Dayside Fe I Emission, Day–Night Brightness Contrast and Phase Offset of the Exoplanet WASP-33b

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Received 2020 December 21; revised 2022 March 4; accepted 2022 March 18; published 2022 May 4

Abstract

We report on Fe I in the dayside atmosphere of the ultra-hot-Jupiter WASP-33b, providing evidence for a thermal inversion in the presence of an atomic species. We also introduce a new way to constrain the planet’s brightness variation throughout its orbit, including its day–night contrast and peak phase offset, using high-resolution Doppler spectroscopy alone. We do so by analyzing high-resolution optical spectra of six arcs of the planet’s phase curve, using Echelle SpectroPolarimetric Device for the Observation of Stars (ESPaDOnS) on the Canada–France–Hawaii telescope and High Dispersion Spectrograph on the Subaru telescope. By employing a likelihood mapping technique, we explore the marginalized distributions of parameterized atmospheric models, and detect Fe I emission at high significance (>10σ) in our combined data sets, located at $K_p = 222.1 \pm 0.4 \text{ km s}^{-1}$ and $\nu_{\text{envelope}} = -6.5 \pm 0.3 \text{ km s}^{-1}$. Our values agree with previous reports. By accounting for WASP-33b’s brightness variation, we find evidence that its nightside flux is <10% of the dayside flux and the emission peak is shifted westward of the substellar point, assuming the spectrum is dominated by Fe I. Our ESPaDOnS data, which cover phases before and after the secondary eclipse more evenly, weakly constrain the phase offset to $+22 \pm 12$ degrees. We caution that the derived volume-mixing ratio depends on our choice of temperature-pressure-profile, but note it does not significantly influence our constraints on day–night contrast or phase offset. Finally, we use simulations to illustrate how observations with increased phase coverage and higher signal-to-noise ratios can improve these constraints, showcasing the expanding capabilities of high-resolution Doppler spectroscopy.

Unified Astronomy Thesaurus concepts: Astronomy data analysis (1858); Exoplanet atmospheres (487); High resolution spectroscopy (2096); Hot Jupiters (753); Exoplanet atmospheric composition (2021); Exoplanets (498); Extrasolar gaseous giant planets (509)

1. Introduction

Our ability to probe the atmospheric properties and compositions of exoplanets has progressed rapidly in the last decade, as the relatively young field of exoplanet observation has shifted from an era of discovery to one focusing on characterization. Perhaps the most exciting advance in atmospheric characterization has been the development of high-resolution Doppler spectroscopy (e.g., Snellen et al. 2010; Brogi et al. 2012; Rodler et al. 2012; Birkby et al. 2013). This has significantly improved our ability to detect exoplanet atmospheres using ground-based observations. High-resolution spectrographs allow individual atomic and molecular lines to be resolved, and the large Doppler shift of planetary lines (due to the orbital motion of close-in planets) allows us to disentangle the planetary signal from the relatively stable stellar lines and telluric absorption. By utilizing high-dispersion data and cross-correlation techniques with model templates, the signals from potentially thousands of resolved lines can be combined to boost the planetary signal.

One of the limiting factors in such characterization, however, is the immense brightness contrast between a planet and its host star, which can prevent any atmospheric emission from being detected. Focusing our attention on the hottest and largest planets known, namely hot Jupiters, improves our prospects.

Hot Jupiters are gas giants that orbit their host stars in a matter of days or even hours, with highly irradiated daysides as a result of tidal locking. Their extreme environment, paired with a planet’s chemical composition, can produce fascinating atmospheric structure, including a stratosphere. Hot Jupiters with effective temperatures $>1600 \text{ K}$ are expected to harbor such thermal inversions due to the presence of gaseous molecules with strong optical opacities, like TiO and VO (Hubeny et al. 2003; Burrows et al. 2007; Fortney et al. 2008). These molecules absorb incident stellar radiation, heating the upper atmosphere.

For hot Jupiters with $T_{\text{eff}} > 2500 \text{ K}$, however, most molecules dissociate and species such as TiO and VO are expected to be less abundant. Instead, other species such as atomic metals, metal hydrides, and H$^+$ opacity may be capable of absorbing enough irradiation to produce a thermal inversion (Lothringer et al. 2018). Neutral iron (Fe I) is of particular interest as a contributor to thermal inversions in ultrahot Jupiters. Below 3000 Å, bound-free transitions absorb high-energy irradiation, while bound-bound transitions absorb significantly above 3000 Å (Sharp & Burrows 2007). As a result, there is an extensive number of Fe I emission lines in the optical, and their detection can be used to directly determine
whether there is a thermal inversion in the planet’s atmosphere. Moreover, given that the abundance of iron is used as a proxy for stellar metallicity, a measurement of atmospheric Fe I could potentially lead to a comparison between planetary and stellar metallicities, though meaningful abundance measurements from observed volume-mixing ratios are difficult.

Only recently has Fe I been detected in the atmospheres of a handful of hot Jupiters. Using high-resolution spectroscopy, Fe I has been found in the transmission spectra of KELT-9b (Hoeijmakers et al. 2019), KELT-20b/MASCARA-2b (Nugroho et al. 2020b; Stangret et al. 2020; Hoeijmakers et al. 2020a), WASP-76b (Ehrenreich et al. 2020), and WASP-121b (Gibson et al. 2020; Cabot et al. 2020; Hoeijmakers et al. 2020b). Additionally, Fe I has been detected in emission from the dayside spectra of three ultrahot Jupiters, KELT-9b (Pino et al. 2020), WASP-33b (Nugroho et al. 2020a), and WASP-189b (Yan et al. 2020). These detections not only suggest that atomic species are common in ultra-hot-Jupiter atmospheres, but the latter emission detections provide direct evidence of thermal inversions in the absence of TiO or VO.

It is worth noting that, in some cases, reports of inversion layers have been debated in the literature. The first claim of a thermal inversion (HD 209458b, Knutson et al. 2008), for instance, was followed by a handful of discrepant results (Diamond-Lowe et al. 2014; Zellem et al. 2014; Schwarz et al. 2015). More recently, reports of a TiO-driven thermal inversion in WASP-33b (Haynes et al. 2015; Nugroho et al. 2017) have either been questioned (Herman et al. 2020) or could not be verified convincingly (von Essen et al. 2015; Serindag et al. 2021). The inconsistencies highlight the necessity of confirming reported detections through independent observation and analysis. We therefore perform an independent search for Fe I emission in the dayside of this ultrahot Jupiter.

1.1. WASP-33b

WASP-33b (Collier Cameron et al. 2010) is an ideal target for atmospheric characterization via high-resolution spectroscopy (HRS), given its incredibly high equilibrium temperature (>3100 K; Smith et al. 2011; de Mooij et al. 2013; Haynes et al. 2015; Zhang et al. 2018; von Essen et al. 2020) and inflated radius (∼1.6 R J; Chakrabarty & Sengupta 2019). The planet orbits its host star with a period of ∼1.22 days. WASP-33, a fast-rotating δ-Scuti A5 star, is also well-suited for HRS due to its brightness (V = 8.14), though its pulsating nature can introduce complications in the analysis (e.g., Nugroho et al. 2020a).

As mentioned, conflicting results have been found regarding a thermal inversion in WASP-33b when analyzing various data sets in different ways. Haynes et al. (2015) first reported evidence of a stratosphere using combined low-resolution transmission data from WFC3/HST and Spitzer, though von Essen et al. (2015) could not rule out an atmospheric model with no inversion based on optical and NIR photometry of the secondary eclipse. Nugroho et al. (2017) used HRS to identify TiO in WASP-33b’s dayside emission, indicative of a thermal inversion, but this detection was not corroborated by Herman et al. (2020), who used HRS to observe the planet in both transmission and emission. Serindag et al. (2021) also reassessed the TiO detection using the original data set of Nugroho et al. (2017) and an alternative line list, and found ambiguous results; they report a slightly weaker TiO signal that is unusually offset in both K p and v sys, shedding more doubt on the detection. Recently, Nugroho et al. (2020a) used their same dayside observations to identify a thermal inversion based on Fe I emission, reporting a 6.4σ signal with K p = 226 km s −1 and v sys = −3.2 km s −1.

In this work, we present confirmation of Fe I emission from multiple dayside observations of WASP-33b using high-resolution Doppler spectroscopy. In Sections 2, 3, and 4, we outline our observations, basic data reductions, and atmospheric emission models, respectively. In Section 5, we describe our search for Fe I using the standard Doppler cross-correlation method, as well as a likelihood-based approach to extract the best-fitting model parameters and their uncertainties. By introducing a brightness variation to this likelihood analysis, we are able to investigate the planet’s day–night contrast and peak phase offset with high-resolution spectra for the very first time. In Section 6 we present our results, including our measurements of the day–night contrast and phase offset, and discuss their implications. In Section 7 we perform the same analysis on simulated spectra to explore the benefits of higher signal-to-noise observations with greater phase coverage. We end with our concluding remarks in Section 8. The included Appendix provides additional details of our model filtering and plots from our likelihood analyses.

2. Observations

We observed WASP-33b on six separate occasions between 2013 and 2015, using two high-resolution spectrographs. In Figure 1 we show the orbital phases spanned by these observations, and below we summarize the parameters for each instrument. Table 1 provides additional details for individual nights.

2.1. ESPaDOnS on CFHT

Five observations of the dayside of WASP-33b were performed using the Echelle SpectroPolarimetric Device for
the Observation of Stars (ESPaDOnS; Donati 2003) on the Canada–France–Hawaii Telescope (CFHT) between September 2013 and November 2014. These data have been previously presented in Herman et al. (2020) and we refer the reader to this work for complete details. To summarize, the data were taken during Queued Service Observing using the “Star+Sky” mode, achieving a resolution of \( \sim 68,000 \). We chose an exposure time of 90 s for all nights, with the total number of exposures varying between nights due to weather, observability, and time constraints. Details are given in Table 1. The observations cover the 3697–10480 Å wavelength range across 40 orders.

2.2. HDS on Subaru

A single observation of the dayside of WASP-33b was performed using the High Dispersion Spectrograph (HDS; Noguchi et al. 2002) on the Subaru telescope on 26 October 2015. These data have previously been presented in Nugroho et al. (2017) and Nugroho et al. (2020a), and we refer the reader to these works for complete details. To summarize, the observations used Image Slicer 3 (Tajitsu et al. 2012) to achieve a spectral resolution of \( \sim 165,000 \), and an exposure time of 600 s with a total of 52 exposures. The observations cover the 6170–8817 Å wavelength range across 30 orders, with a gap from 7402–7537 Å between the blue and red CCD (containing 18 and 12 orders, respectively).

3. Data Reduction

Since our data sets have been previously published, here we provide only an overview of our data reduction procedure. We use the reduced data from HDS (see Nugroho et al. 2017) and the pipeline-reduced data from ESPaDOnS (see Herman et al. 2020). We follow the same procedure for both data sets, as in Herman et al. (2020). For each spectral order, we first apply sigma clipping to mask outliers three times above the standard deviation of each time series. We then correct for the instrument’s blaze response, which is a grating-dependent variation in brightness over time. It also includes other wavelength-dependent effects, such as wavelength-dependent absorption and slit losses. To correct this, we divide each frame by a reference frame (the first frame of the night), bin the frame by 200 pixels, and fit the result with a second-order polynomial, which is then divided out from the full frame. Lastly, we align the extracted spectra to a common wavelength grid in the telluric rest frame by fitting a Gaussian to a spectral line in the \( \text{O}_2 \) \( \gamma \)-band (\( \sim 6300 \) Å) for each frame, and shift the spectra to match the wavelength of our reference frame.

3.1. Removal of Stellar and Telluric Lines

To remove stellar and telluric features from our spectra, we apply the SYSREM algorithm (Tamuz et al. 2005), which has become a standard technique for high-resolution spectroscopy (e.g., Deibert et al. 2019; Gibson et al. 2020; Nugroho et al. 2020a; Herman et al. 2020; Turner et al. 2020). For low numbers of SYSREM iterations, the planetary signal will not be strongly affected as the planet’s radial velocity changes rapidly over the course of the observations, while the stellar and telluric lines remain relatively stable over time.

We use the same SYSREM application as in Herman et al. (2020), performing the iterations on each spectral order separately after converting the flux to magnitudes. For the ESPaDOnS data, we use the pipeline error bars as estimates for the uncertainties, while for the HDS data we use the photon noise. We initially perform 10 iterations on both data sets, and identify the optimal number of iterations for each night by considering the rms of the data. Generally, after 4–6 iterations the rms values in all orders have leveled off and do not decrease noticeably with additional iterations. We list the number of iterations used for each night in Table 1. For our cross-correlation analysis, we convert the detrended data back to flux, and subtract a value of one. An example of the full data reduction process applied to a single spectral order is shown in Figure 2. Note that as in Herman et al. (2020), we exclude the first and last three orders of our ESPaDOnS spectra from the following analysis due to a significant reduction in signal-to-noise ratio at these extremes of the wavelength range.

4. Atmospheric Emission Models

4.1. Generating Models

We use the same model emission spectra as Nugroho et al. (2020a), which are available upon request. Here we provide an overview of the models, and direct the reader to Nugroho et al. (2020a) for complete details.

We model the planetary emission spectra assuming a 1D plane-parallel hydrostatic atmosphere, calculated across 70 pressure layers. We adopt the physical planet parameters from Kovács et al. (2013), where \( R_p = 1.679 \) \( R_J \) and \( M_p = 3.27 M_J \). We then calculate the temperature-pressure (T-P) profile using Equation (29) of Guillot (2010), with an intrinsic temperature of 100 K, an equilibrium temperature of 3100 K, a ratio of the mean visible opacity to the mean infrared opacity, \( \gamma \), of 2, and a mean infrared opacity of 0.01 cm\(^2\) g\(^{-1}\) (e.g., assuming the infrared regime is dominated by H\(^+\) opacity). We determine the cross-section of Fe I using HELIOS-K (Grimm & Heng 2015) assuming a Voigt profile with natural and thermal broadening, and a line wing cut off of \( 10^8 \) times the Lorentz line width.
reduced spectra. We implement the high-pass Butterworth filter to the models.7 This is meant to resemble the effect that SYSREM has on the planetary spectral lines within the data, whereby the continuum and some of the line signal is lost in the process of removing stellar and telluric lines (Section 3.1). As each night of observations experienced different conditions and therefore requires a different number of SYSREM iterations, the parameters of the Butterworth filter applied to the models necessarily change as well. We discuss how these parameters are determined in Appendix A.

The final planetary spectrum model gives the line contrast relative to the stellar continuum, and this can then be interpolated to the wavelength grid of the data in the following cross-correlation steps.

5. Analysis

We conduct a search for Fe I emission from the dayside of WASP-33b by first pre-processing our data with SYSREM, as discussed in Section 3.1, then performing the following Doppler cross-correlation.

5.1. Doppler Cross-correlation

Since our Fe I models contain numerous resolved emission lines, cross-correlating our emission spectra with these models allows the signal from many spectral lines to be combined, increasing the significance of the detection. To perform this cross-correlation, each model is Doppler shifted in steps of 1 km s\(^{-1}\) from -600 km s\(^{-1}\) to +600 km s\(^{-1}\), interpolated onto the same wavelength grid as the data, and then multiplied by our residual spectra, where each data point is weighted by its variance. We then sum over all wavelengths to produce a cross-correlation function (CCF) dependent on both time and velocity. This process is repeated for each spectral order separately, and all orders are then summed together.

We then shift this CCF to the rest frame of the planet, where the planet’s radial velocity at a given orbital phase \(\phi\) (assuming a circular orbit) can be expressed as:

\[
RV = K_p \sin(2\pi \phi) + \nu_{\text{sys}} + \nu_{\text{bary}}.
\]

6 Kp is the orbital velocity of the planet, \(\nu_{\text{sys}}\) is the systemic velocity of the star-planet system, and \(\nu_{\text{bary}}\) is the barycentric correction. We assume a range of orbital and systemic velocities, for a \(K_p\) of 175 to 325 km s\(^{-1}\) and a \(\nu_{\text{sys}}\) of -150 to +350 km s\(^{-1}\), both in steps of 0.25 km s\(^{-1}\). After each frame of the CCF has been shifted to the planet’s rest frame via linear interpolation, the CCF is summed over time. This produces a
$K_p-\nu_{sys}$ map for each night of observation, which can then be summed together.

However, our CCFs are noticeably impacted by the pulsating nature of the host star WASP-33, which is a δ-Scuti variable. These pulsations cause the stellar line profiles to become distorted as a function of time, and since Fe I is also present in the stellar spectrum, cross-correlating with an Fe I model produces an unwanted stellar signal in addition to any planetary signal. If this pulsation signal is included in the summation of the CCF over time, it can produce a signal that could be mistaken for a planetary detection. Luckily, the pulsations are limited to a smaller velocity range in our CCFs than the expected planetary signal at most orbital phases. The stellar and planetary signals in the CCF only begin to overlap near secondary eclipse (and transit), meaning the pulsations can be avoided by limiting the phase range included in our summation over time. We therefore follow the example of Nugroho et al. (2020a), only summing up the CCFs outside of the phase range 0.41 to 0.59.

After this procedure, a clear peak at the expected orbital and systemic velocities can be seen in the resulting $K_p-\nu_{sys}$ map. We may estimate the signal-to-noise ratio (S/N) by dividing this map by its standard deviation, which is calculated by excluding the region $K_p < 275$ km s$^{-1}$ and $\nu_{sys} < +50$ km s$^{-1}$ so as to avoid the planetary signal. As noted by Gibson et al. (2020), this S/N can provide only a rough estimate of the detection significance, as the exact significance will vary slightly, depending on the chosen noise region.

We therefore provide a second estimate of the S/N following the method used in Herman et al. (2020). For each night, we randomly assign a frame to each phase value, then perform the cross-correlation and summation over time. We repeat this procedure 10,000 times, and use the 15.9 and 84.1 percentiles of the resulting distribution to estimate the noise. The strength of the detected signal can then be compared to this to estimate the S/N.

5.2. Likelihood Mapping and Brightness Variation

In addition to cross-correlating our spectra with atmospheric models using the standard approach introduced by Snellen et al. (2010), we also compute the likelihood map, following the approach of Brogi & Line (2019) and Gibson et al. (2020). The latter allows different models to be explored and compared using principled statistical techniques, and can be calculated directly from the cross-correlation map without repeatedly performing the cross-correlation. We employ the generalized form of the likelihood map from Gibson et al. (2020), which is derived using a similar approach to Brogi & Line (2019), but accounting for both time- and wavelength-dependent uncertainties:

$$\ln L = -\frac{N}{2} \ln \frac{\chi^2}{N}$$

where $L$ is the likelihood, $N$ is the total number of data points, and $\chi^2$ is given by

$$\chi^2 = \sum \frac{f_i^2}{\sigma_i^2} + A_p(\phi)^2 \sum \frac{m_i^2}{\sigma_i^2} - 2A_p(\phi) \text{CCF}.$$  

As in the CCF, each sum is performed over wavelength. Here $f_i$ is the mean-subtracted spectrum; $\sigma_i$ is the outer product of the standard deviation of each wavelength and exposure bin, normalized by the standard deviation of the spectra in each order; $m_i$ is the mean-subtracted, Doppler-shifted model; and $A_p(\phi)$ is a phase-dependent term we introduce to account for the planet’s brightness variation throughout the observations, assuming the planetary emission spectrum is dominated by Fe I lines. This takes the form:

$$A_p(\phi) = \alpha (1 - C \cos^2(\pi (\phi - \theta))),$$

where $\alpha$ is an overall scale factor to determine the strength of the planetary signal relative to the model (i.e., to account for any uncertainty in the scale of the model); $C$ is the day-night contrast in the form $1-\left(\frac{F_d}{F_n}\right)$, where $F_i$ is the observed planetary Fe I line emission from the day/nightside measured over the wavelength range of our observations; and $\theta$ is the phase offset of the peak brightness amplitude. Note that the day-night contrast is a bounded parameter limited to values between zero and one, and the phase offset is defined such that a positive offset corresponds to a peak occurring after secondary eclipse.

We recognize that Equation (4) may not perfectly match the planet’s true brightness variation, and note that more complex models could be explored in the future (e.g., Cowan & Agol 2011). We chose this simpler representation largely as a proof of concept: by introducing this variable brightness term, we may shed light on energy recirculation within the planet’s atmosphere. These sorts of parameters have typically only been accessible through photometric phase-curve measurements (e.g., Esteves et al. 2015; Zhang et al. 2018; von Essen et al. 2020), but we show that they can be constrained using high-resolution Doppler spectroscopy as well.

We note, however, that we are specifically constraining the phase offset and day-night contrast of the Fe I signal, which we assume is the dominant emission source over our wavelength range. While this dependence on Fe I may seem like a limitation, it actually demonstrates the power of this technique: by targeting chemical species with different opacities, we may reveal variations in the phase offset and day-night contrast for different molecules/atoms, exploring the atmospheric dynamics at play at different pressure levels. This has a significant advantage over low-resolution spectroscopy, since we will be far less affected by overlapping spectral features, and in the case of WASP-33b, we can minimize the impact of stellar pulsations. We also note that the day-night contrast will predominantly be driven by the change in temperature in the region probed by the Fe I emission lines—since we are operating in the Wien limit, a small change in temperature can significantly impact the flux. The contrast could also be affected by high-temperature cloud coverage, if any, and the condensation of Fe. Of course, a detailed interpretation of $C$ would need to take into account a variable lapse rate as a function of position on the planet. The model we are using is equivalent to many photometric phase-curves, where mostly uniform dayside and nightside brightness are assumed, and the variation is caused by the amount of dayside and nightside visible.

Returning to the likelihood mapping, we note that unlike the standard definition of the CCF, the CCF in Equation (2) is not weighted/normalized. As Brogi & Line (2019) point out, weighting the CCF is no longer required here, as the likelihood contains the data and model variances and thus intrinsically takes the variable S/N of the observations into account.
We compute the log likelihood for $\alpha$ values of 0.5–5 in steps of 0.05, day–night contrasts of 0–1 in steps of 0.05, and phase offsets of $-30^\circ$ to $+60^\circ$ in steps of $1^\circ$. To do so, the second and third terms in Equation (3) are shifted to the rest frame of the planet (assuming a range of velocities as is done for the CCF), then all terms in Equation (3) are added before summing over time and inserting the result into Equation (2). We note that when calculating the log likelihood for each order, $N$ should be equal to the number of pixels multiplied by the number of exposures. The value of $N$ can differ between orders and nights, and if it is not properly computed, the reduced $\chi^2$ will not be correct, which can impact the resulting best-fit values.

After computing the log likelihood for each spectral order, we take the sum over all orders and all nights. The result is a six-dimensional log likelihood map, dependent on log$_{10}$VMR, $K_p$, $v_{\text{sys}}$, $\alpha$, $C$, and $\theta$. To produce the likelihood map from this log likelihood, we first subtract the global maximum, which occurs at the expected $K_p$, and $v_{\text{sys}}$; this is equivalent to normalizing the maximum likelihood to one. We then compute the exponential.

This likelihood mapping technique has the advantage over standard CCF maps in that we are now able to directly compare a range of models, and extract the best-fit parameters and their uncertainties. This can be done by exploring slices of the likelihood map (2D conditional distributions) or sums over various parameters (1D marginalized distributions). To estimate the significance of a detection using this method, we determine the median value of the marginalized likelihood of $\alpha$ and divide by its standard deviation.

### 6. Results and Discussion

We perform the cross-correlation and likelihood mapping described above for our two data sets (ESPaDOnS and HDS), and consider both the separate and combined results. In all cases, we detect dayside Fe I emission at a high significance, confirming the signal reported by Nugroho et al. (2020a). We discuss the details of our constraints in Section 6.2, but first describe the limitations of our analysis below.

#### 6.1. Dependence of Fe I Emission on Wavelength

Interestingly, we find that if spectral orders blueward of $\sim6000$ Å are included in our analysis of the ESPaDOnS data, the Fe I signal is not detectable at a significant level. This has a relatively straightforward explanation: below this wavelength, the line contrast is simply too low to be detected, even with multiple observations combined.

In addition, at the bluest wavelengths our observations are further from the peak of the planet’s emission spectrum, meaning even a small change in the temperature of our model could have quite a significant impact on the detected signal. Any underestimation of scattering processes in the atmosphere would also preferentially affect bluer wavelengths.

We verified this low line contrast explanation with simulated data, in which we injected a model with log$_{10}$VMR = $-3$ and no brightness variation into pure white noise, with the same standard deviation, wavelength range, and phase range as that of each order in the reduced spectra for our first night of ESPaDOnS observations. We Doppler shift the model to the planet’s velocity in each frame, interpolate to the wavelength grid of ESPaDOnS, and multiply the model in via: white noise $\times(1 + F_p/F_3)$. We then cross-correlated this simulated data with the same model, following the procedure of Section 5.1 for each order. Finally, we compared the S/N of all blue orders combined ($\lesssim6000$ Å) and all red orders combined ($\gtrsim6000$ Å).

We found that the S/N of the injected signal in the blue orders was nearly an order of magnitude lower than that in the red orders. This result confirms that the line contrast at bluer wavelengths is simply too low relative to the noise in the ESPaDOnS spectra to produce any significant detection. By including these orders where the line contrast is below the detection limit, we are adding noise to the overall signal when all orders are combined. We therefore exclude the orders below $\sim6000$ Å (orders 1–24) in the cross-correlation and likelihood mapping results presented below. The HDS observations only span wavelengths of 6170–8817 Å, meaning these data are less affected by the decreased line contrast at bluer wavelengths.

This cutoff choice of 6000 Å is largely a balance between the number of Fe I lines available and our wavelength coverage, since eventually the loss of additional lines will instead reduce the significance of our detection. As well, this limit allows us to match the blue ends between HDS and ESPaDOnS. In Section 6.3 we return to this discussion of loss of signal at blue wavelengths, exploring the impact of an alternative temperature structure for our atmospheric models.

| Data Set | Parameter | T-P Profile 1 | T-P Profile 2 |
|----------|-----------|---------------|---------------|
| ESPaDOnS | $K_p$ (km s$^{-1}$) | 224.1$_{-0.5}^{+0.6}$ | 224.0 $\pm$ 0.5 |
|          | $v_{\text{sys}}$ (km s$^{-1}$) | $-5.0 \pm 0.4$ | $-4.6 \pm 0.4$ |
|          | $C$       | $>0.90$       | $>0.90$       |
|          | $\theta$ ($^\circ$) | $+22 \pm 12$ | $+18 \pm 10$ |
|          | log$_{10}$VMR | $-4.1 \pm 0.2$ | $-5.3 \pm 0.2$ |
|          | $\alpha$  | $3.1_{-0.4}^{+0.3}$ | $1.0 \pm 0.1$ |
|          | Significance ($\sigma$) | $>9.1$ | $>9.8$ |
| HDS      | $K_p$ (km s$^{-1}$) | 223.8 $\pm$ 3.4 | 224.6 $\pm 2.3$ |
|          | $v_{\text{sys}}$ (km s$^{-1}$) | $-4.1 \pm 2.4$ | $-5.7_{-1.6}^{+1.1}$ |
|          | $C$       | $>0.97$       | $>0.97$       |
|          | $\theta$ ($^\circ$) | $+44 \pm 6$ | $+40 \pm 6$ |
|          | log$_{10}$VMR | $-4.2 \pm 0.2$ | $-5.2 \pm 0.2$ |
|          | $\alpha$  | $3.6_{-0.4}^{+0.3}$ | $1.1 \pm 0.2$ |
|          | Significance ($\sigma$) | $>8.9$ | $>7.6$ |
| Combined | $K_p$ (km s$^{-1}$) | 222.1 $\pm$ 0.4 | 222.1$^{+0.4}_{-0.5}$ |
|          | $v_{\text{sys}}$ (km s$^{-1}$) | $-6.5 \pm 0.3$ | $-5.9 \pm 0.3$ |
|          | $C$       | $>0.97$       | $>0.97$       |
|          | $\theta$ ($^\circ$) | $+42 \pm 6$ | $+38 \pm 6$ |
|          | log$_{10}$VMR | $-4.1 \pm 0.2$ | $-5.4 \pm 0.1$ |
|          | $\alpha$  | $3.1 \pm 0.3$ | $0.9 \pm 0.1$ |
|          | Significance ($\sigma$) | $>10.4$ | $>10.2$ |

**Table 2.** Results of the Likelihood Analysis

*Note.* We report the median value $\pm 1\sigma$ for the marginalized distributions, with the exception of $C$. For this parameter we report the lower limit, determined from the 84th percentile of the distribution.

$^a$ Due to the limited phase range of the HDS data, this value is likely biased and the uncertainties underestimated (see discussion in Section 7.2).
is bounded, we report only the lower limit, determined from the 84th percentile of the distribution. In the following subsections we discuss the results from the column labeled “T-P Profile 1,” which uses the atmospheric models described in Section 4. In Section 6.3 we describe the results from the column labeled “T-P Profile 2,” where we use models with an alternative temperature structure, for comparison. In Figure 4 we show both the marginalized and conditional distributions for our combined data with T-P Profile 1, and the same figures for the individual data sets can be found in Appendix B.

In Figure 5 we show the $K_p - v_{sys}$ map for the same combined data. It displays the $S/N$ calculated from the standard deviation.
of the map, which is not the same as the significance calculated from the marginalized distribution of the \( \alpha \) parameter. The former can only provide a rough estimate of the detection significance, as it will depend on which part of the map is used to calculate the standard deviation. We find a S/N of 9.0 based on our \( K_p - v_{\text{sys}} \) map, a S/N of 10.1 based on the phase scrambling method described in Section 5.1, and a significance of 10.4\( r \) based on the marginalized distribution of \( \alpha \). Thus we have made a strong detection of dayside FeI emission using both standard cross-correlation and likelihood mapping with a brightness variation term.

6.2.1. Velocity Constraints

In terms of the RV semiamplitude \( K_p \) and systemic velocity \( v_{\text{sys}} \), the values we report in Table 2 are in good agreement between the two data sets, and with previously reported values. We note that the HDS results have larger uncertainties than our ESPaDOnS observations because the latter cover both sides of the planet’s secondary eclipse, allowing for tighter constraints on velocities.

6.2.2. Day–Night Contrast

The lower limits we report for the day–night contrast are also sensible. The most recent phase curve measurements of WASP-33b from the Transiting Exoplanet Survey Satellite suggest a dayside temperature of 3014 K and nightside temperature of 1605 K (von Essen et al. 2020), while measurements with 3.6 \( \mu \)m Spitzer data find an average dayside temperature of 3114 K and nightside temperature of 1757 K (Zhang et al. 2018). To provide a simple estimate of the day–night contrast from these measurements based on our description below Equation (4), we integrate the Planck function in the Wien’s limit, evaluated over the wavelength range of our spectra.\(^8\) In both cases we arrive at a day–night contrast of \( C \approx 0.99 \). Based on the marginalized distribution of \( C \) shown in Figure 4, our data match this result quite well. We emphasize that constraints on bounded distributions are more difficult, however. Since \( C \) is hard bounded at 1, this will will bias recovered values away from 1. This is why we opt to report only the estimated lower limit of the day–night contrast. Even our more conservative lower limit from ESPaDOnS indicates that the nightside flux is at least 10 times less than that of the dayside flux in the wavelength range we consider, assuming FeI is the dominant emission source. In terms of temperature, this contrast of 0.9 indicates that the nightside of WASP-33b is \( \lesssim 2200 \) K, given that our atmospheric models assume a dayside temperature of 3100 K.

6.2.3. Phase Offset

Previous constraints of WASP-33b’s phase offset, on the other hand, have disagreed with each other significantly. von Essen et al. (2020) find a phase offset of \(+28\)°7 westward of the substellar point, which is at odds with the eastward offset of \(-12\)°8 reported by Zhang et al. (2018). von Essen et al. (2020) suggest that this discrepancy could be due to their analysis of systematics in the data, or the effect of the host star’s variability, which plagues the entirety of photometric observations. However, our likelihood analysis also indicates a slight preference for a westward phase offset. Since we exclude phases where the radial velocity of the planet is comparable to that of its host star, our analyses are not impacted by stellar pulsations.

Notably, our constraints on the phase offset differ considerably between the data sets we present. This can easily be explained by the limited phase coverage of our HDS observations. If the peak brightness occurs after the secondary eclipse, it is difficult to constrain the phase at which this peak occurs when observations are only made before the secondary eclipse. We therefore expect the ESPaDOnS observations, which cover both sides of the dayside phase curve, to more accurately constrain the phase offset. Indeed, our ESPaDOnS constraint of \( \theta = +22 \pm 12 \) degrees is comfortably within the uncertainty of the \(+28.7 \pm 7.1 \) degrees reported by von Essen et al. (2020), even though we do not directly observe the phase at which the peak brightness occurs.\(^9\) However, our uncertainty is large enough that our constraint is also within 2\( \sigma \) of zero offset, and is within 2.9\( \sigma \) of the eastward offset reported by Zhang et al. (2018). As mentioned previously, our constraint also assumes that FeI emission dominates the planetary flux in our considered wavelength range. We caution directly interpreting this offset as an offset only in the planet’s hot-spot location, as our observations are mainly sensitive to the contrast between the lines and the continuum, and so variations in abundance and T-P profile could move the location of the peak from the Fe emission away from the hottest point on the planet.

The constraint from our combined data sets is much closer to our constraint from HDS, because our HDS observations have a higher S/N (not to be confused with the detection S/N described in Section 5.1) than all five of our ESPaDOnS visits combined. We further explore the effect of phase coverage and S/N on our ability to constrain the phase offset and day–night contrast in Section 7.

6.2.4. FeI Abundance

Regarding the FeI abundance in \( \log^{10}_{\text{VMR}} \), our constraints are in good agreement with Nugroho et al. (2020a), as expected based on our shared models. These findings suggest that the FeI signal is in emission, as the planet’s atmosphere must experience a thermal inversion at the associated pressures (see Figure 4 of Nugroho et al. 2020a). As previously mentioned, this thermal inversion has been attributed to both FeI (Nugroho et al. 2020a) and TiO (Haynes et al. 2015; Nugroho et al. 2017), but given that TiO could not be detected by Herman et al. (2020) and its existence was debated by Serindag et al. (2021), we question whether both species could be responsible for the thermal inversion simultaneously. Moreover, the dayside atmosphere of WASP-33b may exceed the temperature at which TiO is thought to dissociate (\( T_{\text{eff}} > 2500 \) K), or at the very least be less abundant, based on the findings of Lothringer et al. (2018). We conclude that the high-significance detections of neutral atomic iron in all data sets presented here provide ample evidence for a thermally-inverted atmosphere in this ultrahot Jupiter, though we cannot definitively say that FeI is the cause of the thermal inversion without more detailed modeling.

\(^8\) This is a significant simplification, as the spectral response of the instrument is also wavelength dependent. However, integrating over the efficiency of the instrument is complicated, given that there are numerous overlapping orders in both ESPaDOnS and HDS.

\(^9\) A phase range of 0.41–0.59 would contain a peak with a phase offset between \(-32.4^\circ\) and \(+32.4^\circ\).
We also emphasize that there is a strong degeneracy between chemical abundance and lapse rate \((dT/d\log P; \text{Madhusudhan \\ & Seager 2009})\). An increase in lapse rate can be compensated for by a decrease in abundance, and vice versa, and so we caution against claims of absolute abundance. The abundance constraints we present here are only valid for the specific T-P profile we consider in our atmospheric models.

### 6.2.5. Line Contrast

The recovered \(\alpha\) value in all cases is higher than the constraint from Nugroho et al. (2020a), despite the fact that we use the same planetary emission models. This is because the previous work does not take into account the planet’s expected brightness variation as a function of phase, which decreases the line contrast at phases further from the secondary eclipse. Our constraints may also be higher due to the different filtering method we apply to our models (see Appendix A). Additionally, our constraints suggest a line contrast that is slightly higher than that expected based on the measured secondary eclipse depth from von Essen et al. (2020). However, the line contrast is wavelength-dependent (as mentioned in Section 6.1), meaning our scaling term may also have some wavelength dependence that we do not account for. Investigating the issue further is beyond the scope of the current paper, but it would be informative to explore a wavelength- or order-dependent \(\alpha\) parameter in future studies.

In any case, our constraints on \(\alpha\) still imply that our models have underestimated the strength of the line contrast, as in Nugroho et al. (2020a). There are a few possible explanations for this. Our shared models could have (1) overestimated the abundance of bound-free H, (2) underestimated the temperature of the atmosphere, or (3) underestimated the strength of the thermal inversion. In future works, it would be worthwhile to further investigate the temperature structure and continuum opacity by varying these parameters in our models, but for now we opt to vary only the VMR, since varying additional parameters is computationally expensive. Though the effect is limited, a variable VMR still allows us to probe different temperatures as the atmosphere becomes optically thick at different pressures.

### 6.3. Impact of T-P Profile

As a first step toward determining the impact of the temperature structure on our parameter constraints, we performed another analysis of our data using models with an increased stratospheric temperature. We did this by adjusting the ratio of the mean optical to infrared opacities substantially from 2 to 5.5. We present this second analysis to investigate the impact of the T-P profile on high-resolution spectroscopic observations.

By cross-correlating our data with models using this alternative T-P profile, we found that the Fe I signal was in fact detectable at blue wavelengths in the ESPaDOnS data. The increased stratospheric temperature produces a stronger temperature inversion, and as a result the line contrast of our model below 6000 Å increases, impacting the detected signal. This is in line with our explanation in Section 6.1. Therefore, in the following alternative analysis of our ESPaDOnS data, we include all wavelengths from 4000 to 9225 Å, only excluding the first and last four spectral orders due to noisy data at these outer edges (see Herman et al. 2020 for details).

### 7. Investigating the Recovery of Phase Variations through Simulations

In this section, we produce simulated spectra with higher \(S/\text{N}\)s and greater phase coverage to determine how well the day–night contrast and peak phase offset can be constrained with high-resolution spectroscopy. We perform the same cross-correlation and likelihood analysis on eight sets of simulated data, the details of which are listed in Table 3. Since we are most interested in the effects on the day–night contrast and peak phase offset, and we have shown that the T-P profile has little impact on these brightness variation parameters, in these simulations we employ the atmospheric models used in our main analysis, rather than the models with an alternative T-P profile from Section 6.3.

#### 7.1. Creating Simulated Spectra

For the first and second simulations listed in the table, we first construct white noise (with a mean of 1) with the same

| Sim. Name | Instrument | Orbital Phase | Cadence (min) | No. Frames | S/N |
|-----------|------------|---------------|--------------|------------|-----|
| ESP500    | ESPaDOnS   | 0.3–0.69      | 2            | 440        | 245 |
| HDS500    | HDS        | 0.21–0.54     | 10           | 52         | 330 |
| Comb.     | ESPaDOnS   | 0.21–0.69     | 2 & 10       | 492        | 410 |
| ESP250    | ESPaDOnS   | 0.2–0.8       | 2            | 526        | 250 |
| ESP500    | ESPaDOnS   | 0.2–0.8       | 2            | 526        | 500 |
| ESP750    | ESPaDOnS   | 0.2–0.8       | 2            | 526        | 750 |
| HDS500    | HDS        | 0.2–0.8       | 2            | 526        | 500 |
| HDS750    | HDS        | 0.2–0.8       | 2            | 526        | 750 |

The likelihood results of this second analysis are presented in the last column of Table 2, labeled “T-P Profile 2.” We found that, for all of our data sets, this stronger inversion had no serious impact on the phase offset, day–night contrast, or velocities. Only the \(\alpha\) and \(\log_{10}\)VMR parameters were affected significantly, as expected. In our combined data set, for instance, the Fe I VMR decreases by a factor of 20, while the \(\alpha\) value suggests that these new models better estimate the Fe I line contrast. However, the significance of our detection, based on the marginalized likelihood of \(\alpha\), has decreased slightly. The day–night contrast and peak phase offset, on the other hand, are quite consistent between the two T-P profiles. Our ability to recover these parameters is further explored in our simulations presented in Section 7.

This presents a cautionary tale for high-resolution emission spectroscopy, as the abundances derived are affected by the T-P profile used, as illustrated by the differences in \(\alpha\) and VMR between the two models. A full atmospheric retrieval, which is beyond the scope of this paper, would be required to address this in more detail. On a similar note, in some cases it may be valuable to instead fix the VMR and explore a variable lapse rate or T-P profile instead. However (with the exception of the VMR and \(\alpha\)), our fitted parameters are not greatly influenced by a change to the T-P profile, and therefore fitting for the VMR does not seem to affect our results in a significant way. But it would certainly be beneficial for future works to examine the T-P profile in greater detail.
average standard deviation along the time axis at each wavelength in our reduced data, and the same wavelength range as each spectral order in our reduced data. We do this for each night of ESPaDOnS and HDS observations individually, using the same phase coverage and cadence for each night as listed in Table 1. These simulated data imitate the average noise properties of our observations (since the standard deviation is calculated from our detrended data), but exclude individual contaminating features from stellar and telluric lines, which are not perfectly removed by SYSREM. In general, our use of white noise is largely meant to remove any dependence on the effects of a single night (i.e., poor seeing, weather, etc.), to provide an example of what constraints may be possible for a typical set of observations with a given S/N and phase range.

The third simulation simply combines the data sets from the first two. For the remaining simulations, we create artificial spectra that cover a larger phase range of 0.2–0.8 with a cadence of 2 minutes, to show the constraints we may place with observations with S/Ns of 250, 500, and 750. The S/N of our original observations is estimated via $1/\sigma$, where $\langle \sigma \rangle$ is the average standard deviation along the time axis in a 50 Å window around 6825 Å. We chose this region because it is virtually devoid of stellar and telluric features. From here, we determine the scale factor by which the standard deviation can be multiplied to produce the desired S/N in our white noise simulations, taking into account the increased number of exposures. For the fourth through sixth simulations, we use as our baseline the standard deviation and estimated S/N of night 1 of our ESPaDOnS observations. For the last two simulations, we use the standard deviation and estimated S/N of our HDS observations. We then produce white noise for each case, with the appropriately scaled standard deviation along the time axis and wavelength range of each spectral order.

Next, for all simulations we prepare a model for injection in the same manner as Section 4.2. We convolve the log$_{10}$ VMR = −4.0 model to the resolution of the instrument, and apply a high-pass Butterworth filter. We then Doppler shift this model to the planetary velocity ($K_p = 222$ km s$^{-1}$, $v_{sys} = −6.5$ km s$^{-1}$) for each phase, and interpolate to the wavelength grid of each data set before multiplying the model into the white noise. The multiplied term is $1 + A_p \times F_p/F_\nu$, where $A_p$ is the brightness variation from Equation (4). We use the parameters $\alpha = 2$, $C = 0.99$, and consider three different phase offsets: $\theta = 0^\circ$, $-12^\circ$, $+28.7^\circ$ (from Zhang et al. 2018), and $+28.7^\circ$ (from von Essen et al. 2020). Thus we have a total of 24 simulated sets of spectra.

Finally, after the injection we subtract 1 from the simulated data and perform the same cross-correlation and likelihood mapping as before. Though our simulated data do not retain the stellar pulsations that contaminate our original cross-correlations, we still exclude orbital phases 0.41–0.59 to replicate our original analysis as closely as possible. We also limit our simulated spectra to wavelengths >6000 Å, based on the findings presented in Section 6.1.

### 7.2. Results from Simulations

In Figure 6 we show the marginalized and conditional distributions resulting from our analysis of simulation ESP$_{750}$ with an injected phase offset of $+28.7^\circ$, as an example. These spectra have the resolution and wavelength range of ESPaDOnS, with a 2 minute cadence over phases 0.2–0.8, and a S/N of 750. Based on these results and those of the remaining simulations (which are too numerous to plot in the same manner), we find that the $K_p$, $v_{sys}$, $\alpha$, and log$_{10}$VMR parameters are well constrained relative to their injected values. We further compared the best-fit parameters from our ESP$_{obs}$, HDS$_{obs}$, and Combined simulations to those we report for our real observations, respectively. We found that in all cases the constraints from our simulations, and particularly the uncertainties on each parameter, are generally consistent with the constraints from our real spectra. This suggests that our white noise is a sufficient approximation of the noise in our observations.

Since we are most interested in the feasibility of accurately constraining the brightness variation terms with HRS, we therefore limit our remaining discussion to the recovery of the day–night contrast and phase offset parameters. Figure 7 shows a comparison of our recovered phase offset and day–night contrast with their respective injected values for each simulation. As in Section 6.2, we report the recovered phase offset as the median of the marginalized distribution $±1\sigma$, while for the contrast we report the lower limit, taken as the 84th percentile of the distribution. Our results from the first set of simulations, ESP$_{obs}$, indicate that the recovered phase offsets for all three injected values are quite accurate, albeit with large uncertainties. This lends significant credit to the phase offset we report using our actual ESPaDOnS observations. The lower limits on the day–night contrast from these ESP$_{obs}$ simulations are also similar to the lower limit we report from our real spectra. We again stress that $C$ is hard bounded at 1, which will bias values away from the injected value of $C = 0.99$.

As expected from our analysis of the actual HDS observations, the results from our simulated HDS spectra (labeled HDS$_{obs}$) overestimate the phase offset by more than $20^\circ$. We reiterate that this is because (1) these data only probe the dayside atmosphere on one side of secondary eclipse, and (2) we exclude the phases where the peak brightness would occur in order to avoid stellar pulsations. These limitations make it difficult to constrain the peak phase offset, and exemplify the need for observations on both sides of secondary eclipse. The confidence interval of the phase offset derived from the HDS data (both in our observations and simulations) may also appear relatively high, but it is possible to achieve a relatively tight constraint while having a large systematic offset from the actual value. This is especially true if the peak phase offset is not contained within our phase range, as is the case here. The effect this overestimated phase offset has on the combined spectra (labeled Comb.) is also apparent in our simulation results, reflecting our results from the real observations: the more accurate constraint from simulation ESP$_{obs}$ is slightly outweighed by that of simulation HDS$_{obs}$, due to the higher S/N of the latter. Interestingly, the lower limit on the contrast from simulation HDS$_{obs}$ appears to be dependent on the injected phase offset. This also makes sense for observations with limited phase coverage: An eastward offset is somewhat degenerate with a lower contrast if only phases <0.5 are observed, and vice versa.

To test the bias toward positive phase offsets in greater detail, we ran three additional sets of simulations based on the HDS data with injected offsets of $-35^\circ$, $0^\circ$, and $+28^\circ$, with 25 different realizations of the noise. We kept the other parameters equal to the best-fit model. In general, we found that the rms between the different simulations was larger than the uncertainty we found for our data, but that the bias was always present. However, the magnitude of the bias (both in size and number of simulations) increased with an offset toward the
planet’s morning side, which would imply that the bias is due to the limited phase coverage. From this we conclude that the bias we see in our results is likely real, but that we may be underestimating the uncertainties on the recovered offset.

In more detail, the average uncertainties on the phase offset obtained from our additional simulations were larger than those retrieved from our HDS observations (e.g., ±20°–30° compared to ±6°). Given that an increase in uncertainty could change the nature of any detected phase offset from significant to nonsignificant, this warrants a closer look. The discrepancy between the phase offset uncertainty from our additional simulations and that of our observations is, at least in part, driven by the aforementioned points that bias the results. Furthermore, the increased scatter in our additional simulations appeared to be driven by a few simulations with different noise realizations where a higher value of \( \theta \) was preferred. We also note that in several cases, the fits hit the upper/lower boundary of the parameter grid, which can skew the results slightly, and due to the extensive run time/memory requirements of these simulations, it was not feasible to extend the parameters to a larger range. All of these effects could influence the uncertainty on the phase offset in our additional HDS simulations.

With that said the vast majority of the weight in our combined results, in both our original simulations and observations, originates from the HDS data. Our ESPaDOnS results should have a smaller bias due to coverage on both sides of the dayside phase curve, and therefore the uncertainties on this retrieved phase offset should be less affected.

Continuing with our results in Figure 7, the remaining points show the results for simulations with higher S/Ns and more complete dayside phase coverage. These show that extended observations on both sides of secondary eclipse can greatly improve the accuracy of the recovered contrast and phase offset, particularly compared to the HDS\(_{\text{obs}}\) set of simulations. Observations with higher S/Ns also provide tighter constraints on both the phase offset and day–night contrast. The HDS simulations provide slightly better constraints on the phase offset than the ESPaDOnS simulations at the same S/Ns, which is due to the higher resolution of HDS.

Overall, our HRS observations and simulations both show that, given sufficient phase coverage with high S/N spectra, it is entirely feasible to constrain the day–night contrast and phase offset of a hot Jupiter atmosphere. Such constraints can inform aspects of energy recirculation in a planet’s atmosphere, though the avoidance of stellar pulsations in the CCF is a necessity. If such pulsations can be removed from the CCF around secondary eclipse, we may be able to even better constrain the peak phase offset, because the phase at which it occurs will no longer need to be excluded. This is a complex issue that is outside the scope of this work. Though our simulated spectra do not feature stellar pulsations, we still choose to exclude the affected phases from our analysis, since
injected contrast is kept at models with phase offsets of. The light blue, white, and dark purple points show the results for injected distribution. On the use only the lower limit, taken as the 84th percentile of the bounded spectra remains an open question. Pulsation signals have

Figure 7. Comparison of our recovered phase offset (top) and day–night contrast (bottom) to their injected values for each simulation, plotted as the difference between the recovered and injected values. For the phase offset we use the median of the marginalized distribution ±1σ, while for the contrast we use only the lower limit, taken as the 84th percentile of the bounded distribution. On the x-axis we label the simulations as they appear in Table 3. The light blue, white, and dark purple points show the results for injected models with phase offsets of θ = −1278, 0°, and +287°, respectively. The injected contrast is kept at C = 0.99 in all cases.

the feasibility of removing pulsation signals from emission spectra remains an open question. Pulsation signals have already been successfully removed from transmission spectra (e.g., Johnson et al. 2015; Temple et al. 2017; van Sluijs et al. 2019; though the planetary signal in the latter was artificially injected), but adapting these methods to dayside emission spectra will not be trivial. However, efforts along these lines will be invaluable for future atmospheric investigations of planets orbiting variable stars, such as WASP-33b, β Pic b and WASP-176b/KELT-13b.

8. Conclusions

We have detected Fe I in the atmosphere of the ultra-hot-Jupiter WASP-33b, indicative of a thermal inversion layer produced by an atomic species. Combining optical high-resolution data sets from five nights of observations with ESPaDOnS on CFHT and one night with HDS on Subaru, we make a detection of >10.4σ. By employing a likelihood mapping technique, we are able to constrain the RV semi-amplitude to K_p = 222.1^{+0.8}_{−0.5} km s^{-1} and the systemic velocity to v_sys = 6.5 ± 0.3 km s^{-1}, matching previously reported values. We find that the Fe I signal is only detected above 6000 Å in our ESPaDOnS spectra, and use simulated data to explain that this phenomenon is due to decreased line contrast at bluer wavelengths. By cross-correlating with models with a higher stratospheric temperature, and therefore greater line contrast, we further show that a signal at these wavelengths can actually be detected.

We also introduce a brightness variation term to our likelihood calculations, to explore the day–night contrast and phase offset of the peak brightness from our individual and combined data sets, assuming the planetary emission spectrum is dominated by Fe I lines. By performing the same analysis on simulated spectra, we then explore how well these parameters can be constrained from observations with higher S/Ns and greater phase coverage. We find that our constraint on the phase offset from HDS is likely overestimated due to the limited phase coverage of those observations, and we show that this further affects the constraint from our combined data set, since the S/N of our HDS observations is much higher than that of our ESPaDOnS observations. We therefore suggest that our reported constraint of θ = +22 ± 12 degrees from ESPaDOnS alone is likely a better estimate of the true phase offset of WASP-33b, since these observations cover phases before and after secondary eclipse relatively evenly. We report a day–night contrast of C > 0.90 using the same spectra, indicating that the nightside flux is <10% of the dayside flux in the wavelength range we consider. Using atmospheric models with a stronger temperature inversion, we also show that these brightness variation parameters are not significantly impacted by the T-P profile selected. Given the dependence of our models on the assumed lapse rate, however, our results cannot be directly used to infer the absolute abundance and metallicity of the planet’s atmosphere. A detailed interpretation of the day–night contrast would also need to take into account a variable lapse rate as a function of position on the planet.

Based on both our observations and simulations, high-resolution spectra that cover a large phase range on both sides of secondary eclipse can be used to constrain a planet’s day–night contrast and peak phase offset, even in the presence of stellar variability. This approach provides a new means to confirm or challenge existing measurements from photometric light curves. We encourage further investigation into the removal of stellar pulsation signals from spectroscopic data; this has been done in a few cases (e.g., Johnson et al. 2015; Temple et al. 2017; van Sluijs et al. 2019), but adapting the procedure to dayside emission observations will present unique challenges. We also encourage future studies to examine more complete models of a planet’s brightness variation throughout its orbit. They would facilitate a deeper exploration of energy circulation within a planetary atmosphere, and expand the utility of high-resolution Doppler spectroscopy in characterizing exoplanets.

Some of the data presented herein were obtained at the Canada–France–Hawaii Telescope, which is operated by the National Research Council of Canada, the Institut National des Sciences de l’Univers of the Centre National de la Recherche Scientifique of France, and the University of Hawaii. Our second data set was collected at the Subaru Telescope, which is operated by the National Astronomical Observatory of Japan. The authors also wish to recognize and acknowledge the very significant cultural role and reverence that the summit of Maunakea has had within the indigenous Hawaiian community. We are most fortunate to have the opportunity to conduct observations from this mountain. M.K.H. was supported by funding from the Natural Sciences and Engineering Research Council (NSERC) of Canada.

Appendix A
Model Filtering

As mentioned in Section 4.2, we apply a Butterworth filter to each model prior to cross-correlating, to mimic the effects of
SYSREM on the planetary signal. Each night of observations has unique noise properties, and requires a different number of SYSREM iterations to account for the stellar and telluric features present. The filter parameters that best represent the effects of SYSREM will then be different for each night, and to determine those parameters, we perform a series of injection and recovery tests.

For each injection, we use the same models described in Section 4 but do not apply the Butterworth filter. The model is injected into the extracted spectra (i.e., before blaze correction, SYSREM, etc.) at the same orbital speed as the real Fe signal, but with the opposite sign, so that the real and injected planetary signals do not overlap, but are treated similarly in our data reduction procedure. The model is Doppler shifted to the planet’s velocity for each frame, interpolated to the wavelength grid of each spectral order, and multiplied into the data in the form \(1 + F_p/F_s\). We then apply the same blaze correction and number of SYSREM iterations as are used for each night (Table 1).

Next, we perform the same cross-correlation and likelihood computation as before, this time searching for the injected signal, and fixing the day–night contrast and phase offset to zero. The model with which we cross-correlate (after convolving to the instrument resolution and calculating the planet-star flux ratio) is initially filtered using a minimum window filter with a window of \(\sim 4\,\AA\), to subtract only the planetary continuum from the model. This filtering method is used often with Doppler cross-correlation (e.g., Herman et al. 2020; Nugroho et al. 2020a; Jindal et al. 2020). However, it does not account for the effects that the SYSREM algorithm has on the injected planetary signal, and as a result, the best-fitting \(\alpha\) parameter underestimates the true scale of the injected model—generally by \(\sim 30\%\) or more. This has clear consequences: if we do not address the side effects of SYSREM when dealing with the real planetary signal, the true nature of the underlying emission spectrum cannot be properly understood.

We therefore follow the example of Gibson et al. (2020), and introduce a high-pass Butterworth filter in place of the minimum window filter. We then adjust the parameters of the filter for each night (i.e., the filter order and cutoff frequency). We find that it is possible to recover a value for \(\alpha\) much closer to the true scale of the injection through more aggressive filtering of the model with which we cross-correlate. For our various data sets, this means increasing the cutoff frequency until the recovered \(\alpha\) is within a few percent of the injected value. In Figure 8, we show an example model before any filtering, after applying a minimum window filter, and after applying a Butterworth filter.

Initially, we determined the optimal filter parameters for a given night using a single model for the injection and cross-correlation. However, we confirmed that the chosen parameters were also appropriate for models with different VMRs; in other words the filter order and cutoff frequency were not optimized to recover a specific model. Additionally, this filtering did not have any noticeable impact on the recovery of other injected parameters.

Through these injection tests, we are able to determine the appropriate filter parameters for our models when cross-correlating with the actual planetary spectra for each night, so that the best-fitting \(\alpha\) value is properly estimated. Of course, this singular filtering method cannot perfectly reproduce the complex effects of SYSREM on the planetary signal. We simply consider this to be a first step toward addressing the nuances commonly overlooked in Doppler cross-correlation analyses. As the analysis techniques developed for HRS become increasingly advanced, our data processing methods must evolve as well. Looking forward, an in-depth study of the implications of our treatment of high-resolution data would be well worth the time investment.

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**Figure 8.** An example of the planetary emission model with \(\log_{10}\) VMR = \(-4\), to which different filtering methods have been applied. In the top panel we have only convolved the model to the resolution of the ESPaDOnS data and calculated the planet-star flux ratio. In the center panel we have additionally applied a minimum window filter with a window of \(4\,\AA\) to remove the planetary continuum. In the bottom panel we have instead applied a high-pass Butterworth filter to the model from the top panel, which better accounts for the effect of SYSREM on the planetary signal.
Appendix B
Additional Figures

In Figures 9 and 10, we show the same marginalized and conditional likelihood distributions as Figure 4, but for our individual ESPaDOnS and HDS results, respectively.

Figure 9. The same as Figure 4, but for the likelihood distributions of our ESPaDOnS observations alone. Note that the axis ranges of some subplots differ between these figures.
Figure 10. The same as Figures 4 and 9, but for the likelihood distributions of our HDS observations alone.
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