

Detection of ozone for use as an extrasolar biosignature

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ABSTRACT

While it has previously been proposed that ozone could be a sign of life if detected in an extrasolar planetary atmosphere, detection from the Earth's surface had not been explored as a viable option. Using data from HITRAN, I explore this possibility.

1. Introduction

The ozone in the Earth's atmosphere is indispensable to the existence of life as we know it: it screens out harmful ultraviolet rays that would otherwise be harmful to most life forms. It has been proposed by Schindler & Kasting (2000) that ozone could be used as an extrasolar biosignature, particularly on NASA's proposed Terrestrial Planet Finder (TPF). The only significant abiotic source of O_2 in the Earth's atmosphere is the photolysis of H_2O , producing $\approx 4 \times 10^7$ molecules of O_2 $cm^{-2} s^{-1}$; however this production is overwhelmed by a total volcanic oxygen sink of $\approx 5 \times 10^9$ molecules $cm^{-2} s^{-1}$, through reactions with reduced volcanic gases and oxidation of the Earth's crust (Schindler & Kasting 2000). Thus in an Earthlike atmosphere, if there is a significant amount of O_2 present in the atmosphere, this could likely be explained by the presence of life on the planet's surface. Further, O_3 has a nonlinear dependence on atmospheric O_2 —decreasing from its present level only when O_2 falls below 10^{-1} of its present level (Ratner & Walker 1972)—meaning that if indeed O_2 abundance is a biomarker, it would be accompanied by the more prominent and more easily detected O_3 spectrum, specifically its strong absorption line centered around $9.6\mu m$. In this paper I explore the possibility of whether an atmosphere containing ozone could be detectable through the Earth's atmosphere; if, taking into account shifts from the Doppler effect, it would be feasible to search for extrasolar ozone spectra from the Earth's surface. I used the HITRAN molecular absorption database (<http://cfa-www.harvard.edu/HITRAN/>) to model the ozone spectrum of the Earth and earthlike planets, especially focusing on the optical depth τ and its relation to wavenumber ν .

2. Modeling the spectrum using HITRAN data

Optical depth is a measure of the opacity of an atmosphere, dependent on wavelength, with $\tau=0$ being completely transparent and $\tau \geq 1$ being opaque, so the amount of radiation which is able to pass through a given atmosphere is proportional to $e^{-\tau}$. In order to actually calculate the τ needed above, I turned to the HITRAN molecular database, focusing on the 42258 spectral lines located between 980 cm^{-1} and 1080 cm^{-1} in the ozone spectrum. The following equations from Rothman et al. (1998) were used to manipulate the HITRAN data. To begin, the pressure-broadened line halfwidth $\gamma(p, T)$ [cm^{-1}] is the HWHM of a given broadened transition line centered on $\nu_{\eta\eta'}$:

$$\gamma(p, T) = \left(\frac{T_{ref}}{T} \right)^n (\gamma_{air}(p_{ref}, T_{ref})(p - p_s) + \gamma_{self}(p_{ref}, T_{ref})p_s) \quad (1)$$

where $\gamma_{air}(p_{ref}, T_{ref}) = \gamma_{air}(p_{ref}, T) \left(\frac{T}{T_{ref}} \right)^n \cdot \gamma_{self}(p_{ref}, T_{ref})$ is independent of T, and γ_{air} , γ_{self} (both in units of $\text{cm}^{-1}\text{atm}^{-1}$), and the dimensionless n are found in columns 6, 7, and 9 of HITRAN respectively. This value can then be used to calculate the probability density function in [$1/\text{cm}^{-1}$]

$$f(\nu, \nu_{\eta\eta'}, T, p) = \frac{1}{\pi} \frac{\gamma(p, T)}{\gamma(p, T)^2 + [\nu - (\nu_{\eta\eta'} + \delta(p_{ref})p)]^2}, \quad (2)$$

which describes the broadening distribution of each individual transition line centered at $\nu_{\eta\eta'}$ (column 3 of HITRAN). δ (also in $\text{cm}^{-1}\text{atm}^{-1}$) is found in column 10 of HITRAN. Originally ν was taken to be equal to $\nu_{\eta\eta'}$, which simplifies the computation of τ and produces the correct graph on a large scale, but becomes problematic when dealing with shifts on the order of 10^{-4} such as the Doppler shift due to Earth's revolution around the sun at 29.8 km/sec plus its rotation on its axis at $\approx .5\text{km/sec}$. Regardless, f can then be used to find the monochromatic absorption coefficient k (units of [$1/\text{molecule cm}^{-2}$])

$$k_{\eta\eta'}(\nu, T, p) = S_{\eta\eta'}(T)f(\nu, \nu_{\eta\eta'}, T, p), \quad (3)$$

where $S_{\eta\eta'}(T)$ is the line intensity [$\text{cm}^{-1}/(\text{molecule cm}^{-2})$] given in column 4 of HITRAN. $S_{\eta\eta'}$ is dependent on the temperature of the gas, and so must be reextracted from the

HITRAN data in the event of a temperature change. This is fairly simple using the HITRAN companion program JavaHAWKS. This then ultimately is used to calculate the dimensionless optical depth:

$$\tau_{\eta\eta'}(\nu, T, p) = uk_{\eta\eta'}(\nu, T, p) \quad (4)$$

As ozone is mostly concentrated in the stratosphere, extending from $\approx 11\text{km}$ to 48km , I approximated the height as 30km , giving a temperature T of 227K . This height also gives a value of 21.758 Pa , or $2.147 \times 10^{-4}\text{ atm}$ in p in equations 1 and 2. The partial pressure p_s for O_3 is estimated at $0.07\text{ ppmv} = 1.503 \times 10^{-11}\text{ atm}$. In equation 4, u is the column depth of ozone, taken to be the global average of $8.061 \times 10^{18}\text{ molecules cm}^{-2}$. Ultimately the actual intensity of the radiation which is received from the atmosphere (i.e. the actual amount of energy which passes through plus the energy emitted by the atmosphere itself) will be given by:

$$I_\lambda = I_{\lambda_0}e^{-\tau_\lambda} + S_\lambda(1 - e^{-\tau_\lambda}), \quad (5)$$

where the first term on the right-hand side describes the attenuation due to absorption, and the second term represents the change in intensity due to emission. The initial intensity I_{λ_0} was normalized for simplicity. S_λ is the source function $\frac{\epsilon_\lambda}{\kappa_\lambda}$. A graph of wavenumber versus line intensity can be seen in Figure 1. I designed a program written in C++ to modify the HITRAN data files to replace the line intensity with either the optical depth τ , the percentage of radiation transmitted $e^{-\tau}$, or the percentage absorbed $(1-e^{-\tau})$. These new parameters were then graphed versus wavenumber ν using JavaHAWKS. However, with the real-life column density being used, the graphs of the two latter parameters became too saturated when viewed on a large scale; I focused mostly on the graph of the optical depth (from which the other two could easily be obtained if desired).

Obtaining an accurate model at the degree of precision necessary for very small Doppler shifts requires data out to 10^{-6} , which is the precision of the HITRAN data. For the line broadening equation, I ignored any broadening $> \nu_{\eta\eta'} + 0.005$ or $< \nu_{\eta\eta'} - 0.005\text{ cm}^{-1}$, which gives $\sim 0.001\%$ of the maximum value of τ , simply for (relative) ease of computation. In order to continue graphing using JavaHAWKS, the value of τ must be computed for many points along an individual absorption line; unfortunately this leads to rather large

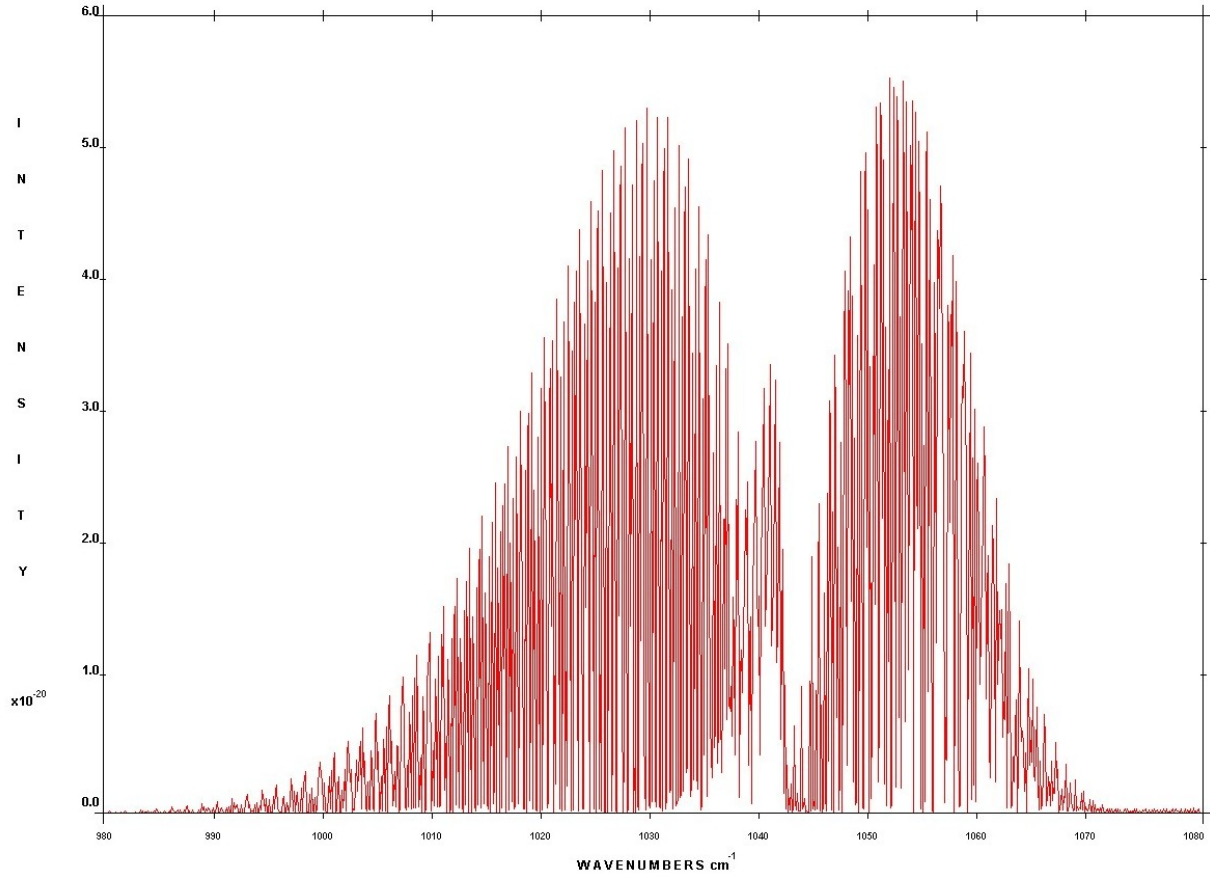


Fig. 1.— The line intensity $S_{\eta\eta'}$ [$\text{cm}^{-1}/(\text{molecule cm}^{-2})$] (given by HITRAN) vs. the wavenumber ν [cm^{-1}]

and unmanageable data files. An alternate graphing system utilizing requiring only τ and ν would be advisable, although none was available to me within the necessary time frame.

For an intensity passing through two identical absorbing columns of gas, the initial I for the second column will be given by the final I for the first column, giving a final intensity of

$$I_\lambda = (I_{\lambda_0} e^{-\tau_\lambda}) e^{-\tau_\lambda} = I_{\lambda_0} e^{-2\tau_\lambda} \quad (6)$$

The final τ can be seen to be the sum of the two separate τ . This can be extended to the more general case:

$$\sum \tau_\lambda = \ln(I_\lambda) = \tau_{\lambda_1} + \tau_{\lambda_2} + \tau_{\lambda_3} + \dots + \tau_{\lambda_n} \quad (7)$$

This is what I ultimately attempted to calculate: with a spectrum shifted an amount d , the optical depth of one line becomes not only the τ of that absorption line added to whatever broadening from other lines may appear at its wavelength, but it will also be added to the optical depth of itself a distance d from its line center. Done properly and accurately, this could include any number of τ , although most would be negligible compared to the optical depth of the line center.

3. Conclusions

I set out to observe the pattern this sort of shifting (periodic in the case of planetary rotation) would produce and to determine if it would be detectable. Ultimately this was not entirely possible due to the precise accuracy necessary and the limited computing capabilities of my program. One point could only be compared to so many others and even with a precision of only 10^{-5} , this produced 1001 data points per absorption line for a total of $\approx 4.23 \times 10^7$ points over the entire absorption band. However, I was able to observe the effect of the shifts on a small scale (Figure 4); obviously more investigation would be necessary, but it remains feasible that extrasolar ozone could be detected from the Earth's surface.

4. Acknowledgments

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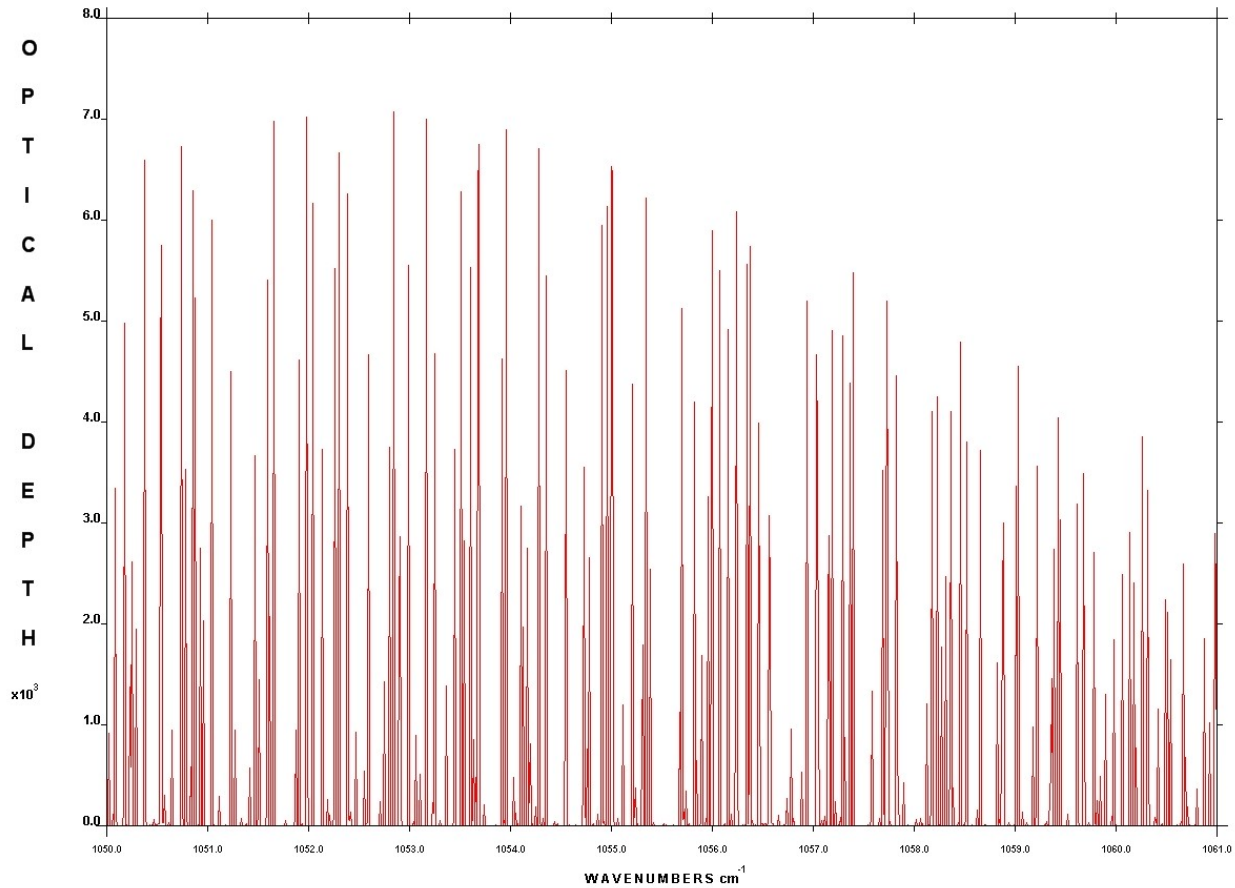


Fig. 2.— The full range of optical depth τ vs. wavenumber for the peak around 1055 cm^{-1} .

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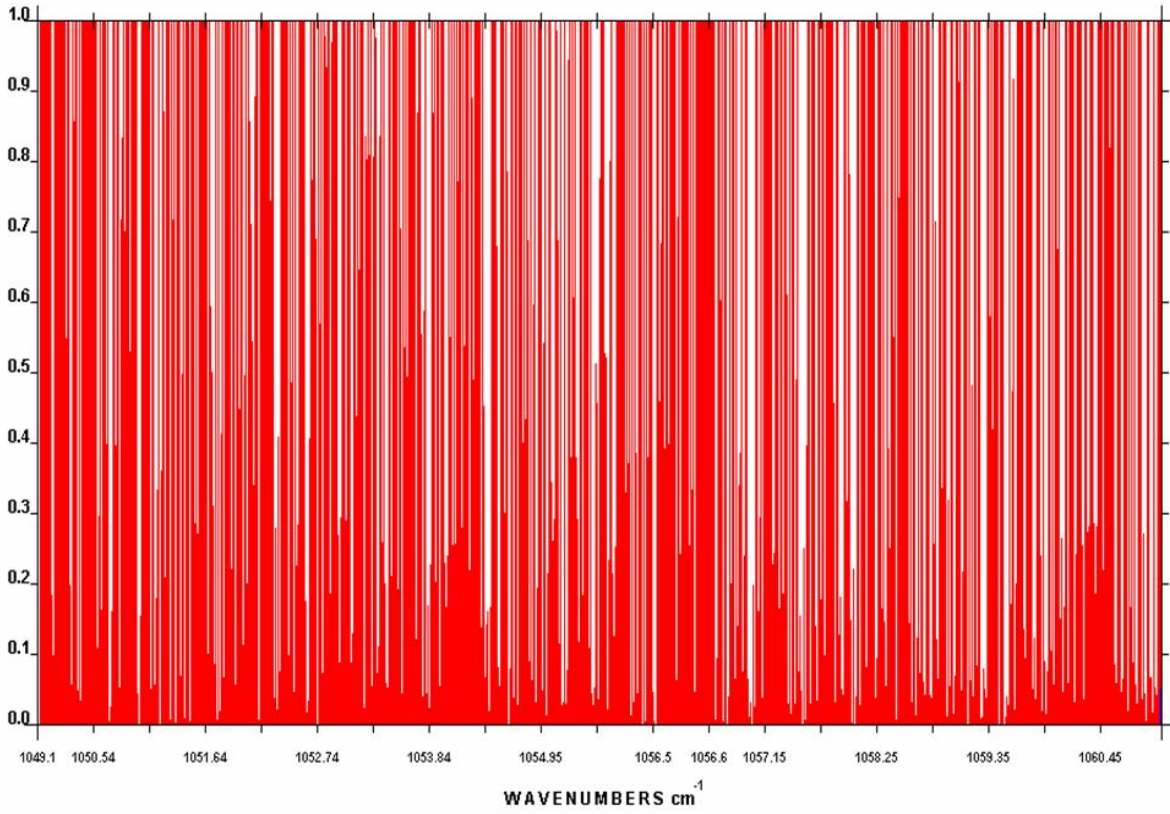


Fig. 3.— τ vs. wavenumber for an optical depth of $0 < \tau < 1$, for which the atmosphere is not opaque

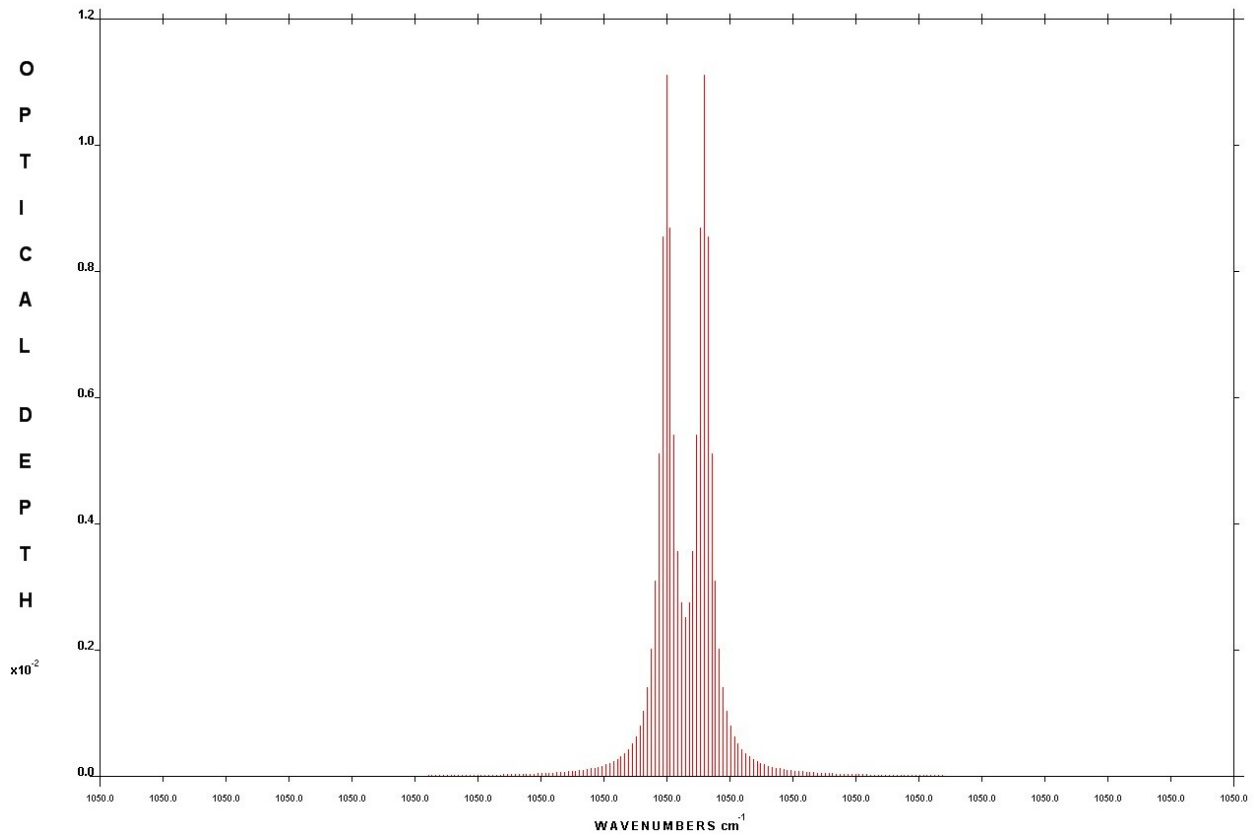


Fig. 4.— A graph of τ vs. wavenumber for only one line shifted against itself a distance of 0.0001 cm^{-1} , with an accuracy of 10^{-5} . The increased absorption in the area of overlap is evident.

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