Searching for atmospheric bioindicators in planets around two nearby stars, *Proxima Centauri* and *Epsilon Eridani* - test cases for retrieval of atmospheric gases with infrared spectroscopy -

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Abstract: We test the ability of thermal infrared spectroscopy to retrieve assumed atmospheric compositions for two types of planet: *Proxima b* (real), and (hypothetical) planets orbiting Epsilon Eridani. Six cases are considered, covering a range of atmospheric compositions, and some diversity in the bulk composition (rocky, water-ocean, hydrogen rich) and the spectral type of the parent star. Planets possess an atmosphere with an assumed composition. In four cases a global mean coupled climate-chemistry atmospheric column model is applied to calculate climate and composition profiles. In two cases the atmosphere structure is assumed. The IR emission is then calculated from line transfer models, and used to investigate retrieval of input atmospheric species. For the six cases considered, no false positive of the triple bioindicator, (H_2O, CO_2, and O_2, in specified conditions), is found. In several cases, results show that the simultaneous acquisition of a visible spectrum would be valuable, especially when the O_3 band is observed but the O_2 abundance cannot be derived from IR data alone. In each case, determining the mass appears mandatory to identify the planet's nature and have an idea of surface conditions, which are necessary when testing for the presence of life.

(*195 words*)

Key words: Exoplanets, atmospheres, spectroscopy, bioindicator, nearby stars, Proxima Cen b.

1. Introduction

In this paper a main focus is to discuss practical issues when assessing for potential life signals during IR spectral retrieval of exoplanetary atmospheres. We present test cases of putative planets with assumed properties (e.g. for atmospheres). Then, we attempt to retrieve these properties using thermal infra-red (IR, 3-18 μm) spectroscopy (Rieke, 2009). We investigate factors affecting S/N, factors influencing the choice of spectral resolution, associated effects upon integration times and methods for constructing the background continuum.

1.1 Two neighboring stars

Performing remote spectroscopy on nearby, cool stars could provide the first chance to discover signs of life outside the Solar System. Proxima Centauri, with a spectral class M6V, is our closest stellar neighbor located 4.3 light years away, and is one of the most prolifically studied M-dwarf stars. It has an effective temperature of 3050 K with a radius and mass of 14% and 12% that of the Sun, respectively. A major recent discovery (Anglada-Escudé et al., 2016) revealed a planet with a minimum mass of 1.3 Earth mass (*Proxima Cen b*) which orbits at a distance of 0.05 AU where it receives ~65% of the net insolation of the Earth. Since the planet is unlikely to transit, its atmospheric characterization is expected to focus on direct imaging, reflection or thermal phase curve variation (Kreidberg and Loeb, 2016). Studies with an atmospheric column model by Meadows et al. (2018) (see also Turbet et al., 2018) suggested habitable conditions if the planet either (1) formed further out (hence avoiding likely desiccation during the early stages), or/and if it (2) possesses a thick, protective H_2 envelope from the protoplanetary disk during its formation. The weak insolation suggests that a strong greenhouse effect would be needed to maintain surface habitability, e.g. via a surface pressure of several bars of CO_2. 3D model studies of Proxima Cen b, Kane et al. (2017), Sparks et al. (2018), Boutle et al. (2017) support this idea.

Epsilon Eridani is a K2V star with a radius and mass of 84% and 85% that of the Sun. It is located 10.5 light years away from us and has at least one gaseous planet (Hatzes et al. 2000). There have been numerous model studies focusing on the potential habitability and biomarkers of hypothetical planets orbiting in the HZ of Epsilon Eridani (e.g. Segura et al. 2003, Grenfell et al. 2007, Godolt et al. 2016, Wolf et al. 2017). These works analyzed photochemical and climate effects in the planetary atmosphere related to a redward shift in the incoming stellar spectrum, compared to that of the Sun.

1.2 Assessing potential signals of life

In exoplanet science the terms “biosignature” and “biomarker” are often used synonymously (see e.g. Grenfell et al. 2007, Kaltenegger et al. 2017) and refer to the inability to account for a given signal without invoking the presence of biologic activity. An example would be the discovery of an Earth-like planet (on a similar orbit as Earth orbiting a G-type star) with an oxygen-rich atmosphere or/and an ozone layer which are similar to those of our home planet. The term “bioindicator” in those works refers to an interesting discovery which could mean life but that requires further information. Given our continuously expanding knowledge of potential abiotic sources, future discoveries of potential life signals are anticipated to trigger a discussion which will evolve with our knowledge of the environmental context (stellar insolation, history, planetary bulk, orbital, interior and atmospheric properties etc.) as summarized in recent reviews by Grenfell (2017), Schwieterman et al., (2018), Meadows et al., (2018).

The present paper uses the term *bioindicator* - defined here as "a set of observable planetary features, such as mass, radius, atmospheric composition, surface temperature, parent star properties and evolution, etc., which our present models cannot reproduce when including known abiotic photo, -physical, and -chemical processes'' (Léger et al., 2011). The latter paper employs the term biosignature for that but we now prefer to use bioindicator since it is more evocative of a conservative pathway towards the detection of life based upon eliminative iteration via step-by-step scientific debate. This philosophy is supported by the comprehensive review papers in exoplanetary biosignature science stemming from the NASA NExSS workshops, see for instance Kiang et al. (2018), which emphasize the approach of interpreting potential signals of life within their full environmental and evolutionary context.

In this paper we also use the term "false positive" and "false negative". *False positive* refers to a set of observations that are falsely interpreted as implying biological activity. Correctly discounting possible false positives is essential when accepting or rejecting a bioindicator. *False negatives* refer to life not found by our search programs.

All the bioindicators we will likely detect in the near to mid-term future are based on global atmospheric changes driven by life. Detecting such life is clearly facilitated if it perturbs its environment on a planetary scale. Clearly, life located only in small niches is likely to be more difficult to detect remotely, or may not be detected at all (a case of false negative). The case of Mars illustrates the challenge of detecting life remotely. Although Mars has been observed from Earth with an accuracy far superior to that which we can hope for any object outside the Solar System, (even sophisticated probes have been sent), yet we still do not know whether life is present on, or under, the Martian surface.

2.0 Model Descriptions

2.1 *Atmospheric model*

We apply several similar models. All are one-dimensional (1D) cloud-free, coupled radiative-convective-climate-photochemical. They calculate the steady-state global mean temperature and concentration profiles of (exo)planetary atmospheres. They are described in Rauer et al., 2011, von Paris et al. 2010 and 2015, and Tian et al 2014. For each test case the model used is specified in Table 1. Models extend from the planetary surface up to *P* = 6.6 x10^{-5} bar (mid-mesosphere for modern Earth conditions, i.e. ~ 65 km), (or up to 100 km). The chemical modules feature over 200 chemical reactions for 55 (or 52) long life chemical species solved with a backwards Euler time-stepping method in 64 model layers (or using a 1 km grid). Initial abundance and temperature profiles are based on the US standard atmosphere (http://www.pdas.com/atmos.html). Long-lived gases O_2, N_2, and CO_2 are set to constant isoprofile abundances, whereas remaining species are calculated either interactively for the longer-lived species or via the steady-state assumption for short-lived species. In the stratosphere, H_2O is calculated by the chemistry module whereas in the troposphere it is determined from the temperature profile assuming a relative humidity, RH, profile. It assumes an atmosphere with: C_{H2O} = RH(z) * $P_{sat,H2O}$(T(z)) / P(z), where C_{H2O} is the volumetric abundance of H_2O, RH(z), the relative humidity profile, $P_{sat,H2O}$ the saturation vapor pressure of H_2O at temperature T(z), and P(z) the atmospheric pressure at height z. RH can be either assumed to be 100% throughout the atmosphere, or chosen to be Earth-like, based on Earth observations (Manabe and Wetherald, 1967). Biomass, volcanic and lightning emissions in the chemistry module are based on the modern Earth. Dry and wet deposition operate at the lower model boundary whereas effusion fluxes of CO and O are applied at the upper boundary to simulate the photolysis of CO_2 in the overlying atmosphere.

The climate module employs a two-stream approach (Toon et al., 1989) in the shortwave (237 nm – 1.0 μm) accounting for absorption and scattering by H_2O, CO_2, N_2, O_2, CH_4, O_3, CO, H_2, He. The longwave (1.0 - 500μm) scheme features the major atmospheric absorbers (H_2O, CO_2, O_3, and CH_4) using the correlated-k approach (von Paris et al. 2015) for surface temperatures below 400 K calculated from the HITRAN 2012 line database (Rothman et al. 2013). For higher temperatures the scheme employs the longwave radiative transfer described in von Paris et al. (2010) assuming a simpler atmosphere accounting only for absorption by H_2O CO_2 and N_2 also using the correlated-k method with absorption coefficients based on the line data of HITEMP 1995 (Rothman et al. 2013). Convective adjustment to the moist adiabatic lapse rate is carried out where applicable.

Table 1

2.2 *Spectral model*

The line-by-line radiative transfer model (LT) model (Li et al. 2016) uses line intensities and half-widths (both self-broadening and air-broadening) in the HITRAN2012 database (Rothman et al. 2013), with temperature and pressure corrections considered, to calculate the transmission, reflection, and emission spectra of exoplanets. By default, the LT model uses a spectral resolution of 0.01 cm^{-1} ($\lambda/\delta\lambda = 10^6$ and 10^5 at 1 and 10 μm respectively). Such a resolution is adequate to resolve all moderately strong lines in the HITRAN2012 database. The high-resolution spectra are reduced to low-resolution spectra using a triangle smoothing function in order to demonstrate results at $\lambda/\delta\lambda = 40$ that are used in the paper. Voigt profiles are used for all lines based on the algorithm in Humlíček (1982). A cut-off distance of 50 times the Voigt halfwidth from line centers is applied. Similar to Rein et al. (2014), the effects of clouds and aerosols are ignored in the model. The wavelength-dependent IR spectra for the Earth calculated in the LT model are in good agreement with those in Des Marais et al. 2002, thereafter quoted as Des+.

3. Method

The paper investigates potentially habitable planets (both hypothetical and real) with assumed atmospheric compositions, orbiting two nearby stars, namely the M-dwarf Proxima Centauri (M6V), or the solar-type star Epsilon Eridani (K2V). Spectral retrieval of atmospheric gases, mainly using thermal infra-red (IR) (3-18 μm) spectroscopy (Rieke, 2009) is subsequently assessed. Several cases address whether the *"triple bioindicator"* (i.e. the detection of the three gases, H_2O, CO_2, and O_2) could be achieved (Selsis et al., 2002) under the following specified conditions: (i) the planet is located in the Habitable Zone (HZ) of its star (Kopparapu, 2013), (ii) it has a surface (rocky or liquid), and (iii) $P_{O2} \gtrsim 10$ mbar (Rosenqvist, and Chassefiere,1995, Kasting 1995, Tian et al. 2014, Meadows et al., 2018). We investigate mainly the IR domain, where we assume that O_3 behaves as a proxy for O_2 (see Segura et al., 2003) which is useful since the former has a strong spectral signature in the IR (e.g. the 9.6 μm fundamental band), whereas O_2 has not (Angel et al., 1986).

First, the user fixes the bulk atmospheric composition (N_2, O_2, CO_2), then the atmospheric models calculate the full composition and climate. Based on this, the spectral models calculate theoretical IR emission spectra. This is subsequently used to investigate retrieval capabilities of atmospheric properties for different assumed spectral resolutions and signal to noise ratios.

The main goal is to illustrate both the capabilities, as well as the limits, of thermal IR spectroscopy. Atmospheric compositions are chosen arbitrarily, in order to explore the diverse range of uncertainty, and aiming to maintain an open mind for the unexpected.

4. Spectral Analysis: how to determine the continuum?

Planetary atmospheres considered in this study are assumed to have IR active gases such as H_2O, CO_2, CH_4, O_3, as well as IR inactive gases such as N_2, O_2, and H_2. To decide whether the IR active gases can be identified in the spectra, one needs to determine a continuum out of which the bands are detected and measured. This determination should be as objective as possible.

For planets with a possible solid or liquid surface, an atmospheric structure analogous to that of the Earth is assumed, i.e. an initial decrease of the temperature with altitude as long as the atmosphere is dense and transparent in the visible. Most of the spectral features are then due to gases acting as absorbers. A possible continuum is a Planck function corresponding to the surface temperature. In some cases, the ground can be observed through spectroscopic windows over which the various atmospheric species have small absorption cross-sections. The continuum is then fitted to pass through these data points.

Using the absorption cross sections given in Fig.1, the usual windows are found in the 8.0 - 9.0 μm, and 10 - 13 μm domains for an Earth-like atmosphere. To investigate the effect of changing spectral resolution the spectrum of an Earth-like planet is computed with different window sizes which result (Fig.2), and then the quality of the derived continuum is estimated. It is generally required thereby that spectral features appear in absorption ("downwards"), and that the derived temperature is close to that given as input. The Planck function has only two fitting parameters, temperature and amplitude. A leastsquares fit is applied to the data points within the different windows. Results indicate that the narrower windows (8.5 - 9.0 μm, 10.5 - 12.0 μm) lead to a better-estimated continuum compared with the broader ones (8.0 - 9.0 μm, 10.5 - 13.0 μm). The former are then adopted whenever a spectrum looks analogous to that of Earth.

For H_2–dominated atmospheres (case 4, Fig.3) the above approach is inappropriate since atmospheric windows down to the surface are lacking. An atmospheric composition close to that of Neptune is assumed in order to simulate the so-called “Mini Neptune Planets (MGPs). In addition to the zero flux condition at 3.0 μm, the rise of the spectrum at short wavelengths (3 – 5 μm) is a main focus since this is a region mainly determined by the temperature of the outer atmosphere, at least for Neptune and the other solar giant planets. The (10 - 11 μm) domain is also a focus because CH_4, a major absorber for the giant planets of our system, has a low absorption in that domain (Fig.1). This approach is illustrated in Fig. 3 for the case of a mini-Neptune in the HZ of eps Eri.

FIGURE 1

FIGURE 2

FIGURE 3

5. Test cases

A range of small planets is considered. Several of these constitute possible examples for *Proxima Cen b,* the planet recently discovered around our nearest star. To explore some diversity regarding the spectral type of the parent star, planets are assumed either to orbit

Proxima Cen (M6V), or *eps Eri* (K2V). The mass, radius, and distance to the star are assumed to be observed as it should be the case for future missions.

All planets are located within, or close to, the HZ of their star. Their parameters are chosen in order to reflect some diversity, although the examples investigated here are far not intended to represent an exhaustive list.

The models used for each case is specified in Table 1.

5.1 Case 1, a rocky planet with no atmosphere orbiting Proxima Cen

The planet is assumed to be rocky with a 4.0 Earth mass and 1.5 Earth radius. For conciseness, these parameters are noted in Earth units: M_{pl} = 4.0, R_{pl} = 1.5. Its distance to Proxima Cen is set such that the mean ground temperature is 300 K. A total absorption of the stellar radiation is assumed in the visible-near IR. In the thermal IR, a ground emissivity is chosen to be that of an Apollo Moon sample 15071 (Donaldson Hanna 2014, Fig.4). The resulting distance to Proxima Cen is 0.043 AU, somewhat closer than the actual *Proxima b* planet (0.049 AU, Anglada-Escudé et al. 2016).

The computed spectrum (model *i*) and Planck fit are shown in Fig. 5. The spectrum confirms the absence of atmospheric gases. The spectral features of the ground are not confused with usual absorbing gases, thanks to the spectral smoothness of the ground assumed emissivity. A possible interpretation of such a spectrum would be a planet stripped of its atmosphere. Within this framework, the Planck fit provides a good estimate (308 K) of the ground temperature (300 K). Some crude indications as to the nature of surface minerals can be derived from the spectrum, even if the spectral features are very broad (see also Hu et al. 2012 for a related discussion).

FIGURE 4

FIGURE 5

5.2 Case 2, a second possible model for *Proxima b*: a Water-ocean planet.

A water-ocean planet (Kushner 2003, Léger et al. 2004, Selsis et al. 2007) is considered in the HZ of *Proxima Cen*. ~~Its features are consistent with those of the actual planet, as we know them today.~~ Internal parameters are $M = 2.0$, $R = 1.5$ (corresponding to: wt. 50% rocks, 50% water, Selsis et al. 2007).

According to Turbet et al. (2016), if the actual planet Proxima b is in synchronous rotation, it could have a partially ice-free ocean due to an estimated huge H_2O equivalent layer (> 10^6 m), even with small amounts of CO_2. A 1D climate-chemistry model, with a 280 K surface temperature (obtained for S = 1.0) allowing water to be liquid, has some legitimacy for a proxy for Proxima b.

The assumed atmosphere has a 1.2 bar total pressure (+ H_2O), its composition is N_2 80%, O_2 20%, plus H_2O assumed to exist at saturation, and very little CO_2 (1 ppm). Note that some O_2, possibly a major part of the total atmospheric inventory could have resulted from water photolysis by the active star irradiation followed by preferential H escape (Luger and Barnes 2015, Tian 2015).

The spectrum resulting from the model used (see Table 1) is shown in Fig.6. It is dominated by H_2O, CO_2, and O_3 absorptions. It looks "Earth-like" and the corresponding spectral windows are used for the Planck continuum fit (see Sect. 4). The fit yields a

284 K surface temperature, close to the input one at the liquid-gas interface, 280 K. This is due to the efficient transparency of water vapor in the windows adopted for a planet having a surface at a moderate temperature (at T_{surf} = 280 K the water vapor pressure is P_{surf} = 10 mbar at saturation).

FIGURE 6

If O_2 is actually abiotic, could this case be considered as a false positive for the triple bioindicator around an active M star? In the thermal IR detection would be H_2O, CO_2 and O_3. The latter indicates the presence of O_2 but not its abundance. Then, the detected gases could not be considered as a false positive because it could not be stated whether P_{O2} is smaller or larger than 10 mbar (see Sect.3). A good S/N spectrum in the *visible* of the planet would allow estimating the O_2 abundance ($P_{O2} \approx 200$ mbar) and then try to apply the triple bioindicator.

The planet's water-ocean nature could only be suspected if its bulk *density* could be estimated at the time when spectroscopy is performed. The planetary radius could be derived from the observed IR spectrum and flux, but its actual *mass* would require the orbital inclination. Accurate differential astrometry (more than one order of magnitude better than Gaia) could achieve this task and perform a full determination of planetary orbital parameters, including the inclination. Unfortunately, to our knowledge, there is no project planned which will focus on this. This is an important piece of information since any biological modifications to the spectrum could be quite different for a water-ocean compared with a rocky planet.

If these two pieces of information - O_2 abundance and planetary density - were available, an intense modeling activity would then be needed to estimate the possible abundance of abiotic O_2 in such an atmosphere, as a result of water photolysis and H escape. Only if a consensual answer "should be significantly lower than P_{O2} ≈ 200 mbar" was to be obtained, could the biological implications of the triple bioindicator be considered.

An interesting point would be to estimate what O_2 surface pressure is consistent with a plausible production by H_2O photolysis and its dissolution in the deep water ocean (50 - 100 km, Léger et al. 2004).

The same applies to the dissolution of CO_2 gas. Noticeable, the vibrational mode of that molecule at 15 µm has a huge oscillator strength (Fig.1). It produces a saturated band even at very low concentrations, typically down to 10^{-2} ppm (~10^{-8} bar), which makes abundance estimations from observed spectra very difficult.

Clearly, the observation of a spectrum similar to that of Fig.6 would trigger exciting exo-geophysical studies.

5.3 Case 3, a third possible case for *Proxima b* : a rocky super-Earth with biotic O_2 and abundant CO_2.

A rocky super-Earth, M = 4.0, R = 1.5, is located at the same distance from Proxima Cen than *Proxima b* (a = 0.049 AU, S = 0.65). CO_2 is abundant in the atmosphere P_{CO2} = 300 mbar, and its greenhouse effect is *assumed* to warms the surface up to 280 K. N_2 is present at level P_{N2} = 500 mbar, and O_2, at P_{O2} = 200 mbar. Oxygen is assumed biotic and O_3 at level of Earth. The computed spectrum is shown in Fig.7.

FIGURE 7

The Planck fit yields a temperature of 219 K, which is significantly lower than the ground temperature, 280 K. This is probably due to the poor transparency of the adopted windows when CO_2 is abundant (Fig.1).

H_2O and CO_2 species are identified. The CO_2 15 μm band is strong and saturated. The observed band at 10.5 μm is interpreted as a CO_2 satellite. It corresponds to much lower an oscillator strength than the 15 μm band, its cross section being four orders of magnitude lower (Fig.1). As it is located in a domain without other major absorption, it allows an estimate of the CO_2 abundance. At the spectral resolution of 40, one measures a ~20% absorption. From the curve of growth (CoG)[1] of the band by Des+, this corresponds to a CO_2 pressure of 30 mbar (Fig. 8). This is a lower limit because the spectral resolution is limited, and therefore is consistent with the input 300 mbar[2].

FIGURE 8

Now, what is the significance of the 9.5 μm band? At the spectral resolution used, this band overlaps with both an O_3 band (9.6 μm) as well as a second CO_2 satellite band (9.3 μm) (Fig. 1). According to the preceding estimate of the CO_2 abundance and the CoG of this band, the CO_2 9.3 μm band alone would have a depth of ~30%, whereas the observed value is ~25%. Then, the observed band can be explained by CO_2 *only* and there is no evidence of an additional O_3 band that would trace the (actual) presence of O_2. This is not therefore a case of false negative for the Triple bioindicator, it is a case where such ideas *cannot apply,* even if O_2 is abundantly present in the input atmosphere. Selsis et al. (2002) came to a similar conclusion when assuming P_{CO2} = 1 bar.

The *visible* spectrum would also be valuable to investigate for this scenario. This could indicate the presence of O_2 and its abundance, two pieces of information that the IR

[1] See for instance: www.physics.sfsu.edu/~lea/courses/grad/cog.pdf
[2] Using the full resolution of the model, $\lambda/d\lambda = 2.5\ 10^5$, the same procedure yields the actual CO_2 pressure, 300 mbar. Such a resolution at these wavelengths is however not generally discussed for currently-planned missions"
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spectrum cannot provide in this particular case (the O_3 band is hidden by a CO_2 band and cannot sign the presence of O_2). In the Earth spectrum, P_{O2} = 210 mbar, the 0.76 µm O_2 band is 50% deep for an average cloud coverage, whereas the 0.69 µm band features 19% (Des+). Although the reflectance spectrum of the considered planet has not been calculated in the present work, it is likely that the spectral features would be analogous for this super-Earth (M = 4.0, R = 1.5) and the Earth because the main difference between their atmospheres is between their height scales (proportional to R_{pl}). These O_2 bands are non-saturated and they would permit a good estimate of O_2 abundance if the S/N ratio of the visible spectrum is sufficient. This remains true in the worse case scenario assuming full cloud coverage[3] because O_2 is present in the high atmosphere, above the water clouds[4]. Detecting a high O_2 abundance would be an indication that it is biotic because an abiotic production is capped at ~10 mbar in these planetary conditions (Tian et al. 2014), far below what would be measured.

However, only a high quality spectrum could do that, typically $\lambda/\delta\lambda \geq 70$ and $S/N \geq 8$ for a 4 σ detection of the strongest O_2 band. The detection of O_3 in the IR would possibly be easier because the needed spectral resolution and signal to noise are less requiring than in the visible ($\lambda/\delta\lambda = 20$ and $S/N = 5$, see Table 2 in Sect.6). If an appropriate IR instrument were built first, such a O_3 detection would likely stimulate building the necessary instrument for observing in the visible, including at the level of getting funds.

It is another case where the simultaneous observation of *both* spectral domains (thermal IR + visible) is highly desirable.

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[3] A full cloud coverage is unlikely situation for a terrestrial planet rotating at a sufficient speed, say a local day shorter than 3 terrestrial days. This is due to the descending parts of the Haley cells that are dry and locally give clear sky (the subtropical deserts on Earth).

[4] The behavior of H_2O bands in the presence of high altitude clouds is different from those of O_2. The 0.94 µm water band moves from a 80% depth without clouds, to only 1% with high altitude clouds (Des+), in agreement with the localisation of most of the water vapour lower than the high altitude clouds (cirrus).

5.4 Case 4, a mini-Neptune in the HZ of Epsilon Eridani

In Case 4, and subsequent cases, planets are considered around the solar type star, Epsilon Eridani (eps Eri).

A mini-Neptune (*M* = 4.0, *R* = 1.8) is located in the HZ of eps Eri at *a* = 0.58 AU (*S* = 1.0). Atmosphere is made of 80% H_2, 19% He, and 1% CH_4, close to that of Neptune (3%) or the other gaseous planets of the Solar system (Guillot and Gautier 2007). The resulting spectrum is shown in Fig.3, Sect 4.

The Planck continuum is fitted to a zero flux at 3.0 μm, and data in (4 - 5 μm) and (10 - 11 μm) windows. It yields T_{cont} = 315 K.

Strong and broad absorption features appear around 6.0 μm and 7.5 μm. They are attributed to CH_4, as in Neptune (Fletcher et al., 2010). They correspond to strong bands in CH_4 spectrum (Fig.1). The 7.5 μm feature corresponds to the umbrella bending mode of this molecule (Jiang *et al.* 2013). The observed spectrum reveals a H_2 rich atmosphere. This is expected for giant exoplanets, provided that their outer atmospheric contain CH_4 as in all the giant planets of the Solar System (by volume: Jupiter ~0.2%, Saturn ~0.4%, Neptune ~3%, Uranus ~3%, Guillot and Gautier, 2007).

5.5 Case 5, a hot water ocean-planet around Epsilon Eridani

A water ocean-planet, M_{pl} = 2.0, R_{pl} = 1.5, (wt 50% water, 50% rocks), is similar to that of Case 2, but orbiting around eps Eri and significantly hotter, *a* = 0.57, *S* = 1.05. Atmospheric abundances are: P_{N2} = 1 bar, H_2O from saturated vapor (at T_{surf} = 413 K, P_{H2O} = 3.6 bars), 1 ppm CO_2, no O_2.

The calculated spectrum is shown in Fig. 9. Contrary to the preceding cases, the Planck fit does not use several data points within atmospheric windows, but instead employs only a few discrete points in order to obtain a continuum from which all features appear downwards. This situation is due to the strong absorption of the thick H_2O atmosphere. Selected points are: dF/dλ(2 μm) is set to zero, the 2 μm wavelength is selected instead of 3 μm to take into account the strong irradiation of the planet; dF/dλ(3.75μm) is set to a data point which corresponds to a local minimum of the spectrum; dF/dλ(12.2 μm) is set to another data point corresponding to another deep minimum for both H_2O and CO_2 (Fig.1). With these points, the fit yields a surface temperature, T_{cont} = 415 K, close to that inserted (413 K) at the ocean surface. This is in agreement with the low cross sections of H_2O vapor at these two wavelengths. Note that total pressure at ocean surface is ≈ 4.6 bars.

A deep absorption is observed in the (4.2 - 9.0 μm) interval, corresponding to the P and R parts of the so-called "6.3 μm" bending mode of water. The central Q band is evident as a reduction in the absorption in agreement with the lower cross section at that wavelength (Fig. 1). The flux decrease at λ < 3.75 μm is faster than that of the Planck function, corresponding to the absorption of the H_2O double stretching modes (so-called "X" band).

The CO_2 absorption around 15 μm is marginally evident, even at such an assumed low abundance of the gas. With these noiseless data, (which do not consider noise sources), results suggest that detailed modeling could permit its detection, especially since H_2O absorption is low in the (12 - 17 μm) domain and would not overlap with the CO_2 absorption (Fig.1). With actual data on the sky and including realistic noise sources, the detection of CO_2 would likely be difficult unless a high signal to noise, S/N $\gtrsim$ 20, were to be obtained.

FIGURE 9

A measurement of the actual mass of the planet is mandatory to establish its water-ocean nature, and to distinguish it from a hot rocky planet with much less water and possibly emerged continents.

5.6 Case 6, a super-Earth in the HZ of Epsilon Eridani, with O_2.

The planet here considered is analogous to Earth but larger, *M* = 4, *R* = 1.5. It orbits around eps Eri at distance *a* = 0.58 AU, so that *S* = 1.0. The atmospheric composition is similar to that of our home planet: P_{tot} = 1 bar (+ H_2O); 78.4% N_2; 19% O_2; H_2O from vapor pressure and profile from that of present Earth (Manabe and Wetherald 1967); 1000 ppm CO_2. O_2 is assumed biotic for the same reason as in Case 3. The larger gravity (17.5 m s^{-2}) makes the atmosphere height (*h*) of the atmosphere more compact than that of Earth.

In that case, no climate calculation is done, an earth like configuration is assumed, and a radiative transfer emission calculation is performed with model (*ii*). It is shown in Fig.10. The Planck continuum gives T_{cont} = 286 K. Spectral features of H_2O, O_3 and CO_2 are observed. As for case 3, the O_2 pressure cannot be derived from the 9.6 μm O_3 band because the band is saturated (Fig. 8).

FIGURE 10

Does this spectrum reveal possible biogenic activity on the planet? In other words, does the *Triple bioindicator* apply? The answer is unfortunately *no*. To be indicative, the bioindicator requires the condition P_{O2} > 10 mbar, a missing piece of information. The spectrum is compatible with a lower O_2 pressure, e.g. P_{O2} = 1 mbar, which could be abiotic (Rosenqvist et al. 1995; Tian et al. 2014). This is another case where a *simultaneous* spectrum of the planet in the thermal IR and in the *visible*, e.g. in the (0.8 - 0.6 μm) domain, would be valuable. The O_2 bands at 0.76 μm and 0.69 μm would appear, and the oxygen abundance could be derived. Explicitly, for an average cloud coverage and P_{O2} = 210 mbar, the maximum depth of the 0.76 μm band at high spectral resolution is 50% (Des+). As for Case 3, an observation at $\lambda/\delta\lambda$ = 70, and S/N = 8 on the continuum, would produce a 4 σ detection of the O_2 band, and the triple bioindicator could apply.

It is interesting to consider the case of that planet with a lower abundance of oxygen e.g. with P_{O2} = 10 mbar, i.e. the minimum abundance for the *Triple bioindicator* to apply (Sect.1.2). The CoG of O_2 (Fig. 8) indicates that its 0.76 μm band would be ~15% deep[5]. A 4σ detection of the band would now require $\lambda/\delta\lambda$ = 70 and S/N = 25 on the continuum, which are demanding requirements.

As mentioned, the 9.6 μm band of O_3 is present over a large range of O_2. A 4 σ detection of the O_3 band would require $\lambda/d\lambda$ ~ 17 and S/N ~ 13, which is easier than conditions for the O_2 band in the visible.

A prior detection of ozone in such a planet would strongly motivate obtaining a high quality spectrum in the visible to measure the oxygen abundance and be able to consider the Triple bioindicator. This is another illustration of the *reciprocal* advantages of having access to both spectral domains.

6. What spectral resolution, what signal to noise ratio?

So far, most analyses have been performed with a spectral resolution $\lambda/\delta\lambda$ = 40, and an infinite signal to noise ratio (S/N), which is of course unobtainable in practice. Now, an optimal set of values for ($\lambda/\delta\lambda$, S/N) will be searched for.

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[5] From Fig.8 for an average cloud coverage, and assuming that the lower atmospheric height of the super-Earth does not change significantly the band depths.

For a given target, the required integration time to detect a spectral feature depends on its relative depth from the continuum, spectral resolution $\lambda/\delta\lambda$, and signal to noise ratio S/N on the continuum (see Fig. 11 caption for a precise definition of S and N). The larger these parameters, the better the discrimination capability, but the longer the required integration time t_{int}. A compromise is necessary.

The Earth-like spectrum of Case 6 is chosen to derive such a compromise. The main spectral features are due to CO_2, H_2O, and O_3. They can be observed at different spectral resolutions and signal to noise ratios. Figure 11 shows four spectra calculated with different combinations of these two parameters, and the corresponding integration times.

FIGURE 11

To qualify the detection of a band, the following criteria are used.

(1) Spectral resolution: at least two data points should be in the FWHM of the band, whatever the relative position of the wavelength grid with respect to the band.

(2) Signal to noise ratio: if A_{band} is the band depth relative to the continuum, and σ_{comb} the standard deviation when combining all the data points within the band, the relation $A_{band} / \sigma_{comb} > 5$ should be satisfied.

Considering the key O_3 band, a set of parameters is searched for that respects the two criteria at a minimum time cost. Table 2 summarizes the parameter sets and indicates whether the criteria are met.

Table 2

Among the four sets, set (c) ***λ/δλ* = 40*,* *S/N* = 20** meets both criteria at minimum integration time, and is proposed as a compromise.

Interestingly, this high spectral resolution set corresponds to an integration time t_{int} = 2 t_0 and fulfills the above criteria, whereas set (b), *λ/δλ* = 20*,* *S/N* = 40, t_{int} = 4 t_0 does not, even if its integration time is twice longer. In some sense, higher spectral resolution is better than high signal to noise.

In the same way, a detailed study by von Paris et al. (2013) concluded that lower values (*λ/δλ* = 20, *S/N* = 10) do not allow reliable detections of H_2O nor O_3 in Earth-like spectra. This is in agreement with our proposed values.

This suggests an instrumental strategy: one should attempt to build an instrument with a spectral resolution that satisfies criterion (1) for all bands of interest. It will retain the possibility of working at high spectral resolution whenever desirable. For broader bands, binning data points for faster observations will always be possible, whereas if the instrumental resolution is low the reverse would not be possible. For detectors the requirement is classical, their should have dark current and read-out noise low enough so that the total noise is dominated by photon noise for most, if not all, observations.

7 Summary and Conclusion

An exercise was performed for testing the ability of thermal infrared spectroscopy to retrieve key components of the atmosphere of a few putative exoplanets, some being different possible cases for the *Proxima b* planet. All were assumed to be in the HZ of their star, or close to it, according to a special interest in the search for planets where water can be liquid, and the *Triple bioindicator* (H_2O, CO_2, O_2, in specified conditions) may be used. Diversity has led the choice of the planets, including diversity in their bulk properties (rocky, water-ocean, hydrogen rich), atmospheric compositions, and spectral types of the parent star.

Planets were considered with an *a priori* atmospheric composition. In four cases, a coupled convective-climate-chemical stationary model of the atmosphere was applied. It also calculated minor species that can be produced by photochemistry, including O_3. In the two others the atmospheric structure was imposed. The IR emission was computed using a radiative transfer model, and the retrieval of input gases was search for.

For the six putative planets considered, no *false positive* of the Triple bioindicator is found when all its criteria are fulfilled, including the impact of the harsh irradiations from an MV star. Notably, in Case 3, a telluric planet with O_2 and abundant CO_2, the abundant presence of the latter gas prevents the observation of the 9.6 μm O_3 band, and consequently the detection of O_2. In Case 4, the spectrum of an assumed H_2 rich planet, pointed correctly to the identification of a gaseous planet.

In several cases, the simultaneous acquisition of a *visible spectrum* would be valuable, especially when the O_3 band is observed in the IR and traces the presence of O_2 but cannot measure its abundance. High quality spectra in the visible are the way to measure O_2 abundance and decide whether the *Triple bioindicator* can apply. The discovery of ozone in the thermal IR requires less stringent spectral resolution and signal to noise ratio and may be somewhat easier. Then, if O_3 were to be detected in a rocky planet's atmosphere, the motivation would be such that gathering funds for building an adequate mission in the visible should be possible.

Finally, the measurement of the *actual mass* of the planet is mandatory in all cases for identifying its bulk composition and have an idea of the conditions at its surface, necessary conditions for any spectroscopic bioindicator study. It is pointed out that *no mission, nor* *ground observation, is foreseen* that can perform this task exhaustively around our neighboring stars, the targets of future spectroscopic observations.

An observing strategy is proposed for the retrieval of key species at a minimum integration time cost, a spectral resolution $\lambda/\delta\lambda = 40$, and a signal to noise ration S/N = 20. It fulfills criteria for the detection of the main species in Earth-like spectra. This approach is preferred over $\lambda/\delta\lambda = 20$ and S/N = 40, which does not always fulfill detection criteria and requires longer integration times. An executive implication results for the concepts of future instruments, they should have, at least, a spectral resolution of 40.

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