Cracking the Puzzle of CO_2 Formation on Interstellar Ices

G. Molpeceres, [1] J. Enrique-Romero,-[2] and Y. Aikawa.[1]

[1]*Department of Astronomy, Graduate School of Science, The University of Tokyo, Tokyo 113 0033, Japan*

[2]*Leiden Institute of Chemistry, Gorlaeus Laboratories, Leiden University, PO Box 9502, 2300 RA Leiden, The Netherlands*

The formation of an ice layer on top of interstellar dust grains is a central topic in astrochemistry. The chemical composition of interstellar ices varies over time [1], and the dominance of polar or apolar fractions in them is important for several surface properties, like adsorption, diffusion or reaction. Among the most abundant components of interstellar ice we find H_2O, CO, CH_3OH or CO_2, to give some examples. These molecules can be formed *in situ* on interstellar ices, as it is the case of H_2O or CH_3OH, or can land on the ices after formation in the gas, like CO. Experiments show that CO_2 mainly forms *via* surface reactions (see, for example [2]), e.g. the CO + OH → CO_2 + H reaction. In this talk I will review our recent calculations on such reaction [3]. I will cover the reactivity on a CO and H_2O ice, showing that the reaction does not proceed directly in neither of them. In reality, the reaction stops at the very stable HOCO radical that may be later transformed into CO_2 via a H abstraction reaction. The H_2O ice is found to be a better substrate for the formation of HOCO, which can be behind the higher abundance of the polar component of CO_2 found in astronomical observations, in comparison with the apolar one [4].

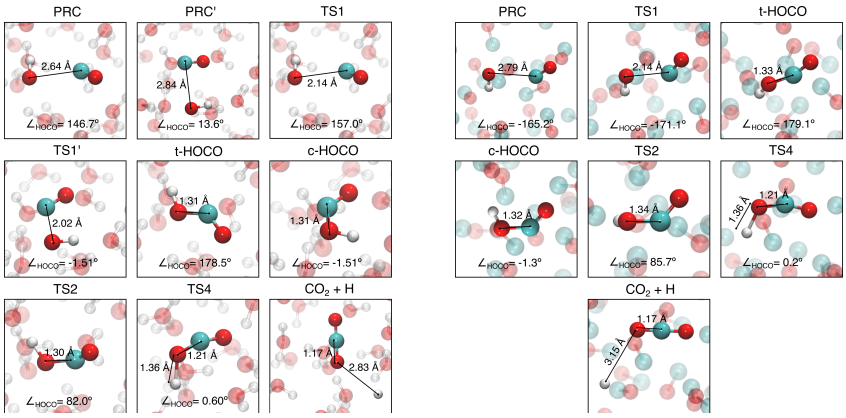

Figure 1: Stationary points in the potential energy surface for the CO + OH → CO_2 + H reaction on water (left) and CO ice (right).

References

[1] Boogert, A.C.A., Gerakines, P.A., Whittet, D.C.B., 2015, Ann. Rev. Astron. Astrophys. **53**, 541–581.
[2] Oba, Y., Watanabe. N., Kouchi. A., *et al*., 2023, Astrophys. J., **712**, 2, L174–L178.
[3] Molpeceres, G., Enrique-Romero, J., Aikawa, Y. 2023, Astron. Astrophys, **677,** A39.
[4] McClure, M.K., Rocha, W.R.M., Pontoppidan, K.M. *et al*., 2023, Nature Astron **7**, 431–443.