# Astro2020 Science White Paper

# Atmospheric disequilibrium as an exoplanet biosignature: Opportunities for next generation telescopes

**Thematic Area:** Planetary Systems

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**Key points**:

- Atmospheric chemical disequilibrium is a potentially useful, generalized exoplanet biosignature that should be considered when designing next generation space telescopes.
- A promising biosignature combination on early Earth-like planets that lack $O_2$ is coexisting $CH_4$ and $CO_2$ (without CO). This disequilibrium combination existed during ~1/3 of Earth's history (4.0-2.5 Ga) due to microbial $CH_4$ production, and it is unlikely that non-biological processes could sustain such an atmosphere on habitable exoplanets. Moreover, the relative simplicity of biogenic $CH_4$ production suggests that this biosignature could be widespread.
- This $CH_4$+$CO_2$-CO disequilibrium biosignature is potentially detectable on nearby transiting planets with JWST. In fact, it is more easily detectable than oxygen/ozone biosignatures with JWST.
- This biosignature gas combination is detectable on nearby transiting planets with next generation instruments. A ~15 m LUVOIR with wavelength coverage extended to 5 µm could readily detect anoxic biosignature detection on transiting planets. Similarly, HabEx with extended wavelength coverage, OST, or a ~8 m LUVOIR may be capable of disequilibrium biosignature detection, but their ability to completely rule out non-biological $CH_4$ production would be limited.

## Introduction

Life produces waste gases that may modify the composition of planetary atmospheres. This raises the possibility of finding life on exoplanets via detecting biogenic waste gases (e.g. Catling et al. 2018). Oxygen and its photochemical byproduct ozone are promising biosignature gases because it is difficult to sustain oxygen-rich atmospheres without photosynthesis (Meadows et al. 2018). Oxygen biosignatures may be uncommon, however. Oxygen production via photosynthesis is a complex metabolism that only evolved once in Earth history (Knoll 2008; Mulkidjanian et al. 2006). Moreover, even if oxygenic photosynthesis evolves frequently, it could take a long time for detectable levels of atmospheric $O_2$ to accumulate. Despite the emergence of oxygenic photosynthesis 3.0-2.5 billion years ago, Earth's atmosphere only attained near-modern oxygen levels half a billion years ago (Lyons et al. 2014). Finally, oxygen accumulation may be even more difficult on M-dwarf planets due to the lower flux of visible wavelength photons (Lehmer et al. 2018).

Other approaches to life detection are desirable. One possible scheme is atmospheric chemical disequilibrium as a sign of life: The coexistence of two or more chemically incompatible atmospheric species could be indicative of biology (Cockell et al. 2009; Hitchcock & Lovelock 1967; Lovelock 1965; Sagan et al. 1993). For example, coexisting $O_2$ and $CH_4$ is a more compelling biosignature than $O_2$ alone because the two species will react, rapidly depleting an atmosphere of $CH_4$ unless it is continuously replenished by life (Prinn et al. 2001; Simoncini et al. 2013). Comparing the atmospheric disequilibria of Solar System planets, the modern Earth has the largest disequilibrium due to the presence of life (Krissansen-Totton et al. 2016). This big disequilibrium is mostly attributable to the coexistence of $N_2$, $O_2$, and liquid $H_2O$, which would dissipate without continuous $O_2$ replenishment from photosynthetic life and an oxidative, $O_2$-influenced biological nitrogen cycle that releases $N_2$ to replace that assimilated into ammonium compounds (Krissansen-Totton et al. 2016).

## Disequilibrium biosignatures on early Earth analogs

Motivated by the expectation that oxygen biosignatures may be uncommon, the disequilibrium biosignature approach has recently been extended to anoxic atmospheres, such as that of the Archean Earth (4.0-2.5 billion years ago). The Archean Earth was inhabited (Knoll et al. 2016), but atmospheric oxygen was virtually absent (Farquhar et al. 2000). Estimates of Archean atmospheric composition imply $CH_4$ and $CO_2$ were out of equilibrium in the early Earth's anoxic atmosphere (Krissansen-Totton et al. 2018b). This disequilibrium combination was biogenic since the dominant source of $CH_4$ was likely microbial production.

Would this $CH_4$+$CO_2$ disequilibrium combination be a biosignature if found elsewhere? Crucially, $CH_4$ has a short lifetime in terrestrial planet atmospheres, and so a $CH_4$-rich atmosphere would not persist without continuous replenishment. Plausible non-biological fluxes of $CH_4$ are insufficient, and so the coexistence of $CH_4$ and $CO_2$ is an excellent biosignature (Krissansen-Totton et al. 2018b). Biogenicity would be especially compelling if $CH_4$ was abundant (>0.1%) because abiotic water-rock reactions—the most plausible "false positive" for methane producing life—are unlikely to yield large quantities of $CH_4$ (Fig 1).

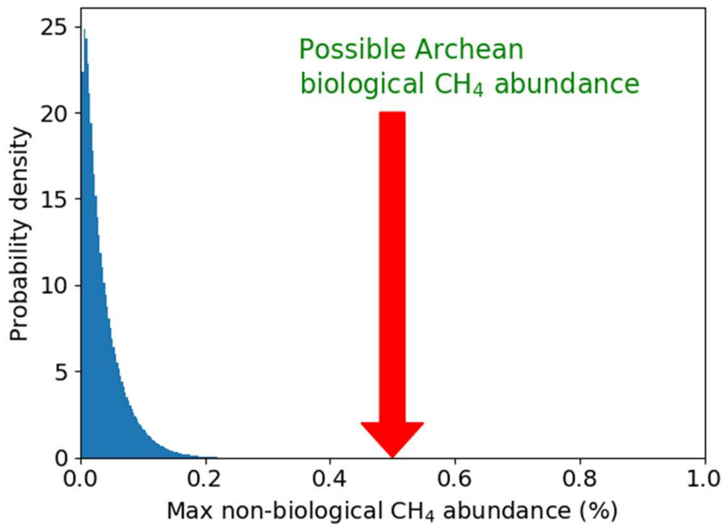


**Figure 1**: Probability distribution for the maximum steady state $CH_4$ abundance from non-biological water-rock reactions. This is calculated assuming surface $CH_4$ fluxes are balanced by photodissociation and diffusion-limited H escape in a temperate, anoxic atmosphere. The red arrow shows a data-driven estimate for the $CH_4$ abundance on the Archean Earth at 3.5 Ga (Zahnle et al. 2019). **The key point of this figure is that $CH_4$ abundances exceeding ~0.1% (in the presence of $CO_2$) are difficult to explain without biological methane production**. This 0.1% threshold for $CH_4$ biogenicity is consistent with previous estimates (Schindler & Kasting 2000). Adapted from Krissansen-Totton et al. (2018b).

Additionally, the $CH_4$+$CO_2$ combination is more likely biogenic if CO is absent. This is because non-biological processes such as volcanic outgassing are unlikely to produce carbon in its most oxidized form ($CO_2$) and carbon in its least oxidized form ($CH_4$) without producing carbon with intermediate oxidation (CO) (Krissansen-Totton et al. 2018b). For example, Earth's mantle is oxidizing and so virtually no $CH_4$ is outgassed except from previously buried biogenic material (Catling & Kasting 2017). Photochemically produced CO may accumulate on M-dwarf hosted planets (Nava-Sedeno et al. 2016). However, microbes can easily reduce CO using water, pulling CO abundance down to very low levels (Kharecha et al. 2005; Krissansen-Totton et al. 2018a). **In summary, the coexistence of $CO_2$ with >0.1% $CH_4$ (plus low or absent CO) in habitable exoplanet atmospheres is a promising disequilibrium biosignature with no known false positives.**

Arguably, this $CH_4$+$CO_2$ (minus CO) biosignature combination is more common than oxygen/ozone biosignatures. In contrast to the complexity of oxygenic photosynthesis, methanogenesis is comparatively primitive and ancient (Weiss et al. 2016; Wolfe & Fournier 2018). The gaseous substrates required for methanogenesis ($H_2$ and $CO_2$) are likely common outgassing products on terrestrial planets.

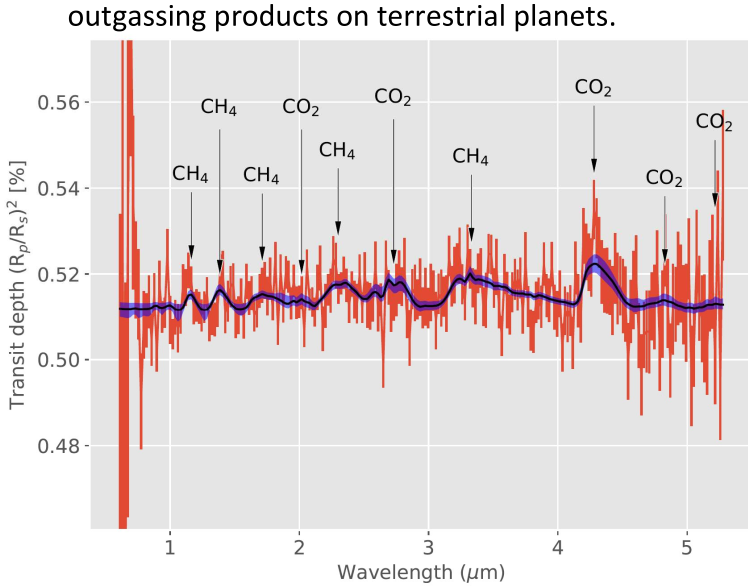


**Figure 2:** Synthetic and fitted transmission spectra for 10 transits of an Archean Earth-like TRAPPIST-1e with the NIRSpec prism instrument on JWST (Krissansen-Totton et al. 2018a). Here, $R_P$ and $R_S$ are the radii of the planet and star, respectively. A typical noisy spectrum (red line), the 95% credible retrieved spectrum (blue shading), and the median retrieved spectrum (black line) are shown. **This figure suggests the $CH_4$+$CO_2$ disequilibrium biosignature combination is potentially detectable after 10 transits.**

## Detectability with the James Webb Space Telescope

Krissansen-Totton et al. (2018a) computed simulated James Webb Space Telescope (JWST) transit retrievals of TRAPPIST-1e (Gillon et al. 2017), the most likely habitable planet in the TRAPPIST-1 system (Turbet et al. 2018; Wolf 2017). TRAPPIST-1e was assumed to be an Archean Earth-like analog with abundant $CH_4$ in combination with $CO_2$, and negligible CO. It was found that ~10 coadded transits may be sufficient to detect anaerobic life on TRAPPIST-1e (Krissansen-Totton et al. 2018a). Fig. 2 shows simulated and retrieved transmission spectra with the NIRSpec prism instrument. $CO_2$ is detectable, the $CH_4$ abundance can be constrained well enough to tentatively rule out abiotic production, and a crude upper limit can be placed on CO (bottom row, Fig. 3). Moreover, this anoxic biosignature combination is easier to detect than biogenic $O_2$/$O_3$ with JWST (Krissansen-Totton et al. 2018a).

Although tentative life detections may be possible with JWST for nearby planets, these will be inconclusive as gas abundances will not be tightly-constrained. Future telescopes will be needed to confirm any detections and broaden the search to more planetary systems.

## Detectability with LUVOIR/HabEx/OST

Biosignature gas detection via direct imaging using LUVOIR or HabEx are discussed elsewhere (Fischer et al. 2018; Gaudi et al. 2018). Detection of the $CO_2$+$CH_4$ disequilibrium biosignature via direct imaging likely requires spectroscopy longward of at least 2.1 μm such that $CO_2$ can be detected by its 2 μm absorption feature.

Here, **we instead focus on the detectability of disequilibrium biosignatures during transit observations**. Specifically, we show simulated transmission spectra retrievals of TRAPPIST-1e with proposed next-generation telescopes such as LUVOIR (Fischer et al. 2018), HabEx (Gaudi et al. 2018), and OST (Cooray et al. 2018). The detectability of Archean Earth-like $CH_4$+$CO_2$ biosignatures is our focus, but the results below are broadly applicable to other terrestrial planet atmospheres and other biosignature combinations. Unless otherwise stated, the methodology used to generate these synthetic retrievals is described in Krissansen-Totton et al. (2018a) where the NEMESIS radiative transfer code was used (Irwin et al. 2008).

Fig. 3 shows abundance constraints from a simulated transmission spectrum retrieval of 10 transits of an Archean Earth-like TRAPPIST-1e. The top row shows abundance constraints using a 15m LUVOIR telescope. Retrievals for both 0.2-2.5 μm (nominal LUVOIR wavelength range) and 0.2-5 μm wavelength ranges are shown. An alternative instrument with this extended wavelength range has been proposed (Fischer et al. 2018). Note that this 0.2-5.0 μm instrument would not require cryogenic cooling; 270 K optics are assumed in Fig. 3. Synthetic retrievals of a similarly equipped 8m LUVOIR telescope are shown in the second row of Fig. 3. **Both 15m and 8m versions of LUVOIR could readily detect $CH_4$+$CO_2$ biosignatures on transiting, Archean Earth-like exoplanets such as TRAPPIST-1e. However, only a 15 m LUVOIR with an upper wavelength limit of 5 μm could constrain CO abundances, thereby ruling out non-biological $CH_4$ production scenarios.** Extending the upper wavelength limit to 5 μm also provides access to prominent $CO_2$ (4.5 μm) and $CH_4$ (3.5 μm) absorption features, and the transit spectrum at these longer wavelengths is less likely to be contaminated by unocculted active regions (Ducrot et al. 2018; Rackham et al. 2018). Note that the presence of an organic haze could further enhance the detectability of biogenic $CH_4$ (Arney et al. 2018).

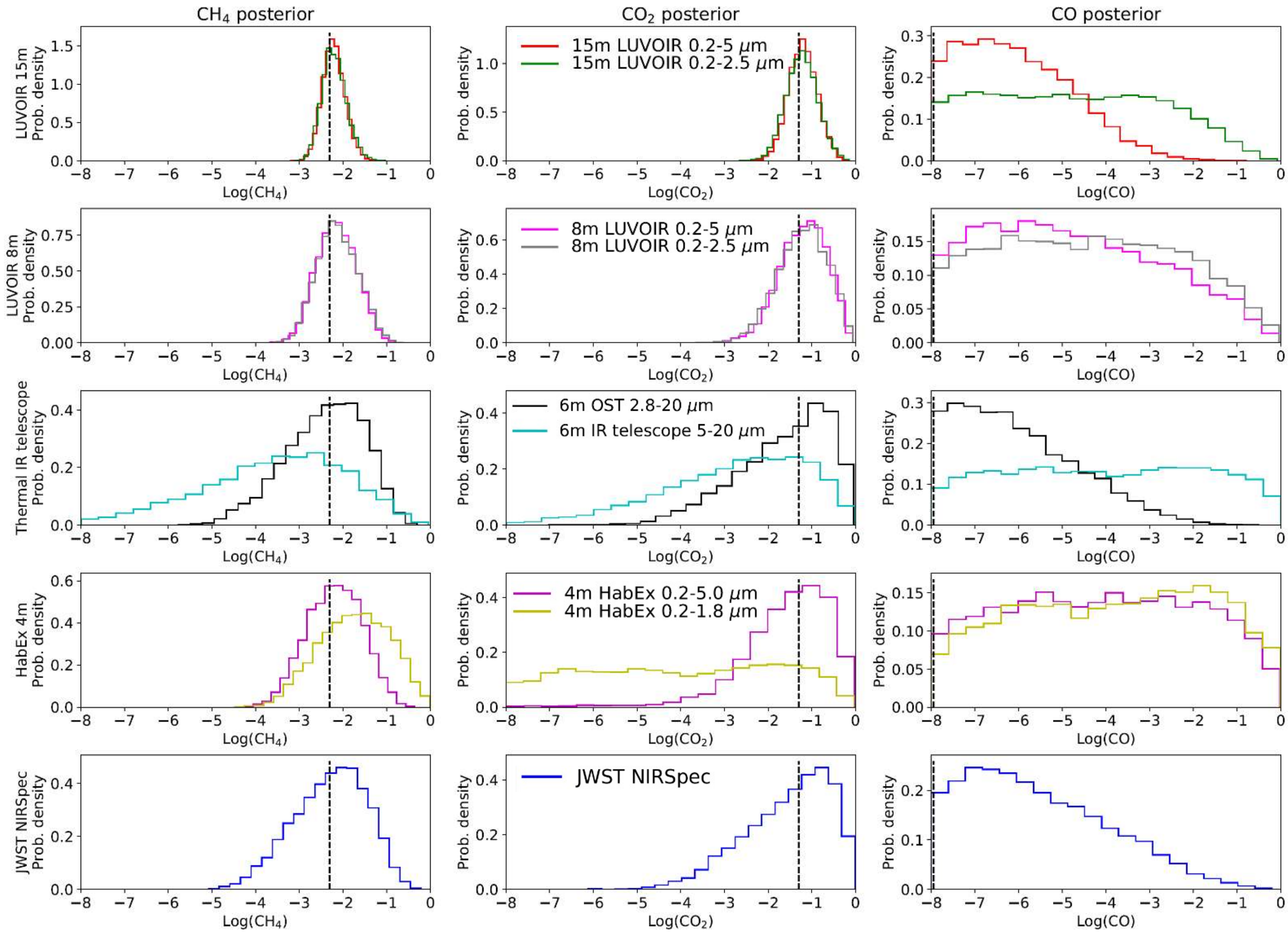


**Fig. 3: Comparison of biosignature detection capabilities of next-generation telescopes.** Retrieved gas abundance posteriors for 10 transits of a cloud-free, Archean Earth-like TRAPPIST-1e using selected next-generation telescopes. The three columns show $CH_4$, $CO_2$, and CO abundance posteriors, respectively. The first row shows 15 m LUVOIR retrievals for both a 0.2-5 µm instrument with no cryogenic cooling (red line), and the nominal 0.2-2.5 µm wavelength range (green line). The second row shows 8m LUVOIR retrievals for both a 0.2-5 µm instrument with no cryogenic cooling (fuchsia line), and the nominal 0.2-2.5 µm HDI instrument (grey line). The third row shows a 6m OST retrieval for the nominal 2.8-20 µm instrument (black lines) as well as a generic 5-20 µm telescope (cyan lines). The fourth row shows 4m HabEx retrievals for both a 0.2-5 µm instrument with no cryogenic cooling (magenta line), and the nominal 0.4-1.8 µm instrument (yellow line). The fifth row shows a JWST NIRSpec simulated retrieval (blue line). **Key point: Archean Earth-like $CH_4$+$CO_2$ biosignature detection is straightforward with LUVOIR, although a long wavelength cutoff of 5 µm is required to constrain CO abundances (ruling out abiotic scenarios). Archean Earth-like biosignature detection is possible with nominal OST and an extended wavelength range HabEx.** Goddard's Planetary Spectrum Generator was used to generate synthetic noise for LUVOIR, HabEx and OST simulations, and PandExo was used for JWST. Vertical, dashed black lines are "true" abundance values: 0.5%, 5%, and 10 ppbv for $CH_4$, $CO_2$, and CO, respectively.

Biosignature detection on transiting terrestrial planets is also possible with OST. Row 3 of Fig. 3 shows abundance posteriors from a simulated retrieval of 10 transits of an Archean Earth-like TRAPPIST-1e with a 5.9 m OST. For the nominal wavelength range of 2.8-20 µm (OST-STDT 2018), $CH_4$ and $CO_2$ detections are possible, although $CH_4$ posteriors are too broad to wholly rule out abiotic $CH_4$ production (Krissansen-Totton et al. 2018b). This is because the OST wavelength range excludes the shorter NIR range available to JWST. Strict upper bounds can be placed on CO abundances, however, which would help to rule out other abiotic $CH_4$ outgassing scenarios. Note that if the wavelength limit of OST were limited to 5.0-20 µm, as was proposed in previous mission concepts (Cooray et al. 2018), then $CH_4$ and $CO_2$ detections are not possible (Fig. 3, row 3), highlighting the necessity of NIR coverage. Increasing the number of transits to 30, which is feasible for OST due to its low noise floor (Cooray et al. 2018), results in a slight improvement in abundance constraints (not shown). Secondary eclipse observations could provide additional constraints, but these are not considered here.

Finally, row 4 of Fig. 3 shows abundance constraints from an Archean Earth-like TRAPPIST-1e using a 4m HabEx. For the nominal instrument range of 0.4-1.8 µm, only $CH_4$ can be detected since neither CO nor $CO_2$ have strong absorption features in this range. Extending the upper wavelength limit to 5 µm would enable $CO_2$ detection, but would still not constrain CO. Even after 30 transits CO is still unconstrained, and the extended wavelength range is required for $CO_2$ detection (not shown). However, HabEx's NIR coverage would allow for better $CH_4$ abundance constraints than for OST, which is crucial for determining $CH_4$ biogenicity.

There are two caveats to these results. First, noise calculations did not include a noise floor. For the cases shown, OST and HabEx noise exceeds plausible noise floors and are thus unaffected. LUVOIR calculations were repeated with a 30 ppm noise floor and abundance constraints do not change significantly. Second, low resolution k-tables were used (0.025 µm) to make retrieval computationally feasible. This smears-out $CO_2$ absorption features at 1.6 µm, and so $CO_2$ detectability for LUVOIR and HabEx may be more favorable than Fig. 3 suggests.

**Conclusions**

Chemical disequilibrium in habitable exoplanet atmospheres could be a sign of life. Specifically, the coexistence $CO_2$ and abundant $CH_4$—plus no/low CO—may be a common biosignature of microbial biospheres. For nearby, transiting Earth-like exoplanets, either a 15m or 8m LUVOIR telescope could detect this biosignature combination. Instruments that extend the wavelength range of transit spectroscopy to 5 µm (with ~270 K optics) would strengthen the case for life by better constraining CO abundances. For OST and HabEx, anoxic biosignature detection on transiting planets may also be possible. With a wavelength range of 2.8-20 µm for transit spectroscopy, OST would be particularly well-suited to constraining CO abundances, thereby ruling out some false positive scenarios. However, it may be challenging to constrain $CH_4$ abundances sufficiently well to exclude low (abiotic) production with OST. In contrast, if HabEx transit spectroscopy is extended upward toward ~5 µm, then biogenic $CH_4$ detection may be easier, but constraining CO abundances will remain challenging. **Based on our understanding of the co-evolution of Earth's life and atmosphere, the $CH_4$-$CO_2$ biosignature is potentially the most common one in the galaxy, and so we strongly recommend that the next generation telescope after JWST has the capability to detect such a biosignature.**

**References**


Arney, G., et al. (2018). Organic haze as a biosignature in anoxic Earth-like atmospheres. *Astrobiology, 18*(3), 311-329.

Catling, D. C., & Kasting, J. F. (2017). *Atmospheric Evolution on Inhabited and Lifeless Worlds*: Cambridge University Press.

Catling, D. C., et al. (2018). Exoplanet Biosignatures: A Framework for Their Assessment. *Astrobiology, 18*(6), 709-738. doi:10.1089/ast.2017.1737

Cockell, C. S., et al. (2009). Darwin-a mission to detect and search for life on extrasolar planets. *Astrobiology, 9*(1), 1-22.

Cooray, A., et al. (2018). *The Origins Space Telescope 2018 Interim Report*. Retrieved from

Ducrot, E., et al. (2018). The 0.8–4.5 μm Broadband Transmission Spectra of TRAPPIST-1 Planets. *The Astronomical Journal, 156*(5), 218.

Farquhar, J., et al. (2000). Atmospheric influence of Earth's earliest sulfur cycle. *Science, 289*(5480), 756-758.

Fischer, D., et al. (2018). The LUVOIR Mission Concept Study Interim Report. *arXiv preprint arXiv:1809.09668*.

Gaudi, B. S., et al. (2018). The Habitable Exoplanet Observatory (HabEx) Mission Concept Study Interim Report. *arXiv preprint arXiv:1809.09674*.

Gillon, M., et al. (2017). Seven temperate terrestrial planets around the nearby ultracool dwarf star TRAPPIST-1. *Nature, 542*(7642), 456.

Hitchcock, D. R., & Lovelock, J. E. (1967). Life detection by atmospheric analysis. *Icarus, 7*(1-3), 149-159.

Irwin, P., et al. (2008). The NEMESIS planetary atmosphere radiative transfer and retrieval tool. *Journal of Quantitative Spectroscopy and Radiative Transfer, 109*(6), 1136-1150.

Kharecha, P., et al. (2005). A coupled atmosphere–ecosystem model of the early Archean Earth. *Geobiology, 3*(2), 53-76.

Knoll, A. H. (2008). Cyanobacteria and earth history. *The Cyanobacteria: Molecular Biology, Genomics, and Evolution, 484*.

Knoll, A. H., et al. (2016). Life: the first two billion years. *Philosophical Transactions of the Royal Society B: Biological Sciences*.

Krissansen-Totton, J., et al. (2016). On detecting biospheres from chemical thermodynamic disequilibrium in planetary atmospheres. *Astrobiology, 16*(1), 39-67. doi:10.1089/ast.2015.1327

Krissansen-Totton, J., et al. (2018a). Detectability of biosignatures in anoxic atmospheres with the James Webb Space Telescope: A TRAPPIST-1e case study. *The Astronomical Journal, 156*(3). doi:10.3847/1538-3881/aad564

Krissansen-Totton, J., et al. (2018b). Disequilibrium biosignatures over Earth history and implications for detecting exoplanet life. *Science advances, 4*(1), eaao5747.

Lehmer, O. R., et al. (2018). The Productivity of Oxygenic Photosynthesis around Cool, M Dwarf Stars. *The Astrophysical Journal, 859*(2), 171-178.

Lovelock, J. E. (1965). A physical basis for life detection experiments. *Nature, 207*(997), 568-570.

Lyons, T. W., et al. (2014). The rise of oxygen in Earth's early ocean and atmosphere. *Nature, 506*(7488), 307.

Meadows, V. S., et al. (2018). Exoplanet Biosignatures: Understanding Oxygen as a Biosignature in the Context of Its Environment. *Astrobiology, 18*(6), 1-33. doi:10.1089/ast.2017.1727
Mulkidjanian, A. Y., et al. (2006). The cyanobacterial genome core and the origin of photosynthesis. *Proceedings of the National Academy of Sciences, 103*(35), 13126-13131.
Nava-Sedeno, J. M., et al. (2016). Carbon Monoxide and the Potential for Prebiotic Chemistry on Habitable Planets around Main Sequence M Stars. *Astrobiology, 16*(10), 744-754.
OST-STDT. (2018). *MISC Transit Spectrometer Fact Sheet*. Retrieved from https://asd.gsfc.nasa.gov/firs/docs/Baseline_instrument_fact_sheet_MISC_20181022.pdf
Prinn, R., et al. (2001). Evidence for substantial variations of atmospheric hydroxyl radicals in the past two decades. *Science, 292*(5523), 1882-1888.
Rackham, B. V., et al. (2018). The transit light source effect: false spectral features and incorrect densities for M-dwarf transiting planets. *The Astrophysical Journal, 853*(2), 122.
Sagan, C., et al. (1993). A search for life on Earth from the Galileo spacecraft. *Nature, 365*(6448), 715-721.
Schindler, T. L., & Kasting, J. F. (2000). Synthetic spectra of simulated terrestrial atmospheres containing possible biomarker gases. *Icarus, 145*(1), 262-271.
Simoncini, E., et al. (2013). Quantifying drivers of chemical disequilibrium: theory and application to methane in the Earth's atmosphere. *Earth System Dynamics, 4*(2), 317-331.
Turbet, M., et al. (2018). Modeling climate diversity, tidal dynamics and the fate of volatiles on TRAPPIST-1 planets.
Weiss, M. C., et al. (2016). The physiology and habitat of the last universal common ancestor. *Nature Microbiology, 1*(9), 16116.
Wolf, E. T. (2017). Assessing the habitability of the TRAPPIST-1 system using a 3D climate model. *The Astrophysical Journal Letters, 839*(1), L1.
Wolfe, J. M., & Fournier, G. P. (2018). Horizontal gene transfer constrains the timing of methanogen evolution. *Nature ecology & evolution, 2*(5), 897.
Zahnle, K. J., et al. (2019). Strange messenger: A new history of hydrogen on Earth, as told by Xenon. *Geochimica et Cosmochimica Acta, 244*, 56-85.