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Photo-thermo-chemistry of hot atmospheres

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Abstract

We have developed a new model to study the atmosphere of exoplanets adapted to the characteristics of the atmospheres of hot Jupiters and hot Neptunes. Such a model appears essential to interpret recent and future observations, to predict the composition and to understand the formation and the evolution of these planetary bodies. As the chemistry of nitrogen compounds is not well constrained, we investigated several sub-networks for nitrogen-bearing species and investigate their impact on the predicted abundances and spectra of HD 189733b. We present these results. An important problem of photochemical models is the lack of high temperature photochemical data. In order to improve this situation, we have begun a campaign of measurement of VUV absorption cross section at high temperature for H_2O, CO_2 and NH_3. We will present the influence of these new experimental data on the thermo-photochemical model.

1. Introduction

In hot Jupiters' atmospheres, high temperatures (typically 500 K - 2500 K), very high UV fluxes (10,000 times the flux received at the top of Jupiter's atmosphere) and strong circulation dynamics coexist. There are observational constraints for few hot Jupiters (HD 209458b and HD 189733b for instance) and hot Neptunes (GJ 436b). Traditional equilibrium models fail to reproduce these observations because they lack mixing and photolyses. Old photochemical models [1, 2] fail because of their incomplete reaction network which lacks endothermic processes and because their reaction rates are inappropriate for high temperature [7]. New models, coupling vertical transport, photolyses and thermochemistry exist now to study these exoplanets [5, 8, 9, 10, 11].

2. Numerical modeling

Our new photo-thermo-chemical model is adapted to the study of hot atmospheres. The chemical scheme comes from an industrial model developed to study car engines combustion [6]. It includes endothermic reactions that are usually neglected when dealing with cooler atmospheres and low temperature kinetics and has been validated in a large range of pressure, temperature and elemental compositions, comparable to the conditions found in both car engines and hot Jupiters. The consistency of this scheme with thermodynamical data allows the kinetic model to reach the thermodynamical equilibrium with a very good accuracy. Our 1D model uses this chemical scheme and accounts for vertical transport and photodissociations coming from a model of Titan's atmosphere [3, 4]. The results of our 1D model applied to HD 189733b show that nitrogen compounds as HCN and NH_3 are abundant and influence the observational spectra. Knowing that nitrogen chemistry is still not-well constrained, we decided to explore other nitrogen sub-networks. Our nominal scheme is the only one that have been validated as a whole. The Figure 1 shows the wide range of results one can obtained for HCN using different nitrogen networks. This is also presented in a submitted paper [11].

3. Experimental measurement

An important source of uncertainty in photochemical models is the temperature-dependency of their parameters: IR absorption coefficients $k_\lambda(T)$, UV absorption cross-sections $\sigma(T)$ and chemical kinetics reaction rates $k(T)$. Usually, available data have been measured at ambient temperature, which is problem-

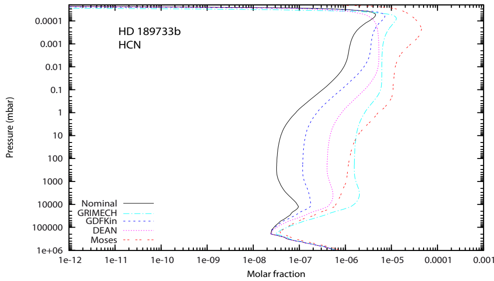

Figure 1: Abundances of HCN in the atmosphere of HD 189733b predicted by different nitrogen sub-networks.

atic for high temperature modeling. In order to improve this situation, we have begun a campaign of experimental measurement of VUV absorption cross sections at high temperature, for some important species of transiting exoplanets atmospheres : water H_2O, carbone dioxyde CO_2 and ammonia NH_3. This experimental work has been done using the BESSY synchrotron facilities (Berlin, Germany). We will show the results of these measurements and their effect on the 1D model (Figure 2)[12].

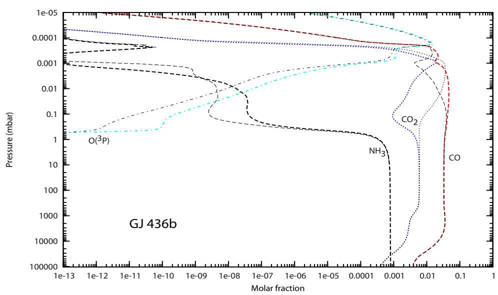

Figure 2: Abundances of some species in the atmosphere of GJ 436b with a model using absorption cross section of CO_2 at 488K (colors) and at 300K (black).

4. Summary and conclusions

Thanks to a validated chemical scheme, coming from an industrial combustion model, we have developed a thermo-photochemical model which is appropriate to study hot exoplanets. We have shown that the nitrogen chemistry is not well constrained and is consequently a source of notable uncertainties. An important work, implying a close collaboration between experimentalists, observers and modelers is necessary to adress this issue. The experimental measurements we are doing for the absorption cross section of some species of the atmosphere is a prerequisite for reproducing correctly the hot atmospheres of these planets.

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