Characterising Exoplanet Atmospheres with High-resolution Spectroscopy

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The search for signs of life elsewhere in the Universe requires the remote detection of molecules in the atmospheres of exoplanets. Recent progress with high-resolution infrared spectra obtained with CRIRES has led to the first ground-based detections of carbon monoxide and water in the atmospheres of hot giant exoplanets. This avenue of exoplanet characterisation has the potential to identify biomarkers in the atmospheres of Earth analogues with the European Extremely Large Telescope. The current detections not only provide evidence for how the composition of a hot giant planet atmosphere can affect its thermal structure and cloud formation processes, but also have the potential to constrain the universal mechanism for planet formation by pinpointing the birth location of the planet in its protoplanetary disc.

The importance of carbon and oxygen in hot Jupiter atmospheres

Recent studies have suggested that the balance of carbon and oxygen in hot Jupiter (HJ) atmospheres may be drastically and unexpectedly different to the composition of their host stars, with HJs being more abundant in carbon (C/O > 1; Madhusudhan et al., 2012). This surprising conclusion was proposed as a solution to the puzzling and seemingly random presence of stratospheres (i.e., temperature inversions) in HJ atmospheres. Other works have proposed either a connection between the intensity of ultraviolet (UV) light from the host star and the existence of stratospheres (Knutson et al., 2010), or a dichotomy of dusty and cloud-free HJ atmospheres (Pont et al., 2013). The latter is partly supported by Evans et al. (2013) who used the Hubble Space Telescope (HST) to detect for the first time a deep blue light reflecting from clouds in the atmosphere of an HJ.

However, measuring the C/O ratio in HJ atmospheres not only has the power to constrain their structure, but potentially has important implications for the theory of planet formation. Intriguingly, Öberg et al. (2011) showed that the C/O ratio in an HJ atmosphere could be directly linked to the location at which it formed within its protoplanetary disc, due to the different condensation temperatures of molecular ice lines for water, carbon dioxide and carbon monoxide. However, only direct evidence for the presence and abundances of the molecules involved in these theories will enable an accurate physical description of these extreme objects.

Tracing the radial velocity shift of molecular features in exoplanet atmospheres with high-resolution spectra

Robust detections of molecular features in the spectra of exoplanet atmospheres are rare because their signals are typically orders of magnitude smaller than the instrumental systematics present in both ground- and space-based observations. The treatment of these systematics has led to a debate of reported detections in the literature (see e.g., Gibson et al. [2011] for a review). However, in 2010, the first robust ground-based detection of carbon monoxide in an HJ atmosphere was made using a technique based on high-resolution spectra at 2.3 μm from the CRyogenic InfraRed Echelle Spectrograph (CRIRES) on the Very Large Telescope (VLT; Snellen et al., 2010). The detection was made by directly measuring the radial velocity shift of the planet, rather than its host star. Crucial to this success was the high spectral resolution provided by CRIRES ($R \sim 100\,000$), which allowed the forest of spectral lines in the carbon monoxide molecular band to be individually resolved. Observing the planet continuously for the duration of approximately one of its transits traces a radial velocity change in the planetary signal on the order of km s^{-1}, which is much larger than the few m s^{-1} change in the velocity of the host star.

The cartoon in Figure 1 illustrates how the individual lines of the planet's spectrum move throughout its orbit. The large wavelength shift of the planet's signal allows it to be separated from the essentially stationary lines of the host star spectrum and from the static spectral absorption features of the Earth's atmosphere. This is achieved by using detrending algorithms. For example, the top panel of Figure 2 shows 48 spectra extracted from CRIRES observations of HD 189733 over the course of five continuous hours just before secondary eclipse, when most of the planet's dayside hemisphere was visible. Each row is a spectrum, and each column can be considered as a wavelength channel with a width of one pixel. The deep, wide absorption bands of the Earth's atmosphere (black regions) are clearly visible. Each column is subject to trends that vary smoothly during the night, such as changing airmass or seeing. By using a principal component-like analysis, such as those commonly used to de-trend transit survey light curves, trends common to all columns can be identified.

The second panel in Figure 2 shows the input to the algorithm, which is simply the extracted spectra with their median value subtracted. The most significant global trend in the columns is identified and then removed from each column (see third panel). In this specific case, the dominant trend closely followed the airmass curve of the target. The algorithm is repeated until no more significant global trends remain (see fourth panel). This column-by-column operation leaves the planetary signal relatively untouched because it is shifting in wavelength during the observations and thus does not constitute a common trend in each column. For illustration, the bottom panel of Figure 2 shows what the fourth panel would look like if we injected a strong model planet spectrum into the data before applying the algorithm. After the telluric features have been removed, the remaining data can be cross-correlated with

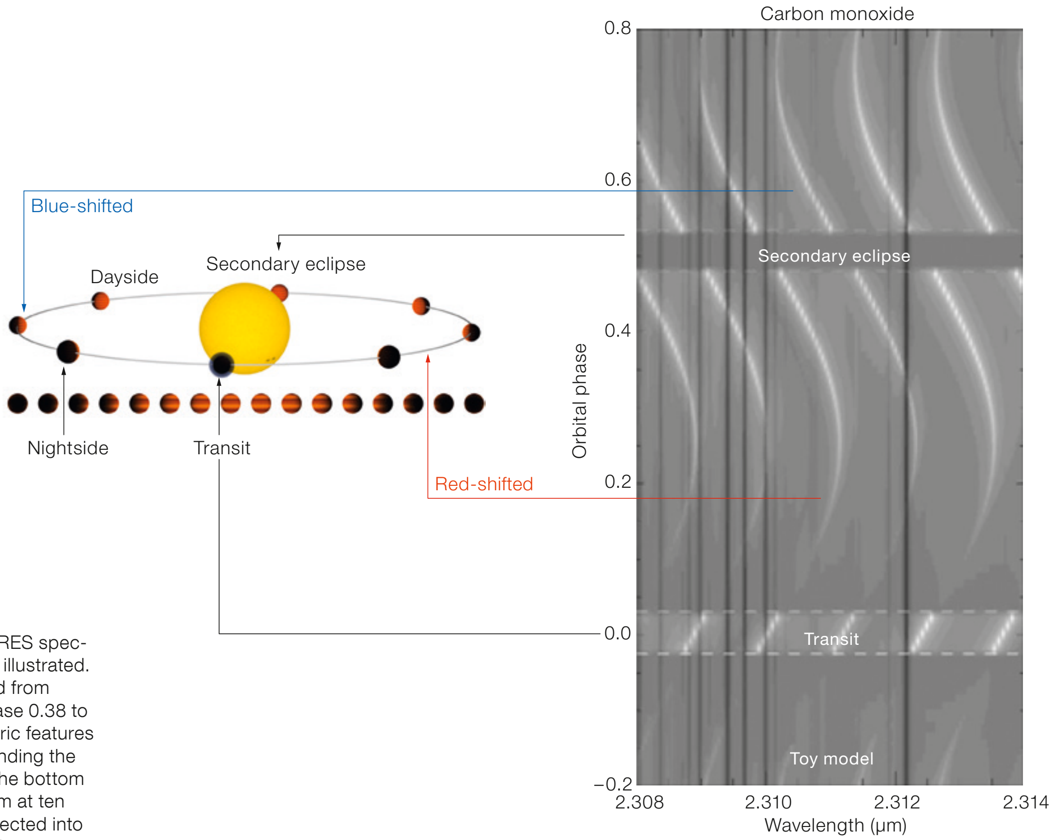

Figure 1. Schematic for detecting molecules in exoplanet atmospheres at high resolution. Each row in the right-hand panel is a spectrum. The white lines trace out the radial velocity curve of individually resolved lines in the carbon monoxide molecular band of a toy model hot Jupiter atmosphere. Throughout the orbit, the lines shift significantly in wavelength compared to the static features of the Earth's atmosphere (dark vertical lines), allowing them to be separated without destroying the planetary signal. This technique works both in transit, as starlight filters through the exoplanet atmosphere and adopts the spectral fingerprint of its molecular constituents, and throughout the phase as thermal irradiation from the planet's dayside and nightside rotate into view, depicted at left.

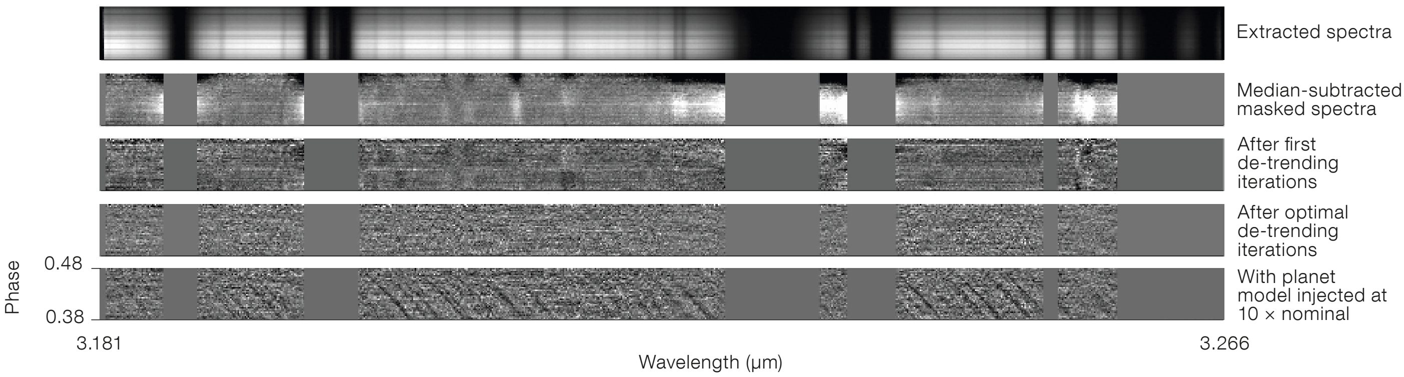

Figure 2. The process of de-trending CRIRES spectra in order to uncover the planet signal is illustrated. The top panel shows 48 spectra extracted from CRIRES observations covering orbital phase 0.38 to 0.48, where each row is a spectrum. Telluric features are removed column by column by de-trending the spectra over time (middle three panels). The bottom panel shows how a model planet spectrum at ten times its nominal value would appear if injected into the extracted spectra before the de-trending process. From Birkby et al. (2013).

high-resolution models of molecular species over a range of planet radial velocity semi-amplitudes (K_p) to trace out the radial velocity curve of the planet (see Figure 3).

In order for any signal to be considered of planetary origin, it must coincide with the total velocity of the system (V_{sys}), which is known from precision radial velocity measurements of the host star. This is a key element in the robustness of the high-resolution technique. In practice, the cross-correlation is carried out over a wide grid of K_p and V_{sys} to reliably reject spurious signals. We have since used this high-resolution technique with observations from our large ESO programme on CRIRES (186.C-0289) to produce a steady stream of ground-based detections of carbon monoxide in the daysides of both transiting and non-transiting HJ atmospheres, opening up the study of atmospheres to the full population of exoplanets (Brogi et al., 2012, 2013; de Kok et al., 2013a).

Adapting the high-resolution technique for use at other wavelengths in more obscured regions of the Earth's atmosphere that contain molecular bands of all the other major carbon and oxygen-bearing species (water, methane and carbon dioxide), has led to the first robust ground-based detection of water in an HJ atmosphere with CRIRES (Birkby et al.,

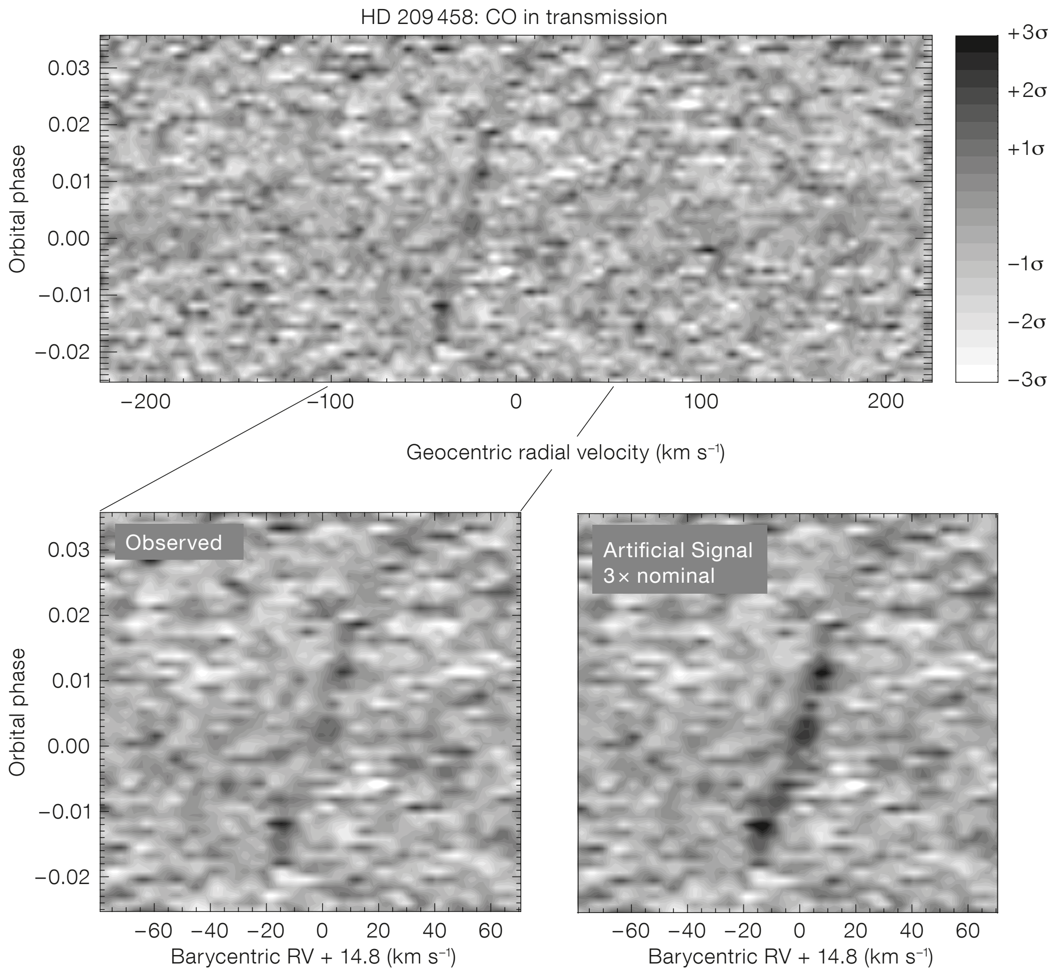

Figure 3. The radial velocity trail of carbon monoxide in the atmosphere of the hot Jupiter HD 209458 b observed during its transit. The signal is blue-shifted by 2 km s^{-1} from the expected V_{sys}, suggesting the presence of a fast, high-altitude wind blowing from the day- to the nightside of the planet. Adapted from Snellen et al. (2010).

	HD 209458 b (Transiting)	τ Boötis b (Non-transiting)	51 Pegasi b (Non-transiting)	HD 189733 b (Transiting)
Molecules detected	CO at 2.3 µm (5.6σ)	CO at 2.3 µm (6σ)	CO at 2.3 µm (6σ) H_2O 3.2 µm (4σ)	CO at 2.3 µm (5σ) H_2O at 3.2 µm (5σ)
Reference	Snellen et al. (2010)	Brogi et al. (2012)	Brogi et al. (2013)	de Kok et al. (2013a) Birkby et al. (2013)
Planet orbital velocity	140 ± 10 km s^{-1}	110.0 ± 3.2 km s^{-1}	134.1 ± 1.8 km s^{-1}	154 ± 4 km s^{-1}
System inclination	86.93 ± 0.01°	44.5 ± 1.5°	79.6° ≤ i ≤ 82.2°	85.71 ± 0.05°
Planet mass	0.64 ± 0.09 MJ	5.95 ± 0.28 MJ	0.46 ± 0.02 MJ	1.162 ± 0.058 MJ
Phase observed	Transit	Dayside	Dayside	Dayside

Table 1. Summary of detections of molecules in exoplanet atmospheres made with CRIRES. The planet masses have been independently derived from the CRIRES measurements and are actual masses, not the minimum mass usually quoted from radial velocity measurements.

2013). The cross-correlation grids showing the detection of these molecular features are shown in Figure 4 and their results are summarised in Table 1. These detections required between 5 and 18 hours of time with CRIRES, which highlights the efficiency of this instrument for exoplanet atmosphere science. Importantly, the measurement of the orbital velocity of the planet in a non-transiting system can be converted to an inclination angle and hence a true mass for the planet, unlike the minimum mass determined from stellar radial velocity measurements alone. This was the case for the well-known non-transiting hot Jupiters τ Boötis b and 51 Pegasi b. The detection of CO in their atmospheres (see Figure 4) revealed that τ Boötis b is inclined at *i* ~ 45 degrees to our line of sight (Brogi et al., 2012), and that the first exoplanet discovered around a Sun-like star, 51 Peg b, was almost a transiting system (Brogi et al., 2013).

What can we learn from high-resolution observations of exoplanet atmospheres?

The detection of molecules at high resolution in exoplanet atmospheres is in itself an important input for atmospheric modelling. In principle, detections at infrared wavelengths that probe the thermal emission of the atmosphere, also make it possible to put constraints on both the abundance of the detected gas and the temperature structure in the

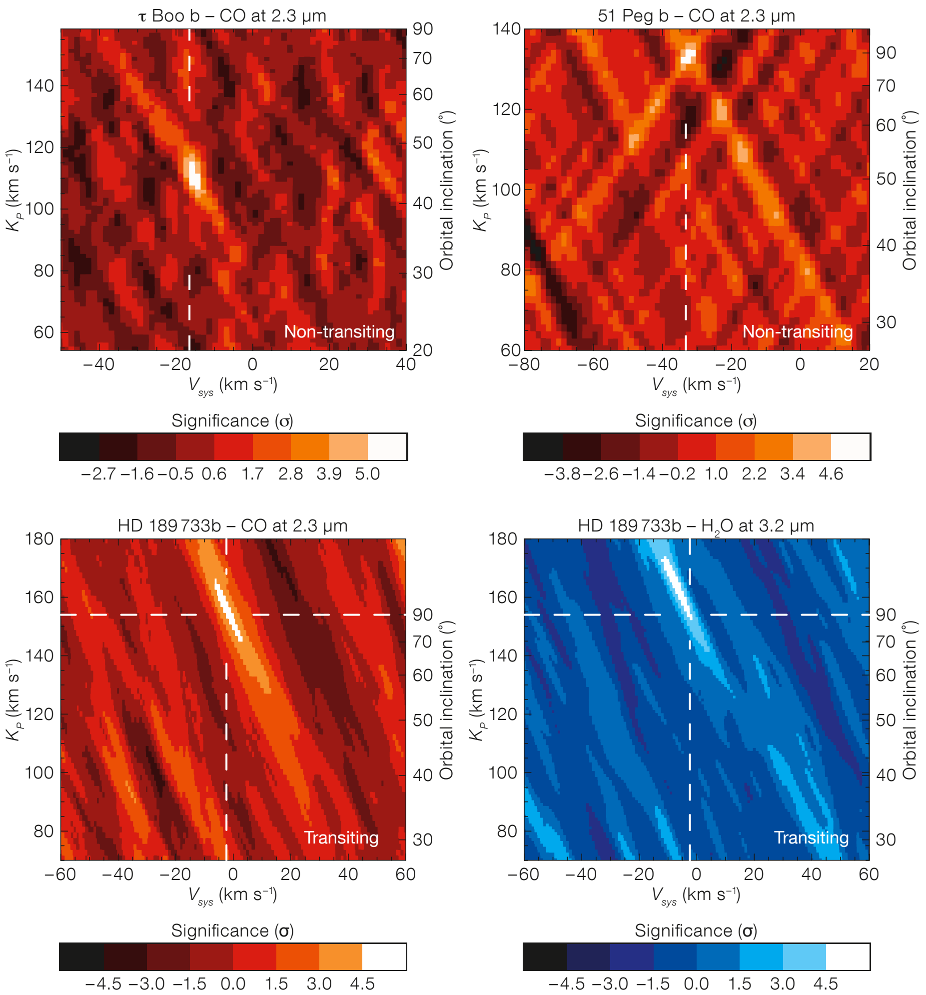

Figure 4. Carbon monoxide (CO) and water (H_2O) detected in the dayside atmospheres of several transiting and non-transiting hot Jupiters using the high-resolution spectra from CRIRES. These figures show the grid of planet radial velocity (K_p) and total system velocity (V_{sys}) explored by the cross-correlation of our processed spectra with model exoplanet atmospheres. The strongest signal is detected at the known total system velocity (dashed vertical white lines) in each case and is thus considered to have planetary origin. The orbital velocity of the planet can also be converted to a system inclination. The CO detection in τ Boötis b used three half-nights of CRIRES spectra, while 51 Peg b used two half-nights, and the detections in HD 189733 b are based on five hours observation each. The colour bars indicate the significance of the detections.

atmosphere. Such constraints can ultimately provide a measurement of the C/O ratio. However, the high-resolution technique is only sensitive to the relative depth of the absorption lines in the planet's spectrum, and not their absolute levels. As a result, many degeneracies exist between the temperature *vs*. pressure (altitude) profile of the atmosphere and the concentration of the gas in question, because different combinations can result in the same relative line depth. Furthermore, if the atmosphere is very cold in its upper layers, or has a very small change in temperature throughout the extent of its atmosphere, the relative line depths for different gas concentrations can be identical.

For transiting planets, additional constraints can be obtained at lower resolution in the same wavelength region from observations of the planet's secondary eclipse, i.e., as it passes behind its host star. This provides a measurement of the absolute flux level of the planet spectrum at the wavelength probed by the high-resolution data, and independently constrains the range of viable temperature–pressure profiles.

For non-transiting planets, where secondary eclipse measurements are not possible, further information can be gained from the simultaneous detection of several molecules in a narrow wavelength range. In this case, the lines all have a very similar continuum level, which removes some of the degeneracies in the models and allows a constraint on the relative gas concentrations. Moreover, detections of the same molecule across a range of wavelengths where the gas absorbs at different levels can further constrain the atmospheric temperature profile, the gas concentrations and even the presence of clouds.

The wavelengths at which different gases are best detected with CRIRES can be simulated in conjunction with the ESO Exposure Time Calculator (ETC). We injected model planet spectra into simulated stellar spectra spanning 1–5 μm obtained from the ETC. Using the same data reduction technique as for the real data, we assessed how well a certain planet signal can be detected at different CRIRES wavelength settings. Figure 5 shows the results of this exercise for a hot Jupiter of a given composition (based on HD 189733 b). The absorption bands in the Earth's atmosphere can clearly be seen to hinder the detection of the planet signal at e.g., 2.7 μm.

The figure also shows that there are wavelength settings that are expected to give a higher signal than the 2.3 μm and 3.2 μm regions in which we have already made carbon monoxide and water detections. In particular, the wavelength setting at 3.5 μm looks ideal for the simultaneous detection of major carbon- and oxygen-bearing gases, given its high sensitivy to water, methane and carbon dioxide, and is the target of our current observations of the dayside atmospheres of two non-transiting hot Jupiters. Interestingly, in the case of high C/O ratios or disequilibrium photochemistry, CRIRES would also be sensitive to hygrogen cyanide and acetylene in HJ atmospheres in the 3.1 μm region.

Exploring the dark side

For HJs, the nightside is expected to be colder than the dayside, as is suggested

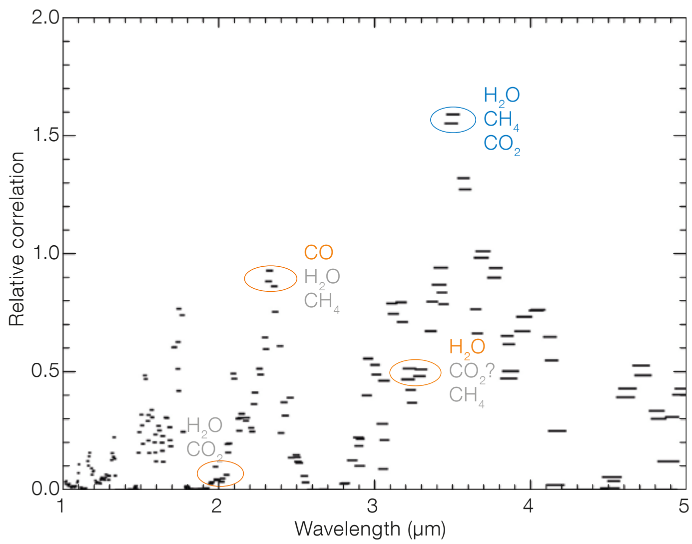

Figure 5. Simulating the sensitivity of CRIRES to different molecules in the atmospheres of exoplanets across its full range of wavelength settings. Orange circles mark regions that we have already observed; orange text denotes molecules detected; while grey text marks species with molecular bands in that region but which were not significantly detected. The blue circle and text marks the 3.5 μm region which we found to be the most sensitive to the simultaneous detection of major carbon- and oxygen-bearing species (de Kok et al., 2013b).

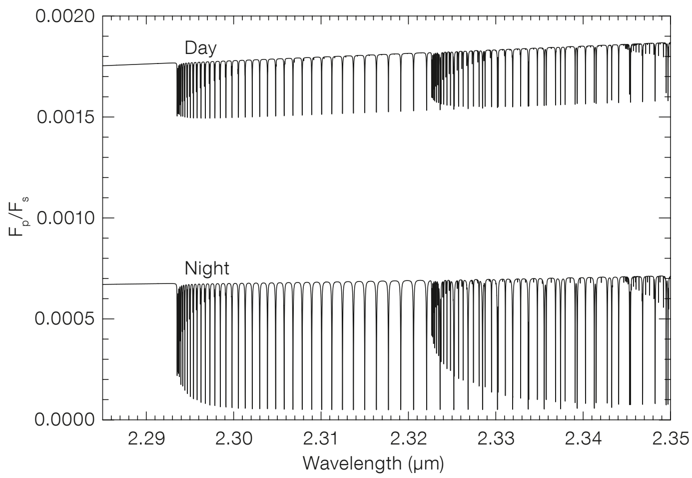

Figure 6. A high-resolution model of CO absorption lines in the day- and nightside of an HJ atmosphere expressed as a fraction of the stellar flux. The nightside produces deeper absorption features which may make it easier to detect them, despite having a lower overall flux (de Kok et al., 2013b).

by infrared phase curves from Spitzer. Despite being darker on their nightside, high-resolution observations can also be used to probe molecules at these phases in HJ atmospheres. In fact, the change in temperature with altitude on the nightside may be larger than on the dayside, and this potentially can result in deeper molecular absorption lines (see Figure 6), making the nightside perhaps even more ideal for hunting for molecules with high-resolution spectra, despite the lower overall flux. A detection of the same molecule in the same wavelength range on both day- and nightsides would allow constraints on the day-to-night heat transfer in the atmosphere, and in particular on its vertical dependence. For instance, a deeper line depth at the nightside can indicate that the highest day-to-night temperature contrast occurs at high altitudes. On the other hand, small line depths on both the dayside and nightside can indicate the presence of a thick global cloud layer.

Exoplanet atmospheres with future high-resolution instrumentation

The imminent upgrade of CRIRES to the cross-dispersed spectrograph CRIRES+ promises to yield a great improvement in the sensitivity of the high-resolution method. Its much larger wavelength coverage and upgraded detectors will greatly improve the correlation signal of detected molecules by significantly increasing the number of individual molecular lines that can be measured. It will also allow the detection of several molecules simultaneously at a relatively high signal-to-noise across a wide region of the planet's spectrum, which will provide information about the atmospheric temperature structure, the presence of clouds, and potential variations of the gas concentrations with altitude. Furthermore, it opens up the possibility of using high-resolution spectra to study the atmospheres of smaller, cooler planets such as warm Neptunes and superEarths at infrared wavelengths. In theory, high-resolution spectra at optical wavelengths can be used in a similar manner to probe for other molecules, such as metal oxides. Therefore, the high-resolution optical spectrograph, ESPRESSO, which is scheduled for first light on the VLT in 2016, will provide another compelling avenue for characterising exoplanet atmospheres.

The greatest step in sensitivity to exoplanet atmospheres with ground-based facilities will be achieved by the European Extremely Large Telescope (E-ELT). The E-ELT will potentially carry two high-resolution instruments: METIS in the infrared *L*- and *M*-bands, and HIRES at visible and near-infrared wavelengths. These E-ELT instruments will allow a detailed chemical census of the full population of exoplanets to reveal the diversity of their atmospheres. Excitingly, simulations have also shown that high-resolution spectra from the E-ELT instruments will be able to detect a potential oxygen biomarker at 0.76 μm in the atmospheres of Earth-like planets orbiting in the habitable zones of M-dwarf stars, in just a few dozen transits (Snellen et al., 2013).

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