Sensitive Probing of Exoplanetary Oxygen via Mid Infrared Collisional Absorption

Thomas J. Fauchez[1,2,3], Geronimo L. Villanueva[1,3], Edward W. Schwieterman[4,5,6,7,8], Martin Turbet[9], Giada Arney[1,3,7], Daria Pidhorodetska[1,10], Ravi K. Kopparapu[1,3,7], Avi Mandell[1,3], and Shawn D. Domagal-Goldman[1,3,7]

[1]NASA Goddard Space Flight Center, Greenbelt, Maryland, USA
[2]Goddard Earth Sciences Technology and Research (GESTAR), Universities Space Research Association, Columbia, Maryland, USA
[3]GSFC Sellers Exoplanet Environments Collaboration
[4]Department of Earth and Planetary Sciences, University of California, Riverside, California, USA
[5]NASA Postdoctoral Program, Universities Space Research Association, Columbia, Maryland, USA
[6]NASA Astrobiology Institute, Alternative Earths Team, Riverside, CA, USA
[7]Nexus for Exoplanet System Science (NExSS) Virtual Planetary Laboratory, Seattle, WA, USA
[8]Blue Marble Space Institute of Science, Seattle, Washington, USA
[9]Observatoire Astronomique de l'Université de Genève, Université de Genève, Chemin des Maillettes 51, 1290 Versoix, Switzerland.
[10]University of Maryland Baltimore County/CRESST II , 1000 Hilltop Cir. Baltimore, MD 21250, USA

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Abstract

The collision-induced fundamental vibration-rotation band at $6.4\ \mu m$ is the most significant absorption feature from O_2 in the infrared (1; 2; 3), yet it has not been previously incorporated into exoplanet spectral analyses for several reasons. Either CIAs were not included or incomplete/obsolete CIA databases were used. Also, the current version of HITRAN does not include

1

CIAs at $6.4~\mu m$ with other collision partners (O_2-X). We include O_2-X CIA features in our transmission spectroscopy simulations by parameterizing the $6.4~\mu m$ O_2-N_2 CIA based on (3) and the O_2-CO_2 CIA based on (4). Here we report that the O_2-X CIA may be the most detectable O_2 feature for transit observations. For a potential TRAPPIST-1e analogue system within 5 pc of the Sun, it could be the only O_2 detectable signature with JWST (using MIRI LRS) for a modern Earth-like cloudy atmosphere with biological quantities of O_2. Also, we show that the $6.4~\mu m$ O_2–X CIA would be prominent for O_2-rich desiccated atmospheres (5) and could be detectable with JWST in just a few transits. For systems beyond 5 pc, this feature could therefore be a powerful discriminator of uninhabited planets with non-biological "false positive" O_2 in their atmospheres - as they would only be detectable at those higher O_2 pressures.

Main

We study the strength of the O_2-X CIA spectral signatures in exoplanets by computing synthetic spectra for various Earth-like atmospheres with the Planetary Spectrum Generator (PSG (6)). The atmospheres are created with the LMD-G (7) general circulation model (GCM) coupled with the Atmos (8) photochemical model (see Methods for details). We focus in particular on planets around M dwarfs such as TRAPPIST-1e. In fact, For modern Earth atmospheric conditions, the $6.4~\mu m$ region is overlapped by a wide H_2O absorption band. However, for a modern Earth-like atmosphere on a tidally locked planet in the HZ of an M dwarf, the terminator region is predicted to be fairly dry (see Supplementary Figure 2). Also, water is mostly confined in a small portion of the atmosphere near the surface and which is under the refraction limit and hidden by clouds (as on Earth, where the troposphere is wet and the stratosphere is dry). Near TOA, H_2O is highly photodissociated (Supplementary Figure 2). The H_2O signature in the transmission spectra of a habitable planet is therefore expected to be very weak (9; 10). While some trace gases such as NO_2 and N_2O also produce opacity in this spectral region, their concentrations are predicted to be orders of magnitude lower than those that would generate confounding impacts on the simulated spectra.

The TRAPPIST-1 system (11), consisting of seven Earth-sized planets orbiting an ultra-cool dwarf star, will be a favorite target for atmospheric characterization with JWST due to its relatively close proximity to the Earth and the depth and frequency of its planetary transits. Therefore, we use TRAPPIST-1e as a case study for our simulated spectra. We employed the LMD-G (7) general circulation model (GCM) and the Atmos photochemical model (8) to simulate TRAPPIST-1e with boundary conditions similar to modern Earth (9). Figure 1 shows TRAPPIST-1e transmission spectra from 0.6 to 10 μm for various Earth-like atmospheres simulated with the Planetary Spectrum Generator (PSG, (6)). The top panel shows the impact of cloud coverage on spectral fea-

2

tures: clouds diminish the strength of all absorption features, but impact the strength of the O_2-X feature much less strongly than they impact shorter wavelength O_2 features like the O_2 A–band or the 1.06 and 1.27 μm O_2 CIA used in **(author?)** (12) (who considered only clear-sky atmospheres). This is because water cloud opacity is stronger at short wavelengths. The middle panel compares the strength of the O_2-X CIA band to the overlapping H_2O absorption band near 6.4 μm for a cloudy atmosphere. O_2-X CIA strongly dominates the absorption in this wavelength range. The bottom panel shows how the strengths of O_2 monomer and CIA absorption features scale as a function of the O_2 atmospheric abundance for O_2 levels ranging from 0.1 times the present atmospheric level of O_2 (PAL) to 2 times PAL. Our results show that the 6.4 μm CIA feature appears to be about three times stronger than the 1.27 μm O_2 CIA feature and is therefore the strongest O_2 signature across the VIS/NIR/MIR spectrum.

Figure 2 shows the number of TRAPPIST-1e transits needed to detect the O_2 A–band, the O_2-O_2 CIA feature at 1.27 μm and the O_2-X CIA feature at 6.4 μm features at a 5 σ confidence level with JWST for a modern Earth-like cloudy atmosphere on TRAPPIST-1e orbiting a TRAPPIST-1-like star at distances from Earth ranging from TRAPPIST-1's true distance (12.1 pc) down to 2 pc. We can see that the 6.4 μm O_2-X CIA feature requires an order of magnitude fewer transits than the two other O_2 features because of the stronger intrinsic O_2-X CIA absorption at 6.4 μm and because cloud opacity is stronger at shorter VIS/NIR wavelengths. The horizontal dashed red line represents the 85 transits that will occur for TRAPPIST-1e during the 5.5 year nominal lifetime of JWST, thus sets up an upper limit on the number of transits observable. Because TRAPPIST-1e orbits a very small M8 star, it offers one of the best SNR a habitable planet can have and therefore represents a best-case scenario in terms of detectability. However, even in this context, none of the O_2 features are detectable at 5 σ at the distance of the TRAPPIST-1 system. However, the 6.4 μm O_2-X CIA feature could be detectable at 5 σ for an analogue system at star-Earth distance closer than 5 pc. Therefore, this simulation shows that the 6.4 μm O_2-X CIA could be the only oxygen feature detectable with JWST for a cloudy modern Earth-like atmosphere for nearby hypothetical TRAPPIST-1 analogue systems.

The O_2-X feature for oxygen could also potentially be used to detect non-habitable conditions, such as a desiccated atmosphere rich in bars of abiotic O_2 generated from massive ocean loss (13; 5; 14; 15; 16; 10). (9) have shown that for an assumed original water content of 20 Earth oceans (by mass), the TRAPPIST-1e, f and g planets may have lost between 3 to 6 Earth oceans resulting in atmospheres with 22 and 5,000 bars of O_2.

Figure 3 shows transit spectra for TRAPPIST-1e assuming conservative 1 bar O_2-only desiccated and isothermal atmospheres ranging from 200 to 600 K. Relative transit depth (ppm, left Y-axis) is the transit depth produced by the atmosphere itself, which can be converted into relative transit atmospheric thickness (km, right Y-axis). These isothermal profiles allow us to test the

3

sensitivity of oxygen spectral features on atmospheric temperature. The atmospheric scale height increases with temperature, and the largest features are seen for the highest temperatures. Note that O_2-O_2 CIA opacities in HITRAN are only provided in the 193 K–353 K temperature range. Therefore, for the isothermal profiles beyond 353 K we used the 353-K CIA coefficients. We can see that the 6.4 μm O_2-O_2 CIA feature is broad ($\sim$ 3 μm) and strong (40 to 90 ppm). The 1.27 μm O_2–O_2 CIA feature reaches a similar relative transit depth but is comparatively narrower (widths of ~ 0.2 μm). In addition, the continuum level for the shorter wavelengths is raised by Rayleigh scattering slope, reducing the NIR CIA relative transit depths to 50 to 80 ppm, respectively. Similarly, the O_2 A–band reaches very high transit depths (up to 110 ppm) but on a high continuum, which reduces its relative strength down to 95 ppm. The larger width of the O_2-X CIA feature at 6.4 μm allows us to bin down the data to a lower resolving power, improving the SNR and therefore compensating for a higher noise floor in the MIRI LRS range. Supplementary Table 1 presents the relative transit depth, 1 transit SNR and number of transits for 3 and 5 σ detections for TRAPPIST-1e assuming 1 and 22 bar desiccated atmosphere on TRAPPIST-1e and Supplementary Figure 3 is similar to Fig. 2 but for the 22 bar O_2 desiccated and isothermal atmospheres.

Interpreting an O_2 detection via the O_2-O_2 CIA band at 6.4 μm will be strengthened by constraining the concentration of O_2, and placing its presence in a broader atmospheric context. For HZ planets with a planet/star contrast comparable to TRAPPIST-1e and within 5 pc from the Sun, next-generation MIR observatories could detect O_2 in concentrations similar to modern Earth using the 6.4 μm O_2-X feature. In combination with detections of other MIR features from CH_4, H_2O, or N_2O, this would represent a strong biosignature with no known non-biological explanations (17). Note that there are 50 red dwarfs within 5 pc from the Sun (http://www.recons.org/TOP100.posted.htm).
For systems farther than about 5 pc and/or HZ planet orbiting earlier M dwarfs, JWST or future MIR observatories may be able to detect the 6.4 μm O_2-X feature only for O_2 concentrations orders of magnitude higher than those on modern-day Earth that would be indicative of a desiccated, O_2-rich, uninhabitable planet.

Detection of this feature for planets within the habitable zone (18; 19; 20) will test the hypothesis that the high luminosity pre-main sequence phase M dwarfs endure can render even current HZ planets uninhabitable (5). Finally, detection of this feature would answer the question of whether planets around M dwarfs can sustain an atmosphere.

Figure 1: Shown are Earth-like transmission spectra of TRAPPIST-1e. Panel A: the impact of cloud coverage on the atmosphere's spectral features. Panel B: a comparison of the strengths of the O_2-X CIA feature and the H_2O absorption band around 6.4 μm for a cloudy atmosphere. Panel C: the strength of O_2 monomer absorptions and CIA features as a function of the amount of O_2 in the atmosphere relative to PAL for a spectrum with clouds included. The O_2-X CIA could be the strongest O_2 feature across the VIS/NIR/MIR spectrum.

Figure 2: Number of TRAPPIST-1e transits needed for a 5 σ detection of the O_2 A–band (R=100), the O_2-O_2 CIA at 1.27 μm (R=100) and the O_2-X CIA at 6.4 μm (R=30) with JWST for the TRAPPIST-1 system moved from its distance to Sun (12.1 pc) down to 2 pc. The atmosphere is composed of N_2, 10,000 ppm of CO_2, 10 ppm of CH_4, 21% of O_2 with a surface pressure of 1 bar. Resolving power (R) has been optimized for each band to maximize the SNR. The horizontal dashed red line corresponds to the number of times TRAPPIST-1e will be observable transiting in front of TRAPPIST-1 during JWST 5.5 years life time (85 transits). The 6.4 μm O_2-X CIA requires much less transits than the O_2 A–band and the 1.27 μm O_2-O_2 CIA and can be detectable at 5 σ for a TRAPPIST-1/TRAPPIST-1e analogue system closer than 5 pc.

Figure 3: Transmission spectra for a 1 bar O_2 desiccated atmosphere on TRAPPIST-1e assuming various isothermal profiles. Depending on the temperature, the 6.4 μm O_2-O_2 CIA feature can reach between 40 to 90 ppm, which is comparable or larger to the O_2 A–band and 1.06 and 1.27 μm O_2 CIA features. No photochemistry is considered here so O_3 is missing in the spectra. Note that the increase of the relative transit atmospheric thickness and relative transit depth is due to the increase of the scale height with temperature.

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Methods

Parameters for TRAPPIST-1e   In this study, TRAPPIST-1e planet's parameters have been set up from (11; 21). The TRAPPIST-1 spectrum of (9) has been used for our photochemical simulations with the Atmos model.

Monomer and CIA pressure sensitivity   Monomer and CIA optical depths can be expressed by the following equations (12):

$$d\tau_{mono} = \sigma \rho dl = \sigma P/T dl \tag{1}$$

$$d\tau_{CIA} = k\rho^2 dl = k(P/T)^2 dl \tag{2}$$

with $d\tau_{mono}$ and $d\tau_{CIA}$ representing the monomer and CIA differential optical depths, respectively; σ and k are the monomer and CIA cross sections, respectively; ρ is the number density of the gas; P is the pressure; T is the temperature; and dl is the path length. $d\tau_{mono}$ is proportional to P and $d\tau_{CIA}$ to P^2, and this difference of sensitivity may be used to estimate the atmospheric pressure (12).

The atmospheric modeling   We use the Atmos (8) photochemical model to self-consistently simulate Earth-like atmospheres with a variety of O_2 partial pressures on TRAPPIST-1e. The terminator temperature, gas mixing ratio, vapor and condensed water (liquid and ice) profiles have been provided from the LMD-G (7) global climate model (GCM) simulations of a 1 bar TRAPPIST-1e

7

modern Earth atmosphere. In Atmos, some of the N_2 has been swapped for O_2 to obtain various O_2 PAL as shown in Fig. 1, both gases having no greenhouse effect except through pressure broadening or CIA, and 10,000 ppm of CO_2 and 10 ppm of CH_4 have been assumed. Due to the terminator atmospheric profiles varying with latitude, Atmos was used to calculate profiles for 98 latitude points, determined by the LMD-G latitude resolution.

Transmission spectra simulations The planetary spectrum generator (PSG, (6)) has been used to simulate JWST transmission spectra. PSG is an on-line radiative-transfer code that is able to compute planetary spectra (atmospheres and surfaces) for a wide range of wavelengths (UV/Vis/near-IR/IR/far-IR/THz/sub-mm/Radio) from any observatory, orbiter or lander and also includes a noise calculator. To compute the noise, PSG takes into account the noise introduced by the source itself (N_{source}), the background noise (N_{back}) following a Poisson distribution with fluctuations depending on $\sqrt{N}$ with N the mean number of photons received (22), the noise of the detector (N_D) and the noise introduced by the telescope (N_{optics}). The total noise being then $N_{total} = \sqrt{N_{source} + N_{back} + N_D + N_{optics}}$. This represents therefore a photon limited situation where N_{source} will largely dominate N_{total}.

For the Earth-like atmospheres, spectra were obtained for each of the 98 Atmos photochemical simulations and an average spectrum was computed. For the 1 and 22 bar O_2 desiccated atmospheres, isothermal profiles from 200 to 600 K were set up with 100% of O_2, ignoring photochemistry. To calculate the SNR and the number of transits needed for 3 and 5σ detection the resolving power has been optimized by adjusting the binning for each O_2 feature to maximize its SNR. SNR is calculated using the highest value in the band minus the nearest continuum value (this value therefore differ between the VIS (Rayleigh slope), NIR and MIR). The number of transits needed to achieve a Xσ detection is computed as the following equation:

$$N_{transits}^{X\sigma} = N_i * (X/SNR_i)^2 \tag{3}$$

with $X\sigma$ the confident level of value X, N_i is the initial number of transit at which SNR_i is computed. If SNR_i is estimated from 1 transit then $N_i = 1$ and the Eq. 3 could be simplified as:

$$N_{transits}^{X\sigma} = (X/SNR_i)^2 \tag{4}$$

O_2-X collision-induced absorption at 6.4 μm. This feature is associated with the fundamental band of O_2, and O_2 collisions with other partners (e.g. N_2, CO_2) can produce additional absorption at these wavelengths. This collision with other gases can be generally written as O_2-X, where "X" refers to the collision partner. Laboratory measurements (1; 23) and atmospheric analysis using Sun occultations (3) have revealed that nitrogen, the major constituent of modern Earth's atmosphere at 78% in volume, produces an O_2–N_2 absorption feature of a similar intensity as O_2–O_2 in the 6.4 μm region. Carbon dioxide

(CO_2) can also produce an O_2–CO_2 feature at these wavelengths, though this feature is weak for modern Earth-like CO_2 atmospheric abundances (approx. 400 ppm) but can be strong for exoplanets with CO_2 rich atmospheres (4). O_2-X CIA can also be produced with H_2O (24) as the collision partner due to the large electric dipole moment of H_2O, but no laboratory measurements exist for this feature.

Parameterization of the 6.4 μm feature   While the 6.4 μm region is known as the fundamental vibration-rotation band of O_2, only the O_2-O_2 CIA band is included in HITRAN (25). Knowing that Earth's atmosphere is mostly composed of N_2 and that the O_2-N_2 CIA have been shown to produce similar absorption to O_2-O_2 (1; 3; 23), it is important to include it in our simulations. We have parameterized the O_2-N_2 CIA in PSG assuming the same absorption efficiency as O_2-O_2 CIA (3) (see Supplementary Figure 1). For O_2-CO_2 CIA at 6.4 μm, we used experimental data of (4) to include that feature in PSG.

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Data availability   The data that support the plots within this paper and other findings of this study are available from the corresponding author upon reasonable request.

Author contributions   T.J.F. led the photochemistry and transmission spectroscopy simulations. G.L.V, E.W.S and M.T. derived parameterizations of the O_2-N_2 and O_2-CO_2 CIAs bands. T.J.F and G.A. wrote most of the manuscript. Every author contributed to the discussions and to the writing of the manuscript.

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