Exploring the Mysteries of CO Ices: Weak Interactions and Vibrational Energy Relaxation

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One of the largest fractions of interstellar ice and gas, carbon monoxide, still remains shrouded in mystery. In particular, models still fail to accurately reproduce the observed ice-to-gas ratio of CO without adding unrealistic tweaks to the models. We previously investigated the binding energy of CO on CO ices, where we found a rather large number of weak binding sites [1]. These weak sites, if incorporated within models, could reduce the discrepancy between observations and models [2]. Additionally, non-thermal desorption mechanisms are being scrutinized to understand their role in non-destructively desorbing molecules. One such novel mechanism speculated by experiments is vibrationally-induced desorption.

Recently, infrared-induced desorption of interstellar CO ice analogs was experimentally performed [3]. However, for it to explain the gas-phase CO abundance, we need to understand the mechanism behind the desorption. We studied the vibrational energy relaxation (VER) of CO ices, with a particular aim of unraveling how desorption could be induced. We find that CO has an extremely slow classical VER timescale and that vibrational to translational energy conversion is extremely inefficient. Furthermore, we do not observe any desorption within the 4700 simulations that we carried out. These results suggest that possible explanations for the desorption seen experimentally are: (i) quantum effects that are not captured by the classical simulations, or (ii) surface or local heating.

References

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[2] Cazaux, S., et al. "CO Depletion: A microscopic perspective." *The Astrophysical Journal* 849.2 (2017): 80.

[3] Santos, J. C., et al. "Resonant infrared irradiation of CO and CH3OH interstellar ices." *Astronomy & Astrophysics* 672 (2023): A112.