

# Probing atmospheric escape and evolution in exoplanets: The feasibility of measuring D/H in exoplanet atmospheres using current and future observatories

Vincent Kofman (1,2) and Geronimo L. Villanueva (1)

(1) NASA Goddard Space Flight Centre, MD, USA, (2) American University, DC, USA. (vincent.kofman@nasa.gov)

## Abstract

The Planetary Spectrum Generator is used to simulate the feasibility of measuring the D/H ratio in different exoplanet atmospheres. We consider a number of current and future observatories. Molecular opacities of H<sub>2</sub>O/HDO and CH<sub>4</sub>/CH<sub>3</sub>D are calculated from most recent *ab-initio* line lists and over a wide range of atmospheric conditions.

## Introduction

The D/H ratio is one of the most important cosmochemical parameters and may be measurable with future observatories. The galaxy's initial D/H ratio is constrained by nucleosynthesis at the formation of the universe, but is locally altered by a number of processes, in particular atmospheric escape, and therefore measuring D/H thus provides a molecular tracer for the physical and chemical evolution of the object investigated.

Measuring the D/H ratio in atmospheres is possible by looking at the absorption/emission features of water or methane in the mid-infrared. Even at natural isotopic abundances, the deuterated isotopes have regions where the absorption surpasses the main isotopes. In exoplanet atmospheres, the absorption features are expected to strongly overlap however, making a critical evaluation of the spectral features necessary. Aside from spectroscopic considerations, accurate geometric and instrumental simulations are required to calculate the sensitivity to the atmospheric D/H ratios.

## Methods

The Planetary Spectrum Generator (PSG) [1] allows users to simulate exoplanet spectra, using geometrical parameters from NASA's exoplanet archive, considering full atmospheric radiative transfer properties, and includes instrument parameters for most current and future observatories.

In order to assess the feasibility of D/H detections, the ro-vibrational opacities of all of the relevant species (i.e. H<sub>2</sub>O/HDO and CH<sub>4</sub>/CH<sub>3</sub>D) have to be very well constrained. *Ab-initio* line lists offer the most complete and accurate way to calculate molecular absorptions. Here, we make use of the most recent line lists [2,3,4,5] to generate molecular absorbances as a function of atmospheric composition, pressure, and temperature. We update PSG with the new line lists, which is used to simulate mid-infrared spectra of transiting exoplanets.

In this study, we investigate the feasibility of D/H detections using HST, JWST, HabEx, LUVOIR, OST, and ELT/GMT/TMT. A number of different atmospheres and planetary sizes are considered, all placed at 10 pc. Included in the calculations are stellar emission spectra, realistic noise components, and photon fluxes.

## Acknowledgments

This work was supported by the NASA's Exoplanets Research (16-XRP16\_2-0071) and NASA's Emerging Worlds Research (15-EW15\_2-0175) programs.

## References

- [1] Villanueva, G. L., Smith, M. D., Protopapa, S., Faggi, S., & Mandell, A. M.: Planetary Spectrum Generator: An accurate online radiative transfer suite for atmospheres, comets, small bodies and exoplanets, *Journal of Quantitative Spectroscopy and Radiative Transfer*, Volume 217, p. 86-104., 217, 86 (2018).
- [2] Polyansky, O. L., Kyuberis, A. A., Zobov, N. F., Tennyson, J., Yurchenko, S. N., & Lodi, L.: ExoMol molecular line lists XXX: a complete high-accuracy line list for water, *Monthly Notices of the Royal Astronomical Society*, Volume 480, Issue 2, p.2597-2608, 480, 2597 (2018).
- [3] Voronin, B. A., Tennyson, J., Tolchenov, R. N., Lugovskoy, A. A., & Yurchenko, S. N.: A high accuracy

computed line list for the HDO molecule, Monthly Notices of the Royal Astronomical Society, Volume 402, Issue 1, pp. 492-496., 402, 492 (2010).

[4] Yurchenko, S. N., & Tennyson, J.: ExoMol line lists - IV. The rotation-vibration spectrum of methane up to 1500 K, Monthly Notices of the Royal Astronomical Society, Volume 440, Issue 2, p.1649-1661, 440, 1649 (2014).

[5] Gordon, I. E., Rothman, L. S., Hill, C., Kochanov, R. V., Tan, Y., Bernath, P. F., Birk, M., Boudon, V., Campargue, A., Chance, K. V., Drouin, B. J., Flaud, J.-M., Gamache, R. R., Hodges, J. T., Jacquemart, D., Perevalov, V. I., Perrin, A., Shine, K. P., Smith, M.-A. H., Tennyson, J., Toon, G. C., Tran, H., Tyuterev, V. G., Barbe, A., Császár, A. G., Devi, V. M., Furtenbacher, T., Harrison, J. J., Hartmann, J.-M., Jolly, A., Johnson, T. J., Karman, T., Kleiner, I., Kyuberis, A. A., Loos, J., Lyulin, O. M., Massie, S. T., Mikhailenko, S. N., Moazzen-Ahmadi, N., Müller, H. S. P., Naumenko, O. V., Nikitin, A. V., Polyansky, O. L., Rey, M., Rotger, M., Sharpe, S. W., Sung, K., Starikova, E., Tashkun, S. A., Auwera, J. V., Wagner, G., Wilzewski, J., Weisło, P., Yu, S., & Zak, E. J. 2017, Journal of Quantitative Spectroscopy and Radiative Transfer, Volume 203, p. 3-69., 3 (2017)