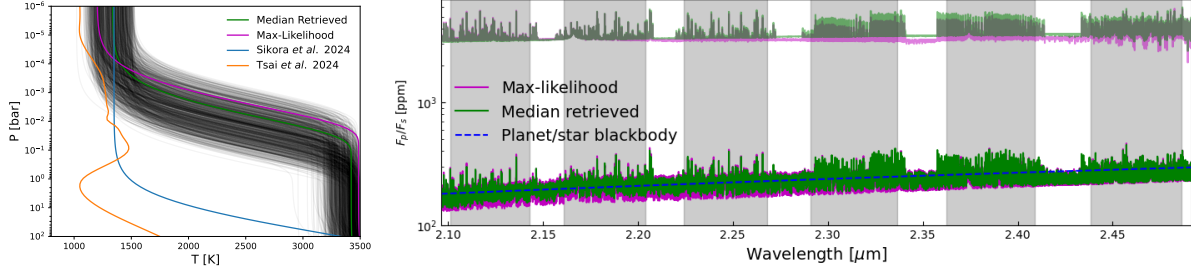


Figure 8.6: Retrieved $P - T$ profiles and spectra for HD 80606 b

$P - T$ profiles (left) and retrieved median/max-likelihood models (right). Purple corresponds to maximum likelihood and green to median values from the retrievals. In the $P - T$ plot, the profile chosen to match the parameters reported in [J. T. Sikora et al. \(2024\)](#) is shown in blue, the profile to match [S.-M. Tsai et al. \(2023\)](#) is in orange, and draws from the posterior in black. In the spectrum plot, the analyzed NIRSPEC orders are shaded, and we plot F_p/F_s assuming the planet is a 1400 K blackbody for comparison. The free $P - T$ profile runs significantly hotter, leading to a significantly greater-than-expected F_p/F_s . This is countered by the larger abundances in the fixed- $P - T$ case producing greater line depth relative to the planet continuum, such that the depth of planet lines relative to the total star+planet continuum does not change as dramatically as the change in planet continuum suggests. A similar phenomenon in a marginal HRCCS detection is presented in Finnerty *et al.*, in prep.

detection (Finnerty *et al.*, in prep.). The HRCCS technique is sensitive to the depths of planet lines relative to the total star+planet continuum level as a result of the continuum being divided out during the data detrending. This can lead to a degeneracy between weak lines at a high planet continuum level and stronger lines at a lower continuum level, as the resulting line depths relative to the host star spectrum can be comparable. The retrieval results are consistent with this scenario, with the hotter $P - T$ preferred by the free retrieval corresponding to significantly lower molecular abundances than in the fixed profile case.

While the detection of HD 80606 b is marginal at best, the presence of a $\text{SNR} \sim 3$ feature in the expected planet reference frame is significant evidence against a strong thermal inversion in the atmosphere of HD 80606 b, which would be expected to result in a significant negative cross-correlation feature in the planet reference frame when cross-correlating the observations with a non-inverted model atmosphere for HD 80606 b. Multiple theoretical studies have suggested a thermal inversion forming around the periastron passage of HD 80606 b (N. Iro & L. D. Deming, 2010; N. K. Lewis *et al.*, 2017; L. C. Mayorga *et al.*, 2021; S.-M. Tsai *et al.*, 2023), but this appears to be at odds with both our results and the *JWST* observations presented in J. T. Sikora *et al.* (2024). This tension between theory and observation is a strong motivator for further observations of HD 80606 b with higher spectral resolutions and/or wider bandpasses in order to obtain a clear detection suitable for retrieval analysis.

8.4.3 Chemical composition

While the retrieved HD 80606 b models are not well-detected in cross-correlation, the retrieval analysis still returns bounded constraints or limits on CO, H₂O, and CH₄. The posteriors from both retrievals give bounded constraints on H₂O, upper limits on CH₄, and a weak preference for small amounts of CO, although the CO posterior in particular is poorly constrained. This is broadly consistent with the *JWST* results from J. T. Sikora *et al.* (2024), who reported $\sim 3\sigma$ detections of these species post-periastris, although omitting the NRS2 detector, which showed strong systematics, resulted in a detection of only CO. CH₄

has weak K band spectral features compared with CO and H₂O, which could explain the upper limit from our observations despite the weak detection from *JWST* data.

Abundance estimation in HD 80606 b is complicated by the possibility of significant vertical abundance gradients. While HD 80606 b does not appear to develop a strong thermal inversion near periastron, the possible presence of CO features does suggest changes in atmospheric chemistry with orbital phase, as at apoastron the dominant carbon species is expected to be CH₄. The rapidly changing stellar flux experienced by HD 80606 b and the apparent discrepancy between theoretical predictions and the observed spectrum suggests a free retrieval approach which incorporates dissociation (e.g. [L. Finnerty et al., 2025b](#)) may be required for accurate abundance constraints.

8.5 Summary and Conclusions

We present post-eclipse K band observations of the highly eccentric planet HD 80606 b from Keck II/NIRSPEC. Retrieval and cross-correlation analysis indicate HD 80606 b is at best weakly detected in these data, with tentative evidence for H₂O and potentially CO absorption features. CH₄ is disfavored, and strong thermal inversions are effectively ruled out by our analysis. These results are consistent with recent results from *JWST* observations ([J. T. Sikora et al., 2024](#)), which also strongly disfavored a thermal inversion and found weak evidence for absorption features of H₂O, CO, and CH₄.

The long period of HD 80606 b poses significant challenges for ground-based observations. Until 2030, only 2026-03-11 (UT) and 2028-12-07 (UT) periastron passages identified in [K. A. Pearson et al. \(2022\)](#) will be accessible to observatories on Mauna Kea. The latter event offers good post-eclipse phase coverage, and Keck/HISPEC ([D. Mawet et al., 2019](#)) is expected to be available during that time, presenting an opportunity to obtain high-resolution observations of HD 80606 b with significantly improved stability, wavelength coverage, and spectral resolution compared with the data presented here.

8.6 Corner Plots

We present the full corner plots for the retrieval freely fitting the $P - T$ profile (Figure 8.7) and using the fixed $P - T$ profile (Figure 8.8).

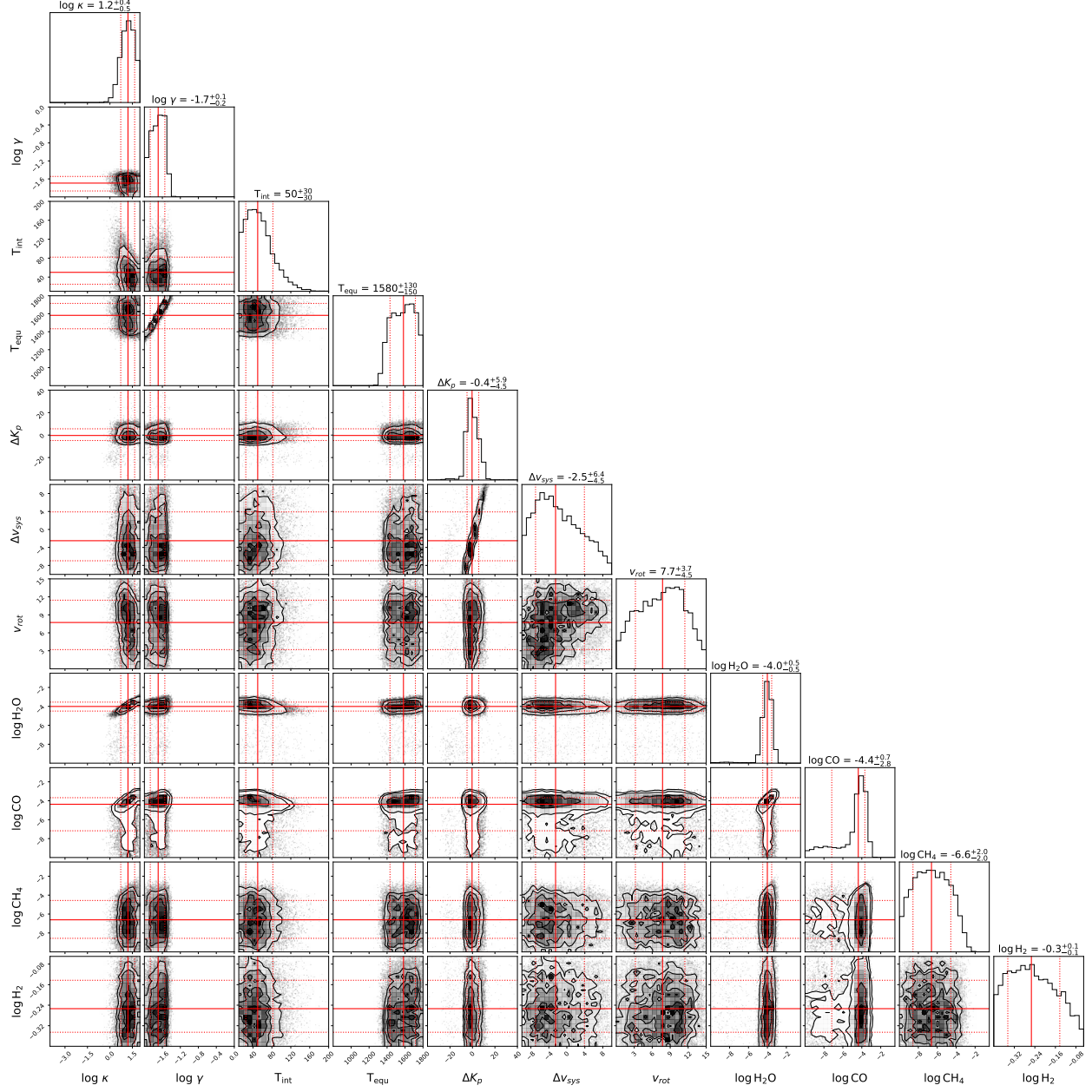


Figure 8.7: Corner plot for the retrieval with free parameters for the $P - T$ profile.

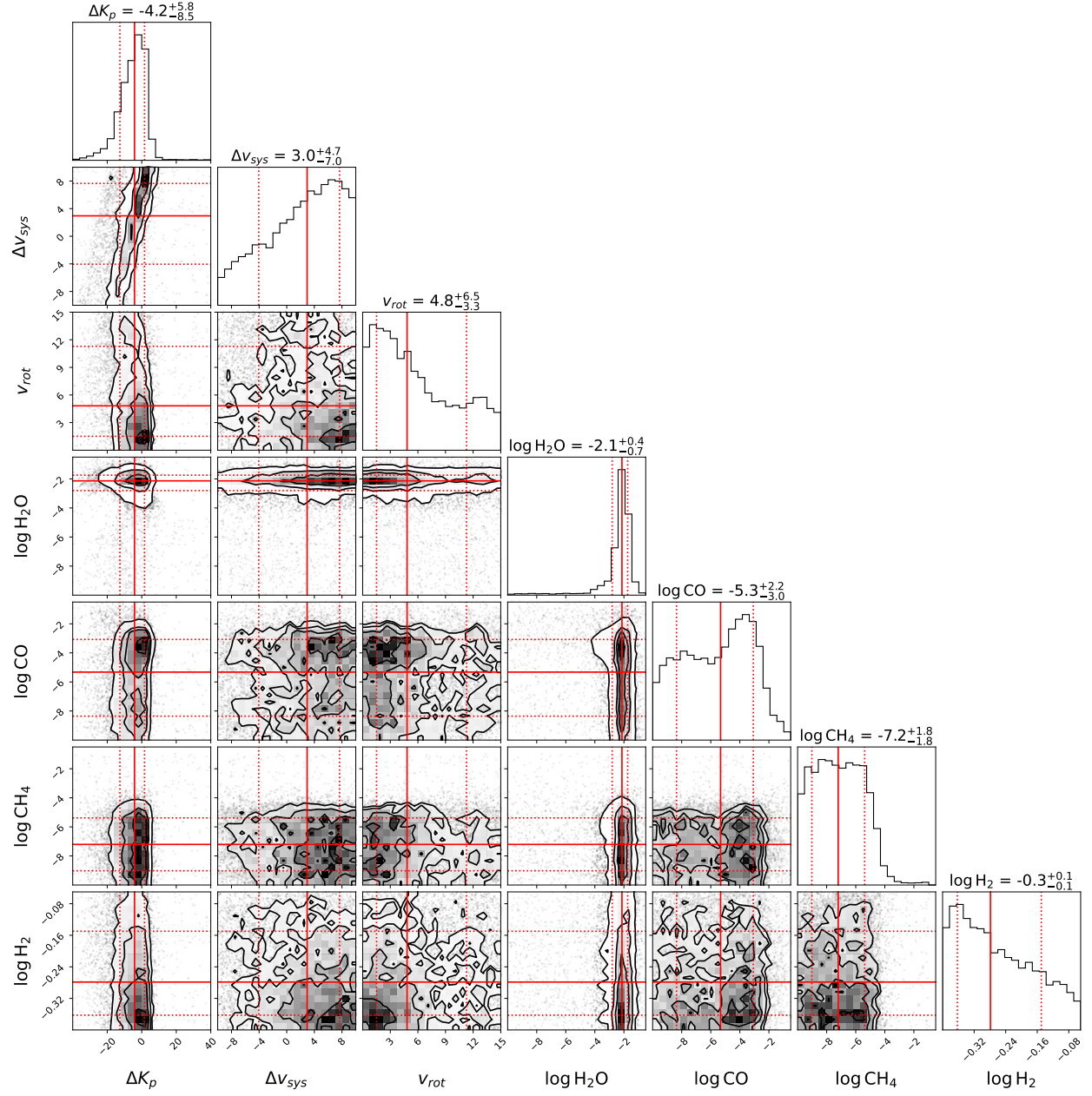


Figure 8.8: Corner plot for the retrieval with the fixex $P - T$ profile.

CHAPTER 9

Possible stratospheric emission in the warm Neptune GJ 436 b

A version of this chapter is in preparation for submission to the *Astronomical Journal* (Finnerty *et al.* 2025e)

Abstract

We present high spectral resolution L band (2.91–3.67 μm) observations of the warm Neptune GJ 436 b from Keck II/KPIC. KPIC’s single-mode fiber feed reduces the L band sky background by a factor of 100, significantly improving sensitivity compared to a seeing-limited spectrometer and enabling a tentative detection of GJ 436 b. In contrast with recent results from *JWST* and high-resolution transmission spectroscopy, our retrieval analysis weakly prefers the presence of CH_4 and H_2O molecular features in emission. The maximum-likelihood planet model is detected at a signal-to-noise ratio of 5, but the broad-band continuum flux associated with this model is substantially higher than expected based on both the ~ 650 K equilibrium temperature of GJ 436 b and previous results from low-resolution spectroscopy. We demonstrate that the loss of continuum information during the processing of high-resolution spectra makes our analysis insensitive to the absolute continuum level of the planet, and that scaling the maximum-likelihood model to match the broad-band flux measured from low-resolution observations of GJ 436 b results in a detection of similar strength in cross-correlation. These results could be explained by a thermal inversion arising above a

haze layer in the upper atmosphere of GJ 436 b. Further observations, ideally post-eclipse in order to break the $K_p - \Delta v_{\text{sys}}$ degeneracy, are needed to clarify this possible planet signal. This work demonstrates the value of L band high-resolution spectroscopy for characterizing significantly smaller and cooler exoplanets compared with hot Jupiters.

9.1 Introduction

GJ 436 b is the archetypal example of the warm Neptune exoplanet population. At the time of its discovery in 2004, it was the lowest-mass exoplanet known, and only the second exoplanet detected around an M-dwarf (R. P. Butler et al., 2004). M. Gillon et al. (2007) subsequently reported the first transit detection of GJ 436 b. As a warm Neptune around a bright host star, GJ 436 b quickly became a popular target for infrared characterization studies. Secondary eclipse spectroscopy from *Spitzer* at $8\ \mu\text{m}$ was quickly used by D. Deming et al. (2007) to confirm the non-zero orbital eccentricity of GJ 436 b. Similar results were reported by B. O. Demory et al. (2007).

Transmission spectroscopy observations from both space and the ground have consistently yielded featureless spectra, suggestive of either high atmospheric metallicity or significant clouds/hazes around 1-10 mbar muting the transmission spectrum (F. Pont et al., 2009; N. P. Gibson et al., 2011; H. A. Knutson et al., 2014; J. D. Lothringer et al., 2018a; N. Grassier et al., 2024). Stellar activity in the M-dwarf primary further complicates the interpretation of transmission spectra, but was helpful in suggesting a misaligned, nearly polar orbit (H. A. Knutson et al., 2011), which has been subsequently confirmed (V. Bourrier et al., 2022). UV transmission observations have been more successful, detecting an extended hydrogen envelope escaping from GJ 436 b (D. Ehrenreich et al., 2015).

Emission observations are less impacted by clouds and hazes, but a consistent interpretation of GJ 436 b observations has remained elusive. K. B. Stevenson et al. (2010) obtained broad-band secondary eclipse measurements in six *Spitzer* bandpasses, finding a very high

planet flux at $3.6\ \mu\text{m}$ and low flux at $4.5\ \mu\text{m}$, suggesting a very high CO/CH_4 ratio as a result of disequilibrium chemistry. A reanalysis of *Spitzer* data by [A. A. Lanotte et al. \(2014\)](#) found somewhat shallower eclipse depths at these wavelengths, still consistent with a high CO/CH_4 ratio but compatible with somewhat lower metallicities ($\sim 50\times$ solar compared with $\sim 200\times$ solar). Subsequent *Spitzer* observations confirmed the lower $3.6\ \mu\text{m}$ and $4.5\ \mu\text{m}$ eclipse depths, and retrievals on the *Spitzer* photometry preferred a non-inverted atmosphere with a metallicity several hundred times greater than solar ([C. V. Morley et al., 2017](#))

Recent low-resolution spectroscopy observations from *JWST* have found a much lower $3.6\ \mu\text{m}$ flux than expected based on the *Spitzer* photometry ([S. Mukherjee et al., 2025b](#)). Reanalysis of the *Spitzer* photometry by [S. Mukherjee et al. \(2025b\)](#) suggests the anomalously high $3.6\ \mu\text{m}$ point may be a detector artifact. Depending on model assumptions, the *JWST* spectra could be explained by a cloudy, very high-metallicity ($> 300\times$ solar) atmosphere, or a clear atmosphere with relatively low ($> 80\times$ solar) metallicity and low internal temperature ([S. Mukherjee et al., 2025b](#)).

In this paper, we present GJ 436 b in *L* band emission with Keck II/KPIC high-resolution spectroscopy covering $2.91\text{--}3.67\ \mu\text{m}$, with significant gaps. By observing in thermal emission at high spectral resolution, our observations are sensitive to weak spectral features arising from above a cloud/haze layer, which may be missed in transmission or at lower spectral resolution. Section [9.2](#) describes the details of our observations, reduction procedure, and retrieval analysis. Results of this analysis are presented in Section [9.3](#), and discussed in the context of previous results in Section [9.4](#). Section [9.5](#) concludes.

Table 9.1: Stellar and planetary properties for the GJ 436 system.

Property	Value	Ref.
GJ 436		
RA	11:42:12.13	Gaia Collaboration (2020)
Dec	+26:42:11	Gaia Collaboration (2020)
Sp. Type	M3V	J. D. Kirkpatrick et al. (1991)
K_{mag}	6.07 ± 0.02	R. M. Cutri et al. (2003)
Mass	$0.44 \pm 0.01 M_{\odot}$	L. J. Rosenthal et al. (2021)
Radius	$0.42 \pm 0.01 R_{\odot}$	L. J. Rosenthal et al. (2021)
T_{eff}	$3600 \pm 40 \text{ K}$	L. J. Rosenthal et al. (2021)
$\log g [\text{cgs}]$	4.84 ± 0.01	L. J. Rosenthal et al. (2021)
$v \sin i$	$0.33 \pm 0.1 \text{ km s}^{-1}$	V. Bourrier et al. (2022)
v_{rad}	$9.6 \pm 0.3 \text{ km s}^{-1}$	D. L. Nidever et al. (2002)
[Fe/H]	0.1 ± 0.08	L. J. Rosenthal et al. (2021)
GJ 436 b		
Period	$2.64389753 \pm 1 \times 10^{-7} \text{ days}$	A. Kokori et al. (2023)
T_{trans}	$\text{JD } 2454873.01582 \pm 4 \times 10^{-5}$	S. Mukherjee et al. (2025b)
a	0.0285 ± 0.0002	L. J. Rosenthal et al. (2021)
e	0.163 ± 0.003	S. Mukherjee et al. (2025b)
ω	$327.3 \pm 1.5^{\circ}$	S. Mukherjee et al. (2025b)
i	$86.70^{\circ} \pm 0.03^{\circ}$	A. Kokori et al. (2023)
K_{p}	117 km s^{-1}	Est.
Mass	$0.067 \pm 0.002 M_{\text{J}}$	L. J. Rosenthal et al. (2021)
Radius	$0.37 \pm 0.01 R_{\text{J}}$	J. D. Turner et al. (2016)
T_{eq}	670 K	Est.

9.2 Observations and Data Reduction

9.2.1 Observations

GJ 436 b was observed using Keck II/KPIC (I. S. McLean et al., 1998; E. C. Martin et al., 2018; R. A. López et al., 2020; J.-R. Delorme et al., 2021; D. Echeverri et al., 2022; N. Jovanovic et al., 2025a) on UT 2024 May 22 from 5:43 to 9:50. The observations covered an orbital phase of 0.42–0.48, during which time the nominal projected orbital velocity changed from 86 km s^{-1} to 58 km s^{-1} . Due to the high and variable slit background in the L band, observations were taken in an ABBA nodding pattern using science fibers 2 and 4, rather than the staring mode used for K -band observations. We used an exposure time of 60 seconds in order to keep the entire detector in the linear regime despite significant thermal background at the red end of the observed spectrum, obtaining 102 frames on science fiber 2 and 104 frames on science fiber 4.

GJ 436 was observed starting just before transiting zenith, with the airmass changing from 1.01 to 1.63 over the observations. Conditions were good and generally stable over the entire observation sequence, aside from a ~ 30 minute patch of poor AO correction around 8:00. Outside of that period, typical counts gradually decreased by $\sim 20\%$ over the course of the observations, roughly tracking the airmass.

9.2.2 Data Reduction

The data were reduced using the modified version of the KPIC pipeline¹ described in L. Finnerty et al. (2025a,b), which uses a variable non-Gaussian model of the trace profile for both flux extraction and the instrumental line-spread function (LSF). While L. Finnerty et al. (2025a,b) used afternoon calibration frames for background subtraction, we found that the L band slit background is significantly different between daytime calibrations and science

¹https://github.com/kpicteam/kpic_pipeline/

operations, and that the background level varies slowly over the course of the night as a result of changes in temperature. We therefore took our observations in an ABBA pattern and performed an A–B subtraction to remove the thermal background.

For wavelength calibration, we observed HIP 62944 before observations of GJ 436 and observed HIP 81497 after. The limited number of existing KPIC *L* band observations necessitated a more manual approach to wavelength calibration. We used the NIRSPEC Echelle Format Simulator (EFS) to obtain a rough estimate of the wavelength solution for each order. This was then refined by manually adjusting coefficients of a second-order polynomial to match a stellar $\times$ telluric model to the data. The resulting initial wavelength solution was then used as a starting point for the KPIC DRP wavelength calibration script. Finally, this wavelength solution was manually checked against the stellar $\times$ telluric model.

Of the seven spectral orders falling on the detector, six were usable, spanning 2.91–3.67 μm , with significant gaps between orders. The seventh order was not usable for analysis due to strong telluric absorption. Subsequent KPIC *L* band observations (e.g. Finnerty *et al.*, *subm.*) have used a different grating/cross-disperser configuration for which all seven orders are usable, spanning 3.03–4.06 μm . The extracted SNR for each 60 second exposure in regions of low telluric absorption is strongly chromatic, ranging from ~ 30 in the bluest order to ~ 100 in the reddest order.

9.2.3 Atmospheric Retrieval

We use the retrieval pipeline described in L. Finnerty *et al.* (2023a, 2024, 2025a,b), using `petitRADTRANS` for radiative transfer (P. Mollière *et al.*, 2019, 2020; E. Nasedkin *et al.*, 2024). We added an additional masking step in the pre-retrieval data processing in order to better handle the saturated telluric features in *L*. After median-dividing each spectrum, any wavelength channel with $< 50\%$ telluric transmission is masked. We then mask the 3% of the remaining wavelength channels with the highest variance, before computing the time series median and dividing the time series for each order by the median spectrum. We then

removed 4 principal components (PCs) for the retrieval analysis. We assess the impact of varying the number of omitted PCs through cross-correlation analysis below.

For the pressure-temperature ($P - T$) profile, we use the [T. Guillot \(2010\)](#) parameterization following [L. Finnerty et al. \(2025a,b\)](#). However, we do not include $\log g$ as a free parameter, as analysis of multiple targets has found $\log g$ and the infrared opacity $\log \kappa$ are strongly degenerate, and that $\log g$ is not constrained by high-resolution spectra alone. We include a gray cloud deck, as multiple studies have found evidence for significant clouds impacting the spectrum of GJ 436 b. We fit for the cloud deck pressure, cloud opacity, and settling parameter f_{SED} .

We fit for vertically constant abundances of H_2O , CH_4 , NH_3 , H_2S , HCN , SO_2 and H_2 , using the default opacity tables included with `petitRADTRANS`. For H_2O , we used the opacities based on the [O. L. Polyansky et al. \(2018\)](#) POKAZATEL linelist. For CH_4 , we use the [R. J. Hargreaves et al. \(2020\)](#) linelist. For NH_3 , we use the [S. N. Yurchenko et al. \(2011\)](#) linelist. H_2S opacity is based on the [A. A. A. Azzam et al. \(2016\)](#) linelist, HCN uses [G. J. Harris et al. \(2006\)](#), and SO_2 uses [D. S. Underwood et al. \(2016\)](#), imported from DACE ([S. L. Grimm & K. Heng, 2015](#); [S. L. Grimm et al., 2021](#)). H_2 opacity is from [L. S. Rothman et al. \(2013\)](#). We also include $\text{H}_2 - \text{H}_2$ CIA opacity from [A. Borysow et al. \(2001\)](#); [A. Borysow \(2002\)](#) and $\text{H}_2 - \text{He}$ opacity from [J. Borysow et al. \(1988\)](#); [A. Borysow et al. \(1989\)](#); [A. Borysow & L. Frommhold \(1989\)](#).

The sampling is performed using the `PyMultiNest` ([J. Buchner et al., 2014](#)) wrapper for `MultiNest` ([F. Feroz & M. P. Hobson, 2008](#); [F. Feroz et al., 2009, 2019](#)). We used 800 live points and a convergence criteria of $\Delta \log z < 0.001$, stricter than our previous retrievals in order to ensure the sampler fully explores the prior space.

9.3 Results

9.3.1 Retrieval analysis

Priors, maximum-likelihood parameters, and retrieved median parameters with $\pm 34\%$ confidence intervals are presented in Table 9.2. None of the parameters included in the retrieval are well-constrained, despite the strict convergence criteria. However, the retrieved posterior shows a weak preference for a thermal inversion and emission from both H_2O and CH_4 , which may be the result of a marginal detection of the planet. The posterior also has a secondary mode without a thermal inversion which prefers a $\sim 40\text{km s}^{-1}$ redshift from the nominal planet rest frame. While the presented data are clearly insufficient for robust parameter estimation, we can use the weak constraints we do obtain as a basis for detection/non-detection hypothesis testing. Such hypothesis testing does not require the same data quality as parameter estimation. Below, we use the maximum-likelihood model from the retrieval as a basis for assessing the possible presence of H_2O and CH_4 in the atmosphere of GJ 436 b.

9.3.2 Cross-correlation analysis

Figure 9.1 shows the cross-correlation signal-to-noise for each frame as a function of the systemic velocity offset, Δv_{sys} and the summed cross-correlation in the nominal planet rest frame in the lower panels. A planet signal is expected to appear as a consistent peak in both fibers near $\Delta v_{\text{sys}} = 0 \text{ km s}^{-1}$. A weak, slightly redshifted peak is seen in each fiber after summing over the time axis, but is not obvious in the frame-by-frame plot. There do not appear to be significant contamination from either the stellar (solid black) or telluric (dashed black) reference frames. In both fibers, there are four orders contributing to the overall signal, with two orders relatively flat, which is consistent with expectations for an atmosphere dominated by CH_4 and H_2O features. Neither time series shows significant features originating near the telluric or stellar reference frames, indicating our detrending process has effectively removed these features from the time series.

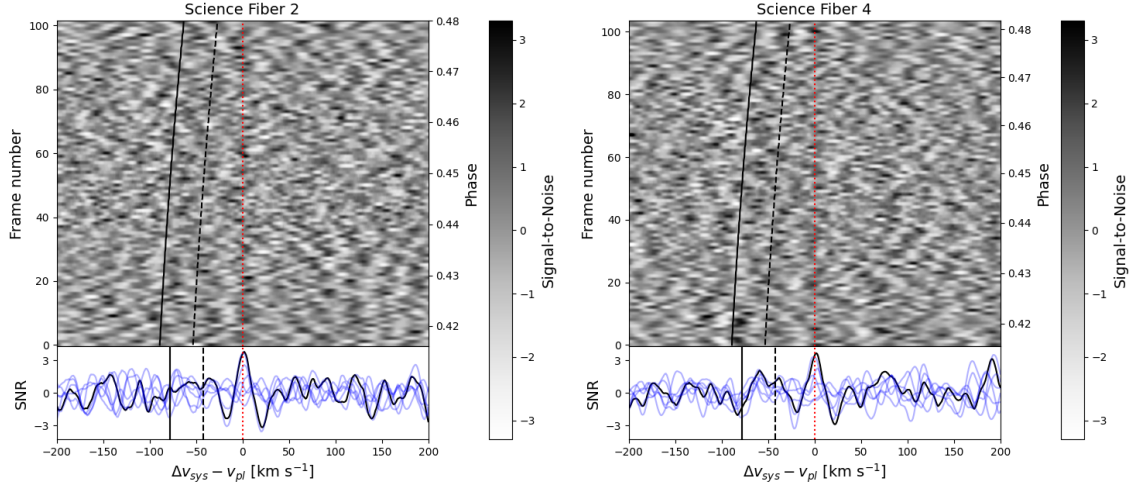


Figure 9.1: Cross-correlation time series for GJ 436 b

Top: Frame-by-frame cross-correlation signal-to-noise for the maximum likelihood model as a function of velocity offset in the planet reference frame. The stellar reference frame is indicated in solid black and the telluric reference frame in dashed black. The planet signal is expected along the dashed red line, but is not clear in either time series. Bottom: Same as top, but summed over the time axis and re-normalized by the standard deviation in the $|\Delta v_{\text{sys}} - v_{\text{pl}}| > 50$ region. Each individual order is shown in blue, and the combination of all orders is shown in black. A weak, slightly redshifted peak is visible in each time series, consistent with a weak detection of GJ 436 b.

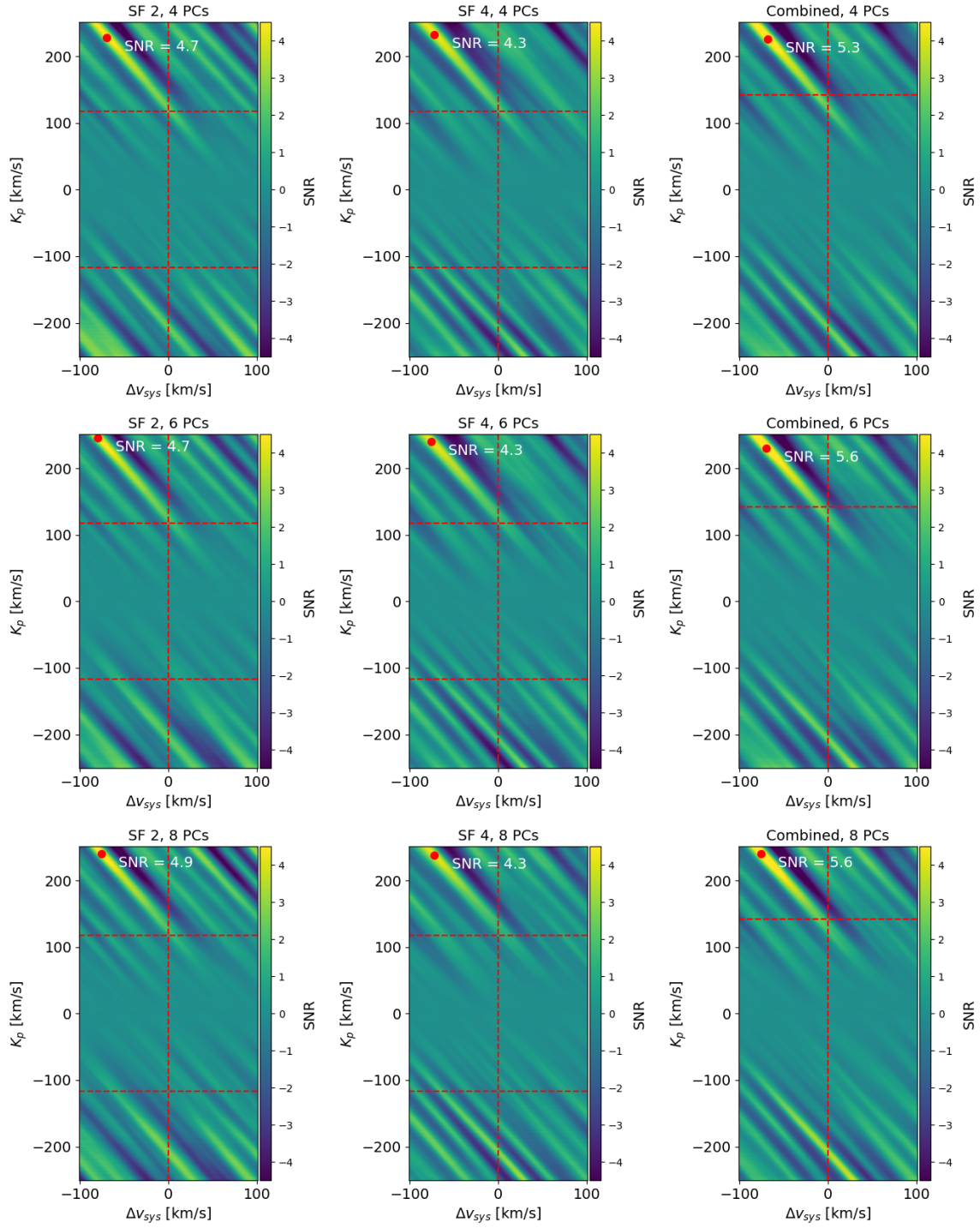


Figure 9.2: $K_p - \Delta v_{\text{sys}}$ diagrams for GJ 436 b

$K_p - \Delta v_{\text{sys}}$ plots for science fiber 2 (left column), science fiber 4 (center) and both fibers (right) for 4 (top), 6 (middle), and 8 (bottom) omitted PCs. The expected K_p and Δv_{sys} are indicated in dashed red.

Table 9.2: List of parameters, priors, and results for atmospheric retrievals.

Name	Symbol	Prior	Retrieved Max-L	Retrieved Median	Inverted test	Non-inverted test
log infrared opacity [$\text{cm}^2 \text{g}^{-1}$]	$\log \kappa$	Uniform($-4, 2$)	-1.2	$-1.5^{+1.4}_{-1.5}$	-0.5	-0.5
log infrared/optical opacity	$\log \gamma$	Uniform($-4, 4$)	2.6	$1.0^{+1.4}_{-2.9}$	1.2	-1.2
Intrinsic temperature [K]	T_{int}	Uniform($10, 500$)	170	170^{+170}_{-110}	150	150
Equilibrium temperature [K]	T_{equ}	Uniform($100, 2400$)	810	1110^{+570}_{-470}	600	600
Cloud settling parameter	$\log f_{\text{SED}}$	Uniform($-2, 2$)	1.6	$0.0^{+1.2}_{-1.3}$	-	-
Cloud opacity	$\log \kappa_{\text{cloud}}$	Uniform($-8, 3$)	-2.9	$-2.5^{+3.4}_{-3.4}$	-	-
Cloud deck pressure	$\log P_{\text{cloud}}$	Uniform($-6, -1$)	-3.0	$-3.5^{+1.5}_{-1.6}$	-	-
K_{p} offset [km s^{-1}]	ΔK_{p}	Uniform($-60, 60$)	54.0	$33.0^{+19.5}_{-48.0}$	0	0
v_{sys} offset [km s^{-1}]	Δv_{sys}	Uniform($-40, 40$)	-32.5	$-9.0^{+21.5}_{-20.6}$	0	0
Rotational velocity [km s^{-1}]	v_{rot}	Uniform($0, 15$)	12.5	$11.0^{+2.5}_{-4.5}$	3	3
log H_2O mass-mixing ratio	$\log \text{H}_2\text{O}$	Uniform($-12, -0.3$)	-1.9	$-4.5^{+2.4}_{-5.0}$	-1	-1
log CH_4 mass-mixing ratio	$\log \text{CH}_4$	Uniform($-12, -0.3$)	-1.3	$-3.5^{+1.9}_{-2.7}$	-0.8	-0.8
log NH_3 mass-mixing ratio	$\log \text{NH}_3$	Uniform($-12, -1$)	-7.0	$-7.2^{+3.1}_{-2.9}$	-2.2	-2.2
log H_2S mass-mixing ratio	$\log \text{H}_2\text{S}$	Uniform($-12, -1$)	-9.8	$-7.1^{+3.1}_{-2.9}$	-2.5	-2.5
log HCN mass-mixing ratio	$\log \text{HCN}$	Uniform($-12, -1$)	-2.3	$-5.9^{+2.3}_{-3.6}$	-10	-10
log SO_2 mass-mixing ratio	$\log \text{SO}_2$	Uniform($-12, -1$)	-1.6	$-6.6^{+3.3}_{-3.3}$	-4.2	-4.2
log H_2 mass-mixing ratio	$\log \text{H}_2$	Uniform($-0.4, -0.05$)	-0.3	$-0.2^{+0.1}_{-0.1}$	-0.3	-0.3
Scale factor	scale	LogNormal($0, 0.1$)	0.3	$0.0^{+0.1}_{-0.1}$	0	0

Note. — No parameters are well-constrained, as can be seen in the corner plot in Section 9.6. The error bars on the retrieved medians correspond to the 68%/1 σ confidence interval. In addition to these priors, we required that the atmospheric temperature stay below 3500 K at all pressure levels.

Figure 9.2 shows the $K_{\text{p}} - \Delta v_{\text{sys}}$ plots for the maximum-likelihood model for each fiber individually and for both fibers together, for 4, 6, and 8 omitted PCs. The Signal-to-Noise (SNR) is estimated by first median-subtracting each row of fixed K_{p} in order to reduce the systematic effects discussed in L. Finnerty et al. (2024, 2025a,b), followed by dividing the entire map by the standard deviation of the $K_{\text{p}} < 0$ region. This results in a $\text{SNR} \sim 4 - 5$ peak in all cases, offset from the expected location of any planetary features. The offset to higher K_{p} values is accompanied by more negative Δv_{sys} values, such that the actual planet velocities are very similar to those expected from the assumed ephemeris. Based on negative injection tests at $-K_{\text{p}}$, discussed in Section 9.4, this offset appears to be a result of the detrending process and/or orbital phase coverage of our observations.

This putative planet peak is seen in both science fibers separately, consistent with the cross-correlation plots shown in Figure 9.1, and gets modestly stronger when the both fibers are combined. Along with Figure 9.1, this suggests that the putative planet peak is not

simply a result of a one-off anomalous frame, which we would expect to produce a peak in the time series for only one fiber. The presence of the putative planet peak in the time series for each fiber at a similar strength suggests it is arising from real features in the observed spectra, rather than a noise-driven false positive. Other features in the $K_p - \Delta v_{\text{sys}}$ space, particularly in the $K_p < 0$ region, are not consistent between the two science fibers.

The potential planet feature is also consistent as the number of omitted principal components is changed. Previous HRCCS studies have demonstrated that false positives at SNRs similar to the possible planet feature can be introduced during the detrending process (e.g. [C. J. Cheverall et al., 2023](#)). In such a scenario, we would expect that the peak strength would vary strongly with the number of omitted PCs. Instead, Figure 9.2 shows that the position and strength of the potential planet feature is not significantly impacted by changing the number of omitted PCs, consistent with expectations for a bona fide detection of GJ 436 b.

9.3.3 Chemical composition

Figure 9.3 presents $K_p - \Delta v_{\text{sys}}$ plots for each molecular species considered in our retrievals. For each species, the planet model was constructed by taking the maximum-likelihood parameters, setting the mass-mixing ratio of the species in question to $10^{-1.5}$, and setting the remaining species to an abundance of 10^{-15} . Only the CH_4 produces a peak in the right location with a strength similar to the all-molecule cases in Figure 9.2.

As discussed in [L. Finnerty et al. \(2023a\)](#), the one-by-one approach to molecular detection is potentially flawed for molecules with high opacity over a wide wavelength range, as these species can effectively create a variable pseudo-continuum which will change substantially when that species is omitted. In the case of the L band data presented here, this occurs for both H_2O and CH_4 , and may be the reason that H_2O is not detected in Figure 9.3 despite the high abundance preferred by the retrieval analysis.

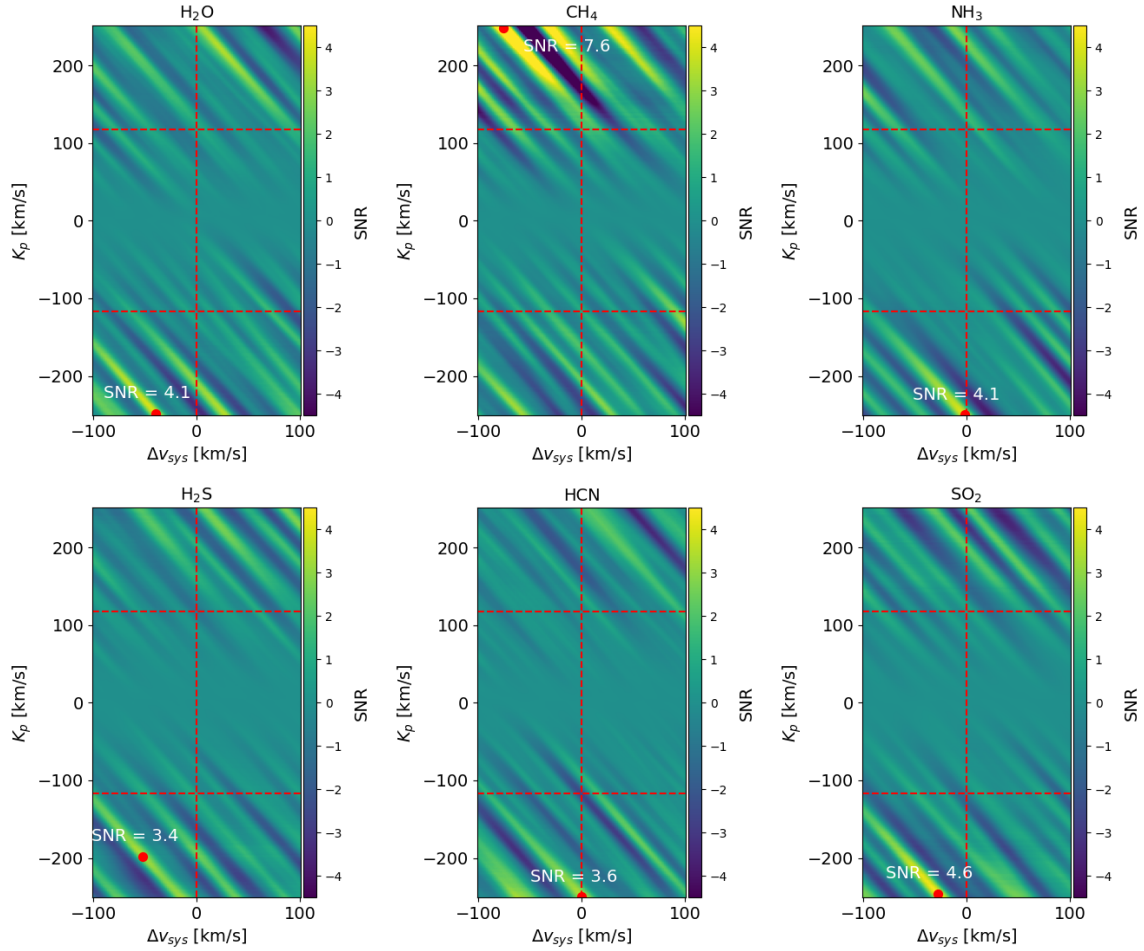


Figure 9.3: Molecular detection maps for GJ 436 b

$K_p - \Delta v_{\text{sys}}$ plots for each molecular species included in the retrieval. For each species, we begin with the maximum likelihood parameters, set the mass-mixing ratio for the species to $10^{-1.5}$, and the mass-mixing ratio of the remaining species to 10^{-15} . Each plot is made omitting 4 principal components and includes the data from both fibers. The only species showing a significant peak is CH_4 , consistent with the high abundance in the maximum-likelihood model.

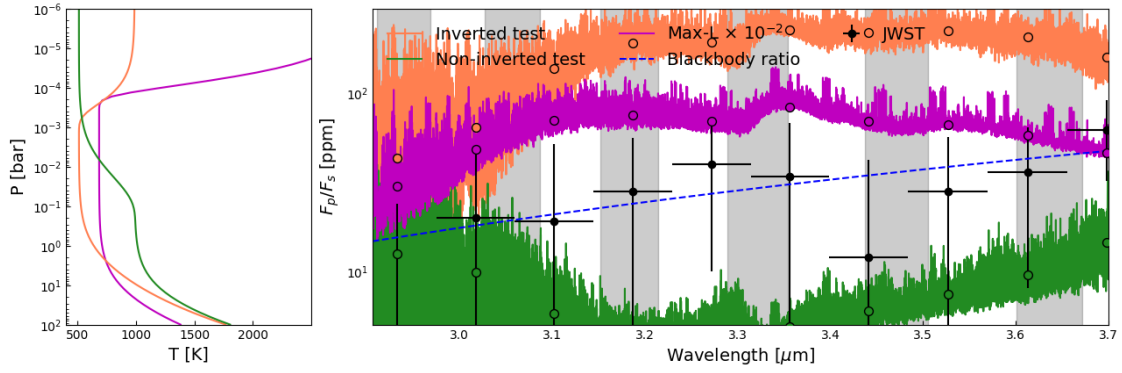


Figure 9.4: Injection models for GJ 436 b

Left: $P - T$ profiles for the planet models used for injection tests. Right: planet spectra used for injection tests, compared with *JWST* photometry from S. Mukherjee et al. (2025b).

The other species included in the retrieval all have substantially lower L band opacities than H_2O or CH_4 . Given the tentative nature of the overall planet detection, we would not expect to see evidence for these species unless they were the dominant constituents of GJ 436 b's atmosphere in the region probed by our observations, which would indicate an atmosphere far from chemical equilibrium and/or would suggest a spurious detection of non-planetary features. A detection based primarily on CH_4 and H_2O features is consistent with expectations for the atmosphere of GJ 436 b under chemical equilibrium.

9.3.4 Injection tests

To assess the robustness of the detected signal, we performed a series of injection tests, where we negative inject a planet model at K_p and re-inject at $-K_p$, and then compute the $K_p - \Delta v_{\text{sys}}$ diagram. The resulting maps are shown in Figure 9.5, along with the $P - T$ profiles and spectra for the injected models. These test give a sense of what planet signals could plausibly be recovered from these data. We consider the maximum-likelihood model from the retrieval, the maximum-likelihood model scaled by 10^{-2} to better match the *JWST* photometry (S. Mukherjee et al., 2025b), a model with a weaker thermal inversion than the retrieved maximum likelihood but higher abundances, intended to mimic an inversion arising

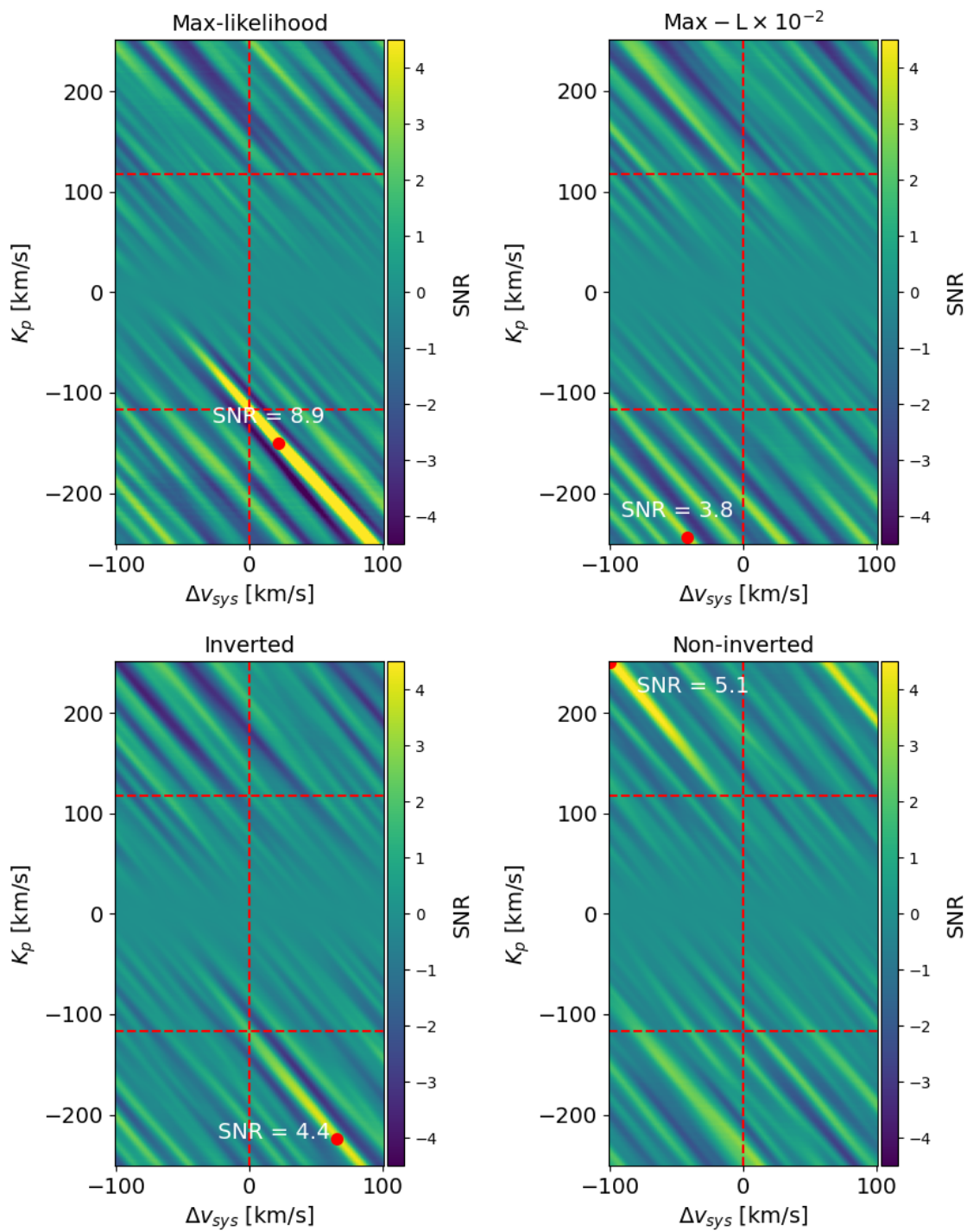


Figure 9.5: Negative injection maps for GJ 436 b

$K_p - \Delta v_{sys}$ plots from negative injection at K_p and reinjection at $-K_p$ for the models described in Section 9.3

above a cloud deck in a high-metallicity atmosphere, and a non-inverted, high-metallicity model. The parameters for these test models are included in Table 9.2. The molecular abundances are based on equilibrium abundances from `easyCHEM` (E. Lei & P. Mollière, 2024) for the inverted $P - T$ profile with $\text{C/O} = 0.6$ and $[\text{Fe/H}] = 1.5$.

The maximum-likelihood model is recovered at $\text{SNR} = 8.9$, while the scaled maximum-likelihood and non-inverted test models are not recovered. The inverted test model appears to be recovered at $\text{SNR} = 3.9$, but comparison with the $K_p - \Delta v_{\text{sys}}$ map for the non-inverted test suggests this feature may be the result of noise, rather than the injected planet model.

The peak associated with the injected maximum-likelihood model is substantially offset to higher magnitudes of K_p , with a higher value of Δv_{sys} countering this to keep the planet velocities similar to the values from the expected ephemeris. As the planet was injected at $(0, -K_p)$, this offset must be a result of our data processing and/or the phase coverage of our observations. This offset is also seen in Figures 9.2 and 9.3, and is of roughly similar magnitude, suggesting that the apparent offsets are consistent with a true planet signal at $(0, K_p)$.

This offset is likely related to the relatively small velocity shift of our observations (28 km s^{-1} compared with a 9 km s^{-1} instrumental resolution) leading to self-division of the planet model during the data detrending. Self-division decreases as K_p increases, and is not a major factor for velocity shifts $> 5 \times$ the instrumental resolution. For smaller velocity shifts, self-division results in the variance of the planet model increasing with K_p . As the M. Brogi & M. R. Line (2019) log-likelihood function depends directly on the model variance, this leads to a systematic change in the log-likelihood with K_p :

$$\log \mathcal{L} = -\frac{N}{2} \log \left[\frac{1}{N} \sum (f^2 + g^2 - 2fg) \right] \quad (9.1)$$

Where f is the data, g is the planet model, and N is the number of pixels, and the g^2 term is the variance of the forward model. If there is significant self-division of the planet model,

g^2 rapidly goes to 0, leading to an increase in the log-likelihood for lower magnitudes of K_p , but a higher variance in the log-likelihood values at higher K_p . This variance suppression at low K_p can be seen in all of our $K_p - \Delta v_{\text{sys}}$ plots. We attempt to account for the overall bias with K_p by median-subtracting each row of constant K_p before we estimate the noise level, as discussed in [L. Finnerty et al. \(2025b\)](#), but this does not address the increased variation with K_p , which will therefore lead to a bias towards higher K_p values when self-subtraction of the planet model is significant.

The greater detection strength obtained in the injection test compared to the real data suggests there is significant model mismatch between the maximum-likelihood model and the true signal. As discussed previously, we expect the omission of clouds not to result in major model mismatch, as the effects of clouds on the final spectra can also be produced by changes in the $P - T$ profile and abundances. In theory, differences in pressure broadening between the cloudy and cloud-free cases could lead to model mismatch, but the emission contribution function in [Figure 9.6](#) indicates the emission is arising above the proposed cloud layer for GJ 436 b. Alternatively, neglecting clouds may lead to changes in the $P - T$ profile in order to match the overall line/continuum ratio, but result in significant discrepancies between the retrieved $P - T$ profile and the actual temperature of the atmosphere of GJ 436 b. The inaccurate temperatures could result in significant model mismatch via differences in relative line strengths.

Alternatively or additionally, linelist errors could be a contributing factor to the better recovery of the injected maximum-likelihood model. The CH_4 and H_2O linelists we use have been extensively validated through near-infrared observations, but the L band has had comparatively little on-sky validation. The cross-correlation detection strength is generally proportional to the square root of the number of detected lines — if enough individually weak lines are slightly incorrect in our opacity tables, the cumulative effect on the detection strength could be significant.

9.4 Discussion

9.4.1 Insensitivity to continuum

A key factor in the interpretation of our results is the insensitivity of HRCCS techniques to the continuum level of the planet. During data processing, the time series is divided by its own median in order to remove stellar and telluric features. In the case of a rapidly moving planet, the resulting time series are in units of F_p/F_s , but in the case of a slowly moving planet where there is some self-division the denominator contains a contribution from the planet spectrum as well. The observations are then compared with a forward model which has been processed in the same way in order to replicate any self-division effects. This comparison is typically done using the cross-correlation coefficient, or a log-likelihood mapping such as the one described in [M. Brogi & M. R. Line \(2019\)](#) (Equation 9.1), which can be re-written in terms of the cross-correlation coefficient. For an observed spectrum f , forward model g , and their associated variances σ_f^2 and σ_g^2 , the cross-correlation is:

$$C = \frac{\sum fg}{N\sqrt{\sigma_f^2\sigma_g^2}} \quad (9.2)$$

Where N is the number of points in the spectra and the sum is carried over a spectral order. The forward model g can be Doppler-shifted to different velocities and C recalculated in order to obtain $C(v)$, and we expect that a planet detection will appear as a peak in $C(v = v_{pl})$, where v_{pl} is the expected radial velocity of the planet based on a prior ephemeris.

A major issue in early cross-correlation analyses is that Equation 9.2 is scale-invariant. Multiplying g by a constant positive value results in no change to C – the top panels of Figure 9.1 are unchanged if the planet model is scaled up or down by a factor of 100. This mathematical shortcoming is addressed by log-likelihood mappings such as [M. Brogi & M. R. Line \(2019\)](#), which have enabled atmospheric retrievals. Even with these mappings, observations over a short bandpass have struggled to retrieve accurate absolute temperatures

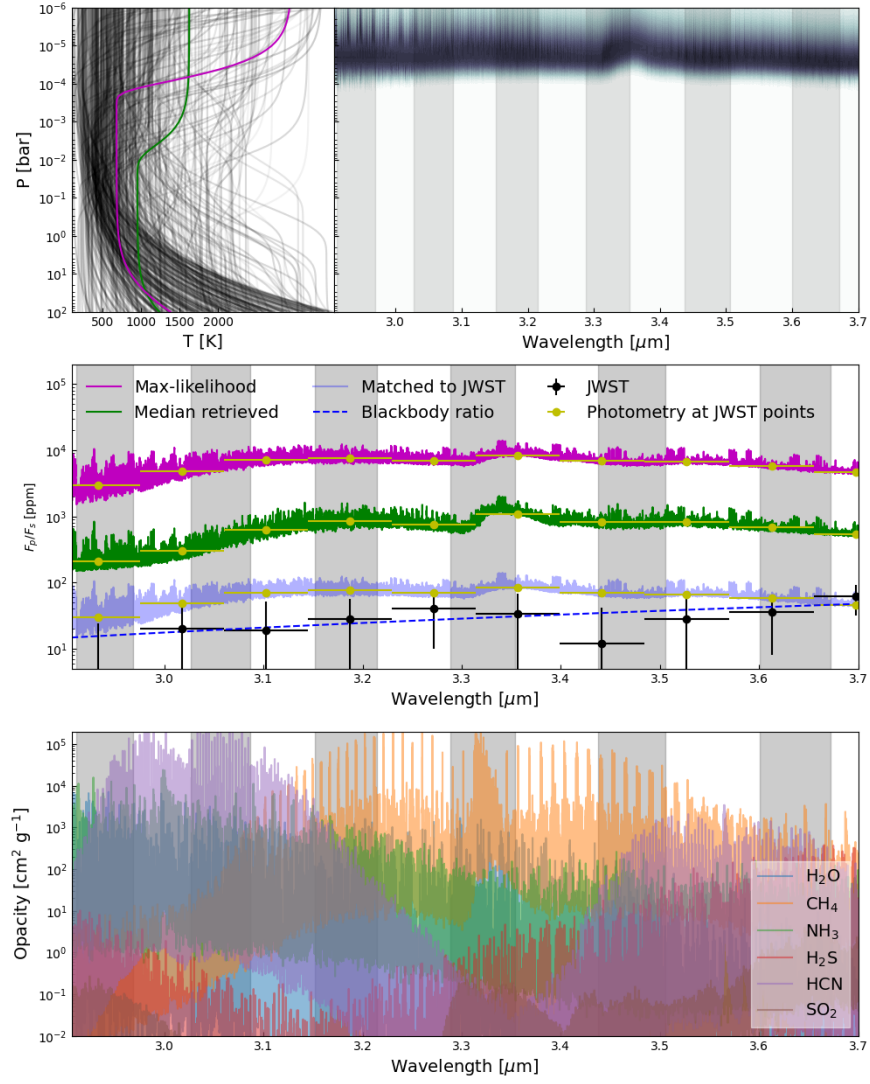


Figure 9.6: Retrieval plot for GJ 436 b

From top left: Retrieved $P - T$ profiles, maximum-likelihood emission contribution function, model F_p/F_s , and opacities. Observed orders are shaded in grey. The F_p/F_s includes the *JWST* low-resolution emission points from [S. Mukherjee et al. \(2025b\)](#), and also the expected F_p/F_s assuming the planet and star are 650 K and 3600 K blackbodies, respectively. For each model, we show the corresponding *JWST* photometry in yellow.

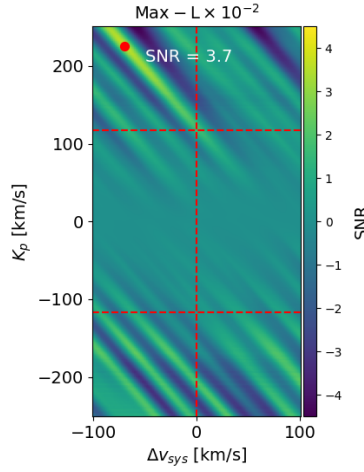


Figure 9.7: $K_p - \Delta v_{\text{sys}}$ diagram for the scaled max-likelihood model

$K_p - \Delta v_{\text{sys}}$ plot for the maximum likelihood model, but multiplying the planet by flux by 10^{-2} in order to match the expected F_p/F_s from the [S. Mukherjee et al. \(2025b\)](#) *JWST* analysis. The tentative planet feature is consistent with the equivalent plot for the full-flux max-likelihood model, demonstrating that the SNR in the $K_p - \Delta v_{\text{sys}}$ space is independent of the planet continuum level.

as a result of degeneracies between scaling factors and $P - T$ profile parameters (e.g. [L. Finnerty et al., 2023a, 2025b](#)). Wider bandpasses become more sensitive to slow changes in F_p/F_s which cannot be well-described by a multiplicative scaling factor, resulting in better constraints on absolute temperature (e.g. [M. R. Line et al., 2021](#), Finnerty et al. *subm.*). In the case of GJ 436 b in the L band, F_p/F_s changes very slowly, suggesting our observations will have very poor sensitivity to the absolute flux level.

Indeed, Figure 9.6 shows that the maximum-likelihood model has $F_p/F_s \approx 100\times$ the expected values from the [S. Mukherjee et al. \(2025b\)](#) analysis of *JWST* secondary eclipse observations, which is consistent with treating the star and planet as blackbodies. This would seem to suggest that the maximum-likelihood model is not representative of a planet detection. However, as Figures 9.6 and 9.7 show, multiplying the maximum-likelihood model by 10^{-2} gives a flux level compatible with [S. Mukherjee et al. \(2025b\)](#) and a detection strength in the $K_p - \Delta v_{\text{sys}}$ space comparable to the original maximum-likelihood model. Further considering the higher detection strength of the injected planet model shown in

Figure 9.5, this strongly suggests that the retrieval analysis is significantly overestimating the strength of planetary lines relative to the continuum through a combination of high abundances and/or large $P - T$ profile contrasts, but that a planet flux level consistent with previous observations is also consistent with the data presented here.

The insensitivity of HRCCS analysis to the continuum level does not apply in the case of injection tests. Rather than scaling one of the data or model by a multiplicative factor, these tests add a synthetic planet model m to the observed spectrum f :

$$C = \frac{\sum(f+m)g}{N\sqrt{\sigma_{f+m}^2\sigma_g^2}} = \frac{1}{N\sqrt{\sigma_{f+m}^2\sigma_g^2}} \left[\left(\sum fg \right) + \left(\sum mg \right) \right] \quad (9.3)$$

The result of this can be seen in comparing the scaled max-likelihood injection test in Figure 9.4 to the direct cross-correlation with the same model in Figure 9.7. While scaling the model does not negatively impact the detection strength, the features of the injected model are too weak to yield a detection. Similarly, the injected planet maximum-likelihood model in Figure 9.4 is recovered at a much greater strength than expected, suggesting that the planet features in the maximum-likelihood model are stronger than the corresponding features in the data.

9.4.2 Thermal structure and clouds

Previous observations of GJ 436 b have favored a non-inverted, high-metallicity atmosphere (C. V. Morley et al., 2017; J. D. Lothringer et al., 2018b; N. Grasser et al., 2024; S. Mukherjee et al., 2025b). Support for clouds and hazes has been more mixed, with C. V. Morley et al. (2017) not seeing significant evidence for either, J. D. Lothringer et al. (2018b) requiring hazes for metallicities $\sim 100\times$ solar but not for higher metallicities, and N. Grasser et al. (2024) favoring a cloud deck with $P < 10$ mbar and metallicity $> 300\times$ solar. Most recently, S. Mukherjee et al. (2025b) favored models with clouds and metallicity $> 300\times$ solar, but also found that cloud-free atmospheres with photochemistry and metallicity $\sim 80\times$ solar

are compatible with the *JWST* eclipse observations. Both the high-resolution observations presented by [N. Grasser et al. \(2024\)](#) and the *JWST* observations presented by [S. Mukherjee et al. \(2025b\)](#) independently support the cloudy, high-metallicity interpretation, and neither analysis is reliant upon the *Spitzer* photometry.

In contrast, our analysis marginally prefers an inverted $P - T$ profile (60% of the posterior draws have an inversion, giving a Bayes factor of 1.5), and the retrieval significantly overestimates the planet flux relative to the values reported by [S. Mukherjee et al. \(2025b\)](#), which are consistent with a blackbody. However, as shown in Figure 9.6, the constraints on the planet flux from these high-resolution data are extremely loose, and there is effectively no constraint on the pressure level or strength of the inversion. While the maximum-likelihood model prefers a strong inversion around 1 mbar, the median model prefers a weaker, higher-pressure inversion that results in an overall lower planet flux. A weaker inversion at a similar pressure to the maximum-likelihood model would lead to a lower planet flux but would still be compatible with the cloud top pressures reported in the literature. Such inversions are permitted in the [S. Mukherjee et al. \(2025b\)](#) *JWST* analysis (see their Figure 5).

In the case of GJ 1214 b, repeated theoretical studies have found that soot hazes can drive thermal inversions and significantly increase the planet flux in the $2 - 4 \mu\text{m}$ band compared with a blackbody. ([C. V. Morley et al., 2015](#); [I. Malsky et al., 2025](#); [M. E. Steinrueck et al., 2025](#)). GJ 1214 b orbits a similar host star to GJ 436 b and receives similar irradiation, but has a significantly smaller mass ($\sim 6 M_{\odot}$). The [S. Mukherjee et al. \(2025b\)](#) analysis preferred very low albedos for GJ 436 b, potentially compatible with such a haze scenario.

While we included a gray cloud deck in our analysis, the posteriors for the cloud parameters are nearly flat. The constant cloud opacity with wavelength is extremely difficult to disentangle from the scaling parameter and/or changes to the $P - T$ profile. Constraining clouds in emission with HRCCS will require broad wavelength coverage and more realistic cloud models to infer the impact of clouds without relying on the planet continuum.

The poor sensitivity of HRCCS analysis to the planetary continuum level creates a de-

generacy between thermal contrast in the $P - T$ profile and molecular abundances, as both larger thermal contrast and greater abundances increase the strength of molecular features. The retrieved maximum-likelihood parameters has a very large thermal contrast ~ 2000 K, but relatively low abundances compared to the values expected for a bulk $[\text{Fe}/\text{H}] \sim 2$. Atmospheres with larger abundances but lower $P - T$ contrast are in better agreement with previous observations (see Figure 9.4), which motivated our parameter choices for the inverted test model (listed in Table 9.2). However, this model does not produce a significant cross-correlation peak in the data, either directly or in negative injection tests, suggesting that the model features are significantly weaker than the features which are being fit by the maximum-likelihood model.

9.4.3 Atmospheric chemistry

The lack of constraints from our retrievals limit our ability to assess the atmospheric chemistry of GJ 436 b. Based on Figure 9.3, the tentative detection is dominated by CH_4 features, although the maximum-likelihood parameters suggest the presence of some H_2O features. Atmospheric opacity dominated by CH_4 and H_2O features is consistent with chemical equilibrium predictions. While previous analyses including *Spitzer* photometry have preferred a high CO/CH_4 ratio based on the $3.6 \mu\text{m}$ flux, suggesting disequilibrium chemistry, this is in tension with results from S. Mukherjee et al. (2025b), who found the high *Spitzer* $3.6 \mu\text{m}$ flux could be a result of instrumental systematics.

9.5 Summary and Conclusions

We present Keck II/KPIC emission observations of the warm Neptune in the L band, covering $\sim 2.9 - 3.7 \mu\text{m}$. While atmospheric retrieval analysis is unable to constrain planet properties, the maximum-likelihood model from the retrieval is weakly detected in the time series from both KPIC science fibers. This model has a thermal inversion and opacity from

CH_4 and H_2O , potentially consistent with an atmosphere roughly in chemical equilibrium with photochemical hazes producing a thermal inversion.

However, the maximum-likelihood model overestimates the planet flux by a factor of ~ 100 compared with recent results from *JWST*. The relatively flat continuum level in the L band presents a particular challenge for HRCCS retrievals, which are only indirectly sensitive to the continuum level. This is further compounded by the small velocity shift of our observations, which leads to shifts of the potential planet peak in the $K_p - \Delta v_{\text{sys}}$ space in injection tests. Additional observations with wider orbital phase coverage are required to validate this potential detection.

This work demonstrates the value of high-stability, high-resolution L band spectroscopy for characterizing smaller and cooler exoplanets via emission spectroscopy. KPIC will be decommissioned at the end of the 2025B observing semester, precluding additional observations with this instrument, and the increased thermal background associated with slit-fed instruments will likely preclude similarly sensitive observations in this bandpass with any existing instrument. Moving forward, warm Neptune characterization is a compelling science case to drive the development of new fiber-fed high-resolution spectrometers operating in the thermal infrared.

9.6 Corner Plots

Figure 9.8 presents the full corner plot from the retrieval. None of the parameters are actually constrained, but there is a weak preference for a thermal inversion and significant quantities of H_2O and CH_4 .

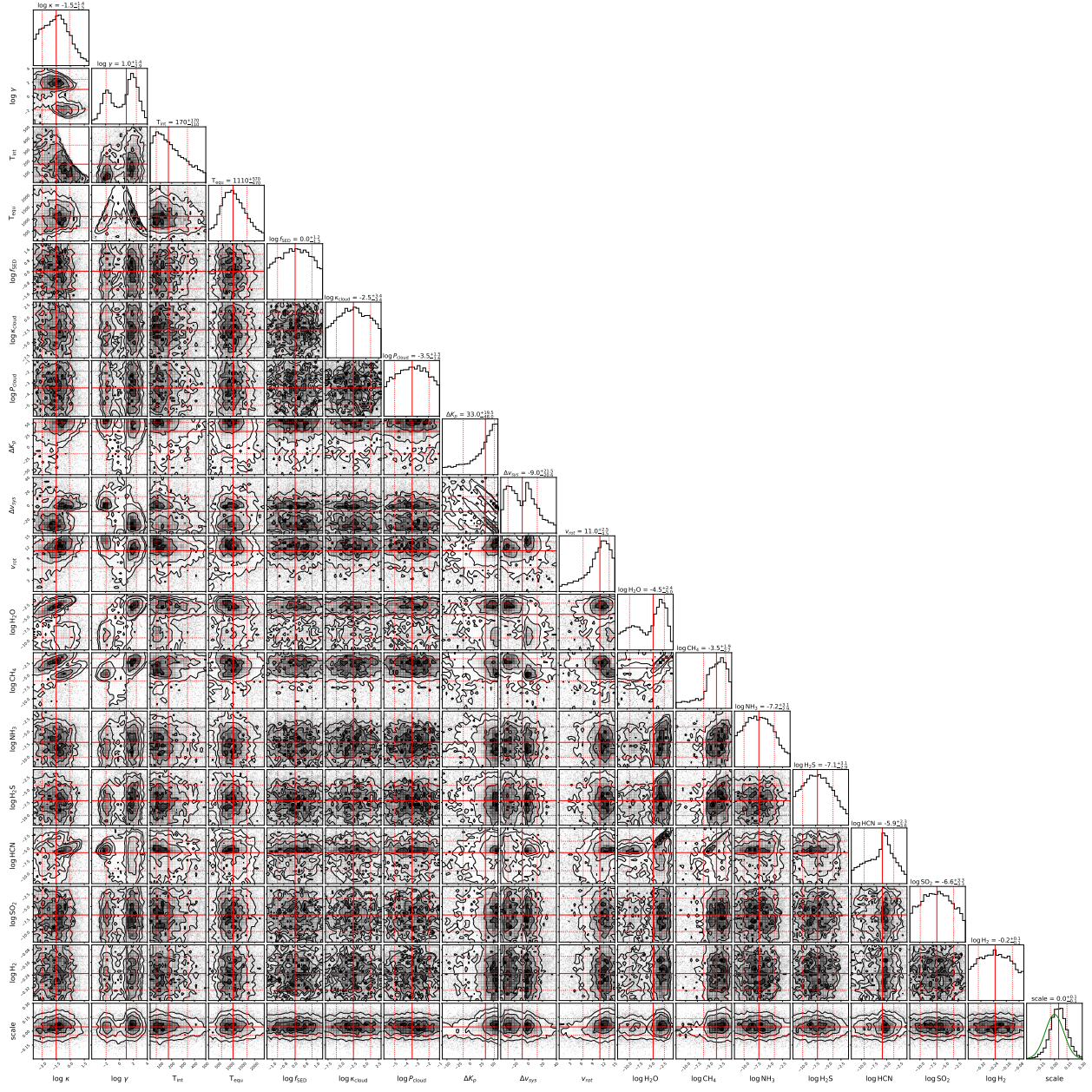


Figure 9.8: Full corner plot for the 4-component retrieval.

CHAPTER 10

Atmospheric characterization of six ultra-hot Jupiters from high-resolution spectroscopy

A version of this chapter is in preparation for submission to the *Astronomical Journal* (Finnerty *et al.* 2025f)

Abstract

We present new Keck/KPIC high-resolution spectroscopic detections of four ultra-hot Jupiters (UHJs) in the K band: KELT-9 b (SNR = 6.4), WASP-189 b (SNR = 9.7), MASCARA-1 b (SNR = 7.1), and TOI-1518 b (SNR = 6.7). We perform a uniform atmospheric retrieval analysis on these objects, as well as previously reported KPIC observations of WASP-33 b (SNR = 13.7) and KELT-20 b (SNR = 13.3), in order to examine trends in atmospheric composition and/or circulation across the UHJ population. The retrieval analysis fits for the atmospheric pressure-temperature ($P - T$) profile, velocity offsets from the nominal planetary ephemeris, planetary $v \sin i$, and abundances of CO, H₂O, OH, and Fe. The free retrieval also includes break pressures to account for molecular dissociation. CO is detected in emission in all six targets, H₂O is detected only in KELT-20 b, and evidence for OH is seen in KELT-9 b, MASCARA-1 b, and TOI-1518 b, despite the limited sensitivity of K band observations to OH. The inability to constrain or obtain limits on the H₂O and OH abundances for most targets limits constraints on the C/O ratio. For all objects, the atmospheric abundances from detected carbon and oxygen species are $1 - 10\times$ solar with no evidence for a

mass-metallicity trend, although with a $\pm 0.5 - 1$ dex uncertainty on each individual object. While H_2O and OH abundances are not well-constrained, we see possible trends between the $\text{H}_2\text{O}/\text{OH}$ ratio and both equilibrium temperature and observed orbital phase. These correlations suggest H_2O features are more strongly disfavored at higher temperatures and pre-eclipse phases, consistent with H_2O dissociation occurring primarily at afternoon longitudes. Additional observations to expand phase coverage for individual objects are needed to confirm this possible trend. Measuring C/O ratios and total volatile abundances will require additional observations at wavelengths with strong H_2O and OH spectral features in order to obtain accurate oxygen abundances in the presence of dissociation.

10.1 Introduction

The hottest giant exoplanets, known as ultra-hot Jupiters (UHJs), present an ongoing puzzle in our understanding of planet formation and a formidable challenge to our models of atmospheric physics and chemistry. Observationally, there is evidence for supersonic winds in UHJs (e.g. [I. A. G. Snellen et al., 2010](#); [D. Ehrenreich et al., 2020](#); [F. Lesjak et al., 2023](#)), which vary with altitude ([A. Y. Kesseli et al., 2022, 2024](#)), and potentially also in time ([A. Pai Asnodkar et al., 2022](#)). However, definitively measuring circulation patterns remains challenging, because large temperature contrasts between the day and night sides of UHJs can lead to condensation ([D. Ehrenreich et al., 2020](#)) and cold trapping ([S. Pelletier et al., 2023](#)), resulting in dramatic changes in atmospheric composition with longitude which can produce net Doppler shifts in the observed spectrum similar to those resulting from winds and rotation. Distinguishing the effects of winds, chemistry, temperature variations, and possible nightside/terminator clouds is a major challenge in interpreting spectroscopy of UHJs (e.g. [A. B. Savel et al., 2022](#)). Constraints on molecules such as CO, which has strong spectral features but minimal 3D abundance variations, even under UHJ conditions, may provide a stable reference point to begin isolating these effects from each other ([A. B. Savel](#)

Table 10.1: Stellar and planetary properties

	WASP-33 A ^e	KELT-9 A ^f	MASCARA-1 A ^g	WASP-189 A ^h	KELT-20 A ⁱ	TOI-1518 A ^j
RA ^a	02:26:51	20:31:27	21:10:13	15:02:45	19:38:39	23:29:04
Dec ^a	+37:33:02	+39:56:13	+10:44:20	-03:01:53	+31:13:09	+67:02:05
K_{mag}^b	7.47	7.48	7.74	6.06	7.42	8.33
Mass [$M_{\odot}$] ^c	1.495 ± 0.031	2.52 ^{+0.25} _{-0.20}	1.72 ± 0.07	2.03 ± 0.07	1.76 ^{+0.1} _{-0.2}	2.54 ^{+0.36} _{-0.64}
Radius [$R_{\odot}$] ^c	1.444 ± 0.034	2.36 ^{+0.08} _{-0.06}	2.1 ± 0.2	2.36 ± 0.03	1.57 ± 0.06	1.82 ± 0.14
T_{eff} [K] ^c	7430 ± 100	10170 ± 450	7550 ± 150	8000 ± 80	8720 ⁺²⁵⁰ ₋₂₆₀	9900 ⁺⁵⁰⁰ ₋₂₃₀₀
$\log g^c$	4.25 ± 0.1	4.09 ± 0.014	4.1 ± 0.2	3.9 ± 0.2	4.29 ± 0.02	4.31 ^{+0.9} _{-0.2}
$v \sin i$ [km s ⁻¹]	90 ± 10	111.4 ± 1.3	109 ± 4	93.1 ± 1.7	117 ± 3	85.1 ± 6.3
v_{rad} [km s ⁻¹]	-0.3	-20.6	8.5	-22.4	-23.3	-13.9

	WASP-33 b	KELT-9 b	MASCARA-1 b	WASP-189 b	KELT-20 b	TOI-1518 b
Period [d] ^d	1.219867 ± 1 × 10 ⁻⁶	1.4810903 ± 4 × 10 ⁻⁷	2.14879 ± 2 × 10 ⁻⁵	2.724031 ± 3 × 10 ⁻⁶	3.4741012 ± 2 × 10 ⁻⁷	1.902608 ± 7 × 10 ⁻⁶
t_{transit} [JD] ^d	2454163.2237 ± 0.0003	2459883.1989 ± 0.0002	2459798.2859 ± 0.0002	2456706.457 ± 0.002	2460337.98638 ± 5 × 10 ⁻⁵	2459854.4146 ± 1 × 10 ⁻⁴
a [AU]	0.0256 ± 0.0002	0.0346 ± 0.001	0.043 ± 0.005	0.0501 ± 0.001	0.054 ^{+0.001} _{-0.002}	0.039 ± 0.001
i [deg]	87.7 ± 1.8	86.8 ± 0.3	87 ⁺² ₋₃	84.03 ± 0.14	86.1 ± 0.3	77.8 ± 0.2
λ [deg]	251 ± 1	84.8 ± 1.4	69.5 ± 3	86.4 ^{+2.9} _{-4.4}	3.4 ± 2.1	240 ± 1
Mass [M_J]	2.8	2.88 ± 0.84	3.7 ± 0.9	2.0 ^{+0.2} _{-0.1}	< 3.37	< 2.3
Radius [R_J] ^d	1.5	1.89 ^{+0.06} _{-0.05}	1.5 ± 0.3	1.62 ± 0.02	1.90 ± 0.05	1.75 ± 0.13
T_{eq} [K]	2690	4050	2540	2650	2210	2920
K_p [km s ⁻¹]	230.9	254	204	200	176	198

References. — ^aGaia Collaboration (2020), ^bR. M. Cutri et al. (2003), ^cK. G. Stassun et al. (2019), ^dM. Guerrero et al. (2021), ^eA. Collier Cameron et al. (2010), ^fB. S. Gaudi et al. (2017), ^gJ. J. Talens et al. (2017), ^hM. Lendl et al., 2020, ⁱM. B. Lund et al. (2017), ^jS. H. C. Cabot et al., 2021

Note. — T_{eq} and K_p were calculated based on the listed parameters. For all other parameters, the corresponding reference is given primarily by row, secondarily by column, if the value does not have a reference specifically indicated

et al., 2023).

Even a simplified 1D approach to UHJ atmospheres can lead to significant biases in inferred abundances due to molecular dissociation. While the CO bond is strong enough that the atmospheric abundance is constant with altitude for all but the hottest UHJs, H₂O is strongly impacted by thermal dissociation, leading to weaker-than-expected H₂O spectral features for a given lower-atmosphere H₂O abundance (V. Parmentier et al., 2018). Observationally, this biases free retrievals of UHJ spectra using vertically fixed abundances towards high C/O ratio and metallicity relative to solar, while retrieval analysis based on equilibrium chemistry models prefers lower C/O ratios and metallicities more compatible with solar values (M. Brogi et al., 2023; S. Ramkumar et al., 2023). Recent analyses have also accounted for dissociation by using an approximate analytic model for the H₂O vertical mixing profile from V. Parmentier et al. (2018), which avoids this bias without requiring a full equilibrium chemistry calculation (S. Gandhi et al., 2024; S. Pelletier et al., 2025), which often entails assumptions about abundance ratios other than C/O. Alternatively, L. Finnerty et al. (2025b) took an entirely numerical approach to dissociation, fitting for a pressure below which the H₂O abundance decays following a power law. This solution naturally accounts for possible vertical mixing effects, which would smooth out the chemical gradients expected under chemical equilibrium.

Despite these challenges, including navigating the variety of approaches to addressing them, UHJs are the most promising exoplanet population for efforts aiming to measure bulk atmospheric composition. The high temperatures of UHJs, while challenging, also leads to nearly all species, including refractory elements, being present in the gas phase and accessible to spectroscopy. For example, S. Pelletier et al. (2023) reported detection of 15 metal species in the atmosphere of the UHJ WASP-76 b, including simultaneous detection of neutral and first ionized states of both calcium and iron. This enables precise measurements of the refractory/volatile ratio in UHJs (e.g. S. Pelletier et al., 2025), which can break degeneracies in formation history which arise from considering only C/O ratio and overall metallicity

(J. D. Lothringer et al., 2021; Y. Chachan et al., 2023).

The formation history of UHJs is a particularly interesting topic. While many UHJs show significant spin-orbit misalignment (e.g. A. Collier Cameron et al., 2010; B. S. Gaudi et al., 2017; G. J. J. Talens et al., 2017; S. H. C. Cabot et al., 2021), this is not universal (G. J. J. Talens et al., 2018). This suggests that either some UHJs are formed through disk migration processes, preserving low inclinations, or that the high-eccentricity migration process believed to be responsible for the misaligned UHJs (S. Naoz et al., 2011) does not always result in inclination excitation.

High-resolution cross-correlation spectroscopy (HRCCS) is a powerful tool for characterizing UHJ atmospheres. UHJs are generally found around hot, rapidly rotating primaries, leading to few and very broad stellar spectral lines. In contrast, UHJs have strong, narrow emission features from a wide range of atoms and molecules, leading to a very large spectroscopic contrast between the planet and host star. The very high orbital velocity of UHJs and short orbital period makes scheduling HRCCS observations comparatively easy and presents opportunities for phase-resolved spectroscopy. While an increasing number of UHJs have been studied using HRCCS (e.g. S. Pelletier et al., 2023; M. Brogi et al., 2023; S. Ramkumar et al., 2023; S. Pelletier et al., 2025; L. Finnerty et al., 2025b), multi-object comparison studies have been comparatively rare (S. Gandhi et al., 2023). Understanding UHJs as a population will require more uniform analyses suitable for cross-comparisons between many objects, including at infrared wavelengths.

As part of the broader KPIC hot Jupiter survey from 2022–2024, we obtained K band observations of six UHJs. WASP-33 b was observed as an initial demonstration target, and the first analysis was reported in L. Finnerty et al. (2023a). Observations of KELT-20 b were reported in L. Finnerty et al. (2025b), where we described a free-retrieval approach to the vertical mixing profiles of OH and H₂O in order to account for dissociation. Here we report the KPIC observations of KELT-9 b, WASP-189 b, MASCARA-1 b, and TOI-1518 b, and perform a re-analysis of the WASP-33 b and KELT-20 b observations with the

Table 10.2: Summary of observations

	UT Date	Wall time [h:mm]	t_{exp} [s]	N_{spec}	Science fibers	Orbital Phase	Airmass	SNR/pixel
WASP-33 b	2021 Nov. 21	3:12	90	46,48	1, 2	0.52–0.63	1.07–1.22	58
KELT-9 b	2022 July 22	3:30	90	35, 35, 35	2, 3, 4	0.36–0.46	1.06–1.54	76
WASP-189 b	2023 May 07	3:18	60	170	4	0.43–0.48	1.69–1.09	120
MASCARA-1 b	2023 July 02	4:30	180	80	2	0.36–0.45	3.05–1.02	116
KELT-20 b	2023 July 30	6:29	300	71	4	0.54–0.61	1.72–1.25	133
TOI-1518 b	2023 July 30	3:00	180	53	4	0.52–0.59	1.50–1.60	63

Note. — N_{spec} is the number of frames in each fiber’s time series after coadding. Integration times and number of coadded frames were chosen to keep the planet velocity shift within the coadded integration time below 4 km s^{-1} while staying well below the non-linear threshold for the NIRSPEC detector. Airmass is given for the start and end of each observation sequence, during which several targets passed through zenith. SNR/pixel is given after extraction, and is not directly comparable across targets due to differences in the integration time.

latest version of our atmospheric retrieval code. This uniform analysis of data obtained with a consistent spectral resolution and wavelength coverage provides a starting point for comparisons between UHJs to explore population-level diversity and trends.

Section 10.2 describes our observations, data reduction, and retrieval setup. Section 10.4 discusses the retrieval results for each object individually. Section 10.4 discusses comparisons between the six objects and broader implications for the atmospheric dynamics and formation/evolutionary history of the ultra hot Jupiter population. Section 10.5 concludes.

10.2 Observations and Data Reduction

10.2.1 Observations

Table 10.2 summarizes our observations with Keck II/KPIC (I. S. McLean et al., 1998; E. C. Martin et al., 2018; R. A. López et al., 2020; J.-R. Delorme et al., 2021; D. Echeverri et al., 2022; N. Jovanovic et al., 2025a). The observations of WASP-33 b were previously described in L. Finnerty et al. (2023a) and the observations of KELT-20 b in L. Finnerty et al. (2025b), and we refer the reader to those papers for further details. The following subsections summarize the previously unreported observations and changes to the previously reported

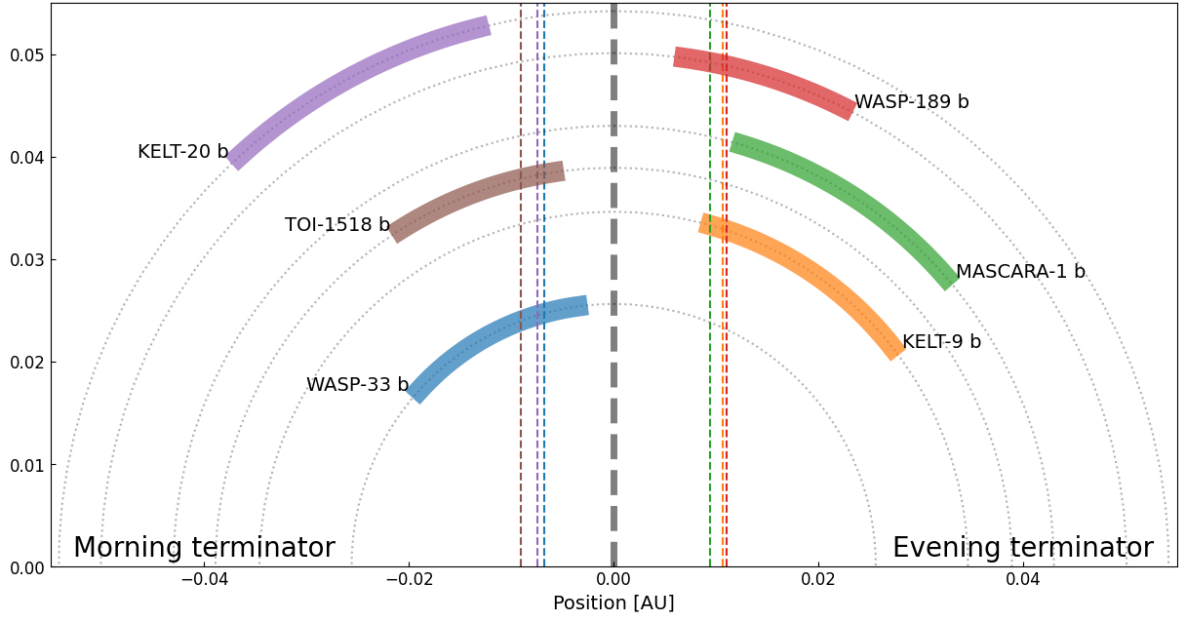


Figure 10.1: Orbital phase coverage of our observations

Semi-major axes are drawn to-scale. All planet orbits are drawn counter-clockwise, and we view the system as seen from the bottom of the plot. The stellar radii are shown as dashed vertical lines in the colors corresponding to each planet to illustrate the start/end of secondary eclipse. We omit portions of the time series for TOI-1518 b, WASP-33 b, WASP-189 b, and KELT-9 b falling within secondary eclipse. WASP-33 b, KELT-9 b, and MASCARA-1 b were observed to significant phase angles.

reduction process as described in [L. Finnerty et al. \(2025b,a\)](#). The orbital phase coverage of our observations is illustrated in Figure [10.1](#).

10.2.1.1 WASP-33 b

These observations were previously described in [L. Finnerty et al. \(2023a\)](#). The science frames were obtained in an ABBA nodding sequence using science fibers 1 and 2 and 90 second exposures. While [L. Finnerty et al. \(2023a\)](#) coadded the science data from the two fibers to create a single time series, for this reanalysis we instead keep the data from each science fiber separate and add the final log-likelihoods. Coadding data from different fibers results in frame-to-frame variations in the line-spread function (LSF) due changes in the measured flux impacting the effective weight of each fiber in the coadded spectrum. Handling each fiber separately eliminates this source of LSF variation. The first 7 exposures in science fiber 1 and the first 8 exposures in science fiber 2 were obtained during the secondary eclipse and are omitted from the log-likelihood calculation. The nominal observed planet radial velocities out of eclipse (in the stellar reference frame) ranged from -57 to -171 km s^{-1} , with a maximum change within a single exposure of 2 km s^{-1} , which is small compared to the 9 km s^{-1} resolution of the spectrograph.

Conditions were good throughout the observations, with typical top-of-atmosphere throughput around 2.5%, close to the maximum value achieved for KPIC phase I. HIP 95771 was observed prior to WASP-33 b for wavelength calibration.

10.2.1.2 KELT-9 b

The science frames were obtained in an ABC nodding pattern between science fibers 2, 3, and 4 with 90 second exposures. As with WASP-33 b, we treat the data from each science fiber as a separate time series and sum the resulting log-likelihoods. The last five exposures in each fiber were taken in secondary eclipse and are omitted from the calculation of the

log-likelihood. The nominal out-of-eclipse planet velocities ranged from 200 km s^{-1} to 90 km s^{-1} , with a maximum change of 2 km s^{-1} within a single exposure.

Conditions were excellent throughout the observations, with top-of-atmosphere throughput up to 5%. The KPIC phase II upgrade (D. Echeverri et al., 2022; N. Jovanovic et al., 2025a) is responsible for the significant sensitivity improvement compared with the KPIC phase I observations of WASP-33 b. HIP 95771 was observed prior to KELT-9 b for wavelength calibration.

10.2.1.3 WASP-189 b

Observations were obtained staring on science fiber 4 with 60 second exposures and no nodding. Afternoon dark frames were used for background subtraction. The last fifty exposures were taken after the start of secondary eclipse and are omitted from the log-likelihood calculation. The nominal star-frame planet velocity ranged from 89 km s^{-1} to 46 km s^{-1} at the start of secondary eclipse, with a maximum change of $\sim 0.5 \text{ km s}^{-1}$ within a single frame.

Conditions were very good throughout the observations, with typical throughputs $\sim 4\%$. Brief patchy cirrus caused some extinction towards the start of the observation sequence. HIP 62944 was observed prior to WASP-189 b for wavelength calibration.

10.2.1.4 MASCARA-1 b

Observations were obtained staring on science fiber 2 with 180 second exposures. The observations ended just before the start of secondary eclipse, and we use the entire observation sequence for calculating the log-likelihood. The nominal planet velocity changes from 154 km s^{-1} to 59 km s^{-1} in the stellar reference frame over the course of the observations, with a maximum single-frame shift of 1.5 km s^{-1} .

Conditions were good throughout the observations, but the large airmass at the beginning of the observation sequence led to relatively poor throughput early on. The top-of-

atmosphere throughput was $\sim 2\%$ at airmass 2.2, but improved to $\sim 4\%$ by the end of the observations when MASCARA-1 b reached its highest elevation. HIP 81497 was observed at the start of the night for wavelength calibration.

10.2.1.5 KELT-20 b

These observations were previously described in [L. Finnerty et al. \(2025b\)](#). Observations were obtained staring on science fiber 4 with 300 second exposures. Observations began after the end of secondary eclipse, and covered nominal planet velocities from -43 km s^{-1} to -119 km s^{-1} relative to the host star. The maximum single-frame velocity shift was $\sim 1.2 \text{ km s}^{-1}$.

Conditions were good throughout the observations, with throughputs ranging from 3-4%. HIP 95771 was observed after KELT-20 b for wavelength calibration.

10.2.1.6 TOI-1518 b

These observations commenced immediately after the end of the KELT-20 b observations, again staring on science fiber 4. The exposure time was reduced to 180 seconds in order to minimize the intra-frame velocity smearing. Observations began as secondary eclipse was ending, and we therefore omit the first three frames from the log-likelihood calculation. The planetary radial velocity changed from -32 km s^{-1} to -107 km s^{-1} relative to the host star reference frame over the observations, with a maximum frame-to-frame change of 1.6 km s^{-1} .

Conditions were similar observations of KELT-20 b earlier that night, but the top-of-atmosphere throughput on TOI-1518 b was somewhat lower, 2.7-3.5%. TOI-1518 b was observed at a significantly higher airmass than KELT-20 b and the primary star is ~ 1 mag fainter, making the AO correction for TOI-1518 b significantly more challenging than it was for KELT-20 b. We use the same observations of HIP 95771 as were used for KELT-20 b for

wavelength calibration.

10.2.2 Data Reduction

We use the modified KPIC DRP¹ described in L. Finnerty et al. (2025b,a) which accounts for the variable line spread function (LSF) of NIRSPEC. In brief, we fit a Gaussian-Hermite model to the trace profile, which is used for optimum extraction. The resulting trace profile is then broadened by a factor of 1.14 based on measurements of OH lines described in L. Finnerty et al. (2022) and used as the instrumental LSF in the forward model. As discussed in L. Finnerty et al. (2025b,a), this scaling factor is somewhat uncertain, leading to a systematic uncertainty in retrieved $v \sin i$ values. For targets which were observed with multiple fibers, a separate spectral time series was created for each fiber in order to eliminate frame-to-frame variations in the LSF due to variable relative flux between fibers. The resulting log-likelihoods from each separate time series were summed during sampling.

Wavelength calibration was performed using the KPIC DRP, which compares observations of a late-type giant star to a stellar $\times$ telluric model. The bluest three orders (37–39, 1.94–2.09 μm) are heavily impacted by telluric CO₂ features and omitted from subsequent analysis, leaving six orders (31–36, 2.1–2.49 μm) for the cross-correlation and retrieval analysis. In the past, orders 35 and 36, which have relatively few strong lines, have been difficult to calibrate. We previously obtained a good wavelength solution for these orders in L. Finnerty et al. (2025a), which provided a basis for obtaining a good wavelength solution for the remaining targets. We verified the resulting wavelength solutions by visual inspection of the wavelength calibration observations with the stellar $\times$ telluric model, and by comparing the coefficients of a 4th-order polynomial fit to the wavelength solution for each order.

The data reduction process produces a flux array ($N_{\text{frame}}, N_{\text{channel}}$) for each order, as well as arrays of the mid-exposure times, barycentric velocities, wavelength solution for each

¹https://github.com/kpicteam/kpic_pipeline/

order, and LSF for each order and channel. These data products are the inputs for our retrieval analysis.

10.2.3 Atmospheric Retrieval

We use the atmospheric retrieval framework described in L. Finnerty et al. (2023a, 2024, 2025a,b). Changes compared with L. Finnerty et al. (2025b) are minor, and primarily focused on improved masking of bad pixels or regions of high telluric absorption. We summarize the retrieval setup below. The full list of parameters and priors is included in Table 10.3. The same set of priors and masking parameters was used for all observations.

10.2.3.1 Data processing

The time series for each order resulting from the data reduction procedure includes frame-to-frame flux variations and the instrumental blaze function, which must be removed before computing the log-likelihood. For each order, we first divide the spectrum from each exposure by its median to remove the frame-to-frame variation in flux. We then mask the 3% of wavelength channels with the highest variance along the time axis, which masks channels strongly impacted by bad pixels or time-varying tellurics. The entire time series is then divided by the median spectrum along the time axis. In the limit of large planet velocity shift, the median spectrum is simply the stellar spectrum multiplied by the average telluric spectrum, $F_s \times \bar{T}$, and this division converts the spectral time series to $F_p/F_s \times T(t)$, where $T(t)$ is the time-dependent change in the telluric absorption spectrum. For smaller planet velocity shifts, the median spectrum may contain some contribution from the planet spectrum, leading to a self-division effect which can reduce the strength of planet features. This is addressed by similarly dividing the forward model $F_p + F_s$ time series by its median to replicate any self-division.

After the median division, we mask the first and last 50 wavelength channels, which have

very low transmission due to the instrumental blaze function. We then mask any points deviating by more than 6 times the Median Absolute Deviation (MAD) from 1, in order to mask any remaining bad pixels.

At this stage, temporal variations in the telluric spectrum remain, and are generally strong enough to hide any planetary emission signals. Consistent with current standard practice in HRCCS analysis (e.g. [M. R. Line et al., 2021](#); [L. Finnerty et al., 2023a, 2024, 2025a,b](#)), we remove this signal through Principal Component Analysis (PCA). For each order, the time series is mean-subtracted and masked data is interpolated over. We then perform the PCA, omitting six components, and re-apply the original masking. Finally, we mask any points deviating by more than four times the MAD. Following [M. R. Line et al. \(2021\)](#), we save the dropped principal components in order to add them to the forward model and project out the same number of components, replicating any distortion of the underlying planet signal resulting from PCA. We also mask any wavelength channels in the forward model with telluric transmission $< 70\%$, in order to ensure that the higher-noise regions of the spectrum are not included in the likelihood calculation. We then compare the forward model and the data, computing the log-likelihood as described by [M. R. Line et al. \(2021\)](#).

We performed retrievals omitting both four and six principal components for all targets. While the optimum number of components is likely different from target to target and order to order, previous studies have found that overly optimizing the number of omitted PCs can lead to false detections ([C. J. Cheverall et al., 2023](#)), and we therefore choose a single number of components to omit for all targets and orders. The posteriors are consistent between the four and six component cases, but in some cases (particularly the last order for WASP-189 b), the four component case left obvious residuals upon visual inspection of the post-PCA time series. We therefore present the six component retrievals as our fiducial runs.

10.2.3.2 Stellar models

For each target, we use a PHOENIX (T. O. Husser et al., 2013) model for the host star, chosen to have the closest T_{eff} , $\log g$, and metallicity in the model grid to the assumed stellar parameters. Each model was rotationally broadened using the fast wavelength-dependent technique described in A. Carvalho & C. M. Johns-Krull (2023) to the respective $v \sin i$ value. For WASP-33 A, we used $T_{\text{eff}} = 9000$ K, $\log g = 4.0$, $Z = 0$, and $v \sin i = 86.9 \text{ km s}^{-1}$. For KELT-9 A, we used $T_{\text{eff}} = 9600$ K, $\log g = 4.0$, $Z = 0$, and $v \sin i = 111 \text{ km s}^{-1}$. For WASP-189 A, we used $T_{\text{eff}} = 8000$ K, $\log g = 4.0$, $Z = +0.5$, and $v \sin i = 93.1 \text{ km s}^{-1}$. For MASCARA-1 A, we used $T_{\text{eff}} = 7600$ K, $\log g = 4.0$, $Z = 0$, and $v \sin i = 109 \text{ km s}^{-1}$. For KELT-20 A, we used $T_{\text{eff}} = 9000$ K, $\log g = 4.5$, $Z = 0$, and $v \sin i = 114 \text{ km s}^{-1}$. Finally, for TOI-1518 A, we used $T_{\text{eff}} = 7400$ K, $\log g = 4.0$, $Z = 0$, and $v \sin i = 85.1 \text{ km s}^{-1}$. Despite the rapid rotation rates of the host stars, we do not include limb or gravity darkening, which may lead to minor offsets in the absolute F_p/F_s values. HRCCS techniques are only weakly sensitive to the absolute F_p/F_s , as discussed in Section 10.4, and we do not expect this omission will significantly impact our interpretation of the retrievals.

10.2.3.3 Planet models

We compute 1D model atmospheres for the planets using petitRADTRANS3 (P. Mollière et al., 2019, 2020; E. Nasedkin et al., 2024). We continue to use 80 log-uniform spaced pressure layers from $10^2 - 10^{-6}$ bar. We adopt the 4-parameter model for the $P - T$ profile from T. Guillot (2010), including the internal temperature following L. Finnerty et al. (2025b). We fix the planetary $\log g$ value to the value corresponding to the nominal mass and radius, after testing found our retrievals were unable to meaningfully constrain $\log g$, which is strongly degenerate with $\log \kappa$.

Dissociation of H_2O is a major process in the atmospheres of UHJs, which significantly impacts interpretation of the K band spectra (M. Brogi et al., 2023; S. Ramkumar et al.,

2023; L. Finnerty et al., 2023a). If not incorporated into the forward model, either through free retrieval of the H₂O and OH mixing profiles or by assuming equilibrium chemistry, dissociation will bias retrieval results towards high C/O ratios, as the only remaining way to match the relative strengths of CO and H₂O features is to reduce the H₂O abundance and/or increase the CO abundance. In the case of KELT-9 b, this may be further complicated by the dissociation of CO at even lower pressures.

We address this by incorporating dissociation and formation pressures into our free retrieval framework, as previously described in L. Finnerty et al. (2025b). For H₂O, OH, and CO, we fit a break pressure, and set the corresponding abundance to decay as $(P/P_{\text{dissoc}})^4$ at lower pressures. For OH, we also fit a formation pressure, with the abundance decreasing as the pressure increases above the formation pressure. This approach allows us to incorporate dissociation without making model assumptions about chemical equilibrium of photochemistry, and also clarifies whether the data quality supports varying vertical abundances.

Again following L. Finnerty et al. (2025b), we use a truncated log-normal prior for the scale factor applied to the planet model with a standard deviation of 0.1. Values above ± 0.75 are rejected for numerical stability. As discussed in L. Finnerty et al. (2025b), the use of this prior somewhat, but not completely, breaks the temperature/scale factor degeneracy which impacts HRCCS observations with limited wavelength coverage.

10.2.3.4 Opacity Sources

The opacity tables used for H₂O, OH, ¹²CO, and ¹³CO were previously described in L. Finnerty et al. (2023a). For H₂O we used the (O. L. Polyansky et al., 2018) partition function and HITEMP 2010 linelist (L. S. Rothman et al., 2010). For both CO isotopologues we used the HITEMP 2019 lists (I. E. Gordon et al., 2022) and the G. Li et al. (2015) partition function. For OH we used the partition function from M. Yousefi et al. (2018) and HITEMP 2020 linelist (I. E. Gordon et al., 2022). Opacities were generated via ExoCross (S. N. Yurchenko et al., 2018) following instructions in the petitRADTRANS documentation. For Fe

and H_2 , we use the default `petitRADTRANS` opacities. The Fe opacity is based on the Kurucz atomic line lists, and H_2 opacity is from [L. S. Rothman et al. \(2013\)](#). We also include CIA opacities for $\text{H}_2 - \text{H}_2$ ([A. Borysow et al., 2001](#); [A. Borysow, 2002](#)) and $\text{H}_2 - \text{He}$ ([J. Borysow et al., 1988](#); [A. Borysow et al., 1989](#); [A. Borysow & L. Frommhold, 1989](#)), and used the scattering mode for `petitRADTRANS`.

While UHJs are in the temperature regime for H^- opacity, and H^- features have been detected in the atmosphere KELT-9 b ([B. Jacobs et al., 2022](#)), we do not include H^- in our analysis, following [L. Finnerty et al. \(2023a, 2025b\)](#). [L. Finnerty et al. \(2023a\)](#) found that including H^- results in a uniform reduction in the strength of planet lines relative to the continuum for KPIC K -band observations. HRCCS analysis has poor sensitivity to the absolute flux level of the planet, and as a result the H^- parameters are unconstrained when included in the retrieval. [B. Jacobs et al. \(2022\)](#) found that H^- opacity results in a turnoff at $1.4\,\mu\text{m}$ in the spectrum of KELT-9 b, suggesting that combining K band observations with additional data at shorter wavelengths would result in sensitivity to H^- .

10.2.3.5 Sampling

We use `MultiNEST` ([F. Feroz & M. P. Hobson, 2008](#); [F. Feroz et al., 2009](#); [J. Buchner et al., 2014](#); [F. Feroz et al., 2019](#)) to estimate posteriors via nested sampling ([J. Skilling, 2004](#)). We use 1200 live points and a convergence criteria $\Delta \log z < 0.01$, similar to our previous HRCCS retrievals. The log-likelihood is computed using the [M. Brogi & M. R. Line \(2019\)](#) mapping for each fiber separately and summed.

10.3 Results

Parameters, priors, and retrieved median/max-likelihood values for each target are presented in Table [10.1](#), along with derived abundance parameters calculated from the retrieved posteriors. Figure [10.2](#) shows the 2D and 1D cross-correlation functions in the planet reference

frames for the maximum-likelihood models for each time series. The corresponding $K_p - \Delta v_{\text{sys}}$ diagrams are shown in Figure 10.3. We assess the detection strengths of CO, H₂O, and OH through a series of leave-one-out tests (see L. Finnerty et al., 2025b, for a discussion of this approach), and present the $K_p - \Delta v_{\text{sys}}$ diagrams leaving each species out in Figures 10.4, 10.5, and 10.6, respectively.

The retrieved $P - T$ profiles for each object are shown in Figure 10.7. The retrieved median and maximum-likelihood spectra are plotted in Figure 10.8, with a comparison to the expected F_p/F_s assuming both star and planet are blackbodies. Figure 10.9 shows the corner plots for the derived abundance parameters, C/O, [C/H], [O/H], and [(C+O)/H]. The full corner plots for the retrievals are included in Section 10.6.

10.3.1 KELT-20 b

The retrieved posterior for KELT-20 b is consistent with the previous analysis described in L. Finnerty et al. (2025b), to which we refer the reader for a more detailed discussion. This consistency establishes that the minor changes in the priors and detrending approach compared with L. Finnerty et al. (2025b) do not impact the retrieved atmospheric properties for a well-detected target.

Figure 10.2 shows a clear detection of the maximum-likelihood model for KELT-20 b, even in the 2D cross-correlation function. Figure 10.3 shows KELT-20 b is the second-strongest detection strength of the six observed targets, at $\text{SNR} = 13.3$. Figure 10.4 demonstrates that the detection is CO-dominated, with the SNR dropping to 4.5 when CO is omitted. Omitting H₂O in Figure 10.5 shows a minor decrease in SNR without H₂O opacity, while Figure 10.6 shows no negative impact from omitting OH. These results are consistent with the retrieved posterior, which constrains CO well, places a lower limit on H₂O, and does not show constraints on OH or Fe.

The dissociation pressure for H₂O is well-constrained by the retrieval ($P_{\text{H}_2\text{O}} = -1.5^{+0.8}_{-1.1}$),

Table 10.3: List of parameters, priors, and results for atmospheric retrievals

Name	Symbol	Prior	KELT-20 b	WASP-33 b	KELT-9 b	WASP-189 b	MASCARA-1 b	TOI-1518 b
log infrared opacity [$\text{cm}^2 \text{g}^{-1}$]	$\log \kappa$	Uniform(-4, 0)	$-2.1^{+0.8}_{-0.6}$ (-2.4)	$-1.3^{+0.7}_{-0.8}$ (-0.1)	$-2.4^{+1.0}_{-0.8}$ (-3.3)	$-1.8^{+1.0}_{-0.9}$ (-2.3)	$-3.1^{+0.7}_{-0.5}$ (-3.9)	$-1.8^{+0.9}_{-0.9}$ (-3.0)
log infrared/optical opacity	$\log \gamma$	Uniform(0, 3)	$1.3^{+0.2}_{-0.3}$ (1.4)	$1.1^{+0.5}_{-0.4}$ (2.1)	$0.8^{+0.4}_{-0.3}$ (0.8)	$0.9^{+0.4}_{-0.3}$ (0.8)	$0.5^{+0.4}_{-0.2}$ (1.0)	$0.5^{+0.4}_{-0.2}$ (0.5)
Intrinsic temperature [K]	T_{int}	Uniform(100, 500)	300^{+100}_{-100} (400)	300^{+100}_{-100} (500)	300^{+100}_{-100} (200)	300^{+100}_{-100} (300)	300^{+100}_{-100} (100)	300^{+100}_{-100} (400)
Equilibrium temperature [K]	T_{equ}	Uniform(1500, 5000)	1800^{+300}_{-300} (1600)	2600^{+600}_{-600} (1800)	2300^{+800}_{-800} (1700)	2200^{+700}_{-700} (1600)	3400^{+800}_{-800} (2200)	3200^{+1000}_{-1000} (4900)
K_p offset [km s^{-1}]	ΔK_p	Uniform(-40, 40)	$-2.4^{+3.1}_{-3.1}$ (-1.2)	$-16.5^{+4.4}_{-4.4}$ (-19.1)	$0.9^{+15.5}_{-9.9}$ (-1.8)	$18.9^{+13.6}_{-19.6}$ (5.8)	$-27.1^{+9.5}_{-7.5}$ (-26.7)	$2.9^{+15.7}_{-14.7}$ (-25.0)
v_{sys} offset [km s^{-1}]	Δv_{sys}	Uniform(-30, 30)	$-2.2^{+1.5}_{-1.5}$ (-1.9)	$-11.5^{+2.3}_{-2.5}$ (-13.2)	$2.2^{+5.6}_{-2.4}$ (2.9)	$-8.2^{+5.8}_{-3.9}$ (-4.3)	$5.8^{+3.5}_{-4.5}$ (4.5)	$7.8^{+4.9}_{-5.2}$ (1.1)
Rotational velocity [km s^{-1}]	v_{rot}	Uniform(0, 15)	$7.8^{+0.7}_{-0.8}$ (8.2)	$9.5^{+1.0}_{-1.1}$ (10.9)	$5.6^{+2.5}_{-2.4}$ (1.1)	$6.3^{+3.2}_{-2.5}$ (5.0)	$11.5^{+2.7}_{-4.7}$ (14.6)	$9.4^{+2.8}_{-4.0}$ (7.4)
log H ₂ O mass-mixing ratio	log H ₂ O	Uniform(-12, -0.3)	$-1.7^{+0.9}_{-1.4}$ (-0.9)	$-5.7^{+3.0}_{-3.8}$ (-9.1)	$-7.4^{+3.1}_{-2.8}$ (-9.3)	$-7.7^{+3.0}_{-2.7}$ (-7.7)	$-7.8^{+2.6}_{-2.6}$ (-4.6)	$-7.0^{+2.9}_{-3.0}$ (-10.4)
log CO mass-mixing ratio	log CO	Uniform(-12, -0.3)	$-1.9^{+0.8}_{-0.8}$ (-2.1)	$-1.8^{+0.8}_{-0.8}$ (-0.8)	$-2.8^{+1.0}_{-1.0}$ (-3.8)	$-2.1^{+0.9}_{-0.9}$ (-1.6)	$-2.3^{+0.8}_{-0.8}$ (-2.7)	$-1.8^{+1.0}_{-1.0}$ (-1.1)
log OH mass-mixing ratio	log OH	Uniform(-12, -0.5)	$-5.2^{+4.5}_{-4.5}$ (-2.3)	$-6.7^{+3.3}_{-3.3}$ (-8.3)	$-2.3^{+1.3}_{-1.3}$ (-1.3)	$-6.6^{+3.4}_{-3.3}$ (-2.4)	$-1.1^{+0.4}_{-0.4}$ (-1.1)	$-6.5^{+3.2}_{-3.2}$ (-2.6)
log Fe mass-mixing ratio	log Fe	Uniform(-12, -1)	$-6.3^{+3.5}_{-3.7}$ (-1.4)	$-6.8^{+3.1}_{-3.2}$ (-8.0)	$-7.3^{+3.0}_{-2.9}$ (-10.3)	$-7.0^{+3.3}_{-3.1}$ (-5.6)	$-7.3^{+2.8}_{-3.0}$ (-2.7)	$-7.4^{+2.9}_{-2.7}$ (-1.5)
H ₂ O dissociation pressure	log P _{H₂O}	Uniform(-6, 2)	$-1.5^{+0.8}_{-1.1}$ (-1.1)	$-1.8^{+2.2}_{-2.4}$ (-1.4)	$-1.5^{+2.3}_{-2.6}$ (-2.4)	$-1.4^{+2.2}_{-2.6}$ (-2.8)	$-1.6^{+2.3}_{-2.6}$ (-0.2)	$-1.7^{+2.3}_{-2.4}$ (-2.5)
OH dissociation pressure	log P _{OH}	Uniform(-6, 2)	$-2.6^{+2.9}_{-2.2}$ (-5.0)	$-1.8^{+2.3}_{-2.5}$ (-5.2)	$-3.1^{+2.2}_{-1.7}$ (-4.8)	$-1.8^{+2.3}_{-2.6}$ (-3.1)	$-3.7^{+1.6}_{-1.4}$ (-3.4)	$-2.0^{+2.4}_{-2.3}$ (-2.2)
CO dissociation pressure	log P _{CO}	Uniform(-6, -2)	$-4.9^{+1.4}_{-1.4}$ (-5.1)	$-4.9^{+1.4}_{-1.4}$ (-6.1)	$-4.6^{+1.5}_{-1.5}$ (-6.9)	$-4.8^{+1.5}_{-1.5}$ (-6.4)	$-4.5^{+1.5}_{-1.5}$ (-4.4)	$-4.7^{+1.5}_{-1.5}$ (-6.6)
OH formation pressure	log P _{formOH}	Uniform(-6, 2)	$-1.8^{+2.4}_{-2.4}$ (1.2)	$-2.1^{+2.5}_{-2.3}$ (-2.9)	$-0.7^{+1.6}_{-1.6}$ (0.4)	$-2.2^{+2.4}_{-2.3}$ (-0.3)	$0.4^{+0.9}_{-1.0}$ (0.5)	$-2.2^{+2.4}_{-2.3}$ (-0.0)
log ¹³ CO/ ¹² CO	log ¹³ CO/ ¹² CO	Uniform(-8, 0)	$-5.3^{+1.8}_{-1.7}$ (-4.2)	$-4.0^{+2.4}_{-2.4}$ (-4.5)	$-3.4^{+2.3}_{-2.8}$ (-1.2)	$-4.1^{+1.9}_{-1.9}$ (-6.5)	$-4.0^{+2.3}_{-2.5}$ (-1.9)	$-5.1^{+1.9}_{-1.7}$ (-5.6)
log H mass-mixing ratio	log allH	Uniform(-0.4, -0.05)	$-0.2^{+0.1}_{-0.1}$ (-0.2)	$-0.2^{+0.1}_{-0.1}$ (-0.2)	$-0.2^{+0.1}_{-0.1}$ (-0.2)	$-0.2^{+0.1}_{-0.1}$ (-0.3)	$-0.2^{+0.1}_{-0.1}$ (-0.2)	$-0.2^{+0.1}_{-0.1}$ (-0.2)
log H ₂ dissociation pressure	log P _{H₂}	Uniform(-6, 2)	$-2.2^{+2.6}_{-2.4}$ (-3.7)	$-1.9^{+2.4}_{-2.5}$ (-0.2)	$-2.2^{+2.5}_{-2.3}$ (1.4)	$-1.9^{+2.3}_{-2.5}$ (-4.4)	$-1.9^{+2.4}_{-2.5}$ (1.0)	$-2.0^{+2.4}_{-2.4}$ (-5.8)
Scale factor	scale	LogNormal(0, 0.1)	$0.04^{+0.08}_{-0.08}$ (0.05)	$0.0^{+0.08}_{-0.08}$ (0.28)	$-0.0^{+0.08}_{-0.08}$ (0.15)	$0.0^{+0.08}_{-0.08}$ (0.24)	$-0.01^{+0.09}_{-0.09}$ (0.06)	$-0.02^{+0.08}_{-0.08}$ (-0.18)

Note. — Values with errors are the retrieved medians and 68%/1 σ confidence interval. Values in parentheses without errors are the values for the maximum-likelihood model. In addition to these priors, we required that the atmospheric temperature stay below 6000 K at all pressure levels. The full corner plots are included in Section 10.6.

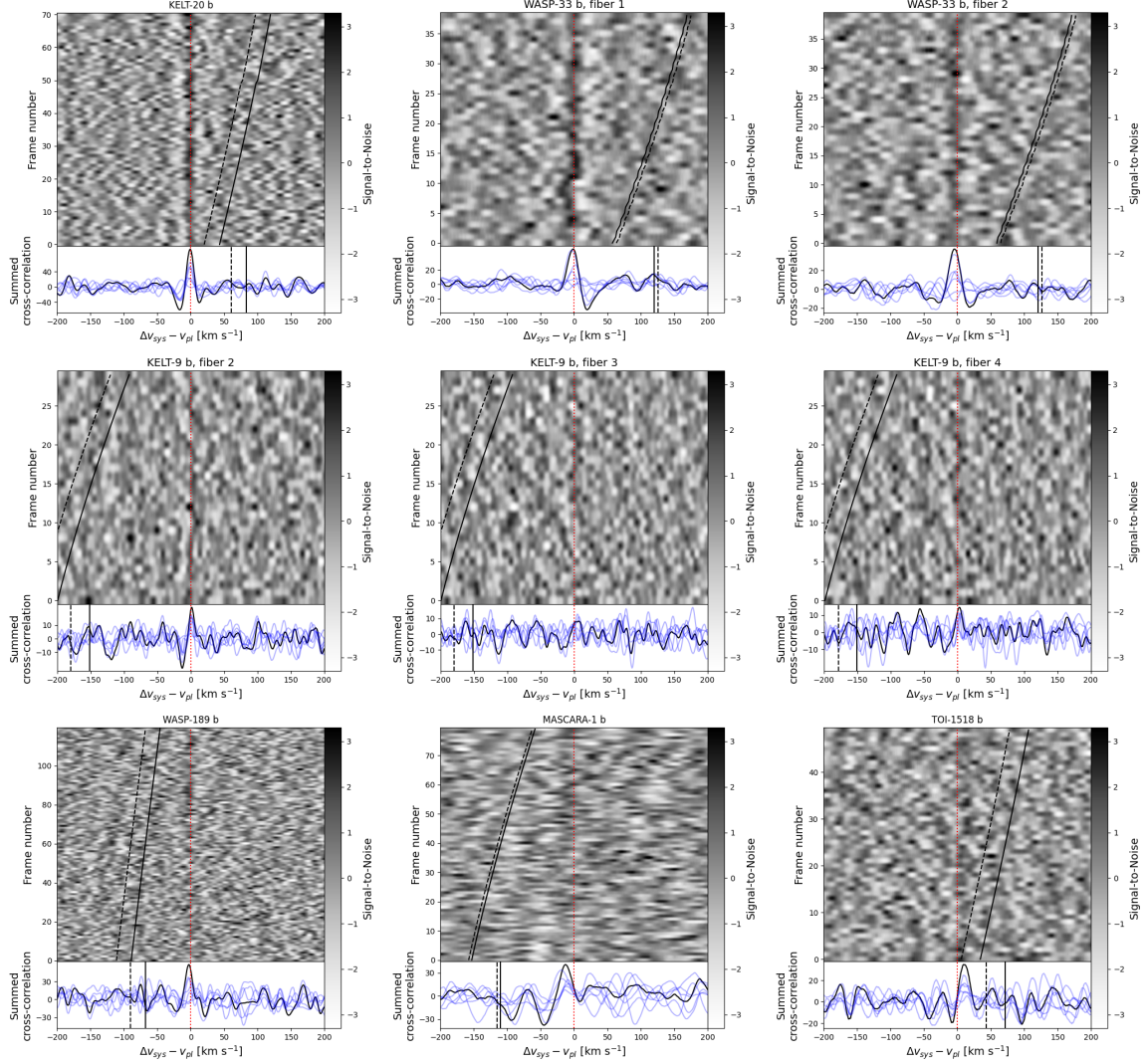


Figure 10.2: Cross-correlation coefficient in the nominal planet rest frame

Top panels show the 2D cross-correlation versus frame number, while the bottom panel shows the CCF after coadding over the full time series for each target and science fiber. The stellar/telluric reference frames are indicated with solid/dashed black lines, respectively, and the nominal planet rest frame is shown in dashed red.

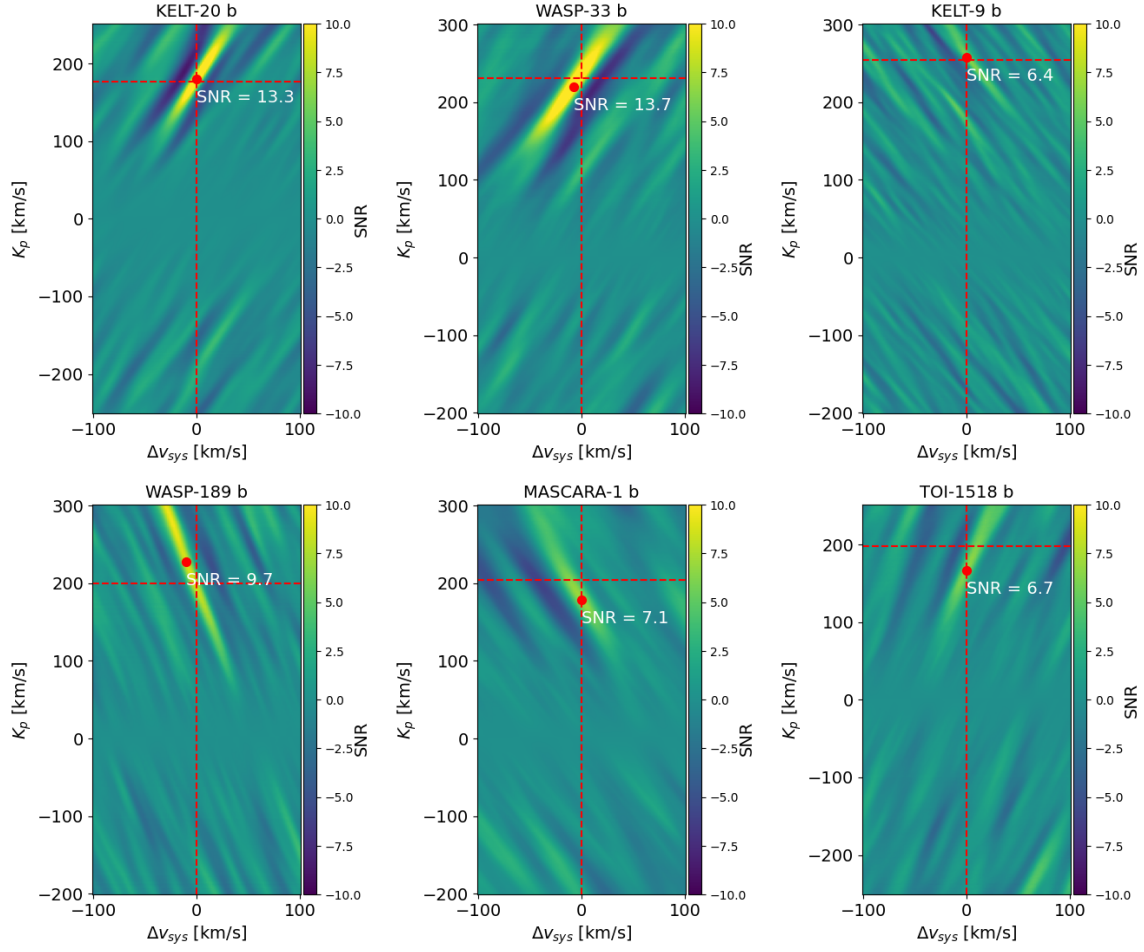


Figure 10.3: $K_p - \Delta v_{\text{sys}}$ diagrams for the maximum-likelihood models

All targets are detected at $\text{SNR} > 6$, with WASP-33 b, KELT-20 b, and WASP-189 b detected at $\text{SNR} \sim 10$ or greater.

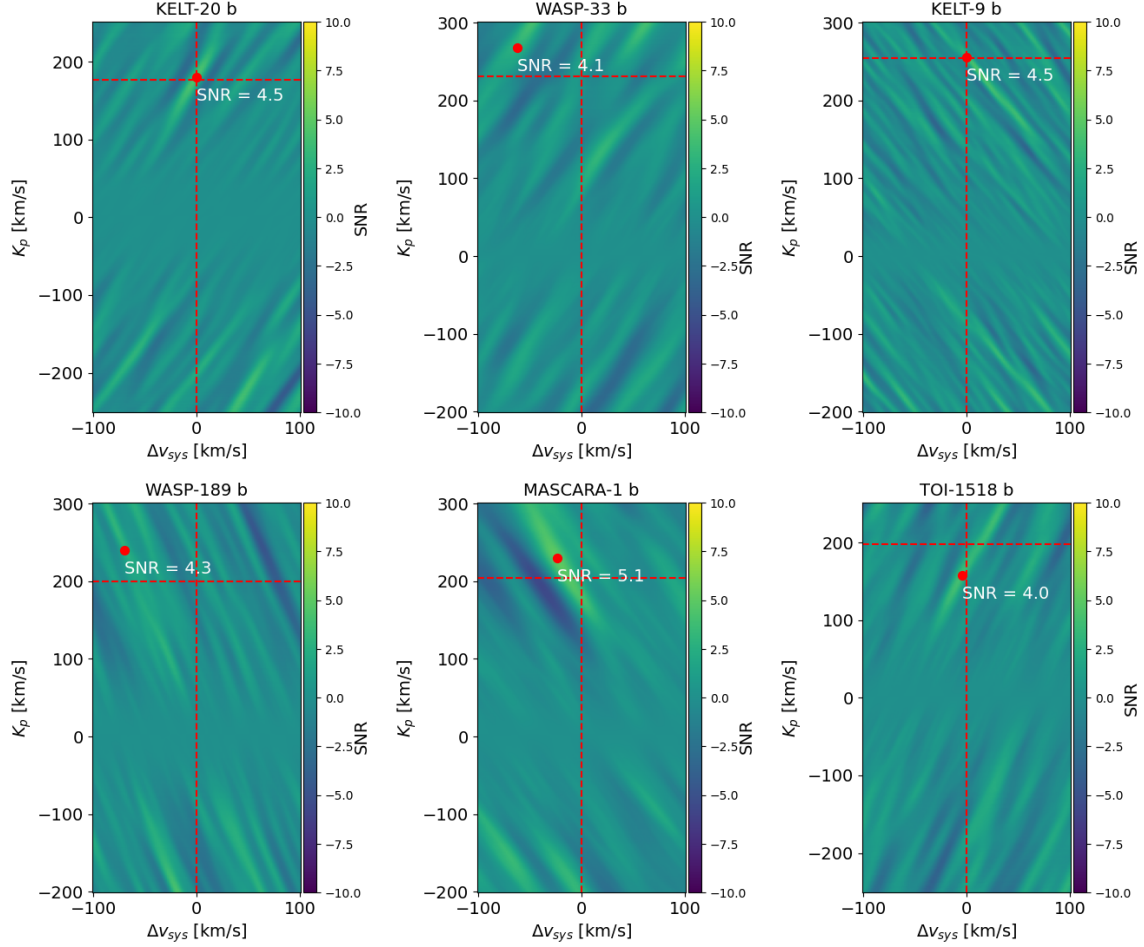


Figure 10.4: $K_p - \Delta v_{\text{sys}}$ diagrams for the maximum-likelihood models omitting CO opacity.

For KELT-20 b, KELT-9 b, MASCARA-1 b, and TOI-1518 b, the strongest feature in the $K_p - \Delta v_{\text{sys}}$ space is consistent with the nominal planet rest frame at $\text{SNR} \sim 4 - 5$, suggesting the presence of H_2O and/or OH in these atmospheres. In contrast, WASP-33 b and WASP-189 b do not show significant cross-correlation peaks in the planet reference frames, indicating these targets do not have detectable quantities of H_2O or OH. For all six targets, there is a significant decrease in detection strength compared with Figure 10.3, indicating CO opacity is contributing to (and in some cases dominating) the atmospheric signal.

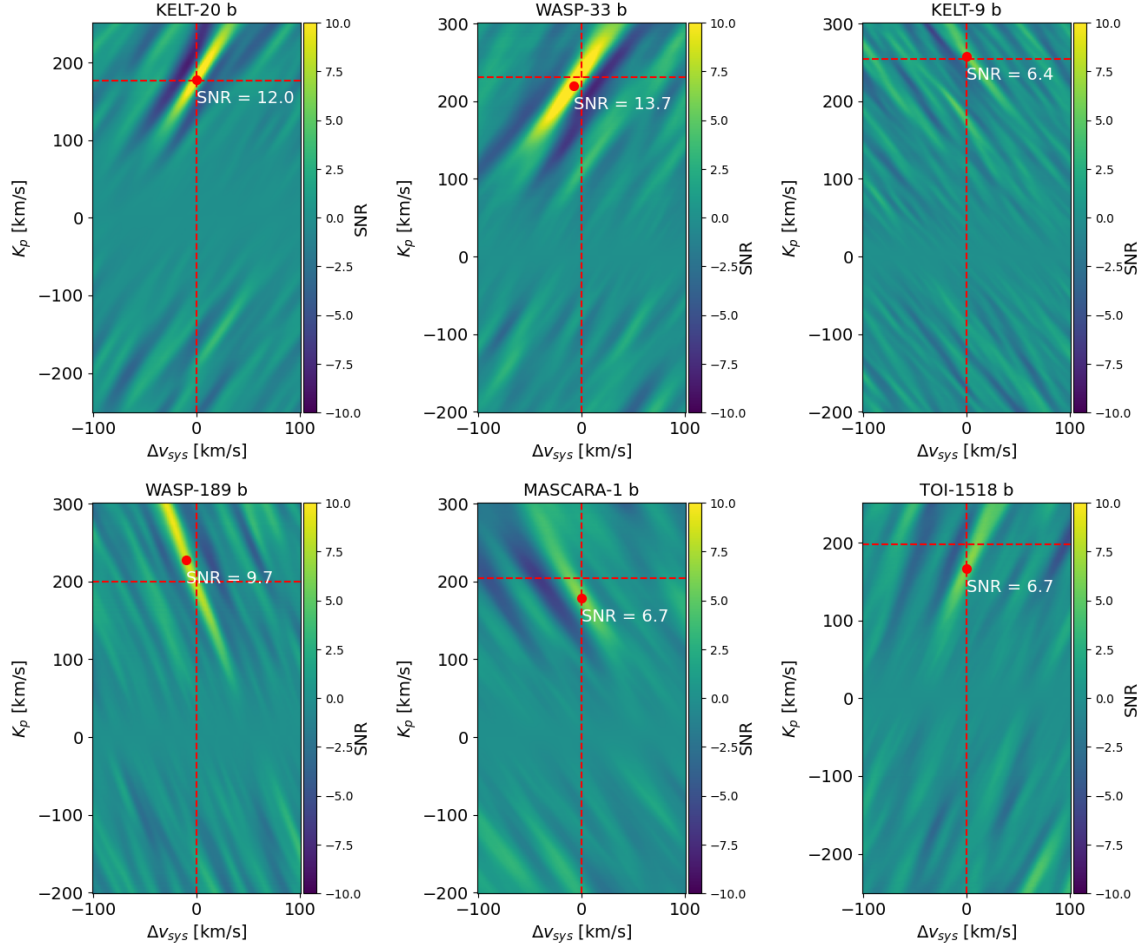


Figure 10.5: $K_p - \Delta v_{\text{sys}}$ diagrams for the maximum-likelihood models omitting H_2O opacity. Compared with Figure 10.3, KELT-20 b and MASCARA-1 b are detected at slightly lower SNR, suggesting H_2O opacity is significantly contributing to the overall detection in these two targets. The other four targets do not show any change in detection strength with the emission of H_2O , indicating a lack of significant H_2O features.

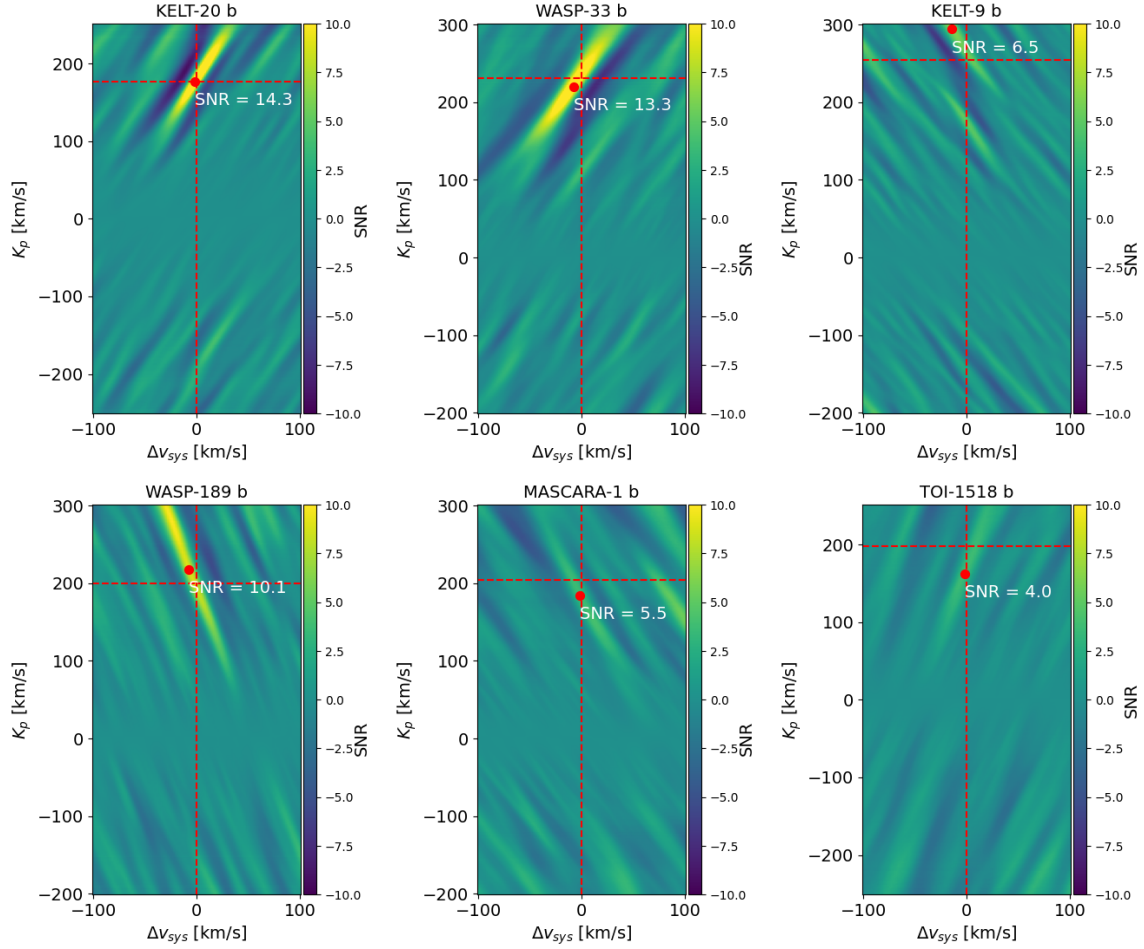


Figure 10.6: $K_p - \Delta v_{\text{sys}}$ diagrams for the maximum-likelihood models omitting OH opacity. TOI-1518 b and MASCARA-1 b show a small decrease in detection strength without OH, indicating OH opacity is contributing to the overall detection of these targets. All other targets are unaffected by the absence of OH.

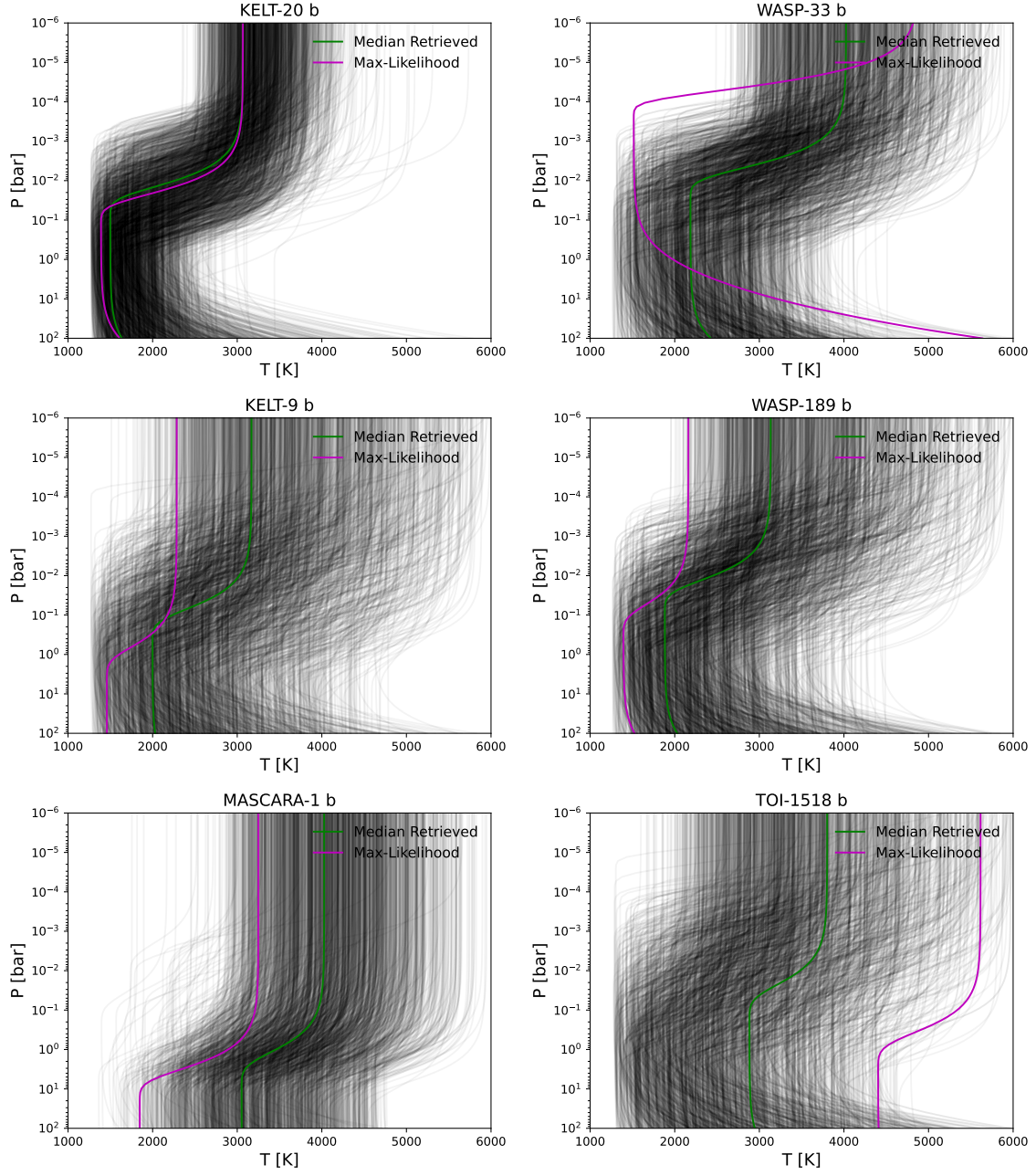


Figure 10.7: Retrieved $P - T$ profiles for each target.

The black lines show 2000 draws from the posterior, in addition to the median and maximum-likelihood values.

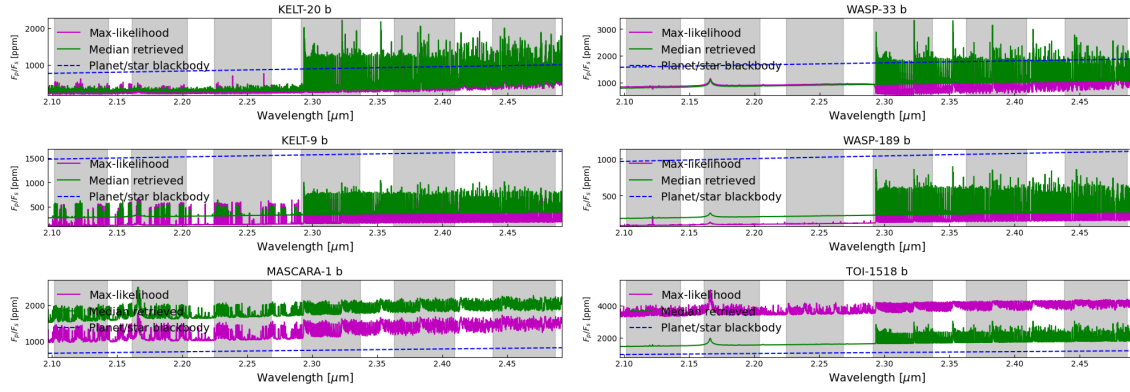


Figure 10.8: Planet/star flux ratios for the retrieved planet models

The expected values for blackbodies are shown in blue, and observed NIRSPEC orders are shaded.

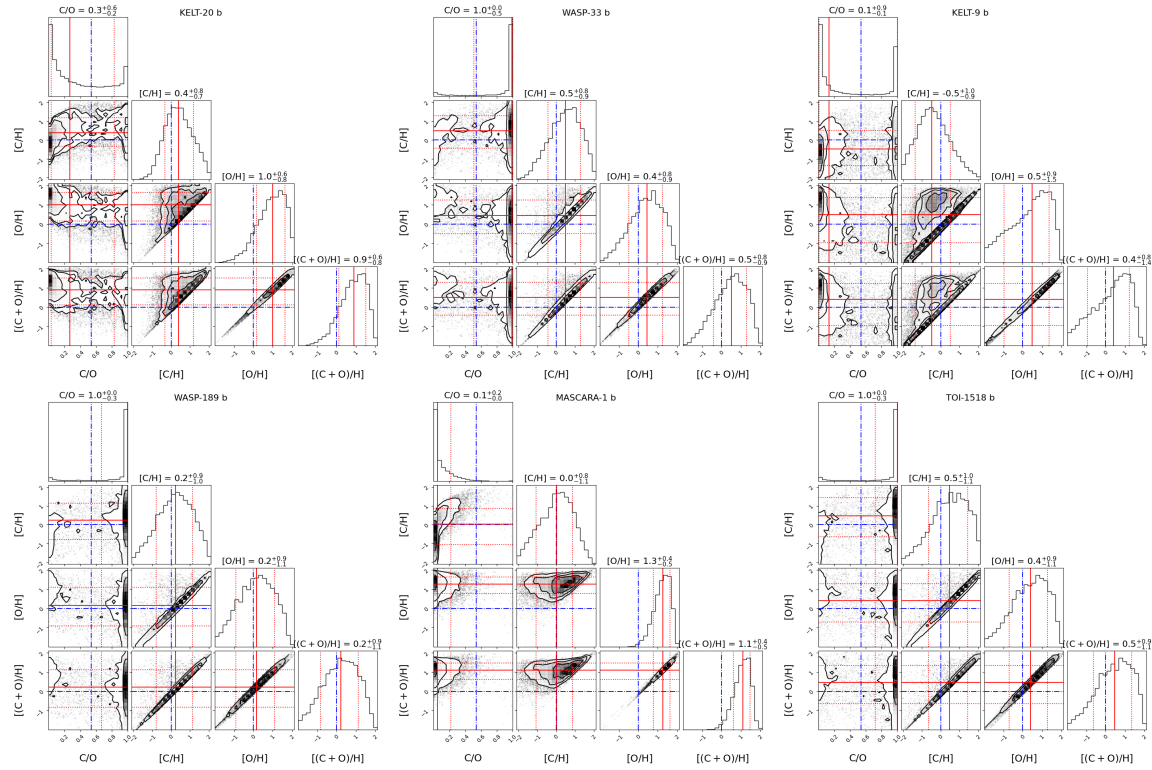


Figure 10.9: Derived posteriors for the C/O ratio, carbon and oxygen abundances, and total volatile abundance.

and there is a significant degeneracy between CO and $P_{\text{H}_2\text{O}}$, previously reported in [L. Finnerty et al. \(2025b\)](#). The median retrieved dissociation pressure is consistent with the location of the thermal inversion (shown in Figure 10.7), in line with predictions from chemical equilibrium models. As a result of this dissociation, the H_2O features in the retrieved spectrum are weak in comparison to CO features, despite the very high H_2O abundance preference, which can be seen comparing the first and last three orders of the retrieved spectra shown in Figure 10.8. As discussed in [L. Finnerty et al. \(2025b\)](#), this results in a degeneracy between the CO abundance and the H_2O dissociation pressure, leading to a secondary high C/O mode in the derived posteriors plotted in Figure 10.9, while the volatile abundance is unimodal, $[(\text{C} + \text{O})/\text{H}] = 0.9^{+0.6}_{-0.8}$, consistent with a moderately volatile-rich composition.

10.3.2 WASP-33 b

The previous analysis of these data, reported in [L. Finnerty et al. \(2023a\)](#), used an older version of the retrieval pipeline used here. Significant changes were made to the detrending/PCA procedures since that analysis, which did not incorporate vertical abundance variations. In this analysis, the maximum-likelihood model produces a clear trace in the 2D cross-correlation plots for both science fibers, and is detected in the $K_p - \Delta v_{\text{sys}}$ space at $\text{SNR} = 13.7$. Figure 10.4 establishes that in the absence of CO opacity, there is no detection of the planet, consistent with the lack of H_2O and OH spectral features in the spectra shown in Figure 10.8. The posteriors for these species are effectively unconstrained. In contrast, [L. Finnerty et al. \(2023a\)](#) constrained the H_2O mass-mixing ratio to $\sim 10^{-4}$ and saw a weak preference for significant quantities of OH in the posterior distribution. This may be a result of the computationally expensive negative injection PCA approach used in [L. Finnerty et al. \(2023a\)](#), and may also explain the lack of isotopologue constraint compared to that work. [Y.-H. Choi et al. \(2025\)](#) recently reported detection of CO, H_2O , and OH emission features using the IGRINS2 spectrograph, which covers the entirety of the H and K bands, yielding much better sensitivity to H_2O and especially OH.

The non-detection of H₂O and OH in WASP-33 b drives the inferred C/O ratio to 1, as CO is the only detected species. However, the C/O ratio posterior has a long tail to low values, as relatively high H₂O abundances are permitted provided the dissociation occurs low enough in the atmosphere for the final spectral features to be minimal. While both the H₂O abundance and dissociation pressures are unconstrained, the corner plot shows the posterior significantly disfavors the combination of high H₂O abundance and low dissociation pressure. The retrieved volatile abundance is $[(C + O)/H] = +0.5^{+0.8}_{-0.9}$, suggesting a roughly solar to slightly super-solar composition.

10.3.3 KELT-9 b

The retrieved maximum-likelihood model provides the first infrared detection of KELT-9 b, at a cross-correlation SNR = 6.4 in Figure 10.3. The cross-correlation trail is not clearly visible in any individual fiber time series, but weak peaks are evident in all three fibers after summing over the time series. Omitting CO opacity reduces the detection strength to SNR = 4.5 in Figure 10.4, suggesting the OH features in the maximum-likelihood model may be contributing to the overall detection. However, Figure 10.6 shows omitting OH opacity has a negligible impact on detection strength when CO is included, suggesting the detection is dominated by CO, despite the weak preference for high OH abundances in the retrieved posterior.

The lack of apparent H₂O features is unsurprising in the case of KELT-9 b, which is hot enough that dissociation produces detectable quantities of atomic oxygen (F. Borsa et al., 2021). The overall detection strength is relatively weak, particularly given the high quality of the KELT-9 b observations, which may be a result of previously reported strong H⁻ opacity muting the observed spectrum.

The CO abundance is constrained, while H₂O is disfavored. The OH posterior is also unconstrained, but has a weak preference for the upper range of the prior. This results in a bimodal distribution in the C/O ratio posterior, shown in Figure 10.9, and a very broad

volatile abundance constraint, $[(\text{C} + \text{O})/\text{H}] = 0.4^{+0.8}_{-1.4}$, compatible with the values reported by [L. Nortmann et al. \(2018\)](#) from *HST* observations.

10.3.4 WASP-189 b

The cross-correlation trail of the maximum-likelihood model is weakly visible in Figure 10.2, appearing somewhat stronger during secondary eclipse. In the $K_p - \Delta v_{\text{sys}}$ space, the maximum-likelihood WASP-189 b model is detected at $\text{SNR} = 9.7$. Comparing figures 10.3, 10.4, 10.5, and 10.6 establishes that this detection is entirely due to CO. Similar to the case of WASP-33 b the retrieved posterior specifically disfavors the combination of high H_2O abundance and low dissociation pressure which can produce significant H_2O spectral features, but high H_2O abundances and deep dissociation are permitted. The OH abundance is also unconstrained, leading the retrieval to a C/O ratio of 1 and a broad $[(\text{C} + \text{O})/\text{H}] = 0.5^{+0.9}_{-1.1}$.

CO emission features have previously been reported from infrared observations of WASP-189 b ([F. Yan et al., 2022](#); [F. Lesjak et al., 2025](#)), while optical observations have reported TiO and a wide range of atomic species ([B. Prinoth et al., 2022, 2024](#)). While these works have not reported an atmospheric metallicity for WASP-189 b, the retrieved $[(\text{C} + \text{O})/\text{H}]$ posterior is consistent with solar to moderately super-solar metallicity, and broad enough to include most physically plausible scenarios.

10.3.5 MASCARA-1 b

The 2D cross-correlation plot for MASCARA-1 b in Figure 10.2 shows a weak, slightly blueshifted trace, which appears to be stronger closer to secondary eclipse. The maximum-likelihood model is more clearly detected in the $K_p - \Delta v_{\text{sys}}$ space, at $\text{SNR} = 7.1$ (Figure 10.3). Figure 10.4 shows an $\text{SNR} = 5.1$ detection even without CO opacity, which appears to be primarily the result of OH features based on Figures 10.5 and 10.6. The posterior provides a bounded constraint on the CO abundance, limits on the H_2O abundance and

dissociation pressure corresponding to an absence of H₂O features, and a lower limit on the OH abundance. The OH formation/dissociation pressures also have lower and upper limits, respectively. The strong preference for OH features but absence of H₂O features is somewhat odd, as OH is expected to be produced by H₂O dissociation, with the OH abundance peaking at a value lower than the deep-atmosphere H₂O abundance at pressure layers just above where H₂O begins to dissociate.

These results are at odds with repeated analyses of VLT/CRIRES+ observations reporting H₂O emission features in the atmosphere of MASCARA-1 b (M. Holmberg & N. Madhusudhan, 2022; S. Ramkumar et al., 2023, 2025). Other observations of OH in UHJs have found strongly blueshifted signals as a result of OH being concentrated at afternoon-evening longitudes and strong day-to-night winds (R. Landman et al., 2021), but the observations presented here cover a very similar orbital phase range as the observations described in S. Ramkumar et al. (2023), so we expect any such 3D phenomenon would impact both analyses. The higher spectral resolution of CRIRES+ may provide greater sensitivity to weak H₂O features, but this still does not explain the preference for very high OH abundances in the KPIC data compared with the apparent absence of OH in the CRIRES+ data.

While S. Ramkumar et al. (2025) report $C/O = 0.7^{+0.11}_{-0.17}$ for joint pre/post eclipse analysis of MASCARA-1 b, the extreme OH abundance preferred by our retrieval drives the C/O ratio to very low values, and $[(C + O)/H]$ to significant volatile enrichment, $[(C + O)/H] = 1.1^{+0.4}_{-0.5}$.

10.3.6 TOI-1518 b

The retrieved TOI-1518 b maximum-likelihood model shows a weak trail in the 2D cross-correlation plot, which becomes a clear, slightly redshifted peak after summing over the time series (Figure 10.2). Figure 10.3 shows the maximum-likelihood model is detected at $SNR = 6.7$ in the $K_p - \Delta v_{sys}$ space. Figures 10.4 and 10.6 show that OH features in the maximum-likelihood model are modestly contributing to this detection strength, despite the unconstrained OH abundance, but Figure 10.5 shows H₂O features are not significant,

consistent with the retrieved posterior.

Figure 10.3 shows our detection of TOI-1518 b is consistent with a significantly lower K_p than expected based on the orbital parameters. While for a non-transiting planet, this would suggest an orbital inclination, the inclination of TOI-1518 b is well-constrained by analysis of the near-grazing transit (S. H. C. Cabot et al., 2021). Significant shifts to lower K_p have been repeatedly observed for TOI-1518 b for a variety of species (S. H. C. Cabot et al., 2021; A. Simonnin et al., 2024; C. Basinger et al., 2025). A. Simonnin et al. (2024) suggests that the observed shifts may be a result of strong magnetic drag in the atmosphere of TOI-1518 b.

The retrieved chemical composition is similar to the values obtained for other targets with only a CO detection – the C/O ratio is driven to 1, and $[(C + O)/H]$ to solar or slightly super-solar values with wide bounds, in this case $[(C + O)/H] = 0.5^{+0.9}_{-1.1}$. The constraints on the $P-T$ profile for TOI-1518 b, illustrated in Figure 10.7, are also significantly broader than those obtained for other targets. TOI-1518 b is the dimmest of the observed targets, and was observed over a relatively small velocity shift, both of which are likely factors contributing to the poor constraints on atmospheric properties.

10.4 Discussion

10.4.1 Planet continuum level

The maximum-likelihood spectra plotted in Figure 10.8 uniformly differ from the expected F_p/F_s assuming both planet and star are blackbodies at their respective equilibrium and effective temperatures. For KELT-20 b, WASP-33 b, KELT-9 b, and WASP-189 b the continuum level is less than the blackbody by a factor $\sim 2 - 4$, while for MASCARA-1 b and TOI-1518 b the retrieved continuum is greater than the blackbody value by a similar factor. Both the retrieved and blackbody continua are nearly flat over the entire observed bandpass, changing by $< 15\%$. This poses a particular challenge for HRCCS due to the

loss of continuum associated with the median division step in data processing. Over wide bandpasses, e.g. combining $H+K$ or $K+L$ data for retrieval, the change in continuum over the bandpass is sufficient to recover the continuum level during retrieval (e.g. [M. R. Line et al., 2021](#), Finnerty *et al.*, *subm.*), but this is not the case for analysis of K band data alone.

The relative insensitivity to continuum has important implications for absolute molecular abundances. HRCCS is sensitive to the strength of planetary lines relative to the stellar continuum. Planetary line strengths are in turn set by both the molecular abundance of the relevant species and by the $P - T$ profile. The $P - T$ profile also sets the planet continuum level, but if this is poorly constrained a degeneracy can arise between $P - T$ profile contrast and molecular abundances. Large $P - T$ contrasts with low molecular abundances can produce line features of similar strength as lower $P - T$ contrasts with high abundances. Further degeneracies may be introduced by dissociation, as the molecular abundance gradient can also lead to the formation of spectral features even for an isothermal $P - T$ profile ([L. Finnerty et al., 2025b](#)). These challenges are reflected in the broad $[(C + O)/H]$ posteriors shown in Figure 10.9, which we discuss in detail in the following Section 10.4.4.

For all of the targets reported here, there are discrepancies in the stellar temperature and radius on the order of 5 – 10% between different published references. For example, for MASCARA-1 [AM. J. Hooton et al. \(2022\)](#) reports $T_{\text{eff}} = 7490 \pm 150$ K and $R_s = 2.08 \pm 0.02 R_\odot$, in good agreement with the values reported in [G. J. J. Talens et al. \(2017\)](#), while the [ExoFOP \(2019\)](#) temperature is 7800 ± 100 K and radius is $R_s = 2.02 \pm 0.06 R_\odot$. For WASP-33 A, the reported effective temperatures are in good agreement, but the reported stellar radii range from $1.444 \pm 0.034 R_\odot$ ([A. Collier Cameron et al., 2010](#)) to $1.602 \pm 0.06 R_\odot$ ([ExoFOP, 2019](#)). TOI-1518 A is an extreme case, with a 2500 K difference between effective temperatures reported in the [ExoFOP \(2019\)](#) and [S. H. C. Cabot et al. \(2021\)](#). This uncertainty in the stellar parameters propagates to the planet radius, which is measured relative to the host star radius, and to the planetary equilibrium temperature, which depends

on the host star temperature, radius, and mass via the the semi-major axis. For WASP-33 b, the reported radii range from $1.497 \pm 0.05 R_J$ (A. Collier Cameron et al., 2010) to $1.63 \pm 0.06 R_J$, corresponding to a $\sim 20\%$ change in the projected surface area of the planet. The accumulation of these potential sources of error could be responsible for a factor $\sim 1 - 2$ discrepancy in the expected F_p/F_s . Furthermore, we did not consider the effects of limb or gravity darkening in detail, which could lead to discrepancies between the model stellar flux and the actual stellar flux incident on the targets.

We also did not include H^- opacity in the atmospheric retrievals. L. Finnerty et al. (2023a) showed that including H^- results in a uniform reduction in the strength of planet lines relative to the continuum of $\sim 10\%$ for WASP-33 b. H^- likely has a stronger impact on the hotter UHJs, particularly KELT-9 b (B. Jacobs et al., 2022), potentially forcing the retrieval to lower abundances in order to match the reduction in line strength caused by H^- opacity. This may also impact the continuum as a result of the previously discussed coupling between line strengths, abundances, and the $P - T$ profile. Obtaining better constraints on H^- opacity in HRCCS analysis may be possible with J and H band observations, as the H^- opacity shows a sharp change at $1.4 \mu m$ corresponding to the change from bound-free to free-free absorption (P. Lenzuni et al., 1991; V. Parmentier et al., 2018).

10.4.2 Molecular dissociation

While the retrievals generally did not provide bounded constraints on the H_2O or OH abundances, we can still use the posteriors to compute ratios of H_2O and OH abundances to each other or to the CO abundance. In the absence of detections, this represents how strongly the posterior disfavors the presence of spectral features from a given species. In Figure 10.10, we plot the retrieved H_2O/OH ratios versus T_{eq} and orbital phase, and the retrieved H_2O/CO and OH/CO ratios versus T_{eq} .

While the error bars on the abundance ratios are large, several possible trends apparent in Figure 10.10. The H_2O/OH ratio versus equilibrium temperature plot shows a possible

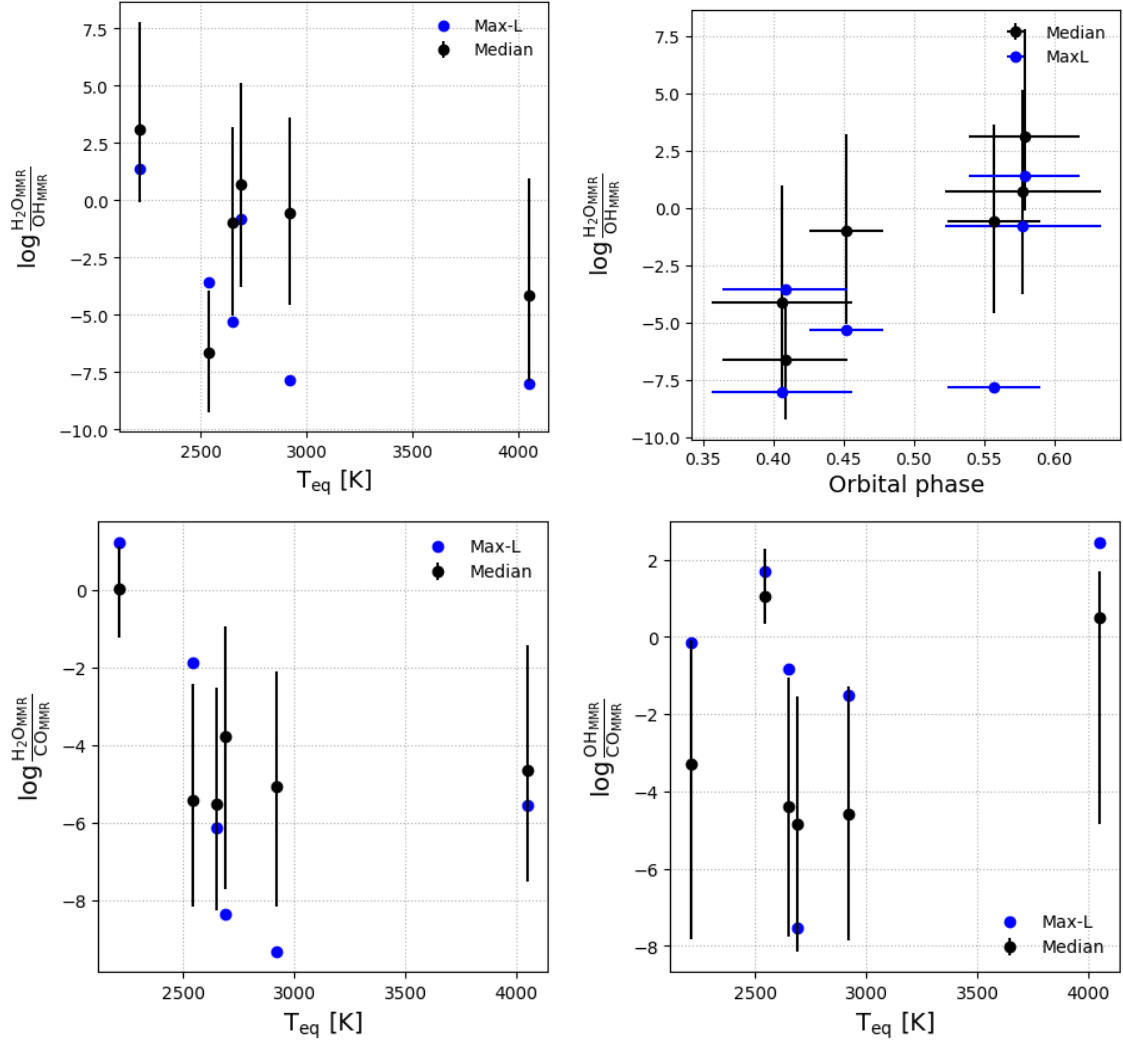


Figure 10.10: Retrieved abundance ratios versus equilibrium temperature or orbital phase.

Maximum-likelihood parameters are plotted in blue, and median parameters in black with $\pm 34\%$ confidence intervals in black. For the orbital phase plot, the x -axis error bars correspond to the phase range of the observations. The $\text{H}_2\text{O}/\text{OH}$ ratio shows a possible negative trend with equilibrium temperature and positive trend with orbital phase, though the error bars are very large. $\text{H}_2\text{O}/\text{CO}$ may also negatively correlate with equilibrium temperature, while OH/CO does not show a similar behavior.

negative correlation, consistent with expectations that H_2O dissociation increasing with temperature. In contrast, the $\text{H}_2\text{O}/\text{OH}$ ratio appears to positively correlate with orbital phase, with pre-eclipse targets more strongly disfavoring H_2O than post-eclipse. The $\text{H}_2\text{O}/\text{CO}$ ratio shows a possible weak correlation with equilibrium temperature, suggesting that H_2O is largely dissociated for equilibrium temperatures above 2500 K. No trend is seen in the OH/CO ratio with the temperature, consistent with the lack of constraint on the OH abundance for most targets.

The potential correlation between $\text{H}_2\text{O}/\text{OH}$ ratio and orbital phase would be consistent with OH being confined to afternoon or evening longitudes. This region is more visible at pre-eclipse phases than post-eclipse, and GCMs generally predict afternoon longitudes to be the hottest regions of UHJs (T. D. Komacek, 2025), which would lead to greater dissociation of H_2O compared with other parts of the planet. However, Figure 10.10 is comparing between different objects, which also differ in equilibrium temperature and bulk composition. The differences in planet properties could be confounding factors in the apparent correlation. Comparing observations of a single target taken pre- and post-eclipse would provide a more clear picture of the OH distribution. KELT-20 b and MASCARA-1 b are particularly promising targets for such followup, as the existing data strongly prefer H_2O in the post-eclipse KELT-20 b spectrum and OH in the post-eclipse MASCARA-1 b spectrum, providing a basis for comparison.

While we attempted to retrieve H_2O dissociation pressures for all six UHJs, constraints were retrieved only for KELT-20 b. KELT-20 b was the best-detected target in the sample, and it may be that retrieving vertical mixing profiles simply requires very high-quality data. KELT-20 b is also the coolest of the observed UHJs, likely leading to less dissociation and stronger H_2O spectral features which can be detected despite the limited wavelength coverage of our observations. For hotter targets, observations of the H and L bands, which include significant H_2O and OH features, may be necessary to obtain constraints on these species.

10.4.3 Atmospheric Circulation

As [L. Finnerty et al. \(2025b\)](#) discusses, obtaining wind speeds from emission observations is challenging due to timing and ephemeris uncertainty, which can lead to Doppler shifts comparable to expected wind speeds in UHJs. In principle, a global day-to-night wind would lead to a net redshift for observations near secondary eclipse. Additionally accounting for planetary rotation (or a super-rotating jet) would slightly increase the redshift prior to eclipse, and slightly decrease the redshift post-eclipse, assuming that the dayside/afternoon longitudes generally dominate the emission spectrum.

Our retrievals reveal no clear kinematic trends indicative of a common global circulation pattern. Using the retrieved median and maximum-likelihood parameters, we calculated the difference in velocity between the assumed ephemeris and the posterior. For KELT-20 b, the planet is blue shifted with respect to the nominal ephemeris by -1.6 km s^{-1} at the start of the observations, decreasing to -0.5 km s^{-1} at the end. For WASP-33 b, the retrieved velocities go from -10 km s^{-1} to $+0.5 \text{ km s}^{-1}$. For KELT-9 b, the velocity offset is a nearly constant 2 km s^{-1} . For WASP-189 b, the offset is 0.2 km s^{-1} to -5.7 km s^{-1} . MASCARA-1 b has a larger offset, -15 km s^{-1} decreasing to -2 km s^{-1} , and for TOI-1518 b the maximum-likelihood offset is $4.8\text{--}14.5 \text{ km s}^{-1}$, while the median is $7.4\text{--}6.3 \text{ km s}^{-1}$. These offsets are generally smaller than the 9 km s^{-1} instrument resolution of KPIC/NIRSPEC, and within the plausible range for ephemeris uncertainties. The largest offset, at the start of the MASCARA-1 b observation, corresponds to an observed airmass of 3, with relatively low throughput. Furthermore, there is no apparent correlation between the velocity offset and the observed orbital phase, which we would expect to see if the offsets were due to a common UHJ circulation pattern.

While we fit for a rotational broadening kernel, the LSF fitting procedure involves systematic uncertainties at the $\sim 10\%$ level, discussed in [L. Finnerty et al. \(2022\)](#); [L. Finnerty et al. \(2025a,b\)](#). While the retrievals consistently provide bounded constraints on the rota-

tional broadening, the physical significance of these values is questionable. Specifically, for KELT-9 b, the retrieved value $v_{\text{rot}} = 5.6_{-2.4}^{+2.5} \text{ km s}^{-1}$ is actually smaller than the expected value of 6.6 km s^{-1} for tidally locked rotation. This suggests that the broadening kernel is not actually fitting rotational broadening in the planet lines, but rather is accounting for errors in measurement of the instrumental LSF. These results demonstrate HRCCS retrievals are sensitive to subtle changes in the shapes of observed spectral lines, but obtaining accurate measurements of rotational broadening will clearly require more precise LSF calibration. Such calibration could be provided in the future by a K -band laser frequency comb.

Our retrievals use a 1D radiative transfer model, which assumes there is no kinematic offset between different species. This assumption has been shown to be false in optical observations of UHJs (e.g. [A. Y. Kesseli et al., 2022](#)), and recently ([J. P. Wardenier et al., 2024](#)) found a $\sim 3 \text{ km s}^{-1}$ velocity offset between CO and H₂O features in transmission observations of the UHJ WASP-121 b, and that the cross-correlation peaks for H₂O and CO vary differently with orbital phase. This suggests that the distinct spatial distributions of H₂O, OH, and CO resulting from dissociation is leading to differences in the radial velocity of the corresponding emission features at the $\sim 3 \text{ km s}^{-1}$ level. While the spectral resolution of our observations is 9 km s^{-1} , this may still lead to subtle model mismatch, biasing inferred abundances particularly for H₂O and OH. Simulation work is needed to assess the effect such kinematic differences will have on atmospheric retrievals, and development of radiative transfer tools which can account for these offsets will likely be necessary for accurate analysis of data from instruments with $R \sim 100,000$.

10.4.4 C/O and metallicity

Without simultaneously constraining CO and one of either H₂O or OH, we are unable to place meaningful constraints on the C/O ratio for any of the observed hot Jupiters, as [Figure 10.11](#) illustrates. We also see no significant trends between the retrieved volatile abundance and either the planet mass or equilibrium temperature. Even if a trend with $[(\text{C} + \text{O})/\text{H}]$

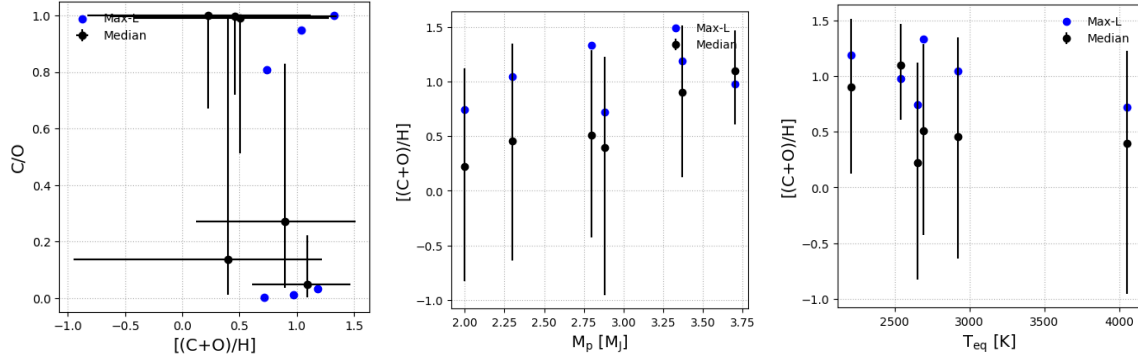


Figure 10.11: Comparisons between volatile abundance and C/O, mass, and temperature.

C/O versus volatile abundance (left), volatile abundance versus planet mass (center), and volatile abundance versus equilibrium temperature (right). None of these parameters appear to be significantly correlated.

was apparent in Figure 10.11, the previously discussed degeneracies arising from continuum mismatches would be a strong caveat.

While in cooler hot Jupiters, K -band observations are sufficient for measuring the C/O ratio (L. Finnerty et al., 2024), these results demonstrate that this is not the case for UHJs. M. Brogi et al. (2023) retrieved C/O and metallicity for the UHJ WASP-18 b using Gemini/IGRINS observations over the H and K bands with similar spectral resolution to our KPIC observations, which suggests that the additional H_2O and OH opacity features in the H band are critical to obtaining such constraints for UHJs. The L band also has extensive H_2O and OH features, potentially providing another avenue for constraining UHJ composition in conjunction with CO measurements from the K band.

While our observations are insufficient to constraint C/O, combining the KPIC data with optical observations may offer some insight into the refractory/volatile ratio for these targets through constraints on transition metal abundances. The wide wavelength coverage of such a joint analysis may also improve constraints on the $P - T$ profile, breaking the degeneracy with abundances. Comparing CO to a refractory species with a similarly uniform global distribution may enable refractory/volatile constraints and formation inferences while sidestepping issues posed by non-homogeneous spatial distributions of other species.

10.5 Summary and Conclusions

We present new Keck/KPIC observations of 4 ultra-hot Jupiters. These targets, as well as two UHJs previously observed with KPIC and published, were all analyzed with a consistent retrieval framework. All six targets were detected, with retrieved spectra dominated by CO emission features. The retrieved continua differ significantly from the values expected for a blackbody, likely due to a combination of stellar model mismatch, H^- opacity, and the intrinsically poor sensitivity of narrow-band HRCCS observations to continuum. This mismatch, and the lack of robust H_2O or OH detections, leads to significant uncertainty in the retrieved absolute abundances.

While we do not obtain bounded constraints for H_2O or OH for any target, the retrieved $\text{H}_2\text{O}/\text{OH}$ ratio appears to show a negative correlation with equilibrium temperature, consistent with greater H_2O dissociation occurring in hotter atmospheres. We also see a potential positive correlation between the $\text{H}_2\text{O}/\text{OH}$ ratio and the observed orbital phase, consistent with an inhomogeneous spatial distribution of OH concentrated at afternoon longitudes. Followup observations of single targets to obtain both pre- and post-eclipse phases may be able to test this.

The inability of our observations to meaningfully constrain either H_2O or OH abundances demonstrates the importance of broad wavelength coverage for measuring bulk compositions in UHJs. Future efforts to combine these data with H - or L -band observations covering strong H_2O and OH features may be able to constrain C/O or metallicity for these targets, using the K -band CO features to constrain the carbon abundance and other bands to measure oxygen. Additionally, combining these observations with optical data may also provide a path to constraining the refractory/volatile ratio.

10.6 Corner Plots

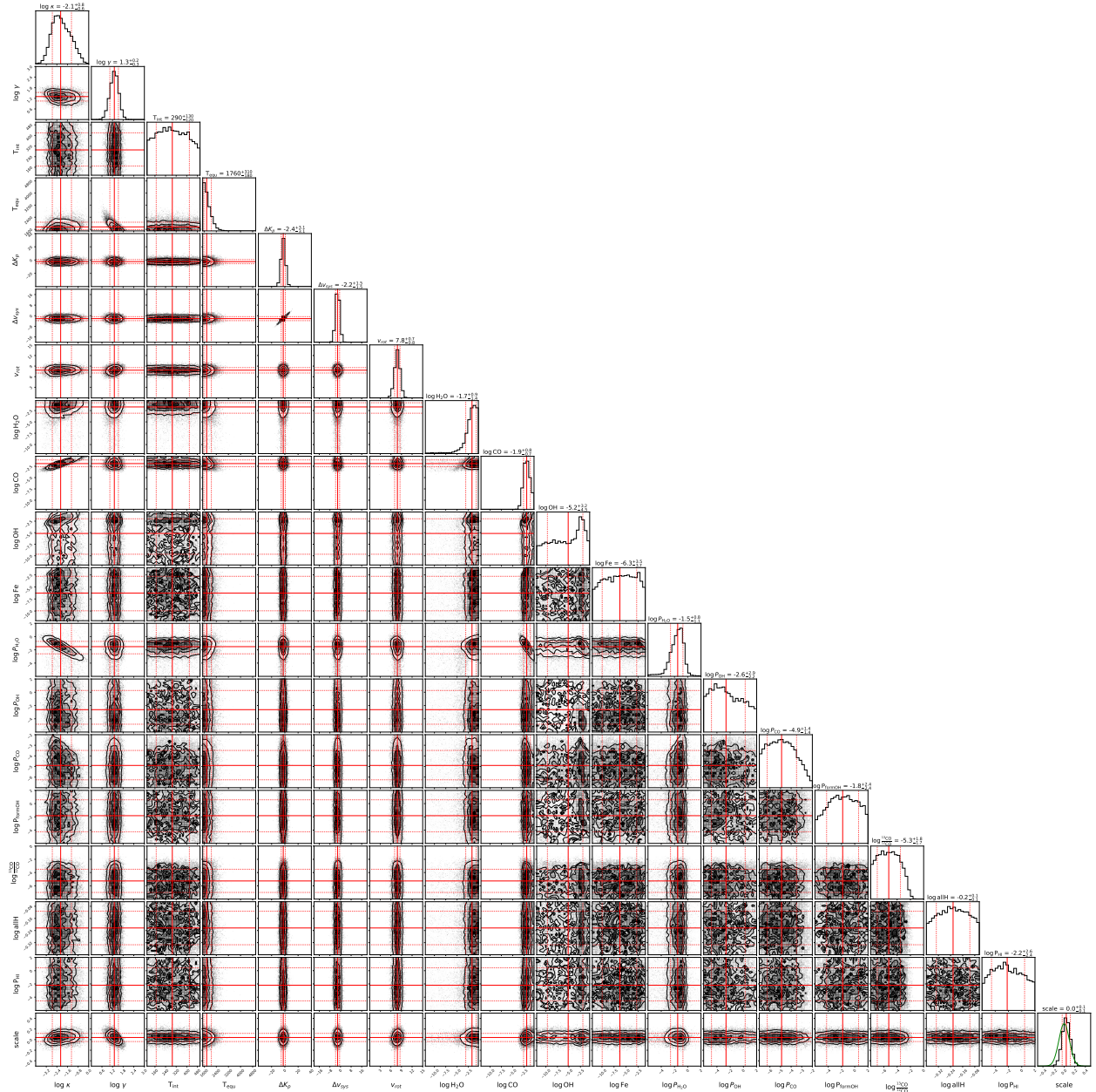


Figure 10.12: Full corner plot for KELT-20 b.

Red solid lines indicate the medians, while red dashed lines indicate the bounds of the marginalized 68% confidence interval. We discuss these results in Section 10.3.

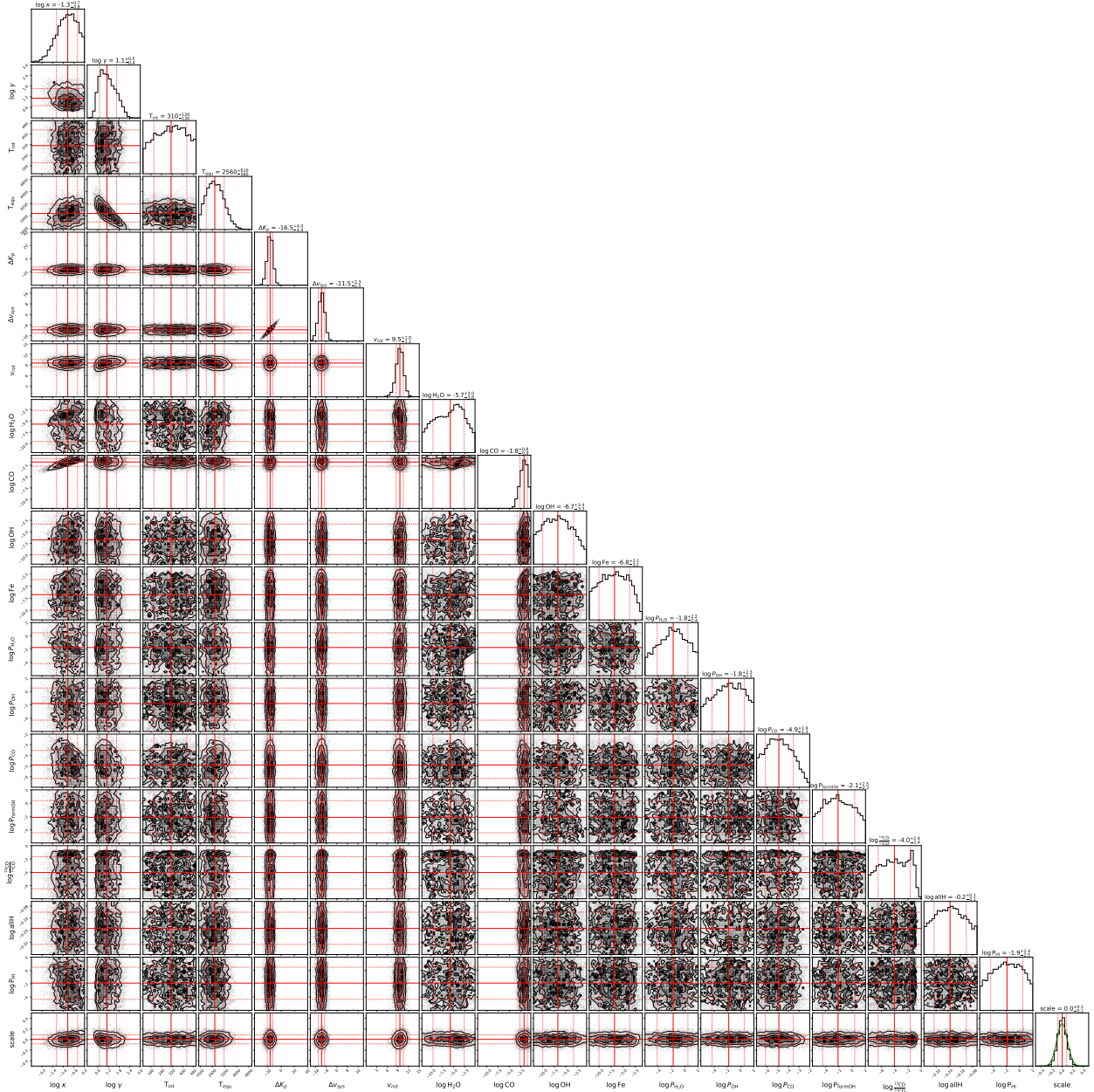


Figure 10.13: Full corner plot for WASP-33 b.

Red solid lines indicate the medians, while red dashed lines indicate the bounds of the marginalized 68% confidence interval. We discuss these results in Section 10.3.

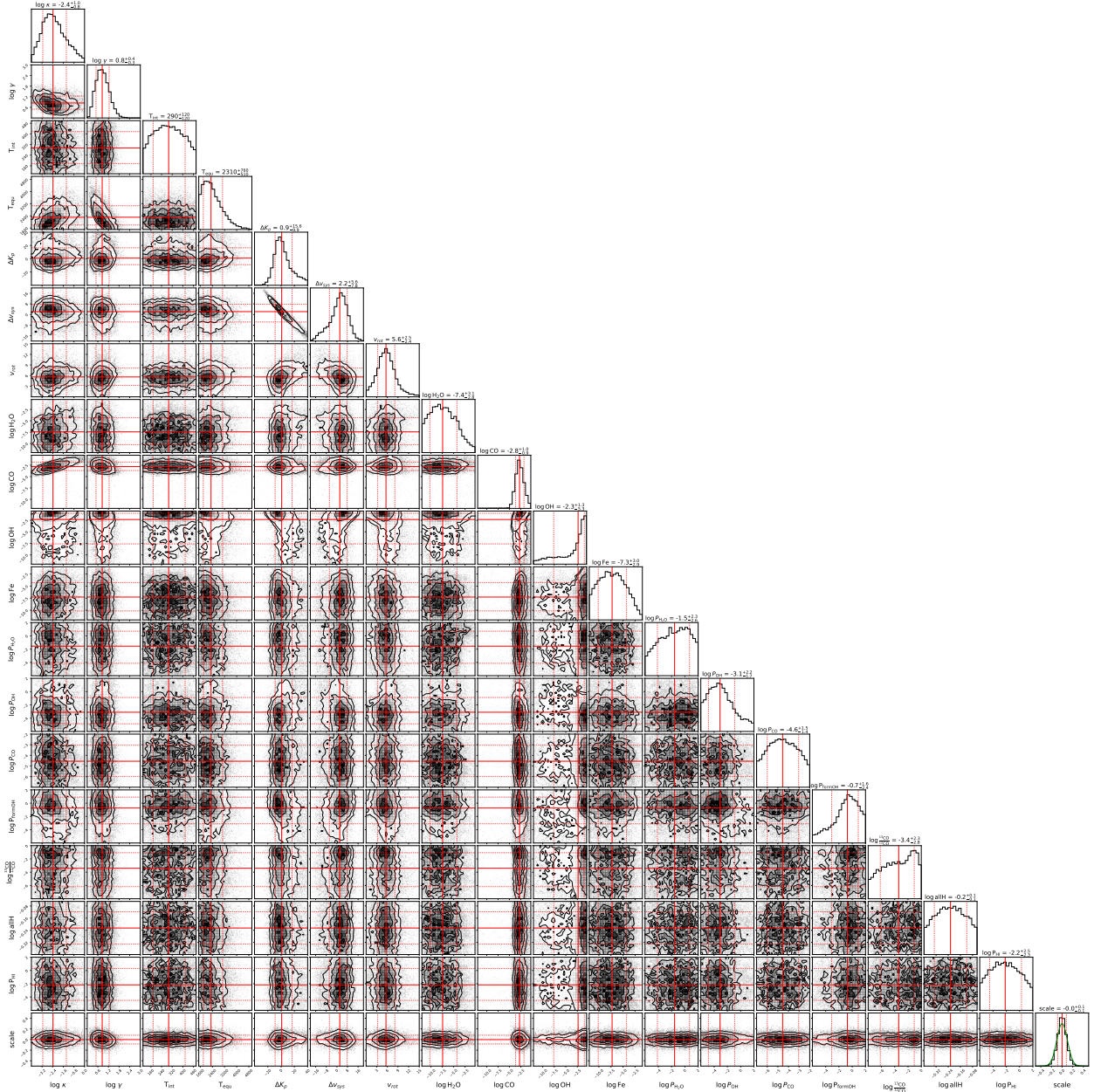


Figure 10.14: Full corner plot for KELT-9 b.

Red solid lines indicate the medians, while red dashed lines indicate the bounds of the marginalized 68% confidence interval. We discuss these results in Section 10.3.

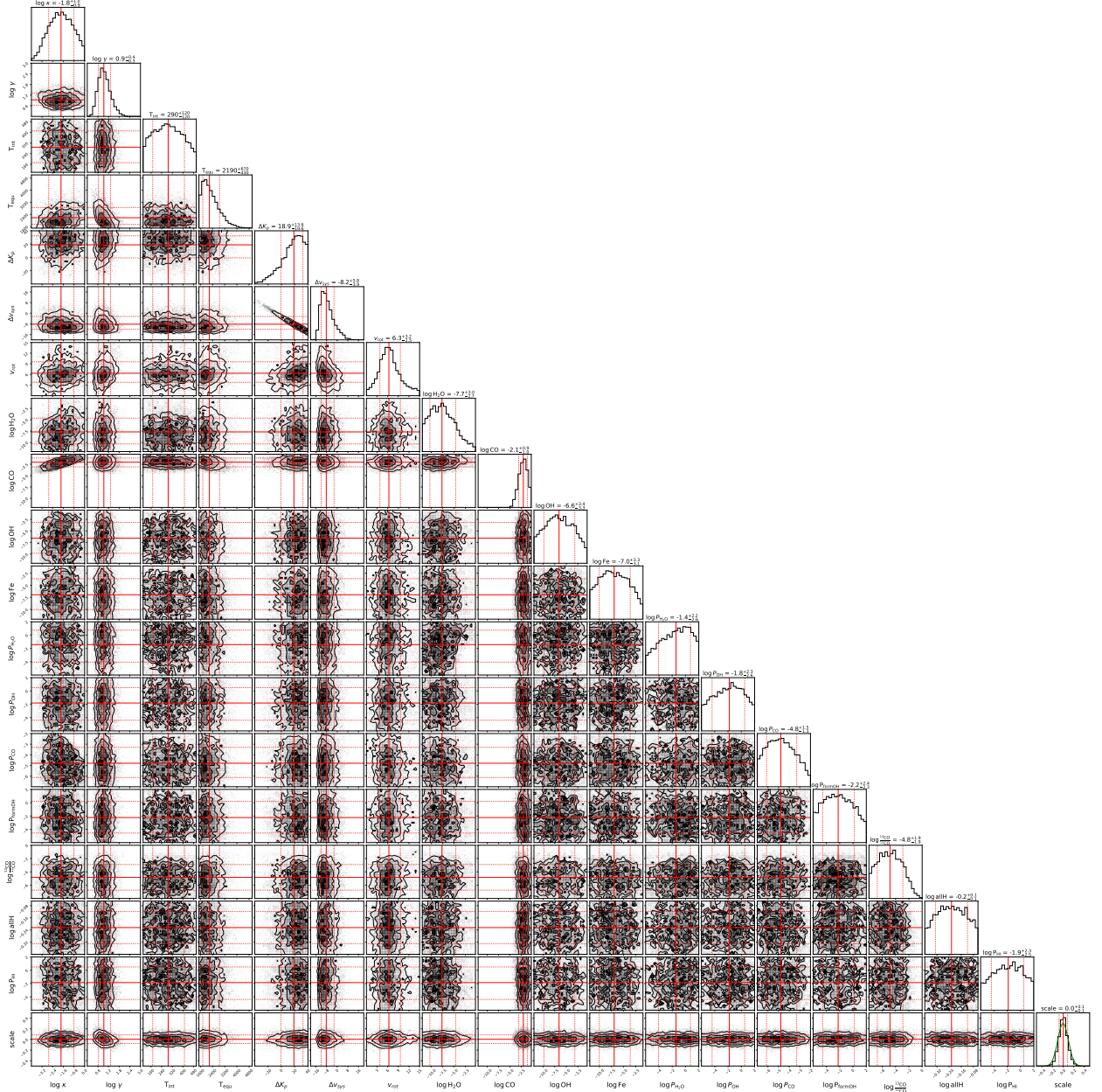


Figure 10.15: Full corner plot for WASP-189 b.

Red solid lines indicate the medians, while red dashed lines indicate the bounds of the marginalized 68% confidence interval. We discuss these results in Section 10.3.

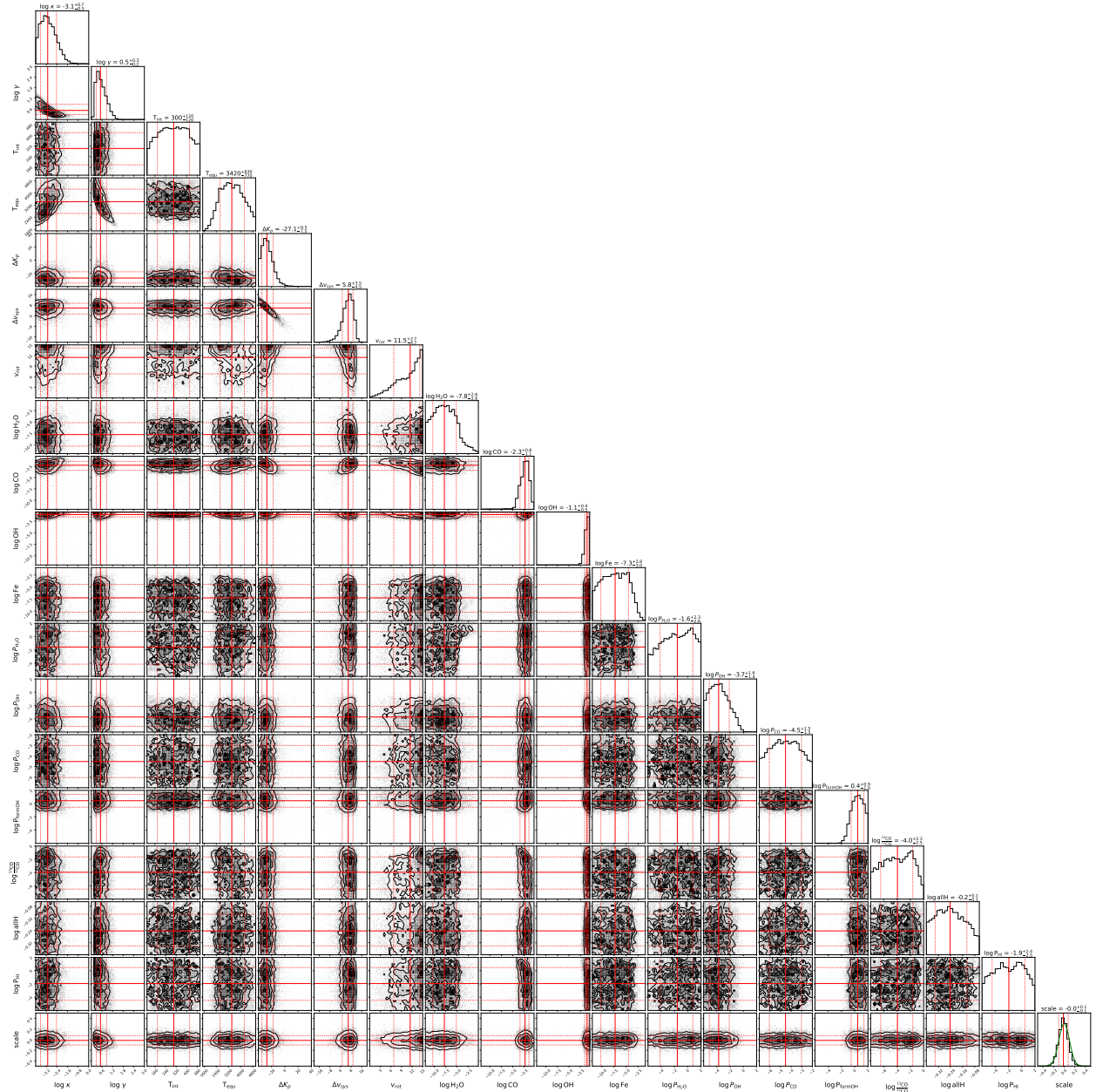


Figure 10.16: Full corner plot for MASCARA-1 b.

Red solid lines indicate the medians, while red dashed lines indicate the bounds of the marginalized 68% confidence interval. We discuss these results in Section 10.3.

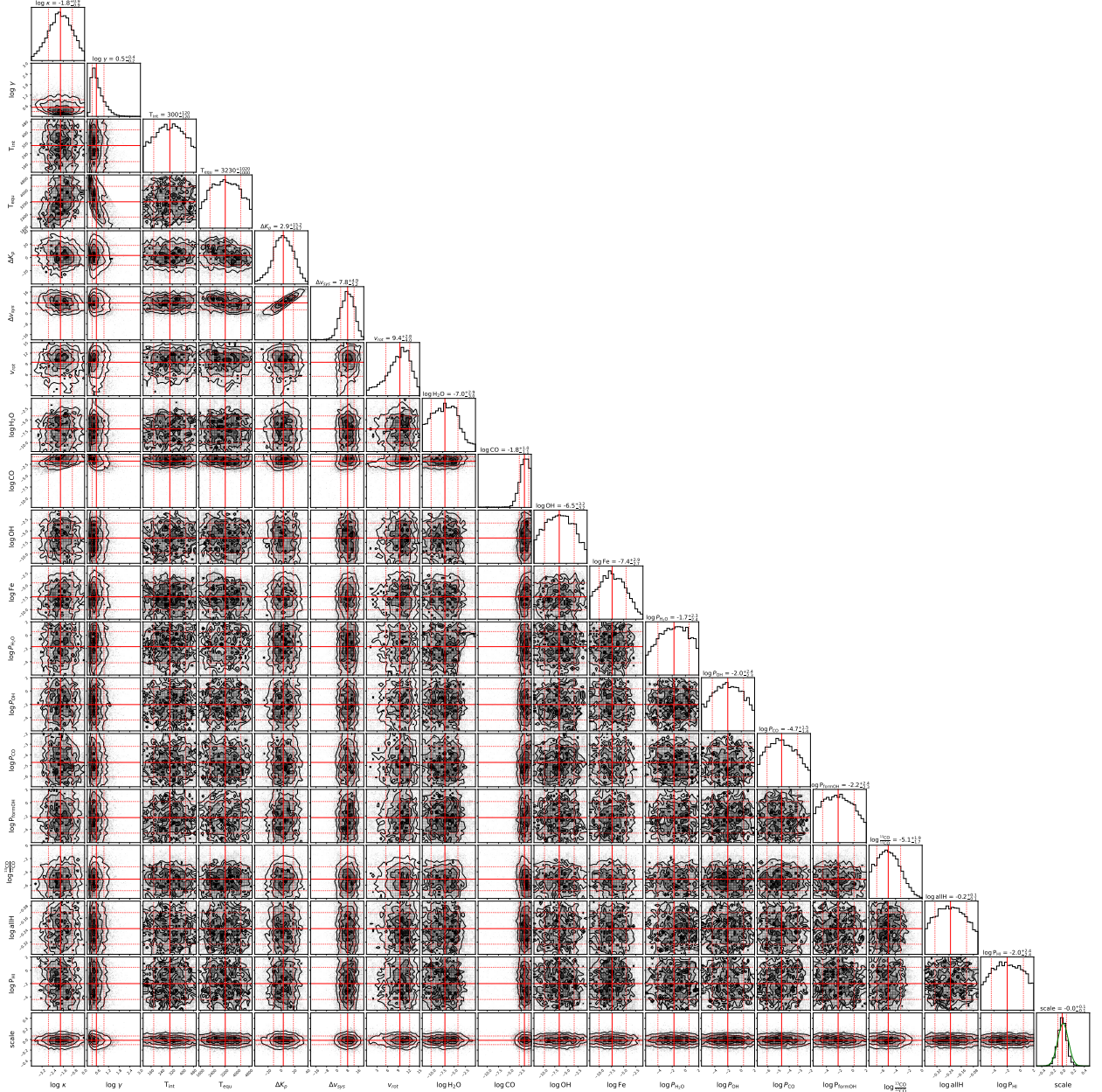


Figure 10.17: Full corner plot for TOI-1518 b.

Red solid lines indicate the medians, while red dashed lines indicate the bounds of the marginalized 68% confidence interval. We discuss these results in Section 10.3.

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