

Introduction

This folder contains results of the simulations performed using the photochemical code presented in Locci et al. 2021, PSJ, submitted. Photochemistry is one of the main processes that drives chemistry out of equilibrium.

Exoplanets form and evolve under the influence of their host stars. During their evolution, their atmospheres arise and change naturally under environmental influence, giving rise to a surprising diversity of compositions and physicochemical conditions. We are mainly interested in studying the effects of high-energy stellar radiation on the outer atmospheric layers of gas giants, as photochemical processes can cause drastic deviations from equilibrium in these regions.

To study these phenomena we assume a planet with a mass equal to half the mass of Jupiter, orbiting a Sun-like star with solar bolometric brightness. We consider a stratified and cloudless atmosphere, in one-dimensional geometry, which is illuminated by a flux of stellar photons in the range between 0.1 and 400 nm, and we derive vertical number density profiles for different chemical species at selected zenith angles.

Chemistry is sensitive to the effects of different types of high-energy radiation. The characteristics of atmospheric chemical evolution emerge from many feedbacks over a wide range of time scales. High-energy stellar emission, in particular X-rays, can cause important changes in the mixing ratio profiles of atmospheric species. The strongest impact on chemistry is expected in planets orbiting young stars, because they have a higher level of chromospheric and coronal activity.

Due to the weak photoelectric cross sections, X-rays can push the ionization of the gas deeper into the atmosphere, reaching pressures inaccessible to lower energy radiation. Although X-rays interact preferentially with metals, they produce secondary electron cascades that can also ionize hydrogen and helium-carrying species by collision, and this occurs at altitudes much lower than those where UV and EUV photons can penetrate.

In particular, one of the major efforts of our investigation was to understand the effects produced by photons in the different spectral bands. These effects frequently appear intertwined and mixed by the interplay of chemical reactions, which provide a non-linear response to irradiation in the resulting molecular abundances. Such a search is made even more difficult by the scaling relationships which link the fluxes in different spectral bands.

The simulation results for our reference case are shown in the main (parent) folder, with the following values of the main parameters:

- X-ray luminosity of the star: 10^{28} erg/s
- Equilibrium temperature at planet surface: 1000 K
- Atmospheric metallicity Z : 1 (solar units)
- Zenith angle: 60°

In the "Spectral components" folder it is possible to see how the vertical profiles of the molecular abundances change taking into account the radiation in the UV, EUV, and X-ray spectral bands.

Another key part of our work was to study the effects on chemistry as stellar activity changes. In the "Luminosity dependence" folder the molecular abundances are shown in the case of different X-ray luminosities, scaling the luminosity in the EUV band as predicted by the empirical relationship of Sanz-Forcada et al. (2011).

We also explored how the effects on chemical profiles due to changes in atmospheric metallicity or temperature are intertwined with the effects due to photochemistry. The results of simulations with

different metallicities are reported in the "Metallicity dependence" folder, while the results with different temperatures are found in the "Temperature dependence" folder.

We have also performed simulations at different zenith angles. Although the temperature profile we use is always isothermal and at the same temperature, varying the zenith angle implies a variation of the optical path of the incident ray of photons, and consequently an influence on the photochemistry. The results of these simulations are reported in the "Zenith-angle dependence" folder.

In each folder a README file explains the correspondence between the lines in the graphs and the various models.