

Chemical signatures in synthetic spectra induced by XUV radiation

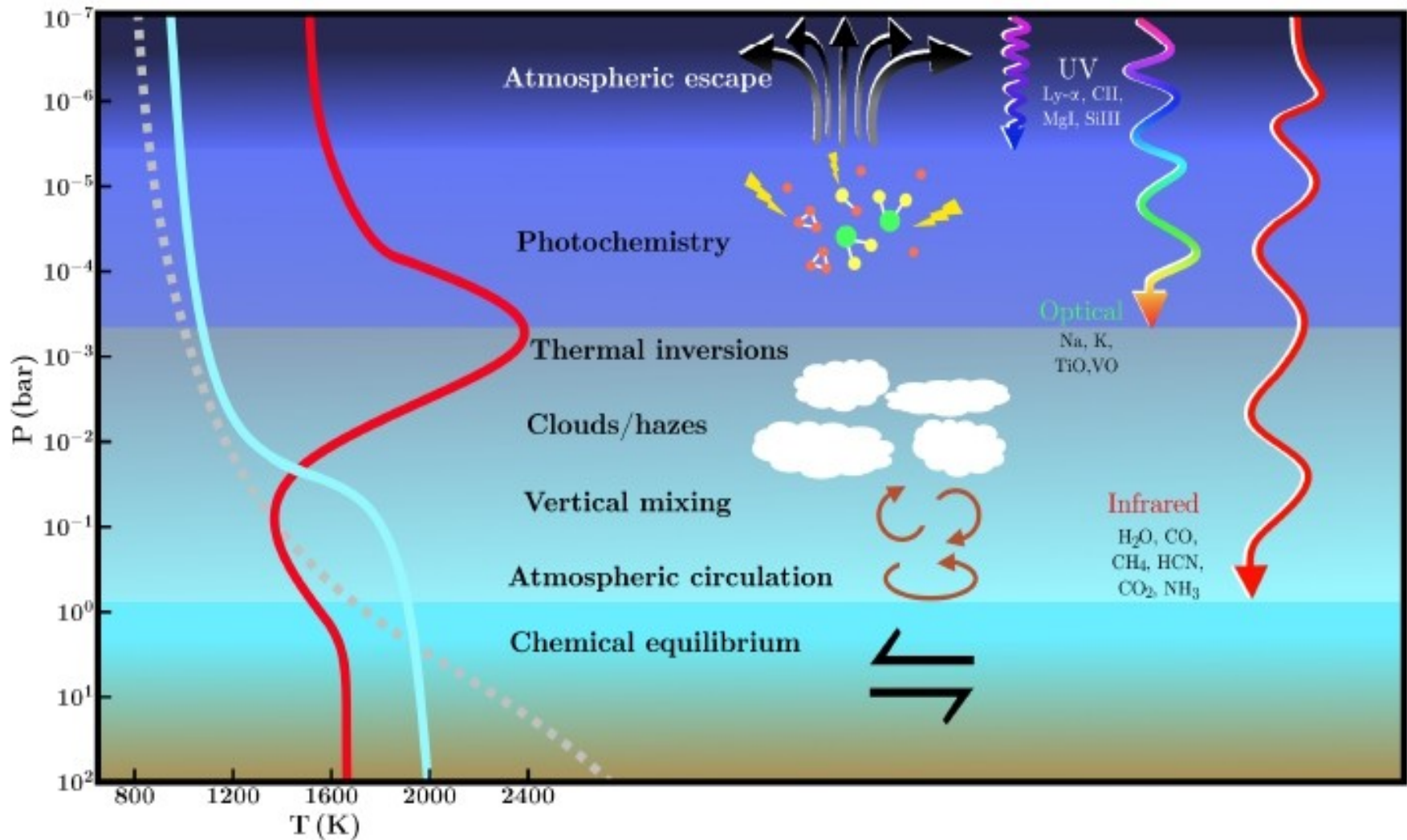
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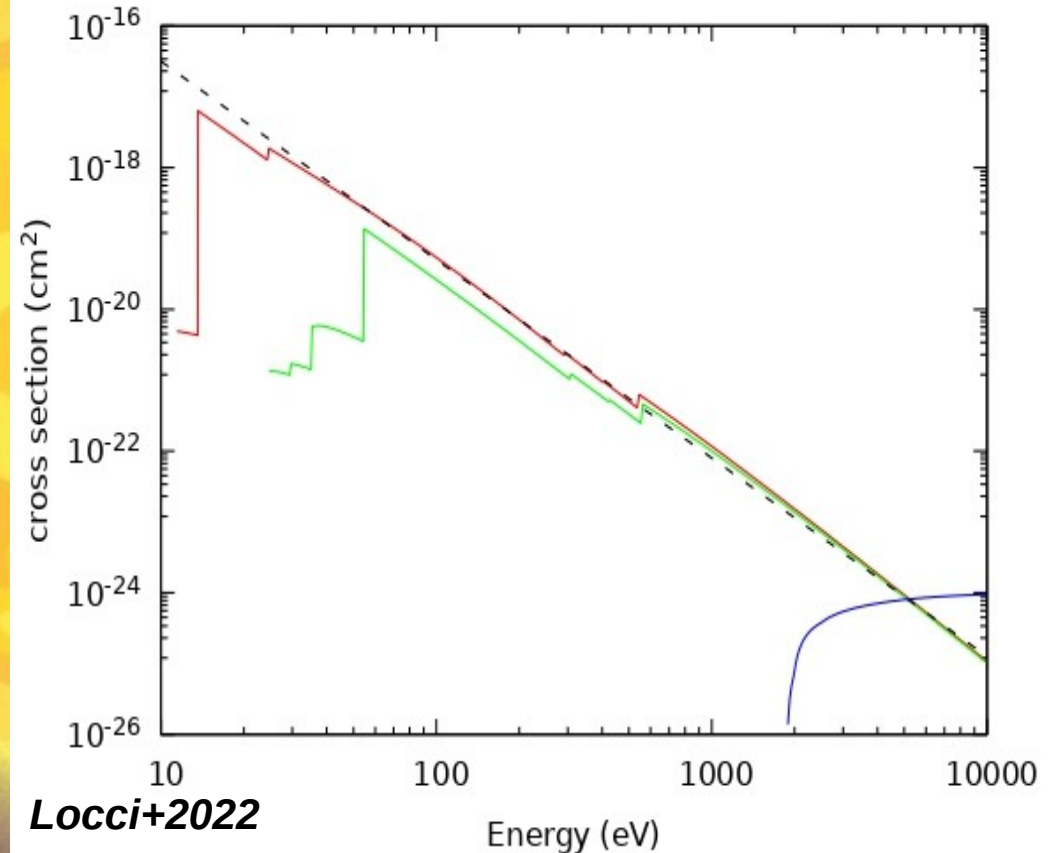
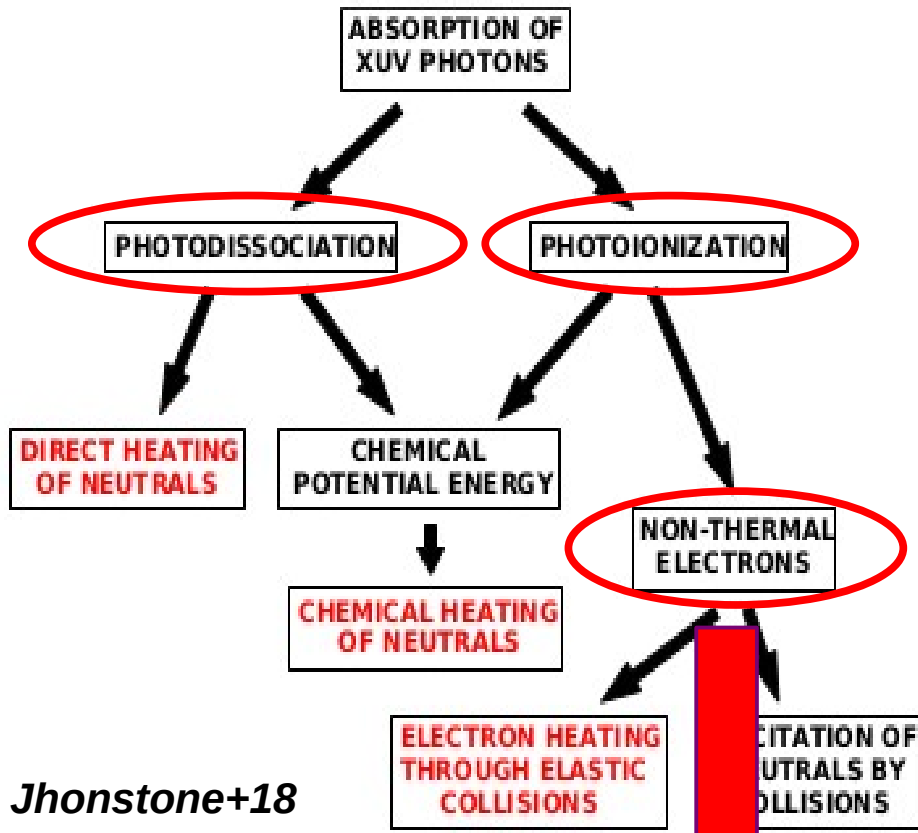
Ariel-It science
26th May 2022



Introduction



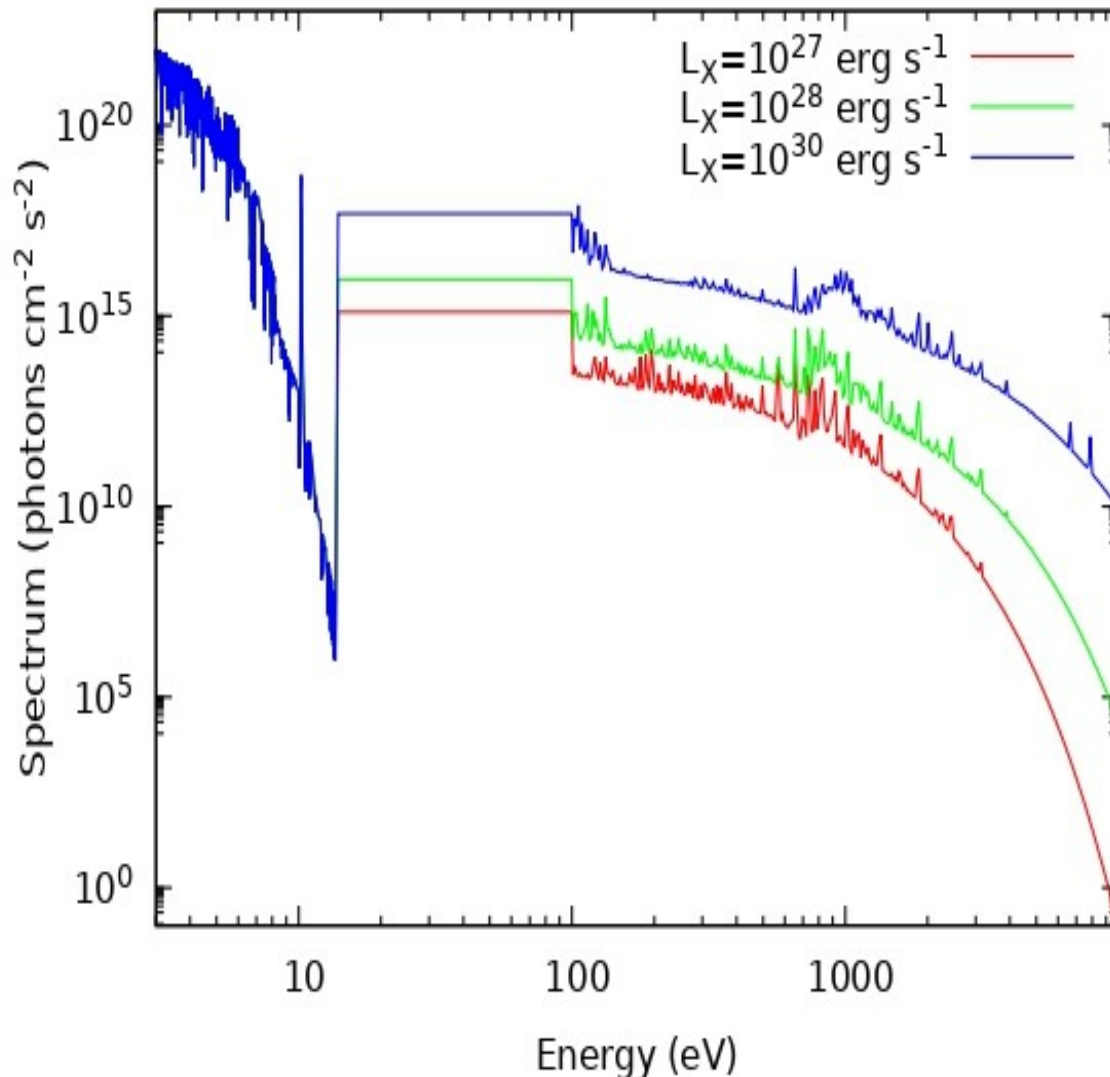
XUV absorption



Secondary ionization

$W(E)$ Energy to make a ion pair
(Cecchi-Pestellini+06)

Adopted spectrum



UV (3 - 13.6 eV)

Stellar spectrum from Phoenix
Lyman- α from *Linsky+20*

EUV (13.6 - 100 eV)

Constant spectral shape

$$L_{EUV} = 6.31 \cdot 10^4 \times L_X^{0.86} \quad \text{Sanz-Forcada+11}$$

X-rays (0.1 - 10 keV)

Emission from a optically thin
plasma *Raymond & Smith+77*

L_X is an input parameter

Chemical network

105 different chemical species plus their ions
2535 chemical and 165 photochemical reactions
Possibility to choose a reduced set of elements

Bimolecular
Termolecular
Thermo-dissociative
Ion-neutral
Photodissociation
Photoionization

Exploratory runs
with ~70 species: H,
He, O, C, N

$$\frac{\partial n_i(r)}{\partial t} + \frac{\partial \varphi_i(r)}{\partial r} = P_i(r) - n_i L_i(r)$$

Exploratory runs

Reference model

Parameter	Value
Mass	150 M \oplus
Radius	12 R \oplus
Temperature	1000 K
Zenit angle	60°
X-rays luminosity	10 ²⁸ erg s ⁻¹



Ionization provided by EUV radiation is the dominant process in the upper layers

Due to the small cross section of atmospheric constituents X-rays penetrate deeper in the atmosphere giving rise to a characteristic chemistry

We found two classes of elements:
Species like hydrocarbons or ammonia that increase their abundance with the increase of X-rays luminosity
Species like water or carbon monoxide that decrease their abundance with the increase of X-rays luminosity

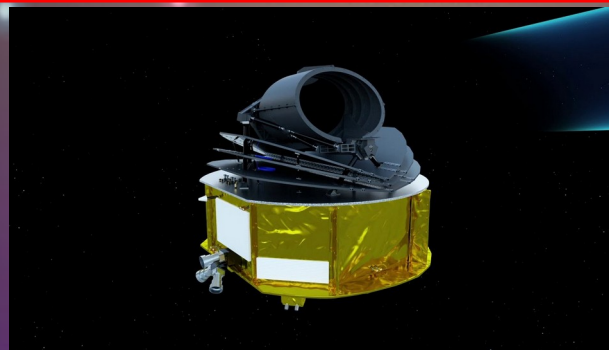
Transmission spectra

(working in progress)

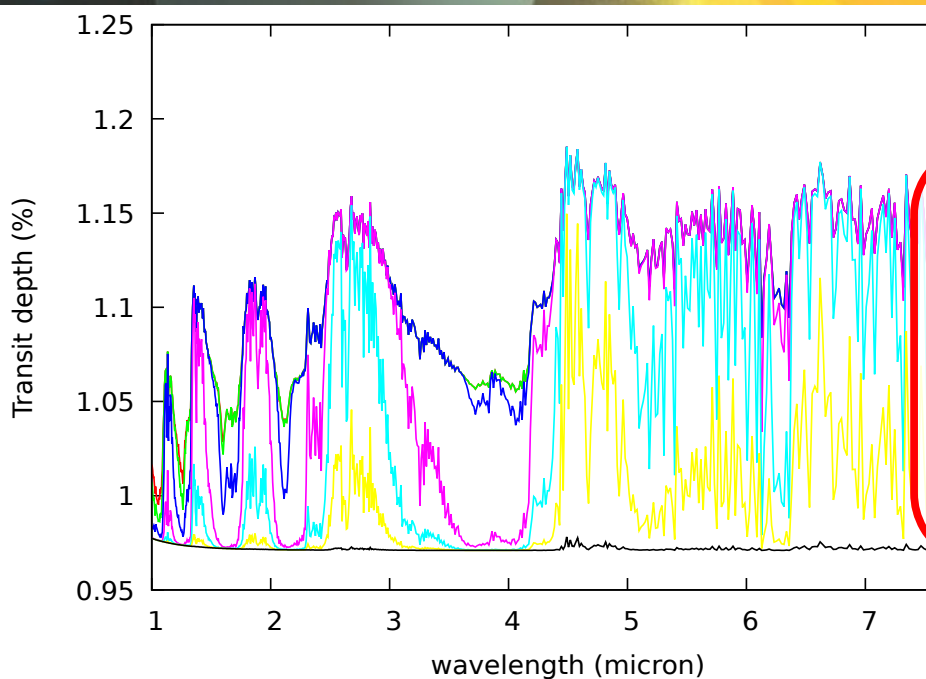
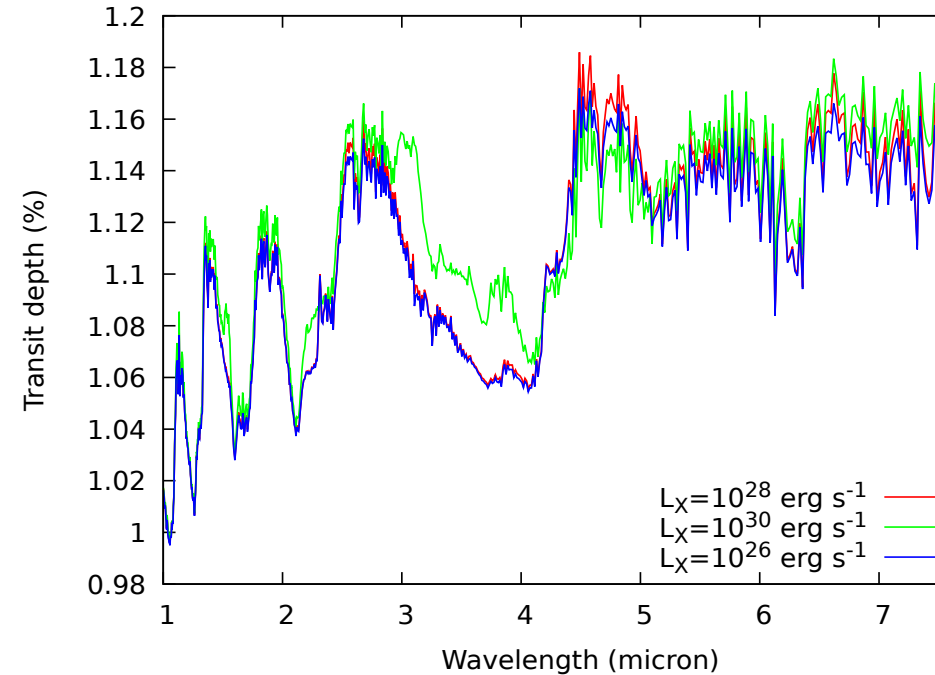
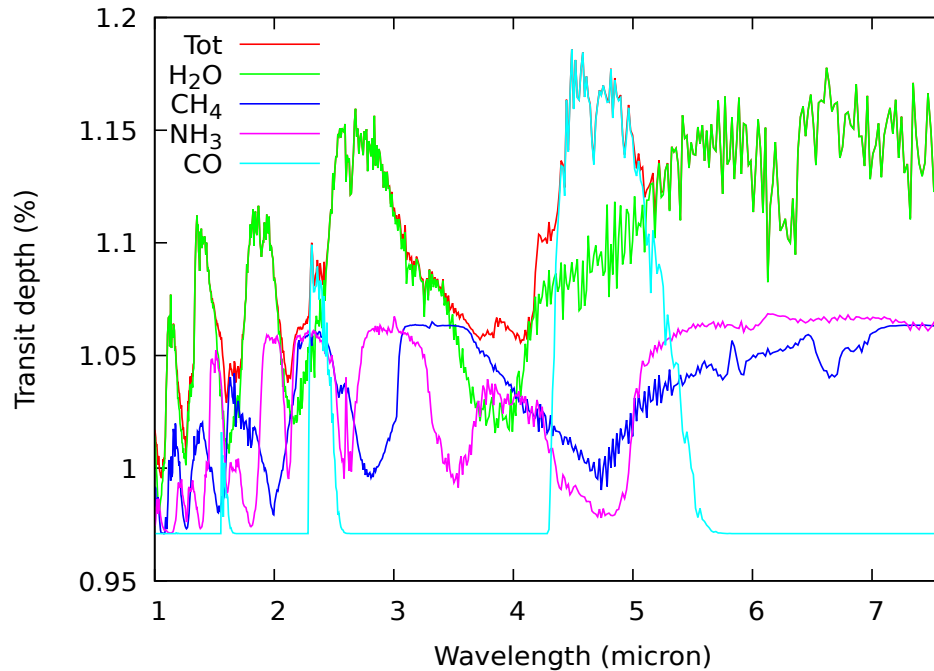
We build up total absorption cross-section taking into account several neutral species such as H_2O , CH_4 and NH_3 and some ionic species such as H_3O^+ , H_3^+

We assembled absorption coefficients exploiting the molecular spectroscopic databases ExoMol and HITRAN in the interval $0.24\text{-}1000\ \mu\text{m}$

Exploiting the chemical code we computed vertical chemical profiles for different values of X-ray luminosity. For each model and for each pressure grid point we calculated absorption cross-sections

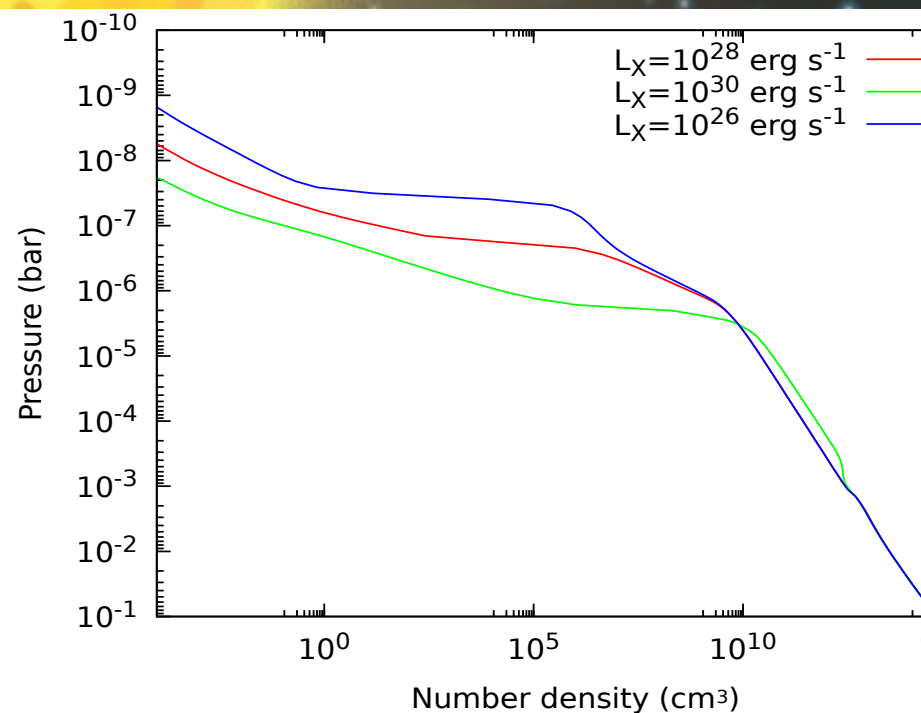
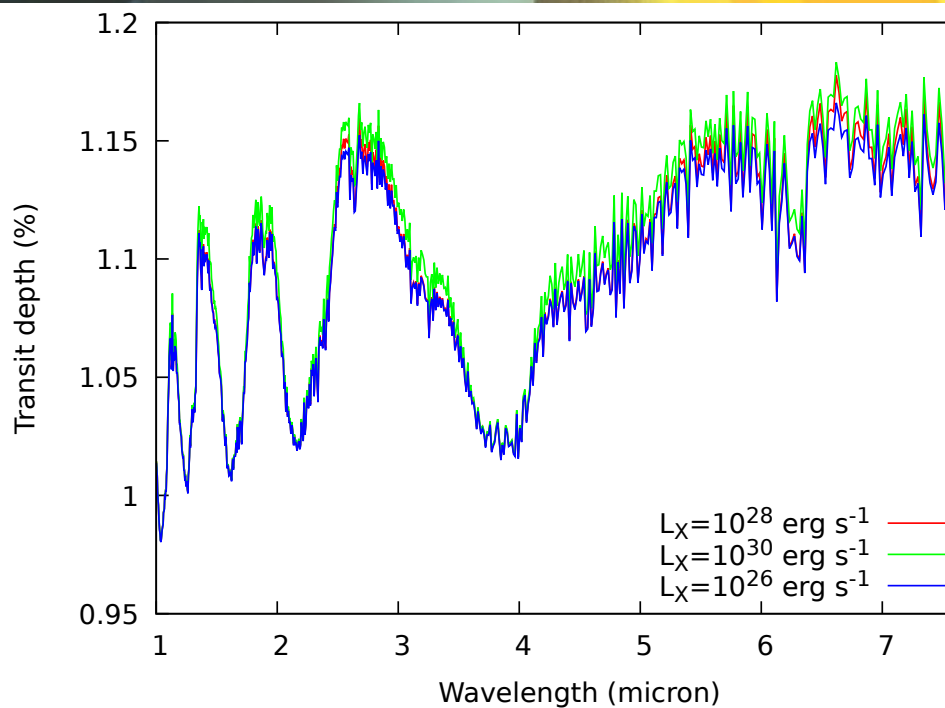
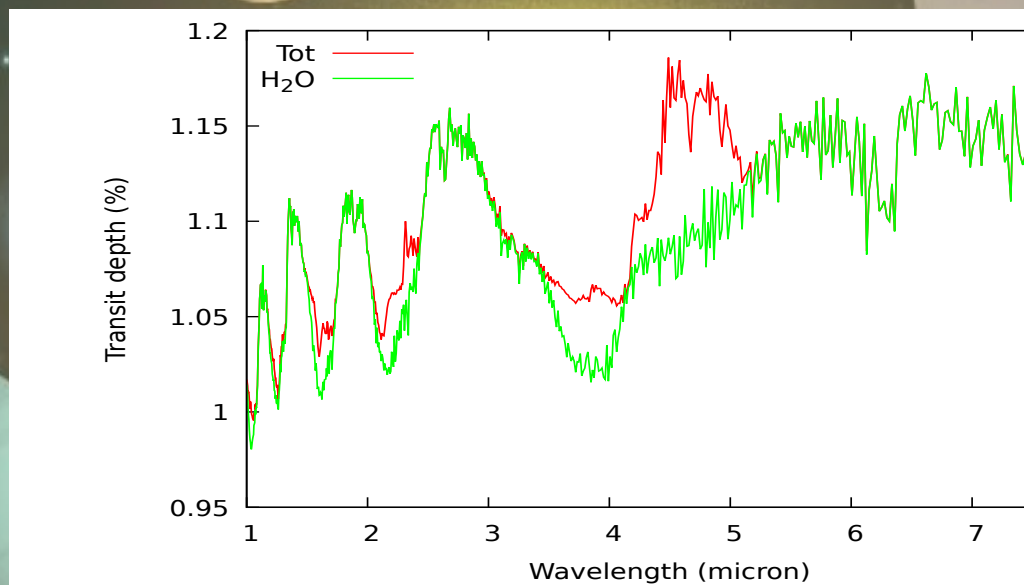


Transmission spectra

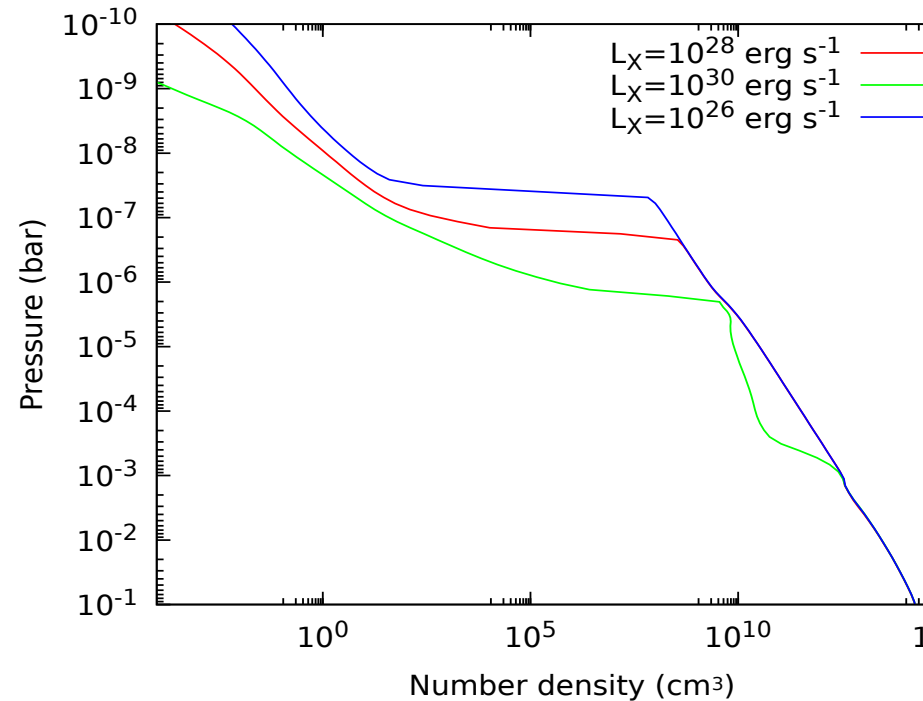
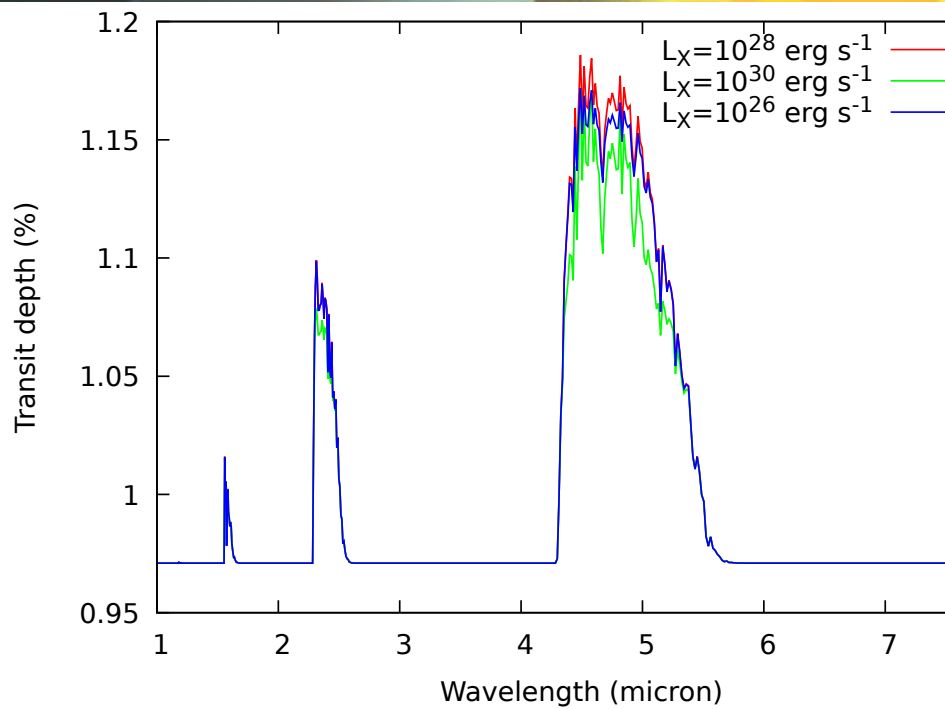
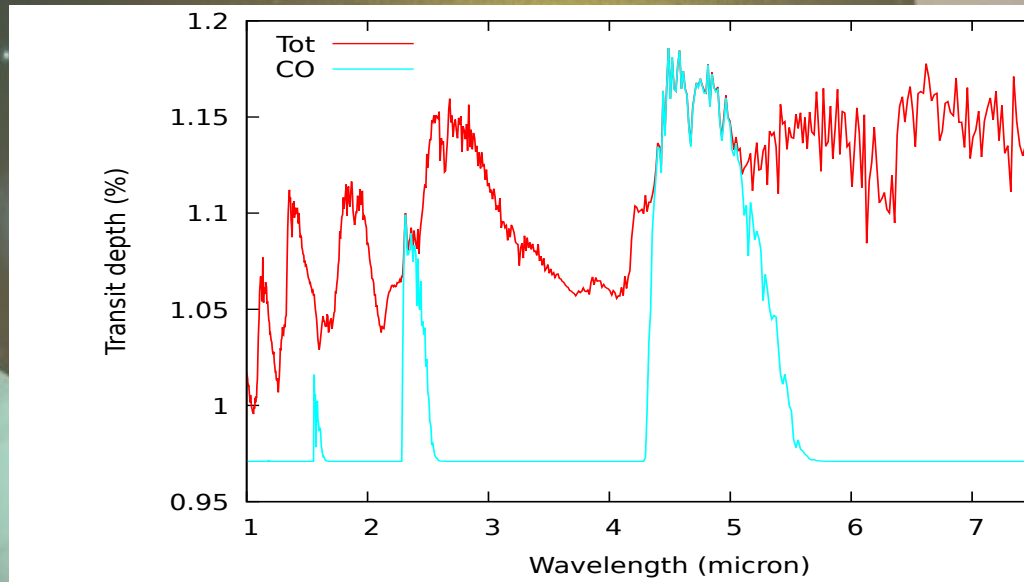


Red: contribution from all layers
Green: contribution from layers with $P < 10^{-1}$ bar
Blue: contribution from layers with $P < 10^{-2}$ bar
Purple: contribution from layers with $P < 10^{-3}$ bar
Light Blue: contribution from layers with $P < 10^{-4}$ bar
Yellow: contribution from layers with $P < 10^{-5}$ bar
Black: contribution from layers with $P < 10^{-6}$ bar

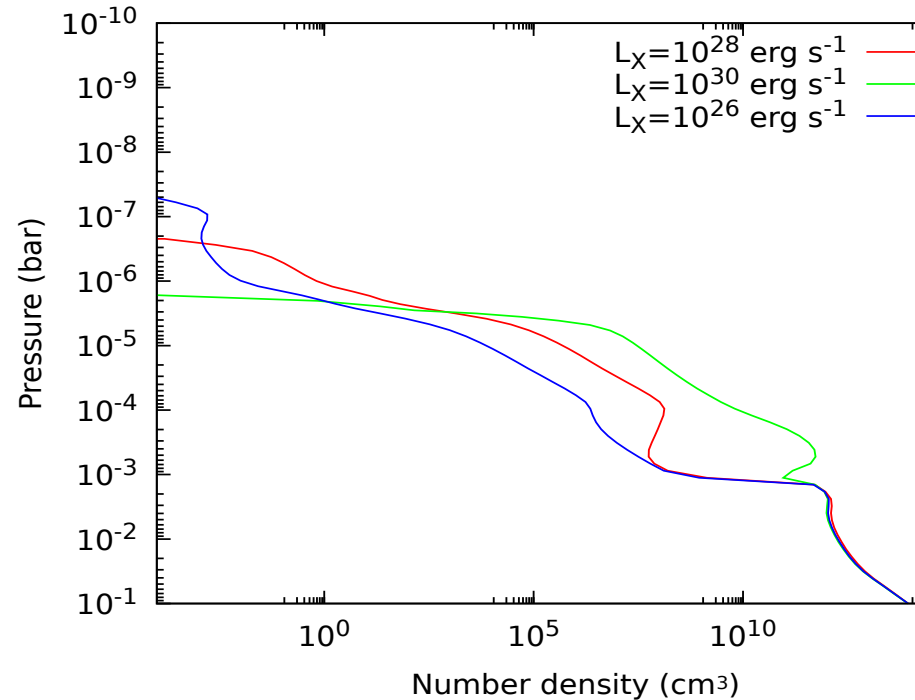
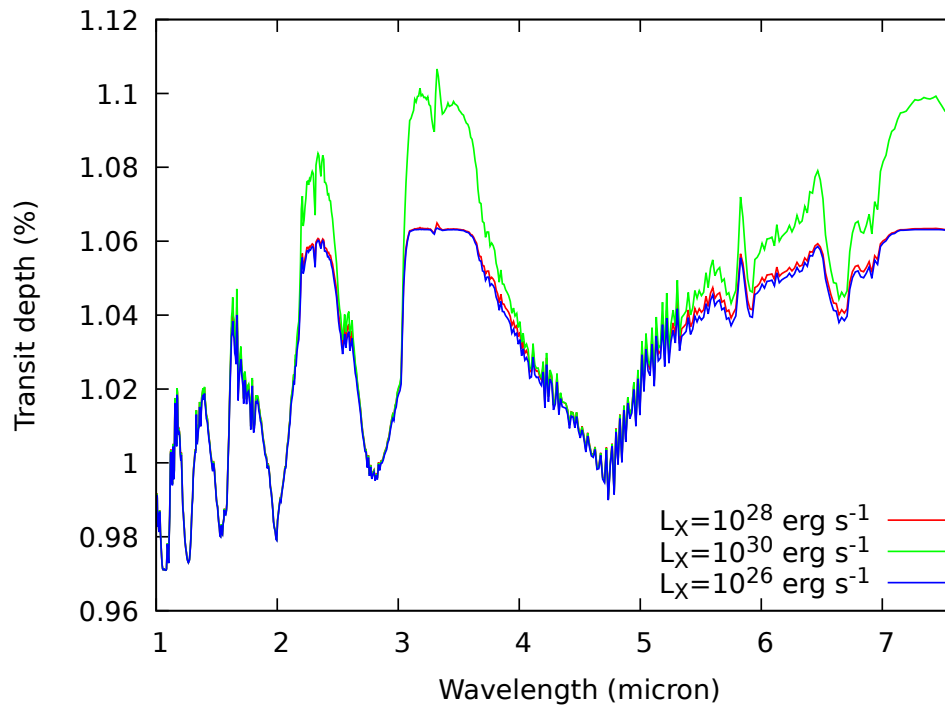
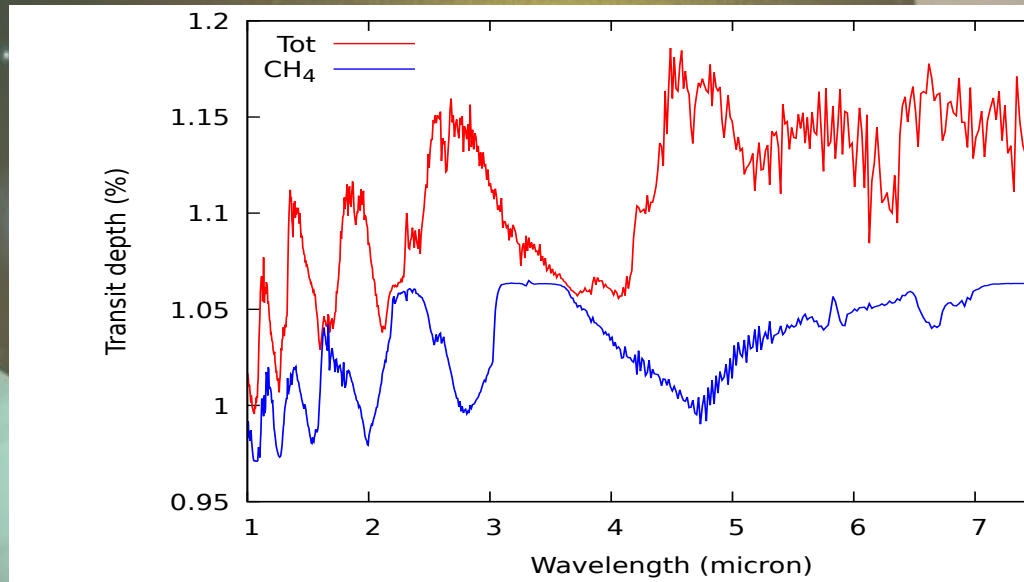
Transmission spectra H₂O



Transmission spectra CO

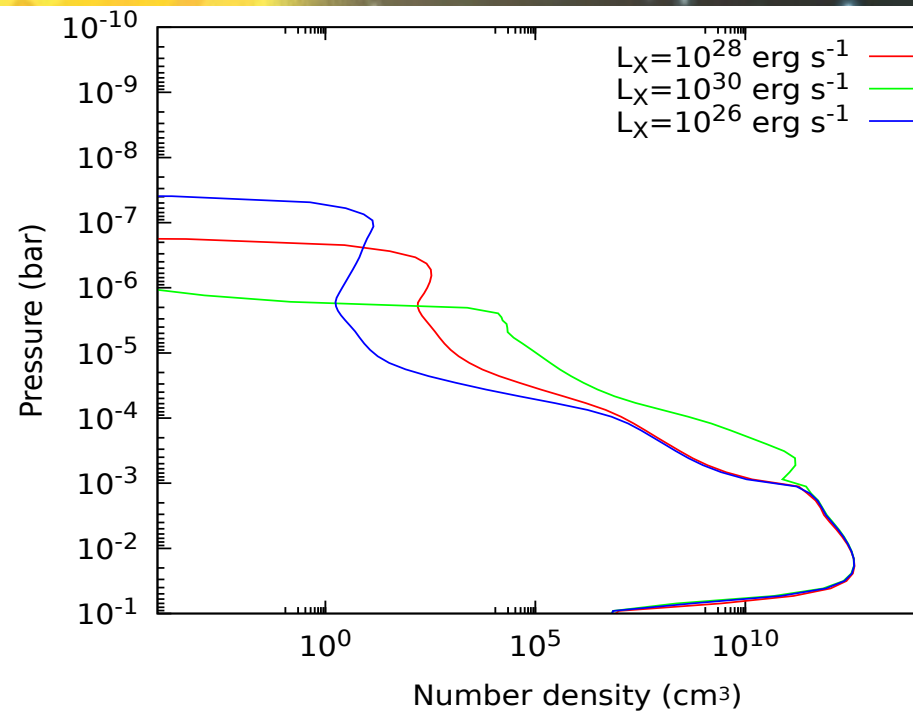
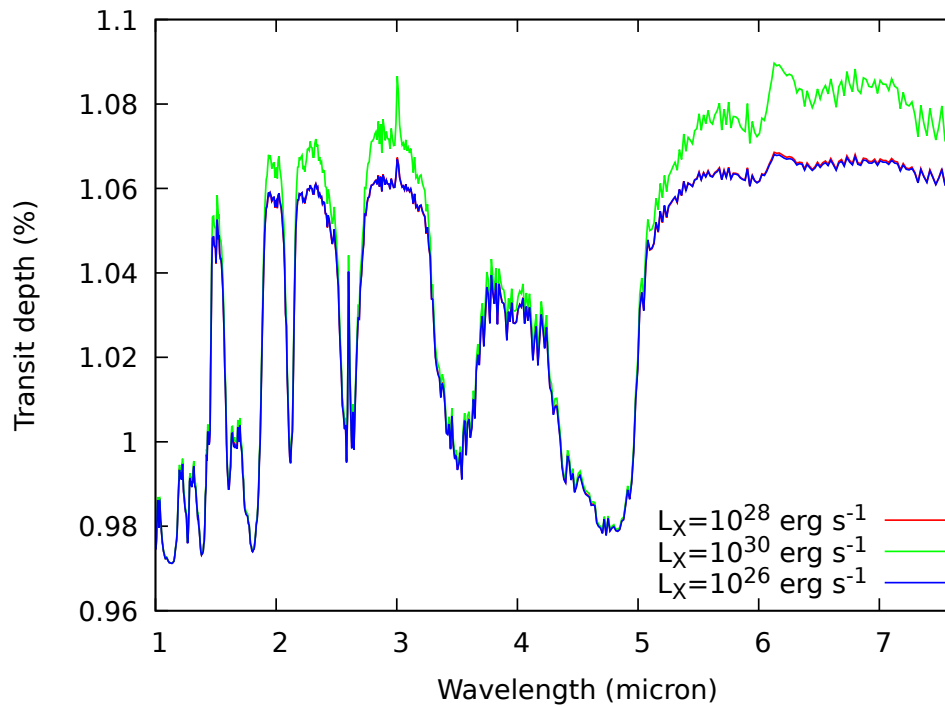
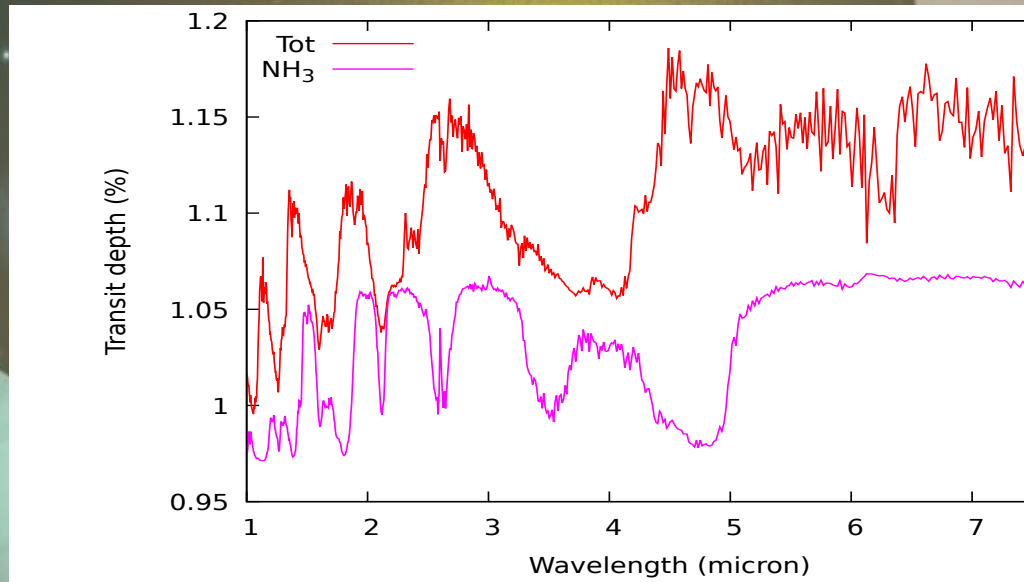


Transmission spectra CH₄



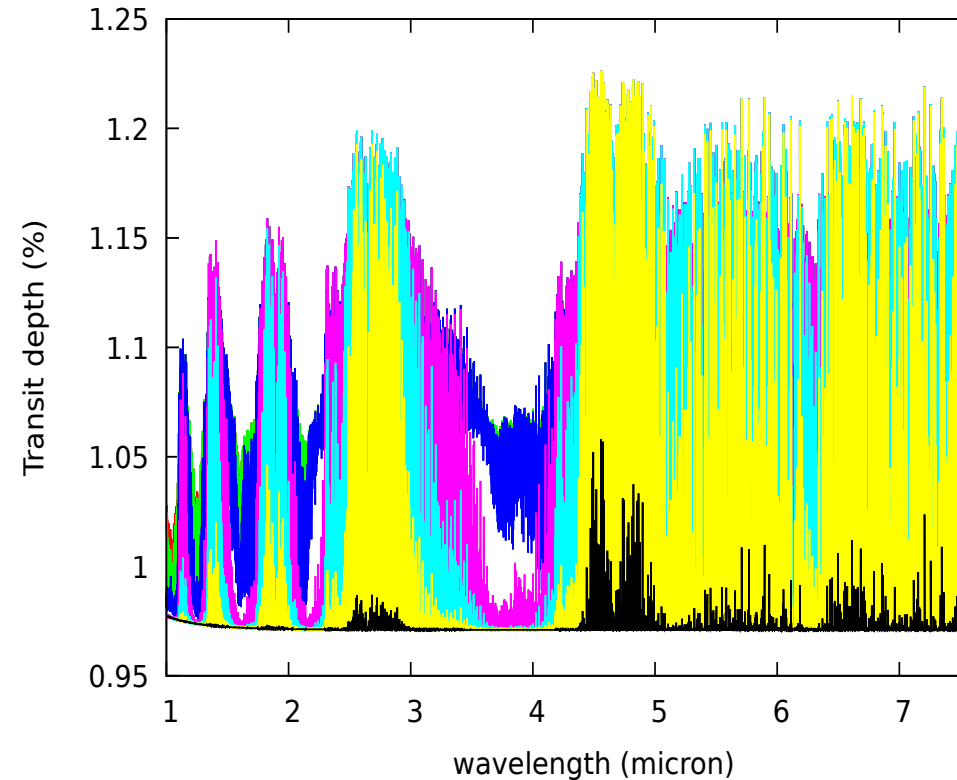
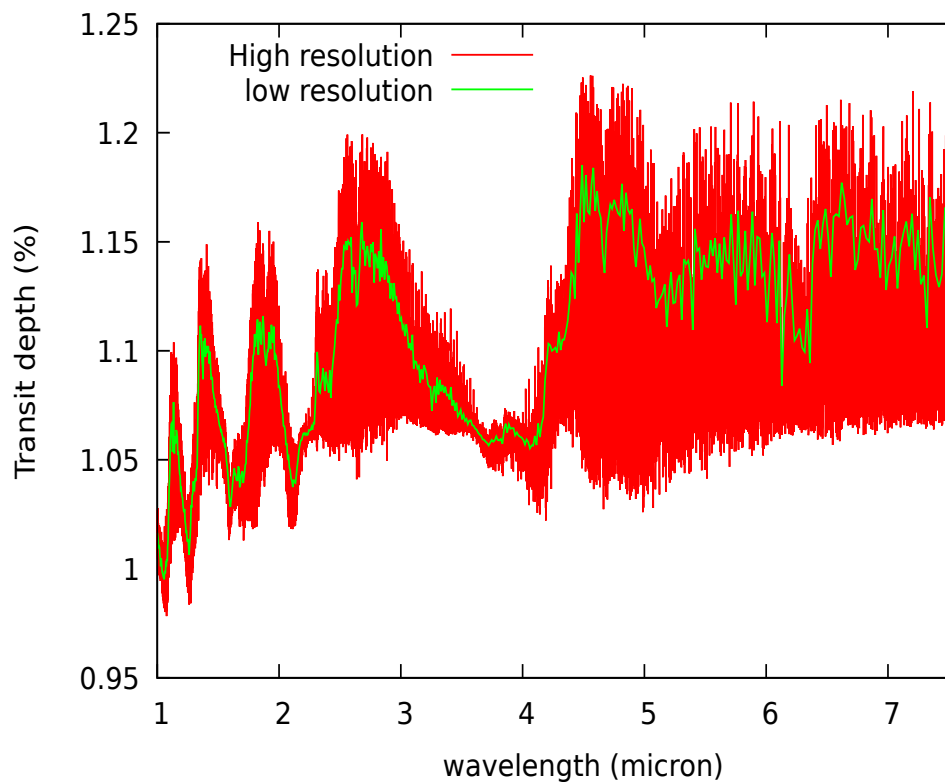
Transmission spectra

NH₃



Transmission spectra

High resolution (R=10000)



Red: contribution from all layers
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Purple: contribution from layers with $P < 10^{-3}$ bar
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Black: contribution from layers with $P < 10^{-6}$ bar

Next steps

Account for vertical mixing

Calculate pressure-temperature profiles and chemical profiles in a self consistent way

Explore the role of metallicity or of C/O ratio

Evaluate if in extreme cases it is possible to observe spectral features due to ionic species