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# An extensively validated C/H/O/N chemical network for hot exoplanet disequilibrium chemistry

## Résumé

**Context :** The reliability of one-dimensional disequilibrium chemistry models in hot exoplanet atmospheres depends on the chemical network used. To develop robust networks, we can rely on combustion studies that provide C/H/O/N chemical networks validated by vast amount of experimental data generated by the extensive research that has been done on hydrocarbon combustion and NO<sub>x</sub> formation in the last decades.

**Aims :** We aimed to build a new and updated C0-C2 chemical network to study the C/H/O/N disequilibrium chemistry of warm and hot exoplanet atmospheres that relies on extensively validated and recent state-of-the-art combustion networks. The reliability range of this network was aimed for conditions between 500 - 2500 K and 100 - 10<sup>-6</sup> bar, with cautious extrapolation at lower temperature values.

**Methods :** We compared the predictions of seven networks over a large set of experiments, covering a wide range of conditions (pressures, temperatures, and initial compositions). To examine the consequences of this new chemical network on exoplanets atmospheric studies, we generated abundances profiles for GJ 436 b, GJ 1214 b, HD 189733 b, and HD 209458 b, using the 1D kinetic model FRECKLL and calculated the corresponding transmission spectra using TauREx 3.1. These spectra and abundance profiles have been compared with results obtained with our previous chemical network.

**Results :** Our new kinetic network is composed of 174 species and 1293 reactions mostly reversible. This network proves to be more accurate than our previous one for the tested experimental conditions. The nitrogen chemistry update is found to be very impactful on the abundance profiles, particularly for HCN, with differences up to four orders of magnitude. The CO<sub>2</sub> profiles are also significantly affected, with important repercussions on the transmission spectrum of GJ 436 b.

**Conclusions :** These effects highlight the importance of using extensively validated chemical networks to gain confidence in our models predictions. As shown with CH<sub>2</sub>NH, the coupling between carbon and nitrogen chemistry combined with radicals produced by photolysis can have huge effects impacting the transmission spectra. This should be kept in mind when adding new elements like sulfur, as only adding a sub-mechanism neglects these coupling effects.

**Mots-Clés:** Astrochemistry, Disequilibrium chemistry, Exoplanets, Chemical Network