# Are we ready to characterize exoplanet atmospheres with the James Webb Space Telescope observations ?

Jean-Loup Baudino<sup>1</sup>, Pierre-Olivier Lagage<sup>2</sup>, Patrick Irwin<sup>1</sup>, Paul Mollière<sup>3</sup>, Pascal Tremblin<sup>2</sup>

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September 22, 2017



Why?



Why?

Future instruments to detect and characterise extrasolar planets



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JWST



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### JWST

spectroscopy in NIR and MIR



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- spectroscopy in NIR and MIR
- high resolution, S/N



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### Analysing observations with something:



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Models



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forward, retrieval



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- spectroscopy in NIR and MIR
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### Analysing observations with something:

Models

- forward, retrieval
- hypothesis, unknowns ???





### October 2018



J-L Baudino et al., Oxford Uni.

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#### October 2018

▶ NASA, ESA, CSA-ASC, 6.5 m





### October 2018

- NASA, ESA, CSA-ASC, 6.5 m
- ► 4 instruments, 4 main topics (including exoplanet)





NASA-C. Gunn

### Exoplanet characterisation





NASA-C. Gunn

### Exoplanet characterisation

Direct imaging (DI) and transit





NASA-C. Gunn

#### Exoplanet characterisation

- Direct imaging (DI) and transit
- photometry and spectroscopy, 0.6-13 microns





NASA-C. Gunn

#### Exoplanet characterisation

- Direct imaging (DI) and transit
- photometry and spectroscopy, 0.6-13 microns
- 2 instruments developed in Europe: NIRSpec and MIRI



# Expected in good cases, for spectroscopy with NIRSpec and MIRI



Baudino et al. submitted to ApJ

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DI: S/N=100 (30 min)



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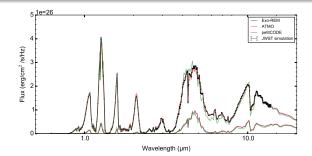
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Emission spectra of VHS 1256-1257 b (top) and GJ 504 b (bottom). The black uncertainties correspond to the combination of simulated NIRSpec/Prism and MIRI/LRS noise level for VHS 1256-1257 b for 0.5 hour of integration.

Baudino et al. submitted to ApJ



### Forward



### Forward

Retrieval



### Forward

compute the thermal and chemical structure of a planet

Retrieval



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- compute the thermal and chemical structure of a planet
- generate spectra and profiles consistent with radiative-convective equilibrium and chemistry

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solve the inverse problem



### Forward

- compute the thermal and chemical structure of a planet
- generate spectra and profiles consistent with radiative-convective equilibrium and chemistry

### Retrieval

- solve the inverse problem
- find the combination of abundances and parameters that reproduces the observations



Various approaches, hypothesis, opacity sources



Various approaches, hypothesis, opacity sources

Identify Find the differences:



Various approaches, hypothesis, opacity sources

### Identify

Find the differences:

emission and transmission



Various approaches, hypothesis, opacity sources

### Identify

Find the differences:

- emission and transmission
- abundances



Various approaches, hypothesis, opacity sources

### Identify

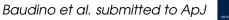
Find the differences:

- emission and transmission
- abundances

### Benchmark

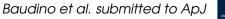
To define a minimal agreement between models to be able to find the differences.







A restrain number of absorbers





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NH<sub>3</sub>, CH<sub>4</sub>, CO, CO<sub>2</sub>, H<sub>2</sub>O, PH<sub>3</sub>, Na, K





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#### Alkali wing shape

Voigt profile



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Elemental abundances Solar (Asplund et al. 2009)



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Solar (Asplund et al. 2009)

same chemical reactions



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#### Alkali wing shape

Voigt profile

#### Elemental abundances

Solar (Asplund et al. 2009)

same chemical reactions

no cloud



### Two kinds of test

Baudino et al. submitted to ApJ



### Two kinds of test

#### Imposed temperature profile

Baudino et al. submitted to ApJ



#### Imposed temperature profile

test of the radiative transfer part

Baudino et al. submitted to ApJ



#### Imposed temperature profile

test of the radiative transfer part

Self-consistent

Baudino et al. submitted to ApJ



#### Imposed temperature profile test of the radiative transfer part

Self-consistent test of the full model

Baudino et al. submitted to ApJ



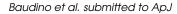
5 given temperature profiles

#### Baudino et al. submitted to ApJ



#### 5 given temperature profiles

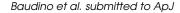
abundance profiles at chemical equilibrium + spectra





#### 5 given temperature profiles

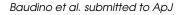
- abundance profiles at chemical equilibrium + spectra
- thermal profiles of Guillot et al. 2010





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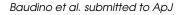
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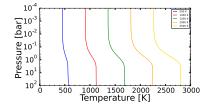
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Input pressure-temperature profiles used in the benchmark



DI

#### Baudino et al. submitted to ApJ



DI

Transit

#### Baudino et al. submitted to ApJ



#### DI

► GJ 504 b T<sub>eff</sub>=510 K, log(g)=3.9, z=0.28 dex

Transit



#### DI

- ► GJ 504 b T<sub>eff</sub>=510 K, log(g)=3.9, z=0.28 dex
- ► VHS 1256–1257 b T<sub>eff</sub>=880 K, log(g)=4.24, z=0.21 dex

Transit



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#### Transit

GJ 436 b, T<sub>eff</sub>=712 K, 0.38 R<sub>Jup</sub>, 0.07 M<sub>Jup</sub>



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#### Transit

- GJ 436 b, T<sub>eff</sub>=712 K, 0.38 R<sub>Jup</sub>, 0.07 M<sub>Jup</sub>
- WASP 12 b, T<sub>eff</sub>=2536 K, 1.736 R<sub>Jup</sub>, 1.04 M<sub>Jup</sub>



### Models used

Forward models, Baudino et al. submitted to ApJ

- ATMO (Tremblin et al. 2015)
- Exo-REM (Baudino et al. 2015)
- petitCODE (Mollière et al. 2015)



### Models used

Forward models, Baudino et al. submitted to ApJ

- ATMO (Tremblin et al. 2015)
- Exo-REM (Baudino et al. 2015)
- petitCODE (Mollière et al. 2015)

#### Retrieval, Baudino et al. in prep.

NEMESIS (Irwin et al. 2008)



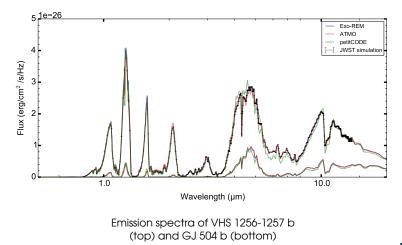
### Difference opacities



Baudino et al. submitted to ApJ

#### Difference opacities

petitCODE (unlike the other models) didn't use  $\rm NH_3$  and  $\rm PH_3$  linelist from Exomol





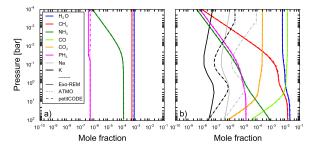
### Differences chemistry

#### Baudino et al. submitted to ApJ



### Differences chemistry

Exo-REM impose a cold-trap (unlike the other forward models) that effect abundance but not spectra



Abundance profiles of the defined molecules for the case with a  $T_{\rm eff}$  =500 K at solar metallicity (a) and 1000 K at 30  $\times$  solar metallicity (b). The curves for the models are often superposed, except for alkalies where *Exo-REM* is not.





**During Benchmark** 



#### **During Benchmark**

1. alkali far wings  $\rightarrow$  first update of the benchmark protocol



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- 2. *petitCODE* was considering calculations without any cut-off. We apply the same profile as *Exo-REM* in *petitCODE* for the benchmark.



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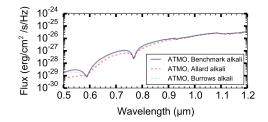
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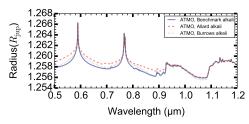
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- 4. CH<sub>4</sub> Hitran vs Exomol
- 5. H<sub>2</sub>-He CIA Hitran not complete before 1 micron



### Alakli



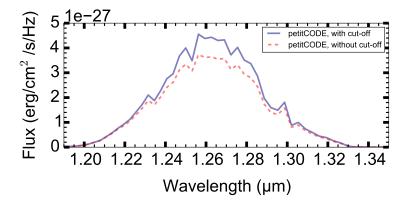
Effects of the different alkali treatments on the emission spectra for the Guillot profile with  $T_{\rm eff}$ =1500K



Effects of the different alkali treatments on the transmission spectra for the Guillot profile with  $T_{\rm eff}$ =1500K



## Far wing lineshape



Emission spectra for GJ 504 b calculated using the nominal temperature structure of the case including sub-Lorentzian far wings. We show the resulting spectrum of the nominal case (blue solid line) as well as the case with full Voigt profiles (red dashed line)





Updates





### Updates

► PH<sub>3</sub>



## NEMESIS

### Updates

- ► PH<sub>3</sub>
- update of the CIA



## NEMESIS

### Updates

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#### To test





#### Updates

- ► PH<sub>3</sub>
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#### To test

radiative transfer in the Benchmark condition



## NEMESIS

### Updates

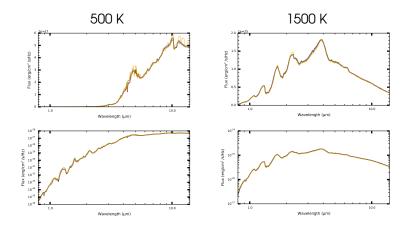
- ► PH<sub>3</sub>
- update of the CIA

### To test

- radiative transfer in the Benchmark condition
- retrieval of the output spectra



## Radiative transfer: Work in progress







Key points



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definition of a benchmark



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- definition of a benchmark
- update of 4 models



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- identification of various approaches with impact on spectrum



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Alkali wing lineshape



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- adding PH<sub>3</sub> in the opacity sources



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- sub-Lorentzian lineshape



#### Key points

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### Approaches with impact on spectra

- Alkali wing lineshape
- adding PH<sub>3</sub> in the opacity sources
- sub-Lorentzian lineshape
- selecting linelists carefully





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Are we ready to characterize exoplanet atmospheres with the James Webb Space Telescope observations ?

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To apply this benchmark on other models !



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- ► To use JWST observations to discriminate the approaches



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- To use the conclusions coming from the observation to update the models



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Do you want to try the benchmark?



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 The paper will be publish with full protocol and the resulting output sources (Baudino et al. submitted to ApJ)



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#### email: jean-loup.baudino@physics.ox.ac.uk twitter: @DrJLoupBaudino

