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A revision of Hydrocarboxyl (HOCO) chemistry under CO_2/CO atmospheres

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In an atmosphere with partial to moderate levels of CO_2, photodissociation reactions will produce CO. Then, based on the water content of the atmosphere the CO+OH reaction produces the Hydrocarbxyl (HOCO) compound. The same product is expected to be formed in an atmosphere with significant CO levels.

In this study we focused of the fate of the HOCO compound by revising its reactivity with radicals likely available in a variety of atmospheres. The study is divided into two sections: a revision of the reaction pathways and kinetic data available in the literature, and the incorporation of the updated chemical kinetics to the PATMO model [1].

The chemical network produced for this model was generated based on the current understanding of the potential chemical reactants (N, O, H derived radicals) and other species that are likely to exist but so far haven't been accounted as potential reactants (SO, S, OH_2, NO, etc). Recent works on the field of creating chemical networks for atmospheric codes have implemented the guiding principle of introducing massive networks automatically generated by data base search algorithms. More sophisticated approaches, have implemented the use of machine learning to fill in missing reaction rate constants. In this study we use as guiding principle reports made in the fields of combustion and the fate of HOCO in current Earth's atmosphere.

The second part of the study is to incorporate the updated chemical network to the PATMO model, this model has been developed to operate under a variety of conditions such current Archean, contemporary Earth, and Free-floating planets [1], [2].

The results obtained so far suggest that the HOCO species may be short or long lived according to specific planetary conditions. More interestingly, the associated compounds produced from the HOCO depletion show a wide variety of organic species.

[1] Danielache et al. (2023). *Geochem. J.* 57, 40-55.
[2] Ávila et al. (2021). *Int. J. Astrobio*. 1−12.