Titanium oxide and chemical inhomogeneity in the atmosphere of the exoplanet WASP-189 b

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The temperature of an atmosphere decreases with increasing altitude, unless a shortwave absorber that causes a temperature inversion exists 1. Ozone plays this role in the Earth’s atmosphere. In the atmospheres of highly irradiated exoplanets, the shortwave absorbers are predicted to be titanium oxide (TiO) and vanadium oxide (VO) 2. Detections of TiO and VO have been claimed using both low- 3–6 and high- 7 spectral-resolution observations, but subsequent observations have failed to confirm these claims 8–10 or overturned them 11–13. Here we report the unambiguous detection of TiO in the ultra-hot Jupiter WASP-189 b using high-resolution transmission spectroscopy. This detection is based on applying the cross-correlation technique 15 to many spectral lines of TiO from 460 to 690 nm. Moreover, we report detections of metals, including neutral and singly ionized iron and titanium, as well as chromium, magnesium, vanadium and manganese (Fe, Fe+, Ti, Ti+, Cr, Mg, V, Mn). The line positions of the detected species differ, which we interpret as a consequence of spatial gradients in their chemical abundances, such that they exist in different regions or dynamical regimes. This is direct observational evidence for the three-dimensional thermochemical stratification of an exoplanet atmosphere derived from high-resolution ground-based spectroscopy.

The ultra-hot Jupiter WASP-189 b has a high equilibrium temperature of $T_{\text{eq}} = 2,641 \pm 34$ K due to its close proximity to its hot A-type host star 14. It is one of the brightest transiting planet systems currently known, making it very amenable for spectroscopic studies of its atmosphere. The system is well characterized, thanks to extensive photometric observations with CHEOPS 16, including a precise measurement of the orbital parameters, which we adopted in this study. In recent years, similar systems have garnered considerable interest within studies that use high-resolution ground-based spectrometers. These have been used to reveal a myriad of absorbing atoms in their emission and transmission spectra 17–32.

We observed time series of the spectrum of WASP-189 during three transit events, with the High Accuracy Radial Velocity Planet Searcher (HARPS) echelle spectrograph at the ESO 3.6 m telescope in La Silla Observatory, Chile (principal investigator Hoeijmakers, programme number 0103.C-0472). In addition, we used one archival HARPS transit observation, previously published by Anderson et al. 14, and one archival HARPS-N observation (principal investigator Casasayas-Barris, programme number CAT19A_97). We corrected for telluric absorption using Molecfit 33,34, masked both outliers and spectral regions affected by residuals caused by strong telluric lines, notably O2, and corrected for the Rossiter–McLaughlin effect (Extended Data Fig. 1). We performed cross-correlation analyses 15 with model spectra of a collection of chemical species, and implemented bootstrap analyses to confirm the statistical robustness of candidate detections (Methods). We observed transit light curves using the EulerCam instrument to rule out stellar activity (Extended Data Fig. 2) and we fitted the spectrum to confirm past measurements of metallicity and equatorial rotation velocity (Extended Data Fig. 3).

Cross-correlation templates were derived from the modelled transmission spectrum of the planet, assuming hydrostatic and chemical equilibrium and an isothermal atmosphere. Each template contains the line opacity of an individual atom, ion or TiO, and the cross-correlation acts to average the spectral lines of each species, weighted by the expected strength of each absorption line as a function of time during the transit event.

Due to the curvature of the exoplanet orbit, absorption signals are Doppler-shifted according to the instantaneous radial velocity of the planet, which scales with the planet’s orbital velocity. High-altitude winds from the dayside to the nightside act to additionally blue-shift any observed absorption line, while planetary rotation and super-rotational winds result in broadening. This type of analysis can thus be used to measure the orbital velocity of exoplanets, as well as dynamics in their atmospheres 15,35–40. We use a template that contains absorption lines of over a hundred atoms and ions to trace the velocity of the planet’s atmosphere as it passes through transit, and obtain a best-fit orbital velocity of $194.1 \pm 4.3$ km s$^{-1}$, consistent with the expected value of $200.7 \pm 4.9$ km s$^{-1}$ as derived from the orbital parameters determined via precise CHEOPS photometry 16 (Extended Data Fig. 4).
For exoplanets that are close to their host stars, the viewing angle varies substantially from the start to the end of the transit event. Corotation of the atmosphere with the tidally locked planet causes absorption lines formed at the leading (morning) or trailing (evening) limbs to be Doppler-shifted in opposite directions. At the same time, there are strong temperature differences between the permanently irradiated daysides and the cooler nightsides of hot Jovian exoplanets due to tidal locking. Atmospheric chemistry being strongly temperature dependent, chemical gradients are expected to exist between the two hemispheres. In addition, the atmospheric scale height decreases with decreasing temperature from the dayside to the nightside, especially in the presence of H$_2$ recombination.

Figure 1 shows a toy-model schematic of how a day-to-nightside temperature gradient is expected to alter the observed cross-correlation signatures—in the absence of any atmospheric dynamics apart from corotation with the tidally locked planet. At the beginning of the transit event, more absorption originates at the leading (morning) terminator, because the line of sight passes through hotter atmospheric regions than at the trailing (evening) terminator. At the leading terminator, the atmosphere is redshifted because the planet rotates in the anticlockwise direction, causing an effective redshift of the observed absorption signal. Towards the end of the transit, absorption at the leading terminator is replaced by absorption at the trailing terminator, which is blueshifted. This effect manifests itself as a decrease in the inferred orbital velocity of the planet, which is a primary observable in analyses of high-resolution spectroscopy of exoplanets. Without a thermal or chemical gradient across the day-to-nightside terminator, the two limbs absorb symmetrically and the resulting signal carries neither a net redshift nor a net blueshift. In the case of a global day-to-nightside wind, the entire absorption signal is blueshifted (that is, the third column of Fig. 2).

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limb by the time of transit centre, implying that Fe condenses out of the gas phase on the planet nightside. The effects on the signature in the cross-correlation functions and in the orbital velocity–systemic velocity ($K_p – V_{sys}$) diagrams were recently explored by Wardenier et al.47, and are explained in Fig. 2.

Our analysis of the HARPS and HARPS-N observations of the WASP-189 system resulted in strong detections of nine species (Fe, Cr, Mg, Mn, Ti, V, Fe$^+$, Ti$^+$ and TiO), as well as tentative detections of five species (Na, Ca, Sc$^+$, Cr$^+$ and Ni) (Table 1, Fig. 3, Extended Data Figs. 5 and 6 and Methods). For most neutral atoms, we observed line depths consistent with models that assume local thermodynamic equilibrium (LTE) and hydrostatic and chemical equilibrium, as revealed by model injection (Extended Data Fig. 7). Strong absorption by metal ions is inconsistent with this class of models, as these are not predicted to be observable. Such departures from model predictions suggest that non-LTE effects, hydrodynamic escape or nightside condensation may be important for ultra-hot Jupiters48,49.

Some species show a significant blueshift compared with the systemic velocity of $-24.452 \pm 0.012 \text{ km s}^{-1}$ (ref. 14), indicative of day-to-nightside flows, as is commonly observed in hot gas-giant exoplanets15,17,20,24,25,29,40,50. These shifts are not all consistent with...
to the nightside condensation, combined with asymmetries in the wind. The apparent orbital velocity and the true planet rest frame are the same.

Overview of the detections of TiO, Ti, and Ti

Fig. 3 | Overview of the detections of TiO, Ti, Ti+, Fe, Fe++, Mg, V, and Mn. Rows 1–5: velocity–velocity (K_p–V_sys) diagrams showing the absorption signals of the detected species in the rest frame of the star. The horizontal opaque dashed lines indicate the orbital velocity at which the signals were extracted; see also Table 1. Rows 2–6: best-fit two-dimensional Gaussian models to the signatures visible in the top panels (Methods). The best-fit orbital velocities including 1σ uncertainties are shown in the panels as white bars. The uncertainty for V corresponds to 1σ.Dashed lines indicate the slopes of the best fit. Rows 3–7: residual K_p–V_vma diagrams after subtraction of the best-fit two-dimensional Gaussian models. Rows 4–8: cross-correlation functions stacked in the rest frame according to the best-fit orbital velocities stated in Table 1. The shaded region indicates the expected 1σ uncertainty. Dashed lines show expected signal strengths, obtained by injecting and recovering the signatures of model spectra, assuming isothermal atmospheres at 2,000 K (red) and 3,000 K (orange). The strong departure from model predictions of the cross-correlation function for Fe++ suggests that non-LTE effects, hydrodynamic escape or nightside condensation may be important for ultra-hot Jupiters.04,47.
of TiO in the transmission spectrum of an exoplanet, and may be the first robust detection of this molecule in the atmosphere of any exoplanet. Importantly, we conclude that, even for planets at high temperatures such as WASP-189 b, TiO may be a major source of stratospheric heating, in addition to atomic metals that absorb efficiently at short wavelengths\textsuperscript{49}.
As more ultra-hot Jupiters are being observed with sensitive high-resolution spectrographs on large ground-based telescopes and space-based observatories such as the James Webb Space Telescope, our observations empirically demonstrate that the three-dimensional nature of these atmospheres and that insights derived from GCMs, atmospheric chemistry and radiative transfer are unified. Observations of hot Jupiters have exhausted the flexibility of one-dimensional models, providing strong motivation for innovations in data analysis techniques, numerical modelling and fundamental atmospheric theory.

Methods

Observations, data reduction and telluric correction. Transit observations with HARPS were performed on the nights of 14 April, 25 April and 14 May 2019. Earlier observations covering a partial transit were performed on the night of 26 March 2018 and have previously been published14. A fifth night of observations covering a full transit was performed on the night of 6 May 2019, using HARPS-N. A log of the observations is provided in Supplementary Table 1.

All science observations are performed with fibre A on the target and fibre B on the sky. Due to weather circumstances, observations on the night of 25 April 2019 started when the planet was already in transit and hence offer no baseline before the transit event. Similarly, the night of ref. 11 covers only half a transit.

All HARPS observations were reduced using the HARPS Data Reduction Software version 3.8. Earth’s atmospheric telluric lines were removed using Molecfit. A moleculine function was applied to the one-dimensional spectra of the night sky to build a model for the telluric transmission spectrum of the entire wavelength range covered by HARPS. This model was run for each exposure in each time series and for all nights individually. Because the HARPS spectra are given in the barycentric rest frame of the Solar System, we used the Earth barycentric radial velocity values to shift each exposure back into the rest frame of the instrument. This step is necessary to ensure correct modelling of the telluric lines with Molecfit. Regions containing strong H2O and O2 absorption lines around 959, 630 and 647.5 nm were used to fit the model, selecting small wavelength ranges that contain telluric lines surrounded by a flat continuum where no stellar lines are present. The telluric models thus obtained were then interpolated onto the same wavelength grid as the individual spectral orders of HARPS and finally divided out to remove telluric effects.

In addition to spectral observations with HARPS, we obtained simultaneous photometric observations with the EulerCam instrument on the Euler–Swiss telescope at La Silla Observatory, during two of the four transit events considered in this study, on the nights of 14 April 2019 and 24 April 2019. Although not expected for hot J stars, these observations were aimed at detecting photometric variability due, for example, to stellar spot crossings or outbursts. The data were reduced using standard methods14. Extended Data Fig. 2 shows the phase-folded light curve, fitted with a standard model15, multiplied by a baseline model consisting of a second-order polynomial in the target peak count level and a linear trend in time, using CONAN. No variability of astrophysical origin was identified, and later observations by CHEOPS also did not reveal significant variability in this host star14.

Preparatory corrections. After removal of telluric lines, further preparatory corrections were made. Individual spectra were Doppler-shifted to the rest frame of the host star by correcting for the Earth velocity around the barycentre of the Solar System as well as the radial velocity of the star caused by the orbiting planet, so that the stellar spectrum had a constant velocity shift consistent with the systemic velocity of —26 km s−1. Following Hoeijmakers et al.17, we corrected 5σ outliers from the spectral time series by applying an order-by-order sigma-clipping algorithm with a running median absolute deviation computed over sub-bands of the time series with a width of 40 pixels. We further manually flagged spectral columns with visible systematic noise caused mainly by residuals of deep telluric lines. For each of the nights, this did not affect more than 1.6% of the total number of spectral pixels in each time series. In the case of TiO, only selected wavelength regions beyond 460 nm were included, where the line list is known to be relatively accurate18. The excluded wavelength ranges were up to 460 nm, 507.2–521.6 nm, 568.8–580.6 nm, 590.9–615.4 nm and 621.0–628.0 nm. Also following Hoeijmakers et al.17, we performed a colour correction by fitting low-order polynomials to approximate the flaring shape of the signatures that is characteristic between strong lines in the cross-correlation templates and the telluric absorption lines obscured by the transitting planet. Because the planet is on a near-polar orbit, these aliases take the form of near-vertical structures in the cross-correlation functions. To remove these, and any other systematic noise constant in radial velocity as a function of time, we fitted and subtracted a polynomial of degree one at each column of the parts of the two-dimensional cross-correlation functions that correspond to in-transit exposures. In addition, we used a Gaussian high-pass filter with a width of 100 km s−1 to remove broadband structures in the spectral direction6,20. The results of these cleaning steps are shown in Extended Data Fig. 1 and Supplementary Fig. 1.

Shift into the rest frame of the planet and fitting. The resulting detrended, cleaned, two-dimensional cross-correlation functions were shifted towards the expected rest frame of the planet, assuming a value for the orbital velocity. To make sure that no Doppler-shadow removal residual unintentionally adds to the signal of the planet, we masked out the overlapping region at the planetary radii. To convolve in-transit cross-correlation functions, they were weighted according to the mean flux of their corresponding spectra, yielding a flux-weighted, time-averaged one-dimensional cross-correlation function for each assumed orbital velocity. This resulted in maps of the cross-correlation of each species in the orbital velocity–systemic velocity space, where the peak of the planetary signal is expected to be located at the true orbital and systemic velocities in the absence of atmospheric dynamics. To combine the cross-correlation functions of the four independent transits we averaged the Ki–Vs maps, similarly weighting them according to the total in-transit flux recorded by HARPS(N) during each observation.

We performed an analysis to extract the line shape, depth and location in Ki–Vs space, by fitting a two-dimensional Gaussian model that allows for correlation between the orbital and systemic velocities via a rotation parameter to the signature in K–Vs space (Fig. 3), with parameters described by low-order polynomials to approximate the flaring shape of the signatures that is characteristic of transit time series. This model is evaluated at steps of 25 km s−1 in K, to

\[
C(v, t) = \sum_{\lambda=0}^{\Lambda} F(\lambda, T(v)) \int_{v_{\lambda}}^{v_{\lambda+1}} \frac{d\lambda}{\Delta \lambda} \int_{t_{\lambda}}^{t_{\lambda+1}} \frac{dT}{\Delta T}
\]

where F(\lambda, T) are the spectra of the time series, that is all spectral points in all echelle orders of the spectrum obtained at a given time t, and T(\lambda) are the corresponding values of the template Doppler-shifted to a radial velocity v. T(\lambda) takes non-zero values within the spectral lines of interest and is normalized such that \(\sum_{\lambda=0}^{\Lambda} T(\lambda) = 1\). This procedure generates the two-dimensional cross-correlation functions for each night of observations and each species. The uncertainty intervals are determined through Gaussian error propagation of the expected photon noise on the individual spectra.

Cleaning steps. Removal of the Doppler shadow. During transit the planet partially obscures areas of the rotating star. This obscured area introduces residual spectral lines when performing differential transmission spectroscopy, which create a spurious cross-correlation signal called the Doppler shadow. Generally, this feature occurs at an apparent radial velocity that is different from the planetary atmosphere, and can thus be removed without affecting the planetary signature. This is especially true for WASP-189 b, which resides on a polar orbit18, resulting in a Doppler-shadow residual that is nearly constant in radial velocity, as also observed for KELT-9b20. We constructed empirical models of the Doppler shadow for neutrals as well as ions using the cross-correlation functions of Fe and Fe+ respectively by fitting a Gaussian profile of which the centroid velocity is prescribed following Cegla et al.19, while the amplitude and width are allowed to vary according to low-order polynomials, to capture variations related to limb darkening and gravity darkening of the host star. We fitted a second Gaussian component to correct for the wide, negative pseudoabsorption inherent to the Rossiter–McLaughlin effect in normalized spectra. These two components form a model that is subtracted from the cross-correlation function of each of the species, multiplied by a scaling factor in a least-squares manner (Extended Data Fig. 1 and Supplementary Fig. 1), following Hoeijmakers et al.17. During this removal we protected the planetary signature by masking out the radial velocity range of the planet at each orbital phase when fitting the Doppler shadow.

Detrending correlated noise and aliases. After removing the Doppler shadow, some correlated structure was still present in the two-dimensional cross-correlation function between the times of ingress and egress, mainly caused by residual telluric correlations between strong lines in the cross-correlation templates and the telluric absorption lines obscured by the transiting planet. Because the planet is on a near-polar orbit, these aliases take the form of near-vertical structures in the cross-correlation functions. To remove these, and any other systematic noise constant in radial velocity as a function of time, we fitted and subtracted a polynomial of degree one at each column of the parts of the two-dimensional cross-correlation functions that correspond to in-transit exposures. In addition, we used a Gaussian high-pass filter with a width of 100 km s−1 to remove broadband structures in the spectral direction6,20. The results of these cleaning steps are shown in Extended Data Fig. 1 and Supplementary Fig. 1.
diminish the strong correlation between values in the vertical direction of the $K_p - V_p$ diagram: in our time series, a change in $K_p$ of 25 km s$^{-1}$ causes a relative shift of 2 km s$^{-1}$ in exposures taken 45 min apart. Given that the cross-correlation function is evaluated in steps of 2 km s$^{-1}$ to eliminate correlation between adjacent cross-correlation function velocity steps, and that the transit duration is 4.3 h, two rows in $K_p - V_p$, space that are separated by 25 km s$^{-1}$ are constructed from cross-correlation function samples of which more than 80% are unique. Because the templates were broadened to a full-width at half-maximum of 2.7 km s$^{-1}$ and the cross-correlation analysis was performed in steps of 2 km s$^{-1}$, only every second data point (that is every 4 km s$^{-1}$) and its corresponding uncertainty were used to fit the Gaussian profile to mitigate correlations between neighbouring cross-correlation points. We therefore treat 25 km s$^{-1}$ steps in $K_p$ and 4 km s$^{-1}$ steps in radial velocity as statistically independent from each other, allowing us to fit a two-dimensional model to the signatures in the $K_p - V_p$ diagram while assuming independently normally distributed uncertainties. At these observed orbital velocities of the signals (Table 1), we extracted the one-dimensional cross-correlation function and fitted a Gaussian to the peak of the cross-correlation function at the location of the systemic velocity to measure the line depth of the detected absorption. The fitting results are shown in Table 1. Even though candidate signals of Ca, Mg, Na, Ni, and Sc are found with confidence larger than 3σ, we conservatively choose to classify these as tentative, on the basis of their having anomalous centre positions or widths, or extended shapes in $K_p - V_p$ space. All species classified as tentative have formal confidence levels less than 5σ, while all claimed detections are at levels of 5σ or greater. Compared with the systemic velocity of $-2.452 \pm 0.012$ km s$^{-1}$ (ref. 19), most spectra are significantly blueshifted, even if the radial velocity of ref. 19 suffered from larger than expected uncertainties, at the level of approximately 0.1 km s$^{-1}$. This indicates the presence of a day-to-nightside wind at the level of several kilometres per second, similar to what has been observed in other hot Jupiters (ref. 20).

Model injection. Following the procedure of Hoeijmakers et al.19, modelled transmission spectra for WASP-189 b were injected at two temperatures (2,500 K, close to the planetary equilibrium temperature of 2,641 K, ref. 11, and 3,000 K, between the equilibrium temperature and the dayside temperature of 3,400 K, ref. 11), assuming the planet’s atmosphere to be isothermal, in chemical and hydrostatic equilibrium and of solar metallicity. The planetary parameters such as the planetary radius and the surface gravity were adopted from Lendl et al.11 (see also Extended Data Fig. 4), assuming a reference pressure of 10 bar at a radius of 1.619 $R_p$. We used FastChem64 to calculate the chemical abundance profiles and followed the radiative transfer procedure as performed in ref. 55.Opacity functions of 128 atomic neutrals and individual ions were included in this model, as well as H$_2$O, TiO and CO. These were computed using the open-source HELIOS K opacity calculator67 from line lists provided by VALD and ExoMol for atoms and molecules, respectively (ref. 68).

The model spectra are full forward models, including continuum and accurate line depths and profiles. No additional normalization is performed for the purpose of injection. The modelled transmission spectra were injected into the observed spectra before cross-correlation, allowing for comparison with the observed line depths. The two-dimensional cross-correlation functions of the observed time series were then subtracted from the injected two-dimensional cross-correlation functions, effectively leaving a residual signature that signifies the predicted line depth of the model. The two models are shown in Extended Data Fig. 7.

Determination of orbital velocity and stellar mass. The orbital velocity is a key observable in the application of the high-resolution cross-correlation technique1,20. For each of the five nights, we fitted a two-dimensional Gaussian model to the $K_p - V_p$ diagram that was obtained using the template containing all 131 considered sources of line opacity at 3,090 K. This fit provided the best-fit combination of both orbital and systemic velocities for each of the nights. In the two-dimensional cross-correlation function, the radial velocity of the planetary absorption lines is expected to occur at $V_{\text{sys}} = V_{\text{sys}} \sin i \phi + V_{\text{rv}}$.

$$V_{\text{sys}} = V_{\text{sys}} \sin i \phi + V_{\text{rv}}$$

where $\phi$ is the orbital phase of the planet and $i$ the inclination of the system. We denoted by $V_{\text{sys}} \sin i = K_p$ the projected orbital velocity as seen from Earth. Using Kepler’s third law and the lever rule $(a u_2 = M/\mathcal{M})$, the sum of the mass of the star and the planet is found to be

$$M_p + M_\star = \frac{P}{2\pi G} \left( \frac{K_p}{K_p} + 1 \right) \frac{\sin i}{\sin i} \frac{1}{3 \sqrt{1 + \frac{1}{3}} \sqrt{\frac{K_p}{K_p}} \sqrt{1 + \frac{1}{3}} \sqrt{\frac{K_p}{K_p}}$$

$$= \frac{P}{2\pi G} \left( \frac{K_p}{K_p} + 1 \right) \frac{1}{3 \sqrt{1 + \frac{1}{3}} \sqrt{\frac{K_p}{K_p}} \sqrt{1 + \frac{1}{3}} \sqrt{\frac{K_p}{K_p}}$$

where $P$ is the orbital period of the planet. Using the centre of mass of the system, the following relationship between the mass of the planet $M_p$, the mass of the star $M_\star$, the orbital velocity $v_{\text{sys}}$ (equal to $K_p$), and the stellar radial velocity amplitude $K_\star$ holds:

$$\frac{M_p}{M_\star} = \frac{K_\star}{K_p}$$

The combination of equations (3) and (4) results in the stellar mass given by

$$M_p = \frac{P K_\star}{2\pi G} \left( 1 + \frac{K_\star}{K_p} \right)^2$$

Supplementary Table 2 summarizes the results for the projected orbital velocity, the systemic velocity and the calculated stellar mass. On the basis of the orbital velocity and assuming a circular orbit, we find a stellar mass of 2.08 ± 0.14 $M_\odot$, which is consistent with the mass reported by Lendl et al.20 (2.030 ± 0.066) as determined via spectral synthesis modelling.

The radial velocity of the planet of $v_{\text{rv}} = -27.2 \pm 0.2$ km s$^{-1}$ is smaller than the true systemic velocity of $-24.452 \pm 0.012$ km s$^{-1}$ as previously measured11, indicating the effect of atmospheric winds blueshifting the atmospheric absorption lines.

The stellar spectrum. To determine stellar parameters of the host star we synthesized spectra using the spectral synthesis code Spectroscopy Made Easy (SME, version 580, private communication)23, and compared them with the observed spectra. SME interpolates in a grid of one-dimensional MARCS atmosphere models24, which are hydrostatic model atmospheres in plane parallel geometry, computed assuming LTE, chemical equilibrium, homogeneity, and conservation of the total flux (radiative plus convective, the convective flux being computed using a mixing-length recipe). This code has the advantage that it includes a flexible $\chi^2$ minimization tool for finding the solution that fits an observed spectrum in a prespecified spectral window. The code also includes a powerful continuum normalization routine able to account for suppressed continuum levels as prescribed by a theoretical model, as it is evaluated against the observed spectrum. In the spectrum of a warm fast-rotating star extra care is needed to normalize the spectrum, as the extreme line broadening can suppress the continuum. Using SME, we find the following stellar parameters: the effective temperature of the star $T_{\text{eff}} = 7,990 \pm 90$ K, the surface gravity log $g = 3.5 \pm 0.3$, the metallicity $[\text{Fe}/\text{H}] = 0.24 \pm 0.15$, the projected stellar rotation speed $v_{\text{rot}} = 96.2 \pm 5$ km s$^{-1}$ and the microturbulent velocity $v_{\text{mic}} = 2.6 \pm 0.3$ km s$^{-1}$. These are consistent with values previously published25. Extended Data Fig. 3 shows the spectrum of WASP-189 b at the position of three out of the 20 analysed Fe lines.

Transmission spectroscopy of the Na doublet. For the extraction of the planetary sodium lines in the observations of the nights of 26 March 2018, 14 April 2019, 25 April 2019 and 14 May 2019, we followed previous work26,27. The spectra were corrected for the blaze, cosmic rays and telluric absorption lines. Telluric sodium is monitored with the detector’s fibre B on the sky and was detected in all four nights of observations. The affected bins were masked during the rest of the analysis. We also masked the entire area occupied by the Doppler shadow of sodium, which is not expected to overlap substantially with the planetary absorption due to the near-polar orbit28. For robustness, the partial transits were not included in the analysis presented here. Extended Data Fig. 6 shows the transmission spectrum of WASP-189 b at the wavelength of the Na D doublet.

The possibility of false positive detections was assessed for each night via a bootstrapping method based on ref. 29, where each run was performed with 15,000 iterations; for further details see previous work27,30. The results are shown in Supplementary Fig. 2.

The false positive likelihood is estimated for the two nights at 0.076% and 0.085% respectively. The combined line depth for the sodium doublet is 15.3 ± 3.1 (x10$^{-4}$), equivalent to 4.9σ, following the calculation of the detection level in ref. 25.

Bootstrap analysis for robustness of candidate signals. To confirm the robustness of detected species, we performed two different types of bootstrap analysis following the approach in ref. 71. The first method tests that the signal originates uniformly from in-transit exposures and that it does not appear in out-of-transit exposures. The second method tests the distribution of candidate signals caused by correlated noise in the cross-correlation functions, essentially ensuring that the detected signal is not the result of systematic noise. Detailed descriptions of the bootstrap methods can be found in Appendix A of ref. 29. We classified the species as a detection only if both bootstrap methods confirmed the robustness. The bootstrap results are shown in Supplementary Figs. 3–10.

In the example of Na, we performed two different analyses, which result in two different bootstrap results (Supplementary Figs. 2 and 9). Supplementary Fig. 9 includes the bootstrap results for sodium based on our cross-correlation analysis. Using cross-correlations only, it is not possible to extract a sodium signal, which is why sodium is classified as tentative (Table 1). Analysing the sodium doublet following previous work27,29,30, we detect sodium at a combined line depth of 15.3 ± 3.1 (x10$^{-4}$), equivalent to 4.9σ, which we do not classify as a robust detection (5σ limit).

Data availability

Raw data as well as pipeline-reduced data from which the findings that are presented in this paper are derived are publicly available from the data archives of the European Southern Observatory (ESO) and the Galileo (TNG). Cross-correlation templates and models are available upon reasonable request. Precomputed opacity functions are publicly available via http://dace.unige.ch/opacity.
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Author contributions

B.P. performed the data analysis (including applying computer code originally written by H.J.H.), produced all of the figures except Extended Data Figs. 2 and 8, co-led the scientific vision and co-led the writing of the manuscript. H.J.H. provided the computer code that was the basis and starting point for the data analysis, mentored B.P. on data analysis techniques, co-led the scientific vision and co-led the writing of the manuscript. D.K. performed radiative transfer calculations used to construct the cross-correlation templates and model spectra. E.S. performed FastChem calculations and produced Extended Data Fig. 8. J.V.S. investigated the fidelity of specific spectral lines, performed supporting EulerCam observations and provided the code, expertise and results to produce Supplementary Figs. 6 and 7. M.L. analysed the EulerCam data and produced Extended Data Fig. 2. N.W.B. cowrote the manuscript. B.T. constructed a model of the stellar spectrum and provided technical support throughout the analysis procedure. H.J.H., D.R.A. and D.B. performed HARPS observations. K.K. performed supporting EulerCam observations. A.G.-M. proofread the manuscript. S.G. provided guidance on optics. H.M.C., M.H., B.M.M. and L.P. provided substantial feedback on the manuscript. H.J.H., D.K., J.V.S., R.A., V.B., H.M.C., D.E., C.F., C.L., S.G., M.O. and K.H. were all coinvestigators on the ESO proposal for open time in observing period 103 that led to the procurement of the data. K.H. co-led the scientific vision, cowrote the manuscript, guided its narrative and formulation and assisted with formatting.

Competing interests

The authors declare no competing interests.

Additional information

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Extended Data Fig. 1 | Illustration of Doppler shadow subtraction and detrending of the cross-correlation function for the time series observed on April 14, 2019, with the Fe template at 3,000 K (see Methods). Top panel: Raw two-dimensional cross-correlation function. During the transit, the Doppler shadow emerges as the positive near-vertical structure. Time of first, second, third and fourth contact as predicted using the ephemeris of Lendl et al. (2020) are indicated as dashed lines. Middle panel: Best-fit model of the Doppler shadow. Bottom panel: Residuals after subtracting the best-fit model from the raw cross-correlation function (top panel) and application of a detrending algorithm in the vertical direction. The absorption signature of the planet atmosphere is visible as the slanted feature, Doppler-shifted to the instantaneous radial velocity of the planet. The residual of the Doppler shadow at the end of the transit is masked during further analysis.
Extended Data Fig. 2 | Phase-folded light-curve as observed with EulerCam on the nights of 2019-04-14 and 2019-04-24. No astrophysical sources of variability are detected.
Extended Data Fig. 3 | Three Fe lines in the spectrum of WASP-189. The black lines correspond to the observed spectrum, the red dashed lines correspond to the best fit using a metallicity of $[\text{Fe/H}] = 0.24$. The blue shaded regions indicate the fit with $\pm 0.15$ metallicity uncertainty.
### Planetary Parameters

| Parameter                          | Value          |
|-----------------------------------|----------------|
| Planet Radius \(R_p\) [\(R_{\text{Jup}}\)] \(^{(a)}\) | 1.619 ± 0.021  |
| Planet Mass \(M_p\) [\(M_{\text{Jup}}\)] \(^{(a)}\)     | 1.99\(^+0.16\)\(\_0.14\) |
| Equilibrium temperature \(T_{\text{eq}}\) [K] \(^{(b)}\) | 2641 ± 31      |
| Day-side temperature \(T_{\text{day}}\) [K] \(^{(a)}\) | 3353\(^+27\)\(\_34\) |
| Surface gravity \(g_p\) [m s\(^{-2}\)]       | 18.8\(^+2.1\)\(\_1.8\) |

### Stellar Parameters

| Parameter                        | Value          |
|----------------------------------|----------------|
| Stellar Radius \(R_\ast\) [\(R_{\odot}\)] \(^{(a)}\) | 2.36 ± 0.030   |
| Stellar Mass \(M_\ast\) [\(M_{\odot}\)] \(^{(a)}\) | 2.030 ± 0.066  |
| Proj. rot. velocity \(v \sin I_\ast\) [km s\(^{-1}\)] \(^{(a)}\) | 93.1 ± 1.7     |
| Systemic velocity \(v_{\text{sys}}\) [km s\(^{-1}\)] \(^{(a)}\) | -24.452 ± 0.012 |

### Orbital and Transit Parameters

| Parameter                          | Value                           |
|-----------------------------------|---------------------------------|
| Mid-transit time \(T_0\) [BJD\(_{\text{TT}}\)-2,450,000] \(^{(a)}\) | 8926.5416960\(^+0.000065\)\(\_0.000064\) |
| Orbital semi-major axis \((a)\) [au] \(^{(a)}\) | 0.05053 ± 0.00098               |
| Scaled semi-major axis \((a/R_\ast)\) \(^{(a)}\) | 4.60\(^+0.009\)\(\_0.012\)     |
| Orbital inclination \((i)\) [\(^{\circ}\)] \(^{(a)}\) | 84.03 ± 0.14                    |
| Projected orbital obliquity \(\lambda\) [\(^{\circ}\)] \(^{(a)}\) | 86.4\(^+2.9\)\(\_4.4\)        |
| Eclipse duration \((T_{14})\) [h] \(^{(a)}\) | 4.3336\(^+0.0054\)\(\_0.0058\) |
| Radius ratio \((R_p/R_\ast)\) \(^{(a)}\) | 0.07045\(^+0.00013\)\(\_0.00015\) |
| RV semi-amplitude \((K)\) [km s\(^{-1}\)] \(^{(a)}\) | 0.182 ± 0.013                   |
| Period \((P)\) [d] \(^{(b)}\) | 2.7240330 ± 0.0000042               |
| Eccentricity \(^{(c)}\)          | 0                               |

### Derived Parameters

| Parameter                      | Value          |
|-------------------------------|----------------|
| Orbital velocity \(v_{\text{orb}} = 2\pi a/P\) [km s\(^{-1}\)] | 200.7 ± 4.9    |
Extended Data Fig. 5 | Signals of Cr\(^+\), Sc\(^+\), Na, Ni and Ca classified as tentative. All of these species have previously been observed in other ultra-hot Jupiters\cite{19,25}. The shaded region indicates the expected \(1\sigma\) uncertainty. Dashed lines show expected signal strengths, obtained by injecting and recovering the signatures of model spectra, assuming isothermal atmospheres at 2,000 K (red) and 3,000 K (orange) respectively.
Extended Data Fig. 6 | Transmission spectrum of WASP-189b at the wavelength of the Na D-doublet. The lines are fit assuming a Gaussian line-shape, resulting in an average line depth of $15.3 \pm 3.1 \times 10^4$, equivalent to 4.9$\sigma$. 
Extended Data Fig. 7 | Two injected models of the transmission spectrum of WASP-189 b at 2,500 K (purple) and 3,000 K (blue). We assumed chemical equilibrium and solar metallicity. The models are sampled at their native resolution as set by intrinsic line broadening, and not additionally broadened to match e.g. the planetary rotation or the instrumental resolving power, although such broadening terms are taken into account when injecting these templates into the data. The inset plot shows the wavelength region between 495.4 and 495.8 nm, where a molecular band head of TiO is visible.
Extended Data Fig. 8 | Model of the abundances of key selected species as a function of pressure (inverse altitude) at a temperature of 2,500 K, assuming thermo-chemical equilibrium and solar metallicity, computed with FastChem\textsuperscript{66}. Solid lines correspond to atomic species, dashed lines to ionised species and the dotted line to TiO.