Glycolaldehyde Formation on Interstellar Water Ice Surfaces. A Computational Quantum Chemical Approach

J. A. Luque-Urrutia, A. Rimola

[1]*Departament de Química, Universitat Autònoma de Barcelona, Spain*

Astrochemists of diverse disciplines aim to unfold the intricate chemical mechanisms that occur in space to get insight on one of the primordial questions we have today: what is the origin of life? To evolve from dead chemical matter into living beings, there are some essential chemical compounds that must be present for that to occur, such as amino acids [1] and complex sugars [2]. Focusing on sugars, glucose is one of the main targets. However, its presence has not been confirmed in space while this is indeed the case of its closest relative, glycolaldehyde (GLA, $HOCH_2CHO$) [3]. In this contribution, we present results dedicated to GLA formation on surfaces of interstellar water ice adopting the formose reaction, $2{\cdot}H_2CO \rightarrow$ GLA, and its radical derivation $H_2CO + CHO^* + H^* \rightarrow$ GLA. Reactions in the gas phase (i.e., absence of water ice) have been used for a benchmarking study, in which CCSD(T) results were compared with those obtained at the more approximated DFT theory level. With the latter, calculations of the GLA formation reactions have been carried out on cluster models for water ice (see Figure 1), in which the energy features of the reactions (i.e., reaction energy and activation energies) are provided. Additionally, simulations also help us to understand the role of the ice surface in this synthetic route.

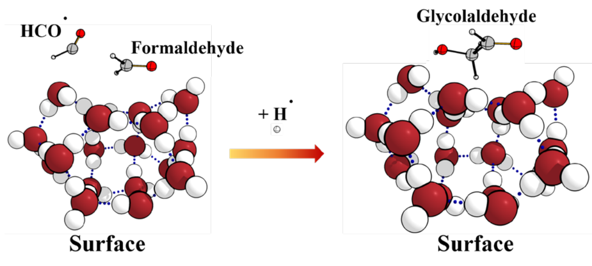

Figure 1: Glycolaldehyde formation by reaction of HCO with H_2CO followed by H addition simulated on a cluster model mimicking the surfaces of interstellar of water ice.

[1] Ehrenfreund, P.; Charnley, S. B. 2000 ARA&A 38, p. 427-83.

[2] Woods, P.M.; Slater, B.; Raza, Z.; Viti, S.; Brown, W.A.; Burke, D.J. 2013 ApJ, 777, p. 90.

[3] Jørgensen J.K.; Favre, C.; Bisschop, S.E.; Bourke, T.L.; Dishoek, E.F.; Schmalz, M. 2012 ApJL 757 L4.