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CHEMICAL CHARACTERISATION OF WARM EXOPLANETARY ATMOSPHERES: REVELATIONS FROM JWST ABOUT WASP-39B AND MUCH MORE

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Abstract. The first observations of WASP-39b by JWST permitted important discoveries concerning exoplanetary atmospheres. With this single target, JWST detected for the first time carbon dioxide, but also sulfur dioxide. Importantly, this latter detection (and its analysis) permitted to obtain the first evidence of photochemical processes in an exoplanet atmosphere. In this context, the EXACT project is particularly timely as it will provide physico-chemical data validated at high temperature enabling reliable modelling of warm exoplanet atmospheres. Such data are mandatory to analyse future data from the next generation of instruments.

Keywords: planets and satellites, stars planetary systems, atmosphere, astrochemistry, techniques spectroscopic

1 Introduction

After a perfect launch on December, 25^{th} and six months of commissioning, JWST began its first scientific operations. In order for the community to become fully familiar with the telescope as swiftly as possible and exploit its full capabilities, the Director's Discretionary - Early Release Science (DD-ERS) program has been set up. The particularity of the observations performed during this program is to be released publicly immediately.

To answer to the call, The Transiting Exoplanet Community (gathering hundreds of researchers) submitted a proposal with the aim of accelerating the acquisition and diffusion of technical expertise for transiting exoplanet observations with JWST. This accepted proposal (ERS Program 1366) is divided in 3 sub-programs, with one target each (Bean et al. 2018):
- Primary transit observation of WASP-39b with NIRISS, NIRCam and NIRSpec
- A single phase curve observation of WASP-43b with MIRI/LRS
- A secondary eclipse observations of WASP-18b with NIRISS

We'll focus in this proceeding on the observations of WASP-39b and the results derived from them (Sect. 2). In view of these discoveries, the EXACT project (funding by ANR) is really timely. We'll present the goal of this project in Sect. 3 and advertise for the very first results.

2 Observations and characterisation of WASP-39b

The warm exoplanet WASP-39b (Faedi et al. 2011) has the mass of Saturn and is slightly larger than Jupiter. It orbits very close (0.048 AU) from his solar-type star. It has been observed by JWST on July 2022. More specifically, observations with NIRSpec PRISM (0.5–5.5 μm) has been performed on July, 10; with NIRCam (2–4 μm) on July, 22–23, with NIRISS (0.6–2.8 μm) on July, 26, and with NIRSpec G395H (3–5 μm) on July, 30–31. The analysis of these different sets of observations lead to a series of six publications (JWST Transiting Exoplanet Community Early Release Science Team et al. 2023; Ahrer et al. 2023; Alderson et al. 2023; Feinstein et al. 2023;

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Rustamkulov et al. 2023; Tsai et al. 2023). The observations of this single planet lead to important results: the first conclusive detection of carbon dioxide (CO_2) and the first detection of a sulfur species, sulfur dioxide (SO_2).

While several other species have been detected in the atmosphere of WASP-39b, a particular focus has been made to understand the origin of SO_2 in this atmosphere. Indeed, this species is not predicted by thermo-chemical equilibrium at such high amount (1–10 ppm) and disequilibrium processes must be invoked to explain such abondances. In Tsai et al. (2023), four different 1D kinetics models have been used in order to reproduce the observations and understand the chemical composition: ARGO (Rimmer & Helling 2016; Rimmer & Rugheimer 2019; Rimmer et al. 2021), ATMO (Tremblin et al. 2015), KINETIC (Moses et al. 2011) and VULCAN (Tsai et al. 2017, 2021). They all used their own chemical network containing sulfur species. From the atmospheric composition derived, the synthetic observations have been calculated with the 3D Monte Carlo radiative-transfer code gCMCRT (Lee et al. 2022). The nominal model reproducing the best the observations is a model assuming a metallicity 10×solar, and a C/O ratio of 0.55 (solar). According to the outputs of all the models, the maximum abundance of SO_2 is found to be at 0.01–1 mbar, with a value of 10–100 ppm (see Fig. 1 of Tsai et al. 2023). This is slightly higher than the values derived from the observations, but still consistent (especially the column-integrated number densities above 10 mbar, see Tsai et al. 2023 for more details).
The analysis of the chemical pathways occurring in the atmospheric models permitted to understand that the production of sulfur dioxide in the upper atmosphere of this planet came from H_2S and was initiated by the photolysis of water, according to:

$$\begin{array}{rcl}
\mathrm{H_2O + h\nu} & \longrightarrow & \mathrm{OH + H} \\
\mathrm{H_2O + H} & \longrightarrow & \mathrm{OH + H_2} \\
\mathrm{H_2S + H} & \longrightarrow & \mathrm{SH + H_2} \\
\mathrm{SH + H} & \longrightarrow & \mathrm{S + H_2} \\
\mathrm{S + OH} & \longrightarrow & \mathrm{SO + H} \\
\mathrm{SO + OH} & \longrightarrow & \mathrm{SO_2 + H} \\
\hline
\mathrm{net: H_2S + 2\,H_2O} & \longrightarrow & \mathrm{SO_2 + 3\,H_2.}
\end{array}$$

This result is very important for exoplanet atmospheric science as it represents the first evidence of photolysis processes in the atmosphere of an exoplanet.
As can be seen on Fig. 1 of Tsai et al. (2023), the several models used in this study do not predict strictly the same abundance of SO_2. The peak of production varies by a factor 10 in term of abundance and by a factor 100 in term of pressure level. These deviations are due to the chemical data used by the models, which are not identical. In particular, the chemical schemes and the UV physico-chemical data are different, because coming from different sources. Indeed, there is no consensus in the community about which data to use and the lack of data at high temperature is an important source of uncertainty (Fortney et al. 2019).

Given the high quality of spectroscopic data that is now provided by JWST, it is urgent to address this point and obtain reliable data at high temperatures. This is the main focus of the ANR project EXACT, presented in Sect. 3.

3 The EXACT project

The EXACT project (EXoplanetary Atmospheric Chemistry at high Temperature, PI: O. Venot) aims at improving the study of warm exoplanet atmospheres. One of the objectives of the project is to reduce the uncertainties of kinetics models by providing physico-chemical data adapted to the high temperatures prevailing in exoplanets such as hot Jupiters and warm Neptunes. On this aspect, the project aims at 1. developing chemical schemes validated in high temperature conditions (Sect. 3.1) and 2. study experimentally the thermal dependency of VUV absorption cross section (Sect. 3.2). All the data developed or obtained in the frame of the project are available on the EXACT website*.

3.1 High temperature validated chemical schemes

Most of chemical schemes used in exoplanetology are developed 'ad-hoc', by picking reactions that seemed relevant from combustion literature, and adding them to existing chemical networks used to study giant planets

*https://www.anr-exact.cnrs.fr/.

(e.g. Moses et al. 2011; Rimmer & Helling 2016). This historically well-used method does not guarantee the completeness of the chemical schemes neither their validity. In an interdisciplinary collaboration with the Laboratoire Réaction et Génie des Procédés (LRGP), an original approach has been adopted, which consists of building comprehensive new chemical networks adapted from combustion studies and validated as a whole (not only individual reactions) against experimental data of the literature. These data correspond to combustion experiments performed on large ranges of temperatures (300-2500 K) and pressures (0.01-500 bars). This unique specificity allows these schemes to be highly robust and reliable. With this approach, several chemical schemes have already been developed (Venot et al. 2012, 2015, 2020). We have recently revisited our last chemical scheme in order to publish the most up-to-date CHON chemical scheme (Veillet et al. accepted, 2023). When used in a kinetic model, this new chemical scheme leads to quite important variations compared to what was obtained with our last chemical scheme (Venot et al. 2020). In particular in the case of warm Neptunes, such as GJ 436b, for which the abundance of CO_2 and HCN are particularly affected (see Fig. 1 and Fig. 5 of Veillet et al. accepted, 2023). This network will serve as basis for developing the first sulfur network validated on experimental combustion points (Veillet et al. in prep.).

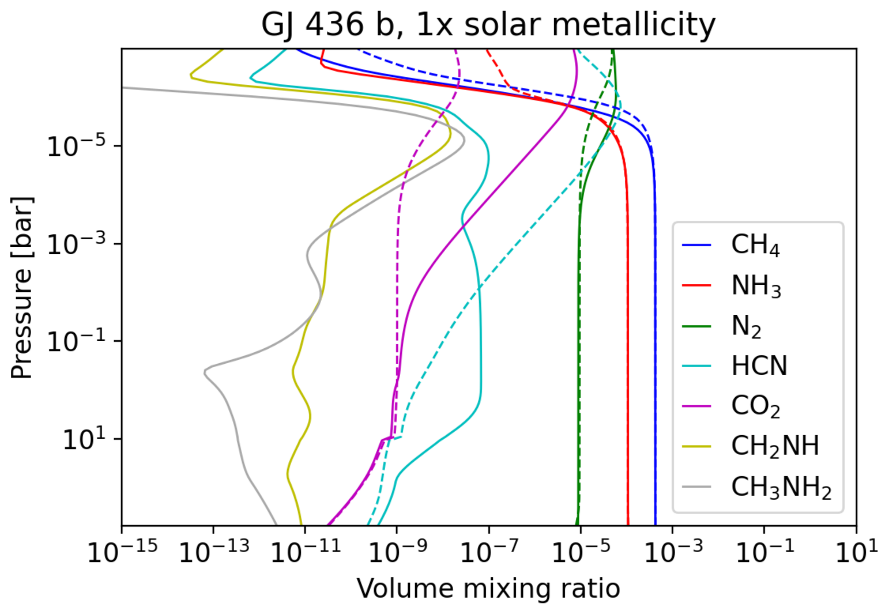

Fig. 1. Abundance profiles of GJ 436 b assuming solar metallicity and a constant eddy coefficient of 10^9 $cm^2.s^{-1}$. Dashed lines are when the kinetic model is using the chemical scheme from Venot et al. (2020), while solid lines are when using the new chemical scheme from Veillet et al. (accepted, 2023). Adapted from Veillet et al. (accepted, 2023).

3.2 Thermal dependency of VUV absorption cross sections

The other source of uncertainty addressed in the EXACT project concerns the VUV absorption cross-sections and their thermal dependency. Indeed, these physico-chemical data, fundamental to calculate the photolysis rates of species and the actinic flux depend on temperature but are poorly known. In the absence of data, room temperature data are often used, which is a major source of uncertainty. Venot et al. (2013, 2018) studied the absorption of CO_2 at various temperatures from 150 to 800 K and observed a strong increase of the absorption with temperature (about four orders of magnitude at 200 nm !). The use of correct data in atmospheric kinetic model has important implication for the chemical composition calculated, modifying by several orders of magnitude the abundance of some (other) species (NH_3, CH_4,...). All the species are indeed linked through chemical reactions, and thus the study of all absorbing species is necessary to have reliable chemical models.
After the study of this first molecule, the EXACT project will permit to study the absorption cross sections of many other molecules, thanks to the VUV spectroscopic platform developed at the Laboratoire Interuniversitaire des Systèmes Atmosphériques (LISA) (Fig. 2). This platform permits acquisition of spectra in the range [50–300] nm with a resolution of 0.01 nm.

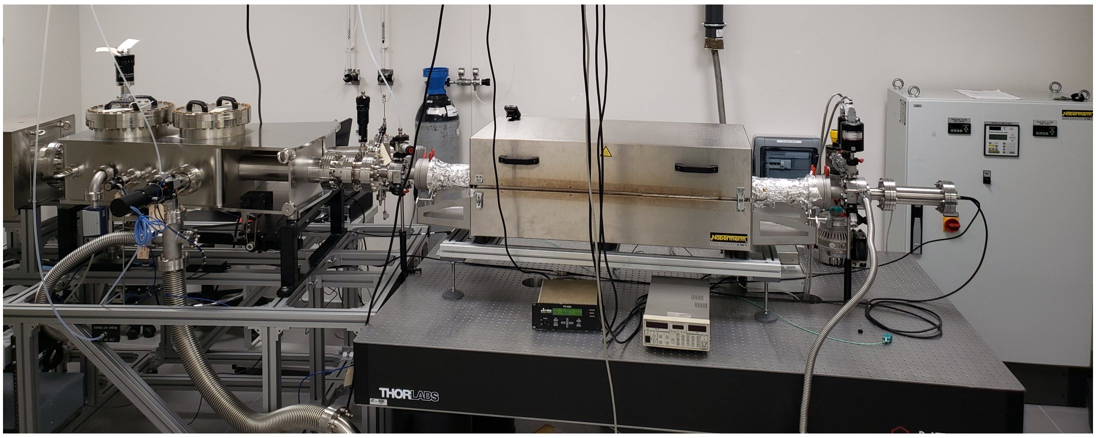

Fig. 2. VUV platform developed at LISA for absorption cross section measurements.

The first molecule for which we studied the absorption cross-section is acetylene (C_2H_2). As expected, we observed that the absorption increases together with temperature (see the Proceeding of Fleury et al. in this Edition and Fleury et al. in prep.).

4 Conclusion

During his first year of life, and with his very first observations, JWST showed us its huge potential. With only one target, the quality of his data and his large spectral covering permits to obtain very important results for exoplanetary atmospheric science : 1) the first firm detection of CO_2 in an atmosphere (JWST Transiting Exoplanet Community Early Release Science Team et al. 2023); 2) the first detection of a sulfur species (Tsai et al. 2023); 3) the first observational evidence of photochemical processes in an atmosphere (Tsai et al. 2023). Given the high quality of JWST data, it is mandatory to have reliable physico-chemical data to study exoplanetary atmospheres. It is the aim of the EXACT project (PI: O. Venot) to provide such data.

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