Carbon monoxide emission lines reveal an inverted atmosphere in the ultra hot Jupiter WASP-33 b and indicate an eastward hot spot

Lennart van Sluijs,1,2,* Jayne L. Birkby,1,2,3 Joshua Lothringer,4 Elspeth K. H. Lee,5 Ian J. M. Crossfield,6 Vivien Parmentier,7 Matteo Brogi,8,9,10 Craig Kuljesa,11 Don McCarthy,11 Keith Powell,12 David Charbonneau3

1Department of Astrophysics, University of Oxford, Oxford, OX1 3RH, United Kingdom
2Anton Pannekoek Institute for Astronomy, University of Amsterdam, Amsterdam, 1098 XH, The Netherlands
3Center for Astrophysics | Harvard & Smithsonian, 60 Garden Street, Cambridge, MA, 02138, USA
4Department of Physics, Utah Valley University, Orem, UT 84058, USA
5Center for Space and Habitability, University of Bern, Gesellschaftsstrasse 6, CH-3012 Bern, Switzerland
6Department of Physics and Astronomy, University of Kansas, Lawrence, KS 66045, USA
7Atmospheric, Oceanic & Planetary Physics, Department of Physics, University of Oxford, Oxford OX1 3PU, UK
8Department of Physics, University of Warwick, Coventry CV4 7AL, UK
9INAF-Osservatorio Astrofisico di Torino, Via Osservatorio 20, I-10025, Pino Torinese, Italy
10Centre for Exoplanets and Habitation, University of Warwick, Gibbet Hill Road, Coventry, CV4 7AL, UK
11Seward Observatory, University of Arizona, Tucson, AZ, USA
12MMT Observatory, University of Arizona, Tucson, AZ, USA

Accepted XXX. Received YYY; in original form ZZZ.

ABSTRACT
We report the first detection of CO emission lines at high spectral resolution in the day-side infrared thermal spectrum of an exoplanet. These emission lines, found in the atmosphere of the ultra hot Jupiter WASP-33 b, provide unambiguous evidence of its thermal inversion layer. Using spectra from the MMT Exoplanet Atmosphere Survey (MEASURE, R ~ 15,000), covering pre- and post-eclipse orbital phases (0.33 < φ < 0.73), we performed a cross-correlation analysis with 1D PHOENIX model atmospheres to detect CO at S/N=7.9 at v_{sys} = 0.15^{+0.64}_{-0.65} km/s and K_p = 229.5^{+1.1}_{-1.0} km/s. However, using the framework of Cross-Correlation-to-log-Likelihood mapping, we further find that the spectral line depths, as probed by the scaling parameter, change with phase: the line contrast is larger after the eclipse than before. We then use the general circulation model SPARC/MITgcm post-processed by the 3D gCMCRT radiative transfer code and interpret this variation as due to an eastward-shifted hot spot. Before the eclipse, when the hot spot is facing Earth, the thermal profiles are shallower, leading to a smaller line depth despite greater overall flux. After the eclipse, the western part of the day-side is facing Earth, where the thermal profiles are much steeper, leading to larger line depth despite less overall flux. We thus demonstrate that even relatively moderate resolution spectra can be used to understand the 3D nature of close-in exoplanets, if assessed within the log-likelihood framework, and that resolution can be traded for photon collecting power when the induced Doppler-shift is sufficiently large. We highlight that CO in ultra hot Jupiters is a good probe of their thermal structure and corresponding dynamics, and does not suffer from stellar activity unlike some atomic species, such as iron, that also appear in the hot host star spectrum.

Key words: planets and satellites: atmospheres – planets and satellites: fundamental parameters – techniques: spectroscopic

1 INTRODUCTION

Ultra hot Jupiters (UHJs) provide the unique opportunity to study gaseous planets in a strongly irradiated environment to learn about their composition and global circulation patterns (e.g. for a review see Showman et al. 2020; Fortney et al. 2021). Their high day-side temperatures above 2200 K provide a unique window to directly detect volatile species in their vapor phase (e.g. Visscher et al. 2010; Parmentier et al. 2018; Hoeijmakers et al. 2018; Lothringer et al. 2018; Kitzmann et al. 2018; Hoeijmakers et al. 2019; Ehrenreich et al. 2020; Merritt et al. 2021; Cont et al. 2021a). Due to their tidally locked rotation, they have an extreme day-to-night-side temperature contrast (e.g. Knutson et al. 2007). Consequently, global circulation models (GCMs) predict strong global jets and hot spots (Showman et al. 2009; Menou & Rauscher 2009; Parmentier et al. 2018; Tan & Komacek 2019). This combined with their relatively high star-planet contrast ratio, makes them ideal targets for atmospheric characterisation with current observing facilities (e.g. Kreidberg 2018; Birkby 2018).

Hydrodynamic simulations and theoretical calculations predict that hot spots occur in ultra hot Jupiters with an eastward offset from the sub-stellar point due to global wind circulation patterns...
(e.g. Showman & Guillot 2002; Dobbs-Dixon & Lin 2008; Menou & Rauscher 2009; Dobbs-Dixon et al. 2010; Rauscher & Menou 2010; Showman & Polvani 2011; Perez-Becker & Showman 2013; Debras et al. 2020). Most observations support this eastward offset hot spot prediction (Harrington et al. 2006; Cowan et al. 2007; Knautson et al. 2007, 2009; Charbonneau et al. 2008; Swain et al. 2009; Crossfield et al. 2010; Wong et al. 2016), but for some UHJs westward offsets have been observed as well (Armstrong et al. 2016; Dang et al. 2018; Jackson et al. 2019; Bell et al. 2019; von Essen et al. 2020; Herman et al. 2022). Several mechanisms including cloud asymmetries, asynchronous rotation and magnetohydrodynamical effects have been proposed to explain these westward offset hot spots (e.g. Hindle et al. 2021).

Thermal inversions of the pressure-temperature profiles (P-T profiles) of UHJs were at first predicted due to the the strong optical/UV absorbing molecules TiO and VO (e.g. Hubeny et al. 2003). Later work found absorption by other atomic and molecular species, in addition to TiO and VO, can also result in thermal inversions (Lothringer et al. 2018; Arcangeli et al. 2018; Gandhi & Madhusudhan 2019). This is due to a combination of short-wavelength stellar irradiation around early type stars and absorption of these wavelengths by continuous opacity sources, metal atoms, metal hydrides and SiO. Analysis of Spitzer and Hubble Space Telescope (HST) secondary eclipse observations support this scenario as they detect emission signatures suggestive of an inverted stratosphere for a handful of UHJs (e.g. Deming et al. 2012; Haynes et al. 2015; Evans et al. 2016, 2017; Sheppard et al. 2017; Arcangeli et al. 2018; Kreidberg et al. 2018; Mansfield et al. 2018; Nugroho et al. 2020a; Yan et al. 2020; Garhart et al. 2020; Baxter et al. 2021).

One well-studied UHJ for which a thermal inversion was predicted by atmospheric modeling is WASP-33 b. This planet orbits every 1.22 days around an A5 star (Collier Cameron et al. 2010). The first observational evidence of a thermal inversion of WASP-33 b's atmospheric profile was excess infrared emission observed by Spitzer from secondary eclipse observations and (Deming et al. 2012; Zhang et al. 2018) and NIR low-resolution HST/Wide Field Camera 3 spectra, possibly due to TiO (Haynes et al. 2015). Furthermore, (Zhang et al. 2018) find a phase angle offset by -12.8 ± 5.8° in the Spitzer 3.6 m-band, indicative of an eastward hotspot. On the contrary, (von Essen et al. 2020) find a 28.7 ± 1.1° phase angle offset in the optical with TESS, suggesting a westward offset hot spot instead, although they mention host star variability may introduce a spurious westward offset. Recently, Herman et al. (2022) report day-to-night brightness contrast variations and a 22 ± 12° westward phase offset from their detection of Fe-I emission lines.

For these low resolution observations, stellar pulsations of the δ Scuti pulsating host star induce variability of the stellar continuum (Herrero et al. 2011), limiting observational constraints as they induce a quasi-sinusoidal trend in transit light curve observations (e.g. Deming et al. 2012; de Mooij et al. 2013; Garhart et al. 2020; von Essen et al. 2019, 2020). Furthermore, stellar pulsations also affect high resolution spectral observations targeting any molecule present in both the stellar and exoplanetary atmosphere due to changes in the spectral line shape (Herrero et al. 2011). For WASP-33 b this has been observed for the detection of neutral iron lines by Nugroho et al. (2020b); Herman et al. (2022).

Pursuits to follow-up the tentative low-resolution detection of TiO in the atmosphere of WASP-33 b using high resolution spectra have led to inconclusive results so far. Nugroho et al. (2017) detected the the optical TiO molecular signature using the High Dispersion Spectrograph on the Subaru Telescope. This detection was later challenged by a re-analysis of the same data by Serindag et al. (2021) who unexpectedly found a slightly weaker signal using the updated TiO ExoMol TOTO line list. Furthermore, Herman et al. (2020) analysed emission and transmission spectra from the Echelle SpectroPolarimetric Device for the Observation of Stars (ESPaDOnS) on the Canada-France-Hawaii Telescope and the High Resolution Echelle Spectrometer (HIRES) on the Keck telescope, but are unable corroborate their observations with a thermal inversion due to TiO.

There is thus a lack of a current consensus regarding the observational evidence for TiO in the atmosphere of WASP-33 b.

Despite the elusive results for TiO, several new detections suggest WASP-33 b must have a thermally inverted atmosphere. Recently, emission signatures of Fe I (Nugroho et al. 2020b; Cont et al. 2021a), neutral Si (Cont et al. 2021b) and OH (Nugroho et al. 2021) have been detected. Nugroho et al. (2021) also marginally detect H₂O, consistent with the theoretical predictions that H₂O molecules dissociate into OH and H⁺ at the temperature regime of UHJs. Other atmospheric detections for WASP-33 b include Ca II (Yan et al. 2019), the hydrogen Hα, Hβ and He Balmer lines (Cauley et al. 2021; Yan et al. 2021; Borsa et al. 2021), evidence for AlO (von Essen et al. 2019), and lastly, Kesseli et al. (2020) place upper limits on the Volume Mixing Ratio (VMR) for FeH based on their null detection. These detections are thus in line with predictions by Lothringer et al. (2018); Gandhi & Madhusudhan (2019) of thermally inverted UHJ atmospheres, regardless of the presence of TiO or VO.

In this paper we report CO emission lines in the atmosphere of WASP-33 b using observations with the MMT in Arizona, USA, equipped with the ARizona Infrared imager and Echelle Spectrograph (ARIES). It is the first detection of CO emission lines detected with high resolution cross correlation spectroscopy (HRCCS) utilizing the large Doppler-shift induced by the planet's orbital motion, and despite the lower resolution of the spectra presented here in comparison to other HRCCS observations, it also reveals information about the planet’s atmospheric dynamics. The observations and the subsequent data reduction are discussed in Section 2. Our models and the methods used to characterise the exoplanet’s atmosphere are described in Section 3. The results are presented in Section 4 and discussed in Section 5. Our main conclusions and recommendations for future work are summarised in Section 6.

2 OBSERVATIONS AND DATA REDUCTION

2.1 Observations

We observed the ultra hot Jupiter WASP-33 b with the ARizona Infrared imager and Echelle Spectrograph (ARIES; McCarthy et al. 1998; Sarlot et al. 1999) in combination with the f/15 adaptive secondary mirror and adaptive optics system at the 6.5-m MMT Observatory on Mt Hopkins in Arizona, USA. The adaptive secondary mirror provides a low thermal background, while augmenting the total throughput of the instrument. ARIES can provide spectral observations using both long slit and echelle spectrograph modes. It can observe in the 1-5 μm range and at spectral resolutions of 2,000-30,000. The observations of WASP-33 b presented in this work are the first of a larger survey called MEASURE (MMT Exoplanet Atmosphere Survey) which contains observations of a diverse set of eleven exoplanets with a wide range of temperatures, masses and radii.

For these observations of WASP-33 b, we obtained echelle spectra in the 1.37-2.56 μm wavelength range during three half nights in October 2016 using the ARIES/MMT combination. In total 211 spectra were obtained with an exposure time of 300 s per frame at a
CO emission lines reveal an inverted atmosphere in the UHJ WASP-33 b and indicate an eastward hot spot

Table 1. Observational parameters of the WASP-33 data set for each night.

| Date (UTC) | Total exposure time (min) | No. spectra | Phase Coverage | S/N* |
|------------|---------------------------|-------------|----------------|------|
| 2016 Oct 15 | 220                       | 44          | 0.331-0.469    | 91   |
| 2016 Oct 19 | 465                       | 93          | 0.461-0.731    | 26   |
| 2016 Oct 20 | 370                       | 74          | 0.337-0.554    | 71   |

*This quantity refers to the median S/N per wavelength bin as measured from the extracted and normalised spectral time series of the 23rd spectral order around the 2.3 μm CO emission region.

2.2 Data reduction: pre-processing

Since this is the first time the MMT/ARIES combination has been used for exoplanet atmosphere characterisation, we developed a purpose-built end-to-end data reduction pipeline that we describe here first. This new pre-processing pipeline will be made publicly available on the author’s GitHub.

An overview of our observed orbital phase coverage\(^1\) is shown in Fig. 1 and our observational parameters and data quality are summarised in Table 1. The layout of the 26 echelle orders of ARIES is shown in the top-left panel of Fig. 2. The three observing nights cover both pre- and post-eclipse orbital phases, but the post-eclipse data covers significantly more of the orbit, almost to quadrature, where the planet shows half its day-side and half its night-side to the Earth.

At the beginning and end of each half night, we observed a set of calibration images. This included a set of dark frames obtained using a blank in the filter wheel and the ARIES entrance covered to prevent any light entering the instrument. We observed flat-fields with the grating in, using an incandescent light bulb arranged such that its light reflected off an aluminumized board into the dichroic of ARIES. We also observed a thorium-argon lamp in a similar manner at the start of the nights to focus the spectrograph, but used the observed telluric absorption lines for simultaneous wavelength calibration.

(i) Cross-talk correction: ARIES experiences cross-talk between the four quadrants of its detector which needs to be corrected. A bright pixel in one quadrant produces distinct, cross-shaped, negative shadows at the same position in all other three quadrants on the detector. This effect is apparent in all dark, flat, science frames. We use the C-based corquad routine provided by the ARIES team\(^2\). Three input parameters define the convolution kernel size for each detector quadrant. The parameter space is explored using a grid-based search to find the best cross-talk convolution kernels, which we define as those that minimize the standard deviation in a 10 × 10 box around a visually identified prominent shadow feature. We apply the corquad routine using the best convolution kernels parameters to all dark, flat and science frames, before any further data reduction.

(ii) Dark correction: we need to remove hot pixels from individual darks and combine them into a master dark. We identify hot pixels as ≥ 3σ-outliers. Like the shadow cross-talk features, they are cross-shaped and we replace them by the median of their neighbours outside of a cross-shaped footing in a 11 × 11 box around each hot pixel. We median combine all frames of identical exposure time into a master dark. We subtract the appropriate master dark from each science and flat frame.

(iii) Flat correction: all flats contain fringes arising from Fabry-Pérot interference between the optical elements of the instrument. Fringes in the flat field introduce modulation in the continuum that would be erroneously divided into the science flat during flat field correction, reducing the sensitivity of our later procedures. To remove the fringes from the flats, we developed a modified version of the flat fringe correction by Stone et al. (2014). The procedure is shown in Fig. 2. We use the getfthrm routine from the publicly available Python package CERES\(^4\) (Brahm et al. 2017) to fit the echelle traces as 4th order polynomials using a 10 pixel wide aperture. We use the solution of all 26 spectral orders to calculate a 2D polynomial transform to dewarp the flat frame. We fit each row by a 7th order polynomial to create a dewarped illumination model, essentially representing the dewarped blaze function. This model is subtracted from the dewarped flat frame to reveal the dewarped flat fringes. Most fringes have frequencies < 0.025 pixel\(^{-1}\). We apply a 6th order Butterworth high-pass filter with a cutoff-frequency \(f_c = 0.025 \text{ pixel}^{-1}\) to create a dewarped fringe model. We then use the inverse 2D polynomial cross-talk. A Python-based version is available at: https://github.com/rabrahm/ceres.

\(^1\) Orbital phases have been calculated using the ephemerides in Table A1, which contains all relevant WASP-33 system parameters used throughout this work.

\(^2\) https://github.com/lennartvansluijs

\(^3\) See http://66.194.178.32/~rfinn/pisces.html to correct for the theoretical instrumental resolution of \(R = 30,000\) using the 1″ × 0.2″ slit and the f/5.6 camera mode. The simultaneously operated ARIES imager was used for in-slit guiding, with occasional manual offsets made to correct any sustained drift during an exposure not corrected by the AO guiding system.

\(^4\) https://github.com/rabrahm/ceres
2.3 Data reduction: post-processing

From the spectral time series we would like to extract the planet spectrum, but it is faint and buried in the noise. Thus we first need to remove the telluric and stellar lines. An overview of all steps of the post-processing procedure for a single spectral order covering the most line dense part of the CO spectrum is shown in Fig. 3. We perform the following steps to post-process the extracted spectral time series for each spectral order in a homogeneous manner:

(i) Bad pixel/column correction (see Fig. 3, panel 2): in each spectral time series, some bad pixel columns or detector artifacts may still be present in the spectral time series. To reveal these anomalies, we normalise each spectra by the median of each row, followed by subtracting the mean of each columns. We iteratively perform the bad pixel and column correction procedure five times to ensure all outliers are corrected.

(ii) Alignment of spectra (see Fig. 3, panel 2): instrumental flexure and changes in air mass cause sub-pixel drift of the spectra across the detector. We need to align the spectra to correct for this effect. We use the first spectrum of every night as a reference spectrum. This reference spectrum is cross-correlated with each frame. We fit a Gaussian to this the cross-correlation function (CCF) to determine the drift on a sub-pixel level for each frame. We then shift each spectra using linear interpolation to align them with the reference spectra.

(iii) Telluric wavelength calibration: after alignment, we perform wavelength calibration using the observed telluric lines. We generate a telluric model using ATRAN\textsuperscript{5} (Lord 1992). For each aligned spec-

\textsuperscript{5}https://atran.arc.nasa.gov/cgi-bin/atran/atran.cgi
tral order we cross-match by-eye telluric lines in the model to the corresponding telluric lines in the median of our observed spectra. We robustly fit a polynomial to all these points for each order to obtain a wavelength solution. Robust here refers to the fact that we iteratively clip $\gtrsim 5\sigma$ outliers and refitting a polynomial until no more outliers are found. By default we fit 3rd order polynomials, but for some orders where there are few absorption lines towards the edges of the detector, we fitted 2nd order polynomials instead, to avoid massive deviation of the wavelength solution towards the edges. All these fits were manually inspected to ensure a proper wavelength solution was obtained. For some orders the wavelength solutions were poorly constrained due to strong residual science fringes and/or weak telluric absorption features. For these reasons we excluded orders 7-9 and 11 from the rest of the analysis.

(iv) Throughput correction (see Fig. 3, panel 3): throughput variations can be caused by variations in airmass and misalignment of the target on the slit. We correct for these variations by dividing by the mean of the brightest 50 pixels per spectrum following the procedure described in Brogi & Line (2019).

(v) Telluric removal (see Fig. 3, panel 4-5): quasi-stationary trends mostly due to the telluric lines are still dominating the spectra. To remove these, Principal Component Analysis (PCA) is used to decompose the spectral time series. In our implementation, we perform a Singular Value Decomposition (SVD) (similar to de Kok et al. 2013; Line et al. 2021). Visual inspection of other ARIES observations from other systems indicates that using seven Principal Components works well to balance telluric removal and retrieve an injected exoplanet signal at a high S/N (as described in Section 3.2.1), so we adopt this also for WASP-33 b. However, we emphasize that we keep the number PCA iterations fixed for all spectral orders and all observing nights to avoid optimisation of order/night specific systematic effects and noise, which can produce artificially large S/N (e.g. Cabot et al. 2020; Spring et al. 2022).

Remaining low-frequency residuals persist due to several effects: (1) throughput variations due to small offsets of the target position on the spectrographs slit entrance; (2) residual airmass variations; (3) echelle traces drift on the detector due to the changing gravity vector during the observations, causing instrumental flexure; and (4) uncorrected science frame fringes. We apply a 6th order Butterworth high-pass filter with a cutoff frequency of 0.02 pixel$^{-1}$ to remove most of these trends.

(vi) Masking (see Fig. 3, panel 6): remaining bad columns in the residual time series are masked. This is done by identifying $> 3\sigma$ outliers in the residual matrix and flagging columns with more than five outliers. We combine flagged columns if there are more than two columns within a five-pixel-wide sliding window. Additionally, the columns in a 50 pixel window from the edge of the detector are masked by default.

The final result of the post-processing pipeline is shown in panel 6 of Fig. 3.

### 2.4 Observed instrument performance

As this is the first time ARIES/MMT is used to characterize an exoplanet atmosphere, we compare the observed performance to the theoretical instrumental performance. We measured the instrumental throughput, resolving power and Precipitable Water Vapour (PWV) directly from the normalised spectral time series. The instrumental throughput is measured directly from the total S/N for each spectra. To measure the observed resolving power and PWV we largely follow procedure described in Chiavassa & Brogi (2019), where we cross-correlate a telluric model with the normalised spectral time series and evaluate the log-likelihood defined by Zuckerman (2003). This method is sensitive to continuum variations and first we correct for them the following way: (1) a median filter removes any possible outliers (2) each spectrum is binned and the maximum of each bin is calculated (3) we fit a low 3rd-order polynomial to these local maxima and (4) we divide out this polynomial fit from each spectra. The TELFIT code is used to compute telluric spectra (Gullikson et al. 2014). We fix the airmass to the logged airmass for each frame which we obtain from the raw FITS-header information, instead of keeping it a free parameter as done by Chiavassa & Brogi (2019). The Markov Chain Monte Carlo (MCMC) PyMultiNest package is used to constrain PWV and $R$.

---

6 https://github.com/kgullikson88/Telluric-Fitter
7 https://johannesbuchner.github.io/PyMultiNest/index. html#citing-pymultinest
3 METHODS

As we use the HRCCS technique to characterise the atmosphere of WASP-33 b, we require forward models for the cross-correlation templates i.e. synthetic spectra of WASP-33 b, which we discuss in Section 3.1, followed by a description of the HRCCS methods used in Section 3.2.

3.1 Models for WASP-33 b

We use several atmospheric modeling codes in this work to address the structure, chemistry, and dynamics of the atmosphere of WASP-33 b. To identify absorption and emission features initially, we used PHOENIX atmospheric models. PHOENIX is a general purpose atmosphere code, well-tested on objects from cool planets to hot stars (e.g. Hauschildt et al. 1997, 1999; Barman et al. 2001, 2011; Allard et al. 2011; Lothringer et al. 2018; Lothringer & Barman 2019). We used both self-consistent atmosphere models in Section 3.1.1 in thermodynamic equilibrium, and a grid of models where the temperature structure and/or the molecular abundances have been manually varied in Section 3.1.2. We then further use the Monte Carlo Radiative Transfer code gCMCRT (Lee et al. 2019, 2021) to model 3D effects and orbital phase-dependent variations of the observed spectra in Section 3.1.3.

3.1.1 Self-consistent PHOENIX models

The self-consistent models used here are similar to the extremely irradiated hot Jupiter models presented in Lothringer et al. (2018). The self-consistent atmosphere models solve the atmosphere structure and composition iteratively, calculating the spectrum at each iteration and comparing it to radiative equilibrium. For our models the radiative-convective boundary is usually below the highest pressure we model and no convective adjustments were made in order to increase speed of convergence. Temperatures are then modified to approach radiative equilibrium after which the chemistry is calculated based on chemical equilibrium and the spectrum is re-calculated. This process is repeated until the temperature corrections are small, indicating that the atmosphere is in radiative and chemical equilibrium. Each spectrum is calculated from 10 to $10^7$ nm using planetary parameters by Haynes et al. (2015) (as summarised in Table 1 of Lothringer et al. 2018) on a grid with varying atmospheric metallicity and a heat re-radiation efficiency $f$ (where $f$ is the parameter as defined in Madhusudhan & Seager 2009). For the metallicity, we explore a grid of models at 0.1×, 1× and 10× Solar metallicity. For the heat re-radiation factors $f$ we explore the values: $f = 1/4$ for day-side and night-side heat redistribution, $f = 1/2$ for day-side-only heat redistribution and $f = 2/3$ for instantaneous heat re-radiation.

These self-consistent models include opacities for TiO and VO, but as explained in Lothringer et al. (2018), TiO and VO are not the sole cause of temperature inversions in extremely irradiated hot Jupiters. Temperature increase at these pressures is likely due to the absorption of short-wavelength radiation by absorbers like atomic Fe and the lack of coolants such as H$_2$O. Such hot temperatures result in the thermal dissociation of most molecules in the atmosphere including H$_2$ and H$_2$O (see Fig A1). The abundance of CO, which exhibits the strongest molecular bond, is also reduced, but to a lesser extent compared to other potential molecular opacity sources. The resulting spectrum, shown in Fig 5, predicts CO emission lines with signatures of H$_2$ and other molecules muted due to thermal dissociation combined with the isothermal lower atmosphere.

3.1.2 PHOENIX models with Modified Structure and/or Abundances

In addition to the self-consistent modeling, we ran a grid of models with varying temperature structures and atmospheric metallicity to further explore the parameter space. Again, we explore metallicities of 0.1×, 1×, 10× and 100× Solar. For the P-T profiles, we use the
CO emission lines reveal an inverted atmosphere in the UHJ WASP-33 b and indicate an eastward hot spot

parameterisation from Madhusudhan & Seager (2009), but modified to have an isothermal upper atmosphere. These simple structures used five parameters to describe the temperature throughout the atmosphere: \( T_1, P_2, T_2, \alpha_2, P_1 \) describes the pressure at the tropopause, above which the temperature was set to \( T_1 \). The temperature then varies until it reaches temperature \( T_2 \) at pressure \( P_2 \), as set by the gradient of the inversion \( \alpha_2 \). We explored a wide range of P-T structures with upper atmosphere temperatures from 2000 to about 10,100 K, shown in Fig. A2. In total we ran 576 forward models.

We also generated a small subset of these models to explore how removing a single opacity source affects the significance of the planet detection i.e we re-run the best matching model without \( H_2O \), without CO, and without OH. We do this in order to identify potential absorbers or emitters in the atmosphere, while keeping the P-T structure fixed. Line lists for the investigated opacity sources were taken from: CO (Goorvitch 1994), OH (Barber et al. 2006) and \( H_2O \) (et al. 2009).

3.1.3 GCM and post-processing modelling

For the 3D GCM models, we use output from a SPARC/MITgcm model (Showman et al. 2009) of WASP-33 b with similar set-up to the simulations performed in the Parmentier et al. (2018) study for UHJs. The GCM output is then post-processed using the gCMCRT 3D RT code (Lee et al. 2021) to provide high-resolution emission spectra that account for variation in the spectra throughout the orbital phases of the observation. We use line-list data from various sources, namely: OH (Hargreaves et al. 2019), \( H_2O \) (Polyansky et al. 2018), \( CH_4 \) (Hargreaves et al. 2020), CO (Li et al. 2015), CO \( _2 \) (Yurchenko et al. 2020), \( NH_3 \) (Coles et al. 2019), HCN (Barber et al. 2014). Cross-sections were calculated using the HELIOS-K opacity code (Grimm et al. 2021) and interpolated between 1.27-2.66 \( \mu \)m at a resolution of \( R = 100,000 \).

The resulting synthetic high-resolution emission spectra include the Doppler shifting of spectral lines due to winds and planetary rotation towards the line of sight for each phase. We include all molecular species listed above as well as CIA H2-H-He pair continuum opacities from Karman et al. (2019) and \( H^+ \) from John (1988).

The resulting GCM phase-dependent model and P-T profiles and the gCMCRT output synthetic spectra are shown in the bottom-left and right panels of Fig. 6. The GCM predicts an eastward hot spot at +5° east from the substellar point, which results in an asymmetry between P-T profiles with an equal longitudinal distance west or east as seen from the sub-stellar point. As the planet rotates in the same direction as it orbits its host star, we see more of the hot spot region pre-eclipse compared to post-eclipse. This results in phase-dependent variations in both the continuum and relative line strengths (see bottom-left panel of Fig. 6). As it is computationally expensive to run a full GCM at all observed orbital phases, we run the full GCM at 9 phases uniformly sampled over the phase coverage during our

Figure 5. WASP-33 b 1D PHOENIX self-consistent synthetic emission spectra. Left panels: PHOENIX self-consistent spectra as a function of the metallicity and re-radiation factor \( f \): \( f = 1 \) for full heat-redistribution, \( f = 1/2 \) for day-side-only heat-redistribution and \( f = 2/3 \) for instantaneous re-radiation. Different metallicity models have been offset by 0.75 along the y-axis with respect to the 0.1×Solar model. The ARIES spectral order wavelength ranges included are indicated by the gray bars. Right panel: corresponding PHOENIX self-consistent P-T profiles.

![Figure 5](image_url)
three observing nights. For spectra observed at intermediate phases, we linearly interpolate these spectra in phase.

To enable comparison and cross-check between the 3D GCM and the 1D PHOENIX model atmospheres, we also created a set of GCM day-side-only models i.e. fixed at orbital phase $\phi = 0.5$ (see top-left panel of Fig. 6). These templates were created by simulating the emission assuming continuum opacity without the effects of Doppler shifting. We also again explore the impact of any single absorber or emitter on the planet signal by creating day-side-only templates with only a single opacity source included i.e. only CO, only H$_2$O and only OH. CO is most prolific in spectral lines in the reddest parts of the ARIES spectra, while OH dominates its shorter wavelengths, and water persists throughout.

### 3.2 High-resolution Cross Correlation Spectroscopy (HRCCS)

The HRCCS technique has been developed in recent years to enable not simply detection of molecular species, i.e. the S/N-method, but into a framework that enables statistically rigorous assessment of atmospheric models that may match the data e.g. Cross-Correlation-to-log-Likelihood (CC-to-log(L)) mapping (e.g. Brogi & Line 2019; Gibson et al. 2020). Both methods have different uses, and we use both in this work to characterise the composition, structure, and dynamics of the WASP-33 b atmosphere, as described below.

#### 3.2.1 S/N method

The S/N-method cross-correlates each observed spectrum with a spectral template and the S/N is calculated from the maximum and standard deviation of the corresponding Cross-Correlation Function (CCF). First the template model is scaled to the expected star-planet contrast ratio using

$$F_{\text{model}, \text{scaled}} = \frac{F_{\text{model}} R_p^2}{R_*^2},$$

(1)

with planet radius $R_p$, stellar radius $R_*$ and assuming a stellar black body flux $F_*$ at the effective stellar temperature (using values in Table A1). A stellar black body is a reasonable assumption for the host star WASP-33 given its hot effective temperature which results in few spectral stellar absorption lines in the wavelength region of interest. Previous works indicate that it is important to match the line shape correctly for HRCCS (e.g. Spring et al. 2022), hence before cross-correlating, we convolve each synthetic spectrum of WASP-33 b to the median observed resolving power for each night (see Fig. 4), using a Gaussian instrumental profile. Since we applied a 6th-order Butterworth high-pass filter at a cutoff-frequency of 0.02 pixel$^{-1}$ to our data, we also apply it to the scaled model template, where we adjust the cutoff-frequency to account for the difference in sampling rate between the model and data wavelength grid. We calculate the correlation coefficient as defined by Brogi & Line (2019) for each observed residual for each spectral order for all observing nights with the scaled template. We explore a radial velocity range of $-31$ to 31 grid in $(v_{\text{sys}}, K_p)$-space around the expected values of $(v_{\text{sys}}, K_p) = (-0.3, 230.9)$ km/s as previously found in the detection of OH by Nugroho et al. (2020b) within the range of $\pm 100$ km/s for $v_{\text{sys}}$ and $\pm 150$ km/s for $K_p$ on a 31x31 grid. For each trial velocity on the grid, we shift the CCF-matrix to $v_{\text{trial}}$ and calculate the combined CCF by taking the mean along the time axis. The S/N is determined by calculating the maximum of the combined CCF and dividing it by the standard deviation of the CCF. Those exposures taken in between the first and last contact of the eclipse of WASP-33 b (see Fig. 1) are excluded from the S/N calculation to avoid dilution of the combined CCF signal. Not all spectral orders are equally sensitive when cross-correlating with the template model. Lower sensitivity is expected for the bluer ARIES orders due to poorer data quality due to lower throughput and stronger spectral fringes and weaker spectral features in the models. To account for both, we use an order-specific weighting scheme in the S/N-method to combine the CCF-matrices, based on the data quality and model. To calculate the weights we follow Spring et al. (2022), where we first inject the model (before PCA cleaning) into the observations using the expected model strength and orbital parameters (based on Nugroho et al. (2020b)). We create a CCF-matrix for each injected order, and then subtract its corresponding observed (no injection) CCF-matrix. For each order we calculate the S/N of this CCF difference. For each order $n$, weights $w_n$ are assigned proportional to this S/N and normalised such that $\sum_{n=1}^{N} w_n = 1$, where $N$ is the total number of spectral orders included. An example of the weighting scheme is shown in Fig. 8. As expected, using the self-consistent PHOENIX model template at $x1$ Solar metallicity with a re-emission factor of $f = 1/2$ as an example, the redder orders around the ~2.3 micron densely-packed CO spectral feature region contribute the highest weights due to the numerous strong spectral lines and higher S/N of the observed spectra.

#### 3.2.2 CC-to-log(L) mapping and model scaling parameter

While the S/N-method is widely used in literature and thus a convenient way to compare the significance of our detection with previous works, it is inherently normalised by definition and therefore insensitive to scaling of the model or observed spectra. This is why there was a need to implement a weighting scheme to combine multiple spectral orders in the S/N-method. The CC-to-log L Bayesian Framework described by Brogi & Line (2019) however does not suffer from this. CC-to-log(L) mapping maximizes the log-likelihood as:

$$log L = -\frac{N}{2} \log (s_f^2 + s_g^2)$$

(3)

with $s_g$ and $s_f$ the variance of model and data, respectively, $R$ the cross-covariance and $N$ the number of spectral channels. When combining multiple nights and spectral orders, we can compute the total sum of their log-likelihood values. There is thus no need to weight each spectral order as this is accounted for in the CC-to-log(L) mapping (Brogi & Line 2019). Moreover, CC-to-log(L) mapping gives us a framework to extract uncertainties on the measured and derived quantities from the modelling.

\[^8\text{https://github.com/shbhuk/barycorppy}\]
**CO emission lines reveal an inverted atmosphere in the UHJ WASP-33 b and indicate an eastward hot spot**

![Figure 6. WASP-33 b GCM (Global Circulation Model) synthetic emission spectra. Top-left panel: GCM day-side-only (i.e. fixed at phase \( \phi = 0.5 \)) spectra with all opacity sources included or only specific molecules included. The different models have been offset by 0.5 along the y-axis with respect to the spectrum at the bottom. The ARIES spectral order window wavelength ranges included are indicated by the gray bars. Bottom-left panel: GCM spectra at different orbital phases. Planck black body curves are plotted at a range of temperatures. The GCM predicts hotter models pre-eclipse compared to post-eclipse due to an hotspot approximately +8° eastward seen from the substellar point. Right panel: GCM P-T profiles as a function of longitude, where 0° is defined as the substellar point and increases towards the eastward direction as seen from the substellar point.](image)

| Parameter                  | Symbol | Prior               |
|----------------------------|--------|---------------------|
| System velocity offset     | \( \Delta v_{\text{sys}} \) | Uniform(-50,50) km/s |
| Orbital velocity offset    | \( \Delta K_p \)     | Uniform(-50,50) km/s |
| Scaling parameter          | \( a \)             | LogUniform(-2,2)    |

Table 2. Priors used in CC-to-log(L) framework. Velocity offsets are given relative to the previous WASP-33 b velocity values of \( (v_{\text{sys}}, K_p) = (-0.3, 230.9) \) km/s as reported by Nugroho et al. (2021).

Our implementation uses PyMultiNest\(^9\) (Buchner et al. 2014b), a generic Python package connected to MultiNest, a Bayesian inference tool\(^10\) (Feroz & Hobson 2008; Feroz et al. 2009, 2019), for all our parameter estimations. Importantly, following Brogi & Line (2019), we also introduce one additional free parameter, the scaling factor \( a \), which allows us to compensate for any potential unknown scaling of the model template, but ideally should be retrieved at \( a = 1 \). We multiply the template by \( a \) after applying the high-pass filter. The multidimensional parameter space is explored using the priors in Table 2.

To statistically compare the models amongst each other we apply Wilks’ Theorem (Wilks 1938). In practical terms, this theorem states that the difference in \( \log(L) \)-values between two models with \( n \) free parameters follows a \( \chi^2 \)-distribution with \( n \) degrees of freedom (for a concise statistical description see Pino et al. 2020). The confidence interval \( p \)-value can now be calculated from the corresponding \( \chi^2 \)-distribution and converted to a familiar \( \sigma \)-value. This way, by its construction, we can only compare models relative to the best trial model.

4 RESULTS

We now present the results using both the S/N-method and the CC-to-log(L) mapping for our four different modelling suites described in Section 3.1. We detect the atmosphere of WASP-33 b and measure its properties to varying significance and confidence for the best matching model in each modelling suite. The key results are summarised in Table 3. The best-matching model from each suite results in the detection the Doppler-shifting spectrum of the planet, as demonstrated by the radial velocity trail in the CCF-matrices shown in Figures 7 and A3. Notably, the trail disappears at the calculated start time of secondary eclipse ingress and reappears at the end of its egress, confirming that the detected signal is associated with the planet’s spectrum as it is obscured by the star during secondary eclipse.

---

\(^9\) https://johannesbuchner.github.io/PyMultiNest/

\(^10\) https://github.com/JohannesBuchner/MultiNest
Figure 7. Cross-Correlation Functions (CCFs) for the best-modified P-T profile detected at a S/N of 7.9σ. Top-left: The CCF for each frame including all three observing nights. Frames are sorted by orbital phase but are not equally spaced, and the blue dotted line marks the post-eclipse frame with symmetric phase to the earliest pre-eclipse frame (see Figure 1). The start/end of ingress/egress are indicated by the white dashed lines labeled TI-TIV for the four contact points. The two red lines are centered around the planet radial velocity trail. Top-right: Same as the top-left panel, but shifted to the planet rest frame. Bottom-left: the mean CCF along the y-axis. Frames where the planet is not fully visible (in between TI-TIV) were excluded when computing the CCF to prevent dilution of the planet signal. Bottom-right: same as the bottom-right panel, but shifted to the planet’s rest frame.

Table 3. Overview of the highest S/N-ratio of the sets of models explored in this work and their corresponding scaling parameter α from the CC-to-log(L) mapping. The final column shows Δ log(α) i.e. the difference between the mean of the pre-eclipse (Nights 1 & 3) scaling parameter and that for the post-eclipse data subset for which we have symmetric phase coverage. The log(α) scaling parameter has a value of zero when the model is a good description of the data. The phase-dependent GCM gives the smallest discrepancy in log(α), indicating that it is accounting for the phase-dependence of the scaling parameter.

| Model                                    | Highest S/N | Δ log(α)           |
|------------------------------------------|-------------|--------------------|
| PHOENIX (1D) modified P-T structure models | 7.9         | 0.21³±0.03         |
| PHOENIX (1D) self-consistent models      | 7.6         | 0.24³±0.03         |
| GCM (3D) day-side-only models (fixed orbital phase φ = 0.5) | 7.1         | 0.27³±0.04         |
| GCM (3D) phase-dependent models          | 7.1         | 0.13³±0.03         |

4.1 Thermal structure and composition

The model that results in the highest S/N detection is a modified PHOENIX model that includes all opacity sources, with the highest likelihood corresponding to at a modified P-T profile with $T_3 = 2000$K, $P_1 = 10^{-3}$ bar, $P_3 = 10^{-6}$ bar, $\alpha_2 = 0.17$ and a metallicity of 10× Solar. As shown in the top row of Fig. 9 this model gives $S/N = 7.9\sigma$ when all nights are combined, and is higher during pre-eclipse orbital phases than post-eclipse. The correspondingly similar results for the PHOENIX self-consistent models are shown in Fig. A4. Although the S/N of the detection varies with phase, this alone is not sufficient evidence to interpret it as due to a planetary feature e.g. an offset hot spot, day-to-night variations in brightness, abundances, or thermal structure. However, we discuss in Section 5.3 the additional evidence supplied by the CC-to-log(L) mapping scaling parameter that could support such interpretations.

The top-left panel of Fig. 10 shows the results from the log(L)-to-CC mapping for the best-matching modified PHOENIX model, giving the posterior distributions for the systemic velocity, orbital velocity, and the scaling parameter. The planet is detected at $v_{sys} = 0.15^{+0.64}_{-0.65}$ km/s and $K_p = 229.53^{+1.11}_{-1.02}$ km/s with this highest S/N model, in agreement with previous literature e.g. $(v_{sys}, K_p) = [-0.3, 230.9]$ km/s (Nugroho et al. 2021). The scale factor posterior distribution, which would have log(α) = 0 for a perfectly matched model, is systematically offset to smaller values indicating that the model does not fully encapsulate all of the physics and chemistry to describe the atmosphere. Similar is seen in the top right panel of Fig. 10 for the best-matching self-consistent PHOENIX model. However, all nights are in agreement with their $(v_{sys}, K_p)$-values within 2σ. We discuss the variation of log(α) in later sections.

We compare the best-matching modified P-T structure PHOENIX model with the rest of the models in the suite, as well as that of the best-matching self-consistent PHOENIX model, to give confidence intervals with respect to the alternative P-T profiles, fixed at 10 x Solar metallicity. This was calculated using Wilks’ Theorem (with 7 free parameters), and is shown in Fig. 11. The best-matching modified P-T structure is slightly cooler than the best-matching self-consistent PHOENIX model, and inverted P-T profiles with an upper and lower
atmosphere temperature difference close to the best-matching model are favoured. Both can be understood by the fact that we are sensitive to the the relative line strength with respect to the continuum, which is set by the upper and lower atmosphere temperature contrast (or equivalently the strength of the inversion layer). On the contrary, we are less sensitive to the absolute temperature due to loss of the continuum information in the HRCCS processing, resulting in a range absolute lower and upper atmosphere temperatures inside the calculated 1σ-confidence interval.

To determine if any one particular species was contributing the majority of the detected signal, we fix the P-T profile to the best-calculated 1σ-confidence interval. Orders 7-9 and 11 were excluded from the analysis in the wavelength calibration step. Orders 23-25 around the CO 2.3μm spectral feature are naturally assigned the highest weights.

![Image](https://example.com/image.png)

**Figure 8.** Weights per spectral order after cross-correlation with the best self-consistent PHOENIX model used in our S/N-method adopted. Weights are calculated from the S/N of the difference between the injected and observed CCF, indicated by the miniature CCF above each order. Orders 7-9 and 11 were excluded from the analysis in the wavelength calibration step. Orders 23-25 around the CO 2.3μm spectral feature are naturally assigned the highest weights.}

4.2 Atmospheric dynamics and longitudinal variation

The post-eclipse phase coverage on Night 2 is longer than the pre-eclipse coverage on Nights 1 and 3. To enable a direct comparison, we split the post-eclipse Night 2 spectra into a subset of data that contains only the symmetric phases corresponding to the pre-eclipse coverage. A comparison of results from Night 2 and this subset of data with the different model suites are shown in Fig. 10 by the grey and green contours respectively, and in the right column of the S/N-maps in Fig. 9. The S/N for the subset data is reduced, but only by ΔS/N=0.7 at most, indicating that the data containing more night side hemisphere contributes less to the overall S/N of the detection. The green contours for the subset of phases are also tighter and better constrained in all cases in the v$_{sys}$ - K$_P$ plots, again indicating a better match with the model when the night hemisphere contributions in the data set are reduced. As shown in Table 3, the scaling parameter from the CC-to-Log(L) mapping differs for the symmetric pre- and post-eclipse phases, indicating a phase-dependence in the observed spectra of the planet due to asymmetry in the disk of the planet caused by e.g. an offset hot spot. To qualify this further, we use the GCM models described in Section 3.1.3.

To first check for general consistency between the GCM models and the results from the PHOENIX 1D models, we perform our two analysis methods using the day-side-only (i.e. no phase dependence) 3D GCM model with all opacities included. This is detected at S/N = 7.1σ, which is slightly lower the PHOENIX models, and found at the expected (v$_{sys}$, K$_P$)-values for all nights combined (see bottom row of Fig. A4 and the corresponding cross-correlation trail is shown in the middle row of Fig. A3). The lower S/N is not necessarily surprising as we explore only a single GCM day-side-only model vs. many PHOENIX models, and we know that the GCM lacks some of the important optical absorbers in its energy balance e.g. atomic iron, such that it cannot produce as strong temperature inversions. We can also assess in the GCM day-side-only model if any single species contributes the majority of the detection. The S/N results for single species models are shown in the right panel of Fig. 12 and the corresponding S/N-plots are shown in Fig. A6. Only CO has significant S/N at 6.6σ. The GCM H$_2$O model has S/N = 3.3σ, which is insufficient for a robust detection in HRCCS as previous work demonstrated spurious signals at a SNR ≤4σ often persist (Cabot et al. 2020; Spring et al. 2022), even though it appears at the expected planet velocity. OH is not detected. The CC-to-log(L) analysis shown in Fig. A7 further highlights the lack of robust detection of any species by CO with this model, in general agreement with the PHOENIX models.

Our main goal is to understand possible phase dependence in log(a). The bottom-left panel of Fig. 10 shows the results from the CC-to-log(L) framework for the GCM day-side-only model. The results are qualitatively similar to the the PHOENIX models, again with offsets in log(a) for the different phase ranges, but with larger error margins. We hypothesize these larger error contours may be due to the broadening of the lines by planet rotation in the GCM model and its overall lower S/N detection. The broad agreement with the trend for offsets in log(a) is confirmed by the day-side-only GCM and thus we proceed to allow the GCM to have phase dependence and determine if this resolves the log(a) scaling discrepancy.

The GCM phase-dependent model provides a different cross-correlation template for each observed spectrum at each phase, where the spectrum corresponds to a P-T profile that a combination of all parameters in the model and the larger number of models explored in the suite.
the profiles from different longitudes visible across the planet disk at that time. The GCM phase-dependent model is similarly detected at $S/N = 7.1\sigma$ at the expected $(v_{\text{sys}}, K_p)$-location for all night combined (the corresponding CCF-matrix and $K_p-v_{\text{sys}}$ maps are shown in the bottom rows of Fig. A3 and Fig. 9, respectively). However, the results from the CC-to-log(L) mapping shown in the bottom-right panel Fig. 10 are notably different for the scaling parameter. The phase-dependent GCM appears to resolve the majority of the $\log(a)$ discrepancy between the pre- and post-eclipse symmetric phases, and brings all the data sets into broad agreement within $2\sigma$. We discuss this further in Section 5.3. Although the GCM gives $\log(a) = 0$ closer to 1 than the PHOENIX 1D models, indicating that the inclusion of 3D dynamical effects such as hot spots and orbital phase brightness variation are a better match to the data, it does not fully describe the atmosphere of WASP-33 b. Additional optical absorbers not in the GCM, such as Fe, Fe+ and SiO would enable greater thermal inversion (Lothringer et al. 2020) likely leading to even deeper lines. While missing physics in the GCM may account for some of the $\log(a) < 0$, it may be that the data reduction process also impacts the overall line shape as discussed in the next section.

5 DISCUSSION

5.1 Thermal structure and composition

The detection of CO emission lines with the modified PHOENIX P-T structures provide unambiguous evidence for a thermal inversion in the atmosphere of WASP-33 b. A non-inverted atmosphere would have exhibited absorption lines instead. This is in agreement with previous observations of other atomic and molecular lines in emission in the atmosphere of WASP-33 b (e.g. Deming et al. 2012; Haynes et al. 2015; Zhang et al. 2018; Nugroho et al. 2020b; Cont et al. 2021a,b; Herman et al. 2022) and expected from atmospheric modelling of UHJ atmospheres (e.g. Lothringer et al. 2018; Gandhi & Madhusudhan 2019). Although, we do not explore non-inverted or isothermal P-T structures, our highest log-likelihood P-T structure (see Fig. 11) shows temperature contrasts with well constrained upper- and lower limits when including a thermal inversion layer.

From all molecular templates investigated in this work, only CO has resulted in a robust detection. This is further supported by the CC-to-log(L) results shown in Fig. A7 where only CO has similar constraints on the velocities compared to when all opacity sources are included: $v_{\text{sys}} = 0.75^{+0.81}_{-0.79}$ km/s, $K_p = 228.74^{+1.26}_{-1.29}$ km/s. Furthermore, only the exclusion of CO had a significant impact on the detection strength of the planet signal. It does remain somewhat puzzling however that we still detect the best modified PHOENIX model without CO at a $S/N = 5.8$ in the first night of pre-eclipse data. This suggests we still detect the combined set of all other opacity sources, besides CO, during the first night, even though we cannot attribute these to H$_2$O or OH alone, and we do not expect significant contributions from iron lines in the ARIES wavelength range either. We do not detect the model without CO during the third night, despite covering similar orbital phases. This may be explained by the better observing conditions during the first observing night relative to the third observing night (see $S/N$ measurements in Table 1). Although there have been many detections of CO in absorption (Snellen et al.
Figure 10. Marginalized distributions from the CC-to-log(L) framework based on Brogi & Line (2019). Results are shown for the best-matching PHOENIX modified P-T structure model (top-left panel), the best-matching self-consistent PHOENIX model (top-right panel), the GCM day-side only model (phase fixed at $\phi = 0.5$; bottom-left panel) and the GCM phase-dependent model (bottom-right panel). The contours indicate the 1$\sigma$, 2$\sigma$, and 3$\sigma$ confidence intervals. All frames with phases during the eclipse have been excluded from this analysis to prevent dilution of the planetary signal. Results are shown for individual observing nights, all nights combined, and for the subset of post-eclipse phases that are symmetrically matched with the pre-eclipse phases (see Fig. 1). The dashed black grid indicates the expected location at $(v_{SYS}, K_p) = (-0.3, 230.9)$ km/s based on the OH detection by Nugroho et al. (2021).
Previous works have indicated both water (Haynes et al. 2015) and OH (Nugroho et al. 2021) in the atmosphere of WASP-33 b, but we do not make a robust detection of CO emission lines using the HRCCS data. To demonstrate that the very weak GCM H$_2$O signal in our data is caused by non-planetary residuals e.g. tellurics, we ran the CC-to-log(L) analysis using only frames obtained when the planet is not visible i.e. during the full eclipse of WASP-33 b. Spurious signals due to telluric or stellar residuals should persist whereas signals originating from WASP-33 b should disappear or move away from the planet’s expected ($v_{\text{sys}}$, $K_p$)-location. For H$_2$O we found that a signal is still retrieved at the same offset ($v_{\text{sys}}$, $K_p$)-position albeit with larger errors, while the CO signal was not obtained at the expected planet ($v_{\text{sys}}$, $K_p$)-position anymore. This supports the interpretation that any H$_2$O signal in the ARIES data is caused by non-planetary residuals.

The non-detection of OH in the ARIES data is not necessarily surprising either when compared to the OH detection by Nugroho et al. (2021) using Subaru/IRD data. The bluer wavelength region (0.97-1.75 $\mu$m) covered by Subaru/IRD with respect to ARIES/MMT contains stronger OH emission lines and Subaru/IRD’s has higher spectral resolution ($R = 70,000$). Thus, the lack of an OH detection with ARIES can likely be explained by the poorer data quality of the spectral orders covering the OH line dense regions compared to CO line dense regions. The synthetic GCM spectrum in the left-top panel of Fig. 6 shows OH line dense regions in the wavelength range of the bluer spectral orders and order 26 at the far red-end. As explained in Section 3.2.1, lower weights are assigned to the bluer ARIES orders which have a lower throughput and contain residual fringing. The redder order 26 falls at the edge of the detector and is consequently of poorer data quality. Lastly, telluric absorption is strong in some OH line dense spectral orders.

Due to the high dissociation temperature for CO, the abundances of CO are approximately constant in- and outside of the hotter and cooler regions of the planet, at the pressures probed by HRCCS (Lodders & Fegley 2002). This makes CO a particularly interesting molecule to target for the characterisation of the thermal structures of UHJs, especially compared to atomic species or other molecules such as OH, H$_2$O or TiO which dissociate on the day-side, resulting in an additional phase-dependent chemical gradient, complicating the interpretation of the line contrast. We therefore advocate for CO as a good probe of the thermal structure and inversions of UHJs compared to H$_2$O in HRCCS.

5.2 Robustness of CO as a temperature tracer in the presence of stellar activity

The CCFs inside the planet radial velocity trail in Fig. 7 are distinct and easily seen even by eye. We do not see contaminating signatures of the $\delta$ Scuti pulsations. On the contrary, the contamination by stellar pulsations can be seen clearly in the cross-correlation analyses neutral iron emission lines (Nugroho et al. 2020a; Herman et al. 2022). This is not exclusive to WASP-33 b; any pulsating star with opacity sources present in both the star and planet will contaminate HRCCS. This contamination limits the available effective orbital phase coverage, as frames obtained at phases close to secondary-eclipse have to be either heavily processed to remove the stellar pulsations (Johnson et al. 2015; Temple et al. 2017; van Sluijs et al. 2019) or disregarded (Nugroho et al. 2020a; Herman et al. 2022; Spring et al. 2022). In contrast to atomic species often present in both the planet and star, CO is dissociated in the hot stellar atmosphere of early-type A/F-stars. These type of stars are also more likely to be pulsating stars due to their location within the Hertzsprung-Russel diagram’s instability strip (e.g. Gautschy & Saio 1996). This highlights a further advantage of using CO in the NIR to probe the atmospheric temperature structure and inversions of UHJ around hot pulsating stars.

5.3 Atmospheric dynamics and longitudinal variation

Hot Jupiter thermal structure is expected to be asymmetric, with the hottest point being shifted away from the sub-stellar point. This shift arises from the competition between heat transport by winds of planetary-scale waves and the radiative cooling of the parcel of gas (e.g. Showman & Guillot 2002; Perez-Becker & Showman 2013). The vast majority of observations and models feature a shift of the hot spot in the direction of the planet rotation, usually defined as an eastward shift. In such a case, the pre-eclipse phases are more dominated by the hot spot than the post-eclipse phases, due to the planet rotation during the eclipse.

Previous evidence for a hot spot on WASP-33 b comes from NIR and optical photometric phase curve observations, where eastward hot spot results in negative phase curve offset. Zhang et al. (2018) report the first evidence of an eastward hot spot on WASP-33 b, measuring a phase curve offset of $-12.8 \pm 5.8^\circ$ in the Spitzer 3.6 $\mu$m band. Conversely, von Essen et al. (2020) found a $+28.7 \pm 7.1^\circ$ westward phase curve offset in the optical TESS light curve, and a range of theories including magnetohydrodynamic effects, non-synchronous rotation, and clouds have been invoked to explain such westward offset hot spots (e.g. Dang et al. 2018; Hindle et al. 2021). Recent work by Herman et al. (2022) further report a $+22 \pm 8^\circ$
**CO emission lines reveal an inverted atmosphere in the UHJ WASP-33 b and indicate an eastward hot spot**

**Figure 12.** S/N results for the models with different opacity sources included or excluded. *Left panel:* results from the best modified P-T structure PHOENIX model for the cases of all opacity sources included and with a single opacity source excluded, respectively models with OH, H$_2$O and CO excluded. All these models fix the P-T profile to the best modified structure PHOENIX model where all opacity sources were included. Only the models without CO result in a significant drop of the S/N when compared to the all included case. *Right panel:* Results from the GCM day-side-only opacity templates for the cases of all opacity sources included and respectively with only CO, only H$_2$O and only OH included. From all opacity sources, only CO remains robustly detected.

**Figure 13.** Confidence intervals for the PHOENIX self-consistent model grid for all observing nights combined using Wilks’ Theorem. The best model, the one with the highest log-likelihood, is indicated by the star-marker. By definition of Wilks’ Theorem, all confidence intervals here are with respect to this best model. Models with $f \geq 1/2$ and metallicity $\geq 1 \times$ Solar are all within $1 \sigma$.

It is important to note that the phase-dependence detected in this work and in *Herman et al.* (2022) is found via a model scaling parameter ($a$ in this work, and a similar $A_P(\phi)$ in equation 4 of the other study). Both studies detect that a larger scaling is required to best model the observations just after eclipse. *Herman et al.* (2022) interpret the larger $A_P(\phi)$ post-eclipse as an overall brightness variation, indicating more flux west from the sub-stellar point and hence a westward hot spot. This is the typical interpretation for photometric phase curve measurements, which are sensitive to absolute flux as a function of phase. Instead, we highlight that because the HRCCS we use in this work divides out the continuum, that the scaling parameter is a measure only of line contrast i.e. that the lines in the planet spectrum are larger just after eclipse, as shown in Figure 14.

The phase-dependent line contrast can then be understood in the context of our GCM model. First, the eastward hot spot results in a hotter continuum and thus greater overall brightness for pre-eclipse phases as shown in the bottom-left panel of Fig. 6. But, since our post-processing of the high resolution spectra removes the continuum information we argue we are insensitive to these variations. Fig. 6 then shows that the GCM predicts thermal profiles that are shallower in the eastward-shifted hot spot and steeper on the western part of the day-side. Overall, this leads to a disk-integrated temperature gradient that is shallower during pre-eclipse when it contains the eastward hot spot (where our line-of-sight is centered on longitudes $\sim 17^\circ$ $-$ $61^\circ$ east of the sub-stellar point), and steeper during post-eclipse when it contains more of the western day-side hemisphere (where our line-of-sight is centered on longitudes $\sim 277^\circ$ $-$ $341^\circ$ east of the sub-stellar point). Consequently, the average line contrast associated with these temperature gradients will be shallower during pre-eclipse and stronger during post-eclipse. We therefore conclude that the data can be well described by an eastward offset hot spot. We do not find significant evidence for a relative blue-shift pre-eclipse compared to post-eclipse that would further indicate eastward hot spot. Such net Doppler shifts are predicted of $\sim$1-3 km/s as the hot spot rotates in and out of the observers view over while orbiting its host star (*Zhang*...
et al. 2017). However, our velocity sampling is ~4–6 km/s for the best self-consistent PHOENIX model for the individual observing nights. Thus we cannot resolve such Doppler shifts at our spectral resolution. We note that when including all orbital phases out to quadrature in the post-eclipse night, the scaling parameter prefers shallower lines (see grey contours in Fig. 10), despite the strong line contrasts shown in Fig. 14. While these later phases give only a small addition to the overall S/N, the change in line contrast may be explained by missing physics in the GCM e.g. clouds close to quadrature phases that flatten out the continuum, reducing the overall line contrast.

We further find a systematic bias towards small scaling parameter \( \log_{10} a < 0 \) in all models. Rather than missing physics, we consider that the data cleaning steps of the HRCCS can affect the line shape and strength of planetary signal. PCA likely degrades more of the planetary signal at lower resolution, where the lines spread across multiple pixels. Applying PCA to our template in every iteration of our CC-to-log(L) PyMULTINEST implementation is computationally expensive. As an alternative, we investigated these effects by injecting the model at \( a = 1 \) into the frames observed during the eclipse of WASP-33 b. We still found a bias towards \( a \)-values < 1 for the recovered signals, albeit much closer to one. This result supports our hypothesis that our data cleaning steps cause at least part of the bias towards lower scale factors. Given that we apply the data processing in a homogeneous way to all data sets, and while we do not give large weight to the absolute values of \( \log(a) \), we still give weight to the interpretation of the relative differences. Novel new model-filtering techniques such as the one introduced by Gibson et al. (2022) may alleviate these issues in future work.

### 5.4 Low resolution limit for HRCCS technique

For the HRCCS technique in the photon-limited regime, to first order the S/N is given by:

\[
\frac{S}{N}_{\text{planet}} = \left( \frac{S_p}{S_*} \right) \frac{S/N_{\text{star}}}{\sqrt{N_{\text{lines}}}},
\]

where \( \frac{S_p}{S_*} \) is the planet-to-star contrast ratio, \( S/N_{\text{star}} \) the stellar S/N-ratio, and \( N_{\text{lines}} \) the number of spectral lines resolved (Snellen et al. 2015; Birkby 2018). For the close-in UHJs, we cannot be aided by High Contrast Imaging to spatially resolve the exoplanet and increase our planet-to-star contrast ratio. We thus rely solely on disentangling the exoplanet’s lines from its Doppler shift induced by its orbital motion. We can thus increase our exoplanet’s S/N in two ways: Firstly, we can increasing our photon collecting power such that \( S/N_{\text{star}} \) increases or secondly increase the total number of spectral lines observed by either expanding our instantaneous wavelength coverage or our spectral resolving power.

Since S/N is proportional to \( \sqrt{N_{\text{lines}}} \) it is crucial to have a sufficiently high spectral resolution to resolve more lines. Conservatively, Birkby (2018) placed a lower limit of \( R = 25,000 \) on the use of the HRCCS method based on the detection of water vapour in the atmosphere of \( \tau \) Boo with pre-upgraded NIRSPEC1.0/Keck combination reported by (Lockwood et al. 2014). Other evidence for a detection of the thermal spectrum of HD 88133 b, also with NIRSPEC1.0/Keck was reported by Piskorz et al. (2016) using a multi-epoch approach, but later on disputed (Buzard et al. 2021). Our detection with ARIES/MMT pushes this to a lower limit at \( R = 14,000 \) = 16,000.

Our detection of WASP-33 b at this lower spectral resolution provides proof-of-concept HRCCS is still possible at lower resolving power given a sufficiently large orbital Doppler shift. Although less and diluted spectral lines are observed at a lower spectral resolution, more photons are collected per resolution element. Therefore one can trade off spectral resolving power for photon collecting power. This is particularly interesting for short period exoplanets where we do not need a high spectral resolving power to resolve their large orbital Doppler shifts. Examples include other UHJs (for example KELT-9b) or terrestrial lava worlds (for example CoRoT-7b) as both have orbital velocities of similar order of magnitude as WASP-33 b.

---

**Figure 14.** Line contrast (flux - mean(flux)) of a single CO line (2.314-2.316 \( \mu m \)) in the GCM phase-dependent model as function of orbital phase (\( \phi \)) coverage. The phase-dependent variations show shallower lines pre-eclipse compared to post-eclipse for symmetric phases around the secondary eclipse. This is due to a shallower average temperature gradient in the pre-eclipse phases compared to post-eclipse.
6 CONCLUSIONS

In this work we presented the first high resolution spectroscopy observations from the NIR spectrograph ARIES mounted behind the MMT targeting WASP-33b. We develop public pre-processing pipeline for ARIES to extract a spectral time series from the raw detector images. We use the HRCCS technique with PCA to characterise WASP-33b’s atmosphere using both the S/N-method and CC-to-log(L) mapping. The primary conclusions of this work are the following:

(i) We present the first robust detection (7.9σ) of CO emission lines using HRCCS in an exoplanet atmosphere. The detection of CO emission lines in the atmosphere of WASP-33 b is unambiguous evidence of an inverted P-T profile.

(ii) The best PHOENIX self-consistent atmospheric models prefer day-side-only heat redistribution.

(iii) The modified P-T structure PHOENIX models show we are sensitive to the temperature gradient of the inversion layer, but less sensitive to the absolute temperatures of the lower atmosphere.

(iv) The CC-to-log(L) mapping reveals a phase-dependent scaling factor, which shows that the planet spectral line contrast is greater just after secondary eclipse than before. We demonstrate that the P-T profiles from a GCM that includes an eastward offset hot spot can explain the majority of the phase-dependence in log(α). We emphasise that inclusion of a scaling parameter in the CC-to-log(L) mapping can reveal the longitudinal phase-dependent thermal structure of the atmosphere, even in spectra that lack the resolving power required to detect the additional induced Doppler shift caused by the offset hot spot.

(v) We find no evidence of stellar pulsations affecting our detection of CO, in contrast to previous detections of atomic emission lines in the optical. We advocate that CO is therefore an advantageous and good probe of the thermal atmospheric structure of UHJs at pressures seen with HRCCS.

(vi) At a measured resolving power of R ~ 15,000, this detection of CO in emission pushes the HRCCS technique to its lowest resolution limits when using only the large Doppler-shift induced by the exoplanet’s orbital motion to disentangle its spectrum from its host star and tellurics. Thus spectral resolving power can be traded for photon collecting power in cases where the induced orbital Doppler shift is sufficient move the planet spectrum over multiple pixels such as expected for close-in terrestrial lava planets and ultra hot Jupiters.

ARIES is currently being upgraded into the MMT: AO exoPlanet characterization System (MAPS)\(^\text{11}\). It will have an updated AO system, broader instantaneous wavelength coverage and modes at a higher spectral resolution. A modified version of the ARIES data reduction pipeline presented in this work may prove helpful in analysing future output from MAPS as well.

Finally, future low-resolution observations of WASP-33 b with the James Webb Space Telescope can be combined to with ground-based high-resolution observations to mitigate the effects of stellar pulsations and give tighter constraints on the P-T profile and chemical abundances of OH, H₂O, CO, and CO₂ (Beichman & Greene 2018). UHJ have the additional benefit that refractory elements can be measured as well (Lothringer et al. 2021). Combined this will enable calculation of abundance ratios which can in turn be used to constrain different planet formation pathways (e.g. Öberg et al. 2011; Madhusudhan 2012; Crisland et al. 2016, 2017, 2019; Khorshid et al. 2021). Finally, combining phase-dependent low resolution data, for example the recently observed diurnal variations in the atmosphere of WASP-121b (Mikal-Evans et al. 2022), and high resolution data using the CC-to-log(L) (Brogi et al. 2016a; Brogi & Line 2019; Gibson et al. 2020, e.g.) mapping will greatly improve our understanding of the longitudinal chemical and thermal phase-dependence.

ACKNOWLEDGEMENTS

JLB extends special thanks to all the MMT Observatory staff, particularly the telescope and AO operators, for their assistance and valuable advice in carrying out the MMT Exoplanet Atmosphere Survey. This research is part of the exoZoo project that has received funding from the European Research Council (ERC) under the European Union’s Horizon 2020 research and innovation program under grant agreement No 805445. Observations reported here were obtained at the MMT Observatory, a joint facility of the Smithsonian Institution and the University of Arizona. This work was performed in part under contract with the Jet Propulsion Laboratory (JPL) funded by NASA through the Sagan Fellowship Program executed by the NASA Exoplanet Science Institute.

DATA AVAILABILITY

All the original data will be made publicly available in the author’s Github repository.

REFERENCES

L. S., et al., 2009, J. Quant. Spectrosc. Radiative Transfer, 110, 533
Allard F., Homeier D., Freytag B., 2011, in Johns-Krull C., Browning M. K., West A. A., eds, Astronomical Society of the Pacific Conference Series Vol. 448, 16th Cambridge Workshop on Cool Stars, Stellar Systems, and the Sun. p. 91 (arXiv:1011.5405)
Arcangeli J., et al., 2018, ApJ, 855, L30
Armstrong D. J., de Mooij E., Barstow J., Osborn H. P., Blake J., Saniee N. F., 2016, Nature Astronomy, 1, 0004
Barber R., Tennyson J., Harris G., Tolchenov R., 2000, Monthly Notices of the Royal Astronomical Society, 368, 1087
Barber R. J., Strange J. K., Hill C., Polansky O. L., Mellau G. C., Yurchenko S. N., Tennyson J., 2014, MNARS, 437, 1828
Barnar T. S., Hauschildt P. H., Allard F., 2001, ApJ, 556, 885
Barman T. S., Macintosh B., Konopacky Q. M., Marois C., 2011, ApJ, 733, 85
Baxter C., et al., 2021, A&A, 648, A127
Beichman C. A., Greene T. P., 2018, Observing Exoplanets with the James Webb Space Telescope. Springer International Publishing. p. 85, doi:10.1007/978-3-319-55333-7_85
Bell T. J., et al., 2019, MNARS, 489, 1995
Birkby J. L., 2018, arXiv e-prints, p. arXiv:1806.04617
Borsa F., et al., 2021, A&A, 653, A104
Brahm R., Jordán A., Espinoza N., 2017, PASP, 129, 034002
Brogi M., Line M. R., 2019, AJ, 157, 114
Brogi M., Snellen I. A. G., de Kok R. J., Albrecht S., Birkby J., de Mooij E. W., 2012, Nature, 486, 502
Brogi M., de Kok R. J., Birkby J. L., Schwarz H., Snellen I. A. G., 2014, A&A, 565, A124
Brogi M., Line M., Bean J., Desert J.-M., Schwarz H., 2016a, preprint, (arXiv:1612.07008)
Buchner J., et al., 2014a, A&A, 564, A125
Buchner J., et al., 2014b, A&A, 564, A125

\(^{11}\) More information can be found here: https://www.as.arizona.edu/~ktmorz/maps.html

MNRAS 000, 1–19 (2022)
CO emission lines reveal an inverted atmosphere in the UHJ WASP-33 b and indicate an eastward hot spot

Serindag D. B., Nugroho S. K., Mollière P., de Mooij E. J. W., Gibson N. P., Snellen I. A. G., 2021, A&A, 645, A90
Sheppard K. B., Mandell A. M., Tamburo P., Gandhi S., Pinhas A., Madhusudhan N., Deming D., 2017, ApJ, 850, L32
Showman A. P., Guillot T., 2002, A&A, 385, 166
Showman A. P., Polvani L. M., 2011, ApJ, 738, 71
Showman A. P., Fortney J. J., Lian Y., Marley M. S., Freedman R. S., Knutson H. A., Charbonneau D., 2009, ApJ, 699, 564
Showman A. P., Tan X., Parmentier V., 2020, Space Sci. Rev., 216, 139
Smith A. M. S., Anderson D. R., Skillen I., Collier Cameron A., Smalley B., 2011, MNRAS, 416, 2096
Snellen I. A. G., de Kok R. J., de Mooij E. J. W., Albrecht S., 2010, Nature, 465, 1049
Snellen I., et al., 2015, A&A, 576, A59
Spring E. F., et al., 2022, arXiv e-prints, p. arXiv:2201.03600
Stone J. M., Eisner J. A., Salyk C., Kulesa C., McCarthy D., 2014, ApJ, 792, 56
Swain M. R., Vasisht G., Tinetti G., Bouwman J., Chen P., Yung Y., Deming D., Deroo P., 2009, ApJ, 690, L114
Tan X., Komacek T. D., 2019, ApJ, 886, 26
Temple L. Y., et al., 2017, MNRAS, 471, 2743
Visscher C., Lodders K., Fegley Bruce J., 2010, ApJ, 716, 1060
Wilks S. S., 1938, The Annals of Mathematical Statistics, 9, 60
Wong I., et al., 2016, ApJ, 823, 122
Wright J. T., Eastman J. D., 2014, PASP, 126, 838
Yan F., et al., 2019, A&A, 632, A69
Yan F., et al., 2020, A&A, 640, L5
Yan F., et al., 2021, A&A, 645, A22
Yurchenko S. N., Mellor T. M., Freedman R. S., Tennyson J., 2020, MNRAS, 496, 5282
Zhang J., Kerzhenet E. M. R., Rauscher E., 2017, ApJ, 851, 84
Zhang M., et al., 2018, AJ, 155, 83
Zucker S., 2003, MNRAS, 342, 1291
de Kok R. J., Brogi M., Snellen I. A. G., Birkby J., Albrecht S., de Mooij E. J. W., 2013, A&A, 554, A82
de Mooij E. J. W., Brogi M., de Kok R. J., Snellen I. A. G., Kenworthy M. A., Karjalainen R., 2013, A&A, 550, A54
van Sluijs L., et al., 2019, A&A, 626, A97
von Essen C., Mallonn M., Welbanks L., Madhusudhan N., Pinhas A., Bouy H., Weis Hansen P., 2019, A&A, 622, A71
von Essen C., Mallonn M., Borre C. C., Antoci V., Stassun K. G., Khalafinejad S., Tautvaišienė G., 2020, A&A, 639, A34

APPENDIX A: ADDITIONAL TABLES AND FIGURES

For transparency, completeness and reproducibility of this work, we include some additional figures and tables here.

This paper has been typeset from a TeX/LaTeX file prepared by the author.
| Quantity                  | Value   | Unit   | Reference                                      |
|--------------------------|---------|--------|-----------------------------------------------|
| Stellar mass             | 1.495   | M⊙     | Collier Cameron et al. (2010)                 |
| Stellar effective temperature | 7400    | K      | Collier Cameron et al. (2010)                 |
| Stellar radius           | 1.444   | R⊙     | Collier Cameron et al. (2010)                 |
| Primary transit time     | 2454590.17936 | BJD | Smith et al. (2011)                           |
| Eccentricity             | 0.0     | -      | Smith et al. (2011)                           |
| Semi-major axis          | 0.02558 | au     | Smith et al. (2011)                           |
| Orbital period           | 1.21986967 | days | Smith et al. (2011)                           |
| Orbital inclination      | 87.7    | degree | Lehmann et al. (2015)                         |
| Planetary radius         | 1.603   | R_Jup  | Lehmann et al. (2015)                         |
| Impact parameter         | 0.21    | -      | Chakrabarty & Sengupta (2019)                 |
| Expected system velocity | -0.3    | km/s   | Nugroho et al. (2020b)                        |
| Expected orbital velocity| 230.9   | km/s   | Nugroho et al. (2020b)                        |

Table A1. An overview of relevant WASP-33 system parameters used in this work.

Figure A1. Mixing ratios in chemical equilibrium as functions of pressure for different species in the self-consistent PHOENIX model atmospheres of WASP-33 b. This is for the day-side-only heat redistribution model $f = 0.5$ at $\times1$ Solar metallicity.
Figure A2. Overview of all modified PHOENIX P-T structures explored in this work.
Figure A3. Similar to Fig. 7, but for the highest SNR PHOENIX self-consistent model, GCM day-side-only model (middle panel) and GCM phase-dependent model (bottom panel).
CO emission lines reveal an inverted atmosphere in the UHJ WASP-33 b and indicate an eastward hot spot

**Figure A4.** Same as Fig. 9 but shown for the best PHOENIX self-consistent model (top row), best GCM day-side-only model (bottom row).

**Figure A5.** Similar to Fig. 9, but for the PHOENIX modified P-T structure models with all opacity sources included except CO. The detection of $5.7\sigma$ for the first night suggests we are still sensitive to some of the other opacity sources in the atmosphere of WASP-33 b.
Figure A6. Similar to Fig. 9, but for the GCM day-side-only templates with respectively: all opacity sources, only CO, only H$_2$O and only OH included. Amongst the opacity sources, CO is the only molecule that is robustly detected at 6.6$\sigma$.

Figure A7. Same as the panels in Fig. 10, but results shown for the GCM day-side-only models for different opacity sources included. All results are shown for all nights combined.