This work was written as part of one of the author's official duties as an Employee of the United States Government and is therefore a work of the United States Government. In accordance with 17 U.S.C. 105, no copyright protection is available for such works under U.S. Law. Access to this work was provided by the University of Maryland, Baltimore County (UMBC) ScholarWorks@UMBC digital repository on the Maryland Shared Open Access (MD-SOAR) platform.

Please provide feedback

Please support the ScholarWorks@UMBC repository by emailing scholarworks-group@umbc.edu and telling us what having access to this work means to you and why it’s important to you. Thank you.

nature astronomy

SUPPLEMENTARY INFORMATION

https://doi.org/10.1038/s41550-019-0977-7

In the format provided by the authors and unedited.

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, MD, USA. [2]Goddard Earth Sciences Technology and Research (GESTAR), Universities Space Research Association, Columbia, MD, USA. [3]GSFC Sellers Exoplanet Environments Collaboration, Greenbelt, MD, USA. [4]Department of Earth and Planetary Sciences, University of California, Riverside, CA, USA. [5]NASA Postdoctoral Program, Universities Space Research Association, Columbia, MD, 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, WA, USA. [9]Observatoire Astronomique de l'Université de Genève, 51 chemin de Pégase, Sauverny 1290, Switzerland. [10]University of Maryland Baltimore County/CRESST II, Baltimore, MD, USA. *e-mail: thomas.j.fauchez@nasa.gov

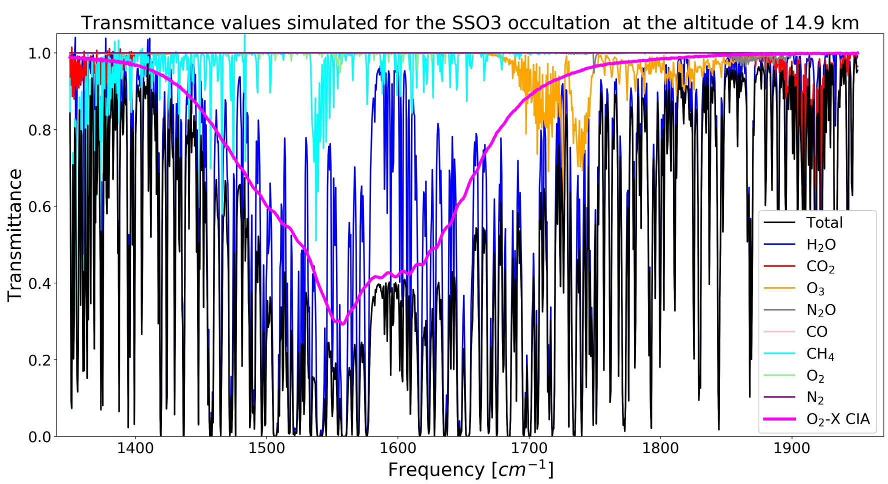
Supplementary materials for: Sensitive Probing of Exoplanetary Oxygen via Mid Infrared Collisional Absorption

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

November 7, 2019

Overview of previous works on O_2 spectral features for exoplanet's studies. Because O_2 is one of the most detectable and robust indicators of global biological activity, concepts for telescopes that would attempt to search for life on exoplanets all include the ability to detect O_2 or its photochemical byproduct, O_3. O_2 absorbs at several wavelengths in the visible (VIS) at 0.63, 0.69 and 0.76 μm and near-infrared (NIR) at 1.27 μm. The O_2 A–band at 0.76 μm has often been considered the most viable spectral feature for oxygen detection in transmission (1) and reflectance spectra (2). (1) showed that it could be possible to detect the O_2 A–band in the atmosphere of an Earth twin with the future Extremely Large Telescopes (ELTs). However large unknowns remain to disentangle the exoplanet O_2 signal the from the telluric O_2. Meanwhile, (3) showed that O_2–O_2 collision induced absorption (CIA) features at 1.06 and 1.27 μm were present in Earth's transmission spectrum during lunar eclipse and produce more absorption than the O_2 A–band monomer feature. CIA features are produced through inelastic collisions in a gas. In the case of the O_2–O_2 CIA features, the two O_2 molecules interact forming transient multipole-induced dipoles producing broad spectral features distinct from the individual underlying O_2 molecule. (4) showed that the 1.06 and 1.27 μm O_2–O_2 CIA features may be detectable (for SNR > 3) with the James Webb Space Telescope (JWST) for an Earth analogue orbiting an M5V star at a distance of 5 pc. (5) proposed that the 1.06 and 1.27 μm transit features could be used to identify the high O_2 partial pressures predicted to be associated with abiotic O_2 atmospheres, which should be significantly higher than for the modern Earth case. More recently, (6) have shown that the 1.06 and 1.27 μm O_2 CIA features could be detectable with JWST at a SNR of 5 in just few transits for the TRAPPIST-1 planets with O_2 desiccated and dense (10 and 100 bars) atmospheres.

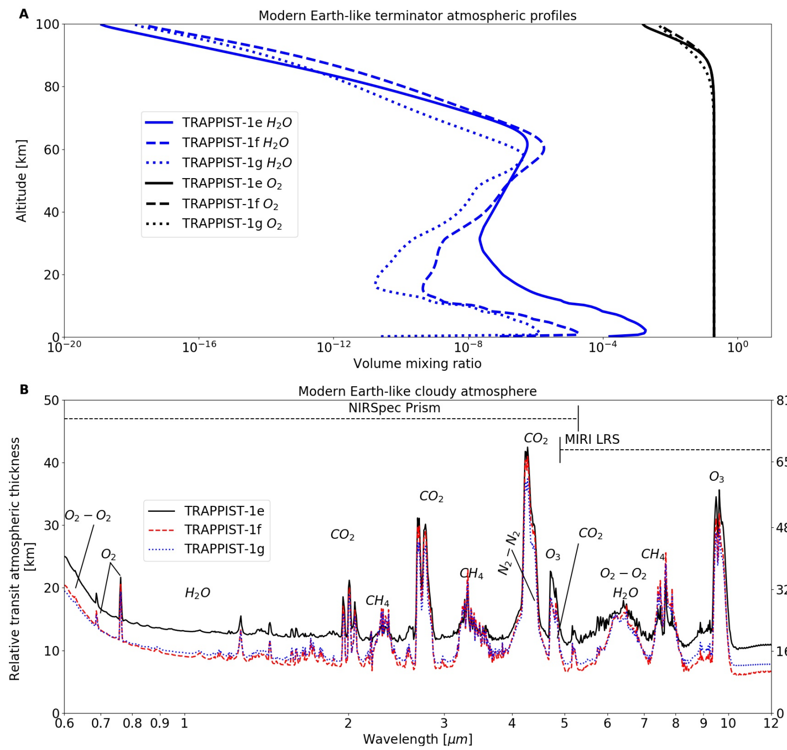


Supplementary Figure 1: Simulation with PSG of the SSO3 occultation observed by (7) April 30, 1985 at an altitude of 14.9 km over the latitude 32.3°N and longitude 290.6°W. Simulation of the 6.4 μm O_2-X CIA is in very good agreement with observation data from (7).

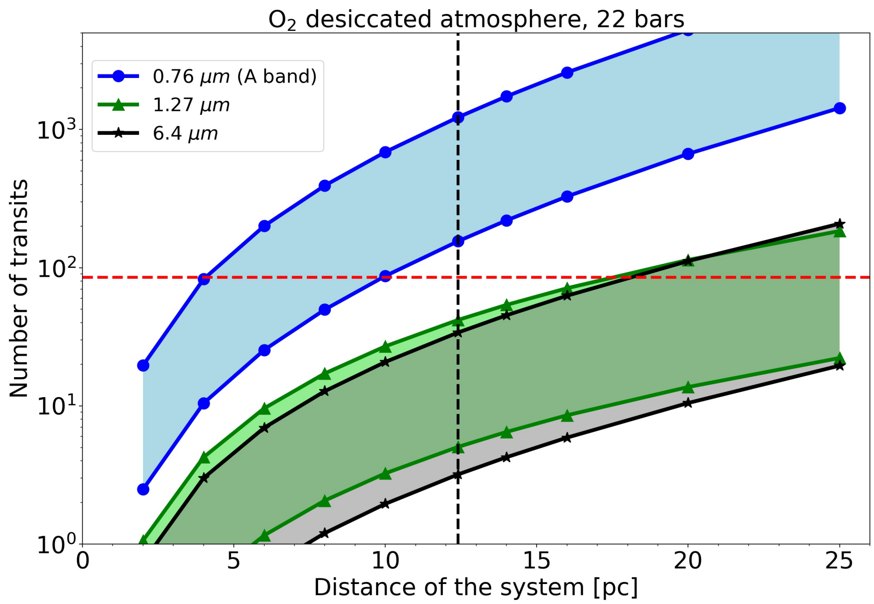
Supplementary Figure 1 shows the simulation of the Sun occultation SSO3 observed by (7) (figure 3) on April 30, 1985, at an altitude of 14.9 km (13 km over the Himalayas). Our simulation and the observation data are in very good agreement, showing the validity of our O_2-X CIA parameterization at 6.4 μm.

Supplementary Figure 2 shows the terminator H_2O and O_2 atmospheric profiles with a modern Earth-like atmosphere composition for TRAPPIST-1 planets in the habitable zone, namely 1e, 1f and 1g (top panel) and their transmission spectrum with clouds included (bottom panel). Boundary conditions for the photochemistry are those described in (8) Table 8. We can see that the terminator region is very dry, with volume mixing ratios near the surface reaching the maximum value 10^{-3} for TRAPPIST-1e decreasing down to 10^{-6} for 1g. However, as we can see in the spectra this region of maximum H_2O concentration is below the continuum level because of clouds and atmospheric refraction. Note that above $\sim$ 60 km H_2O is strongly photodissociated. As a results, the contribution of H_2O at 6.4 μm is very largely dominated by the O_2-X CIA and this domination increase for dryer planets TRAPPIST-1f and 1g.

Supplementary Figure 3 is similar to Fig. 2 but for the 22 bar O_2 desiccated and isothermal atmospheres presented in Table 1. We can see that the O_2-O_2 1.27 μm CIA and O_2-X 6.4 μm CIA features require significantly fewer transits than the O_2 A–band monomer band and would be detectable at up to about 25 pc (except for the coldest isothermal atmosphere beyond 20 pc). Note that in the case of a desiccated, O_2-rich planet with aerosols, the 6.4 μm band would require significantly fewer transits than the 1.27 μm for the same reasons as for the habitable case.



Supplementary Figure 2: Panel A: H_2O and O_2 atmospheric profiles at the terminator of TRAPPIST-1e, 1f and 1g planets in the habitable zone with a modern Earth-like atmosphere. Panel B: Corresponding transmission spectra for the three planets. We can see that H_2O volume mixing ratio is tiny by comparison to O_2 and that the wetter region near the surface is below the continuum level of the spectra because of the atmospheric refraction and/or clouds. O_2-X largely dominates over H_2O in the 6.4 μm region.



Supplementary Figure 3: 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=20) and the O_2-X CIA at 6.4 μm (R=10) with JWST for the TRAPPIST-1 system moved from 2 to 25 pc away from the Sun. The atmosphere is exclusively composed of O_2 with surface pressure of 22 bars. For each wavelength the shaded area correspond to various isothermal profiles from 600 K (lowest line) to 200 K (highest line). 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 transits during JWST 5.5 years life time (85 transits). The vertical dashed black line denotes the distance of the TRAPPIST-1 system with respect to the Sun. The O_2-O_2 CIA at 1.27 μm and the O_2-X CIA at 6.4 μm are detectable up to 25 pc away, except for the coldest atmospheres beyond 20 pc.

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. 22 bars is based on a conservative estimate of O_2 retention by (8). We can see that the difference in transit depth between the 1 and 22 bar cases increase with temperature (because the refraction limit is at higher pressures) and that the strength of O_2 A–band is relatively insensitive to pressure. The O_2-X CIA feature at 6.4 μm requires fewer transits to achieve 3 or 5 σ detection and is therefore the most promising indicator of a massive O_2 desiccated atmosphere potentially observable with JWST.

Supplementary Table 1: Relative transit depth (ppm), signal-to-noise ratio for 1 transit (SNR-1) and number of transits to achieve a 5 σ and 3 σ detection of O_2 assuming O_2 desiccated and isothermal atmospheres on TRAPPIST-1e (8). The numbers at the left of the "–" mark are for the 1 bar atmosphere while the numbers at the right are for the 22 bar atmosphere. (-) represent the cases for which more than 100 integrated transits are needed. For each feature, the wavelength and resolving power (R) are mentioned.

Feature	A–band	O_2-O_2	O_2-O_2	O_2-X
Wavelength [μm]	0.76	1.06	1.27	6.4
R	100	40	20	10
Temperature		200 K		
Depth [ppm]	44–44	38–37	42–41	67–66
SNR-1	0.25–0.25	0.66–0.65	1.16–1.14	1.33–1.31
N transits (5σ)	(-)	57–59	19–19	14–15
N transits (3σ)	(-)	21–21	7–7	5–5
Temperature		300 K		
Depth [ppm]	68–68	52–62	57–71	88–107
SNR-1	0.39–0.39	0.90–1.07	1.59–1.98	1.75–2.13
N transits (5σ)	(-)	31–22	10–7	8–6
N transits (3σ)	59–59	11–8	4–3	3–2
Temperature		400 K		
Depth [ppm]	91–99	63–88	71–107	110–162
SNR-1	0.52–0.57	1.10–1.54	1.97–2.97	2.18–3.22
N transits (5σ)	93–77	21–11	6–3	5–2
N transits (3σ)	33–28	7–4	2–1	2–1
Temperature		500 K		
Depth [ppm]	114–127	74–108	83–132	129–197
SNR-1	0.65–0.73	1.28–1.88	2.31–3.65	2.56–3.91
N transits (5σ)	59–47	15–7	5–2	4–2
N transits (3σ)	21–17	6–3	2–1	1–1
Temperature		600 K		
Depth [ppm]	137–156	83–136	95–174	147–264
SNR-1	0.79–0.89	1.44–2.37	2.63–4.83	2.93–5.23
N transits (5σ)	40–32	12–5	4–1	3–1
N transits (3σ)	14–12	4–2	1	1–1

References

[1] Snellen, I. A. G., de Kok, R. J., le Poole, R., Brogi, M. & Birkby, J. FINDING EXTRATERRESTRIAL LIFE USING GROUND-BASED HIGH-DISPERSION SPECTROSCOPY. *ASTROPHYS J* **764**, 182 (2013). URL `https://doi.org/10.1088%2F0004-637x%2F764%2F2%2F182`.

[2] Fauchez, T., Rossi, L. & Stam, D. M. The o2 a-band in the fluxes and polarization of starlight reflected by earth-like exoplanets. *ASTROPHYS J* **842**, 41 (2017).

[3] Pallé, E., Zapatero Osorio, M. R., Barrena, R., Montañés-Rodríguez, P. & Martín, E. L. Earth's transmission spectrum from lunar eclipse observations. *Nature* **459**, 814–816 (2009). `0906.2958`.

[4] Misra, A., Meadows, V., Claire, M. & Crisp, D. Using Dimers to Measure Biosignatures and Atmospheric Pressure for Terrestrial Exoplanets. *Astrobiology* **14**, 67–86 (2014). `1312.2025`.

[5] Schwieterman, E. W. *et al.* Identifying Planetary Biosignature Impostors: Spectral Features of CO and O_4 Resulting from Abiotic O_2/O_3 Production. *ASTROPHYS J* **819**, L13 (2016). `1602.05584`.

[6] Lustig-Yaeger, J., Meadows, V. S. & Lincowski, A. P. The detectability and characterization of the TRAPPIST-1 exoplanet atmospheres with JWST. *ASTRON J* **158**, 27 (2019). URL `https://doi.org/10.3847%2F1538-3881%2Fab21e0`.

[7] Rinsland, C. P., Zander, R., Namkung, J. S., Farmer, C. B. & Norton, R. H. Stratospheric infrared continuum absorptions observed by the atmos instrument. *J GEOPHYS RES-ATMOS* **94**, 16303–16322 (1989). `https://agupubs.onlinelibrary.wiley.com/doi/pdf/10.1029/JD094iD13p16303`.

[8] Lincowski, A. P. *et al.* Evolved Climates and Observational Discriminants for the TRAPPIST-1 Planetary System. *ASTROPHYS J* **867**, 76 (2018). `1809.07498`.