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ATMOSPHERIC CHARACTERIZATION OF EXOPLANETS WITH THE SPECTROMETER AT MEDIUM RESOLUTION ON JWST/MIRI

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Abstract. Direct observations are needed to constrain the physical properties of long-period exoplanets. The current generation of ground-based instruments allows to observe young, giant, long-period planets : a favorable configuration to minimize contamination by diffracted starlight. The James Webb Space Telescope (*JWST*), launched in December 2021, is equipped with a mid-infrared instrument (MIRI). At these wavelengths, the flux ratio between the star and the planet is more favorable than in the near IR, also providing access to relevant molecular signatures to characterize the atmosphere of exoplanets. Our objective is to evaluate, for the Medium Resolution Spectrometer (MRS), the potential detection of molecules with the method known as "molecular mapping", which allows to distinguish spectrally and spatially the signal of the planet and the signal of the star. We present performance estimates based on simulations of observations. Finally, we present a parametric analysis of the detection capability of the MRS studying the impact of stellar spectral type, planet temperature and angular separation. Once combined with near-IR or coronographic data, the MRS of MIRI would have the ability to improve the characterization of exoplanetary atmospheres and infer constraints on planetary formation.

Keywords: Exoplanets, atmospheric characterization, James Webb Space Telescope, mid infrared

1 Introduction

As of now, about twenty exoplanets have been directly imaged. This method represents a real challenge as it requires to achieve very high contrasts at small angular separations. So far, exoplanet imaging is doable with specialized instruments for high angular resolution combined to coronagraphs, together with post-processing methods to attenuate the starlight. Planetary systems must have favorable features to be imaged: the planet must be far enough from its star so that the planetary signal is not polluted by starlight. Also, it is necessary to observe young giant planets so that they are still warm due to their recent formation and thus emit more light. Finally, the observation in the infrared allows to observe with a reduced contrast and in a spectral range in which the planet is brighter. Such planets have been already observed from the ground in the near-IR (ex: SPHERE, SINFONI, NACO at the VLT), but it is now important to obtain observations in the mid-infrared to further constrain atmospheric parameters. However, mid-IR is more difficult to observe from the ground due to atmospheric absorption. In that context, space instruments are inevitable to provide access to this spectral range, and they also have the advantage of not being impacted by the atmospheric turbulence (better image quality) nor telluric residuals (better for spectroscopy). MIRI, onboard the JWST, provides access to the first direct imaging data above 5 μm which features signatures of molecular species that have never been observed before. In addition, at these wavelengths, the contrast between the star and the planet is even smaller than in the near IR. The MRS is an integral field spectrometer with a resolution up to 3700 (at the shortest wavelength) and covering a wide spectral range from 5 to 28 μm. It has four integral field units, each representing a channel with a different part of the wavelength range and each being subdivided into subchannels (also called bands). As there are 3 sets of gratings, it is necessary to make 3 observations in SHORT, MEDIUM, LONG configuration to get the full wavelength range. Hence one pointing yields 12 cubes, which will be treated individually or reconstructed by channel (Wells et al. 2015)

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2 Molecular mapping method

To characterize the atmosphere of exoplanets and in particular to detect molecules with the future MRS data of MIRI, we used the method called "molecular mapping" introduced by Hoeijmakers et al. (2018). This method uses the fact that the spectra of stars and planets are different to spectrally and spatially disentangle the light of the star from that of the planet. In each spaxel (spectral pixel) we perform a cross-correlation with a synthetic spectrum (using Exo-REM atmospheric models Charnay et al. 2018) of a planet and plot the 2D map of the correlation value retrieved in each spaxel. We obtain values close to 0 at the position of the star and higher values at the position of the planet. The same method can be applied using a synthetic spectrum with the contribution of a single molecule to detect the molecules present in the data. Cross-correlation adds up the individual molecular lines to increase the S/N. To apply this method and simulate MRS data, we used MIRISim (Klaassen et al. 2020) that is supposed to represent the best knowledge of the instrument. The JWST pipeline * is used to correct the simulated raw data for the detector effects, to perform the calibration and cubes reconstruction. Before applying the correlation, we need to subtract the stellar contribution : we filter the low frequencies on each spaxel using a simple Gaussian filter. The low frequencies correspond more to the stellar contribution while the high frequencies components are due to molecular lines present in the planetary atmosphere Ruffio et al. (2019). Afterwards, we can apply the correlation and plot the correlation map. This method has many advantages when used with the MRS, and some results are presented hereafter.

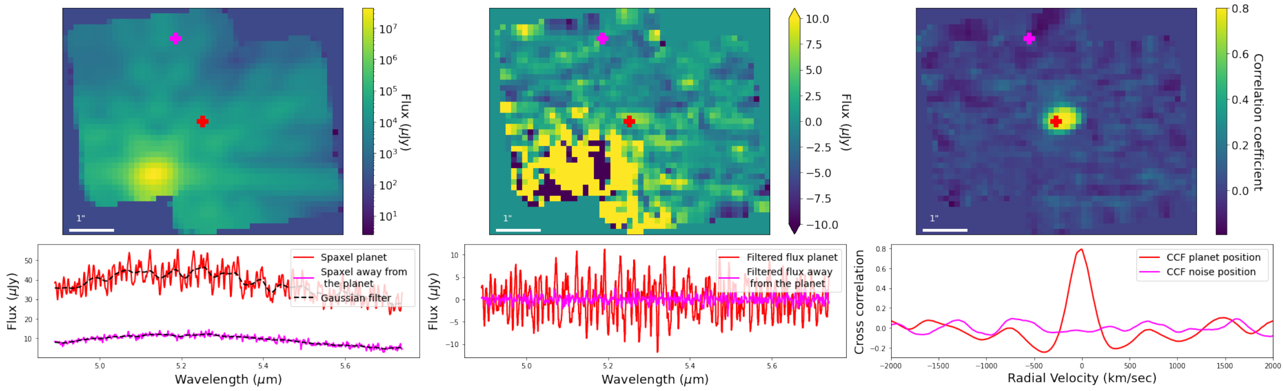

Fig. 1. Top : Simulation in channel 1A for a star ($T = 6000\,K$) and a planet ($T = 1000\,K$) separated by $1.8''$. From left to right: direct image resulting from four dithered positions, the star being offset in the bottom left corner (sum over the wavelengths of the channel); high frequency residuals after subtraction the spectral Gaussian filter in each spaxel; correlation map with the very same template spectra as injected into the simulation for $\delta V = 0$. The red cross indicates the planet position. Bottom : Illustration of the molecular mapping technique in two spaxels, one at the planet's position (red) and the other at a position away from the planet (pink), for channel 1A ($4.885 - 5.751\,\mu$m). From left to right: we display the combined spectra and the Gaussian filter (black) in both spaxels, the high-frequency component after subtraction, and the cross-correlation function for $\delta V = [-2000; +2000]$ km/s.

3 Results on simulated MRS data

3.1 Detection of molecules

GJ 504 is one of the best targets as it is a cold planet (550 K) with a variety molecular signatures in the mid-IR. It is bright and quite far from its star (2.5") (Bonnefoy et al. 2018). The system is simulated by offsetting the star outside of the field of view at coordinates (2.0, -2.5)$''$. Indeed, since this is a nearby system, the star is too bright for the MRS and the detector would saturate in a few groups per integration. After processing the simulated data with the molecular mapping method, we obtain the correlation maps shown in Fig. 2, which displays the S/N for each detection. Molecules are detected by looking at the part of the wavelength range (band or reconstructed channel) that corresponds to the location where the molecular signature is most

* https://jwst-pipeline.readthedocs.io/en/latest

prominent and is not hidden by other molecules. H_2O is detected in channel 1 ($S/N = 57.1$), CH_4 in channel 2 ($S/N = 16.2$), CO in band 1A ($S/N = 9.1$), NH_3 in channel 2 ($S/N = 25.6$), HCN in channel 3 ($S/N = 8.0$), and PH_3 in the band 2B ($S/N = 7.0$), which is a molecule that have not been yet detected in any exoplanet's atmosphere.

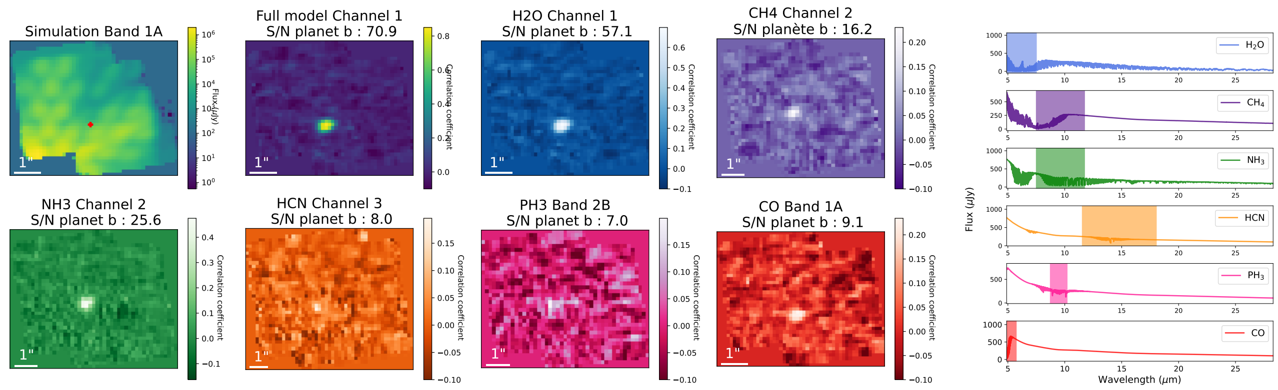

Fig. 2. Left: Correlation maps for the simulated system GJ 504 with ExoREM full template and molecular template. Each molecules is shown in the channel / band where the S/N is the highest. **Right:** Exo-REM molecular template spectra GJ 504, the corresponding part of the spectrum from channels/bands shown are highlighted.

3.2 Disentangle between atmospheric parameters

The detection of molecules can be also an indicator of the temperature of planets. 2M 1207 b is a good example to show the interest of mid-IR wavelengths. The atmospheric properties of this object are not well constrained, so the MRS observations can break the degeneracy between two radically different models. On the one hand Barman et al. (2011) proposed a temperature of 1000 K, log g = 4 and 1.5 R_{jup} and on the other hand Patience et al. (2010) found a best-fit model at about 1600 K and log g = 4.5 with a smaller radius of 0.5 R_{jup}, the two being based on near IR data. Considering the model at 1000 K, we obtained a detection of H_2O ($S/N = 51.3$), CO ($S/N = 9.9$), and NH_3 ($S/N = 10.7$). The planet is well detected ($S/N = 56.6$) with the full model. For the model at 1600 K, the planet is less detected ($S/N = 8.1$) with the full atmospheric model, the detection of H_2O is much lower ($S/N = 3.9$) and CO is undetected because the planet is simply smaller than in the first case. NH_3 is not detected, as expected for such a planet temperature. Since the star is an M8 brown dwarf, the warmer planet scenario represents an extreme case for the molecular mapping method. In this case, the MRS has the ability to provide a definitive answer about the planet temperature. The detection of NH_3 is an indicator for the temperature of the planet.

4 Parametric study

Many directly imaged planets could be observed with the MRS. To test the detection limits of this method, we run a group of simulations of systems with varying properties. First, we kept the contrast between the star and the planet constant and fixed the separation to explore the impact of the temperature of the planet and the star. As the method relies on the fact that the spectra of stars and planets are different, we first check the impact of the spectral lines. We conclude that the stellar spectral type has a weak impact (even if we still have a weaker detection for a planet around a cool star), however the planet's temperature has a more important impact : planets hotter than 1500 K are more difficult to detect and to characterize (Fig. 3, left).
Secondly, we fixed the same star and the planet radius (only the temperature of the planet varies, so the colder planets have a lower flux). We conclude that the planets closer than 1" are more difficult to characterize, and we can again see that those at 2000 K are less well detected (even if they are the brightest in the sample) and those at 500 K as well, because their flux is much lower than the others planets, but they are still detected even if they are very faint (Fig. 3, right). Two aspects are highlighted here: the flux level and the spectral type of the planet will have an impact on the detection level. If we look at the detection of molecules in each case : the further away the planet is from the star (and the colder the planet), the better the molecules can be detected.

Molecules with less spectral features are better detected in the case where the planets are further away from their host star.

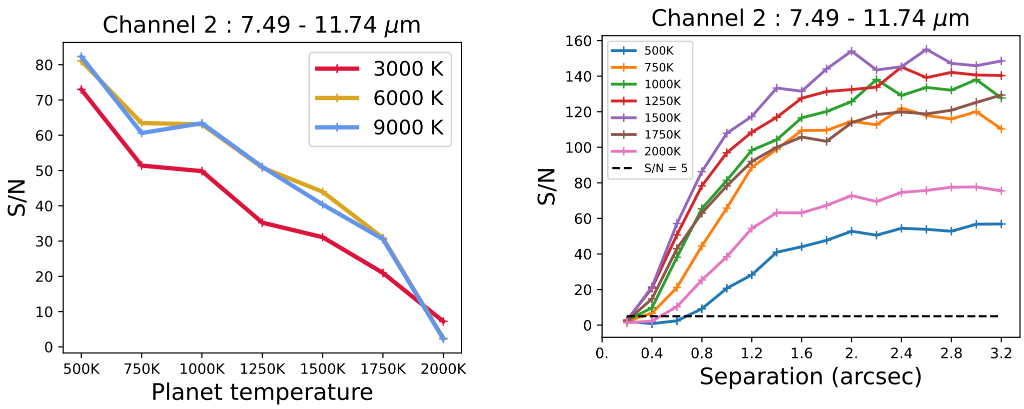

Fig. 3. Left: S/N obtained for planet's temperature ranging between 500 K and 2000 K and stellar temperature of 3000 K, 6000 K and 9000 K. **Right:** S/N obtained for the same temperature range and varying the angular separation with the host star in each case. Both examples in the channel 2 of the MRS.

5 Conclusions

Simulated MRS/MIRI data show that we would be able to detect molecules in the atmospheres of directly imaged planets using molecular mapping. We simulated and analyzed known directly imaged systems, which could be good targets for future JWST observations. This work shows the possibility of detecting molecules such as CO, CH_4, NH_3, H_2O, HCN and PH_3. Then, we defined detection limits and thus concluded that molecular mapping is globally better for characterizing planets colder than 1 500 K and angular separation larger than 1". Future stellar subtraction methods would improve the performance of detection and characterization of planets closer that 1". Using complementary coronographic data (GTO MIRI) and bayesian analysis, we would be able to better define the constraints on the atmospheric parameters.

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