Computational Investigation on the Potential Energy Surface of the Formation Route of Formamide from Reaction between NH_2 and H_2CO on Interstellar Water Ice Surface

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Formamide has a key role in prebiotic chemistry as it is the simplest molecule containing the four most important atoms from a biological point of view: hydrogen, carbon, nitrogen and oxygen. But also, because it is the simplest molecule containing the amide bond O-C-NH, the group that join amino acids forming peptides [1]–[3]. Since it was first detected and due to its importance, different pathways leading to its interstellar formation has been studied considering both the gas-phase scenario and on ices of dust grains[2]–[4]. In the present contribution, computational simulations based on quantum chemical calculations are presented, focusing on the energetics of the NH_2CHO formation from reaction of NH_2 with H_2CO (a channel proposed to occur in the gas phase [3]) on water ice surfaces. To model the water ice surfaces, a periodic approach has been adopted, in which both a crystalline and an amorphous model has been used. Different DFT functionals have been employed to obtain accurate energy values for the mechanistic steps involved in the reaction.

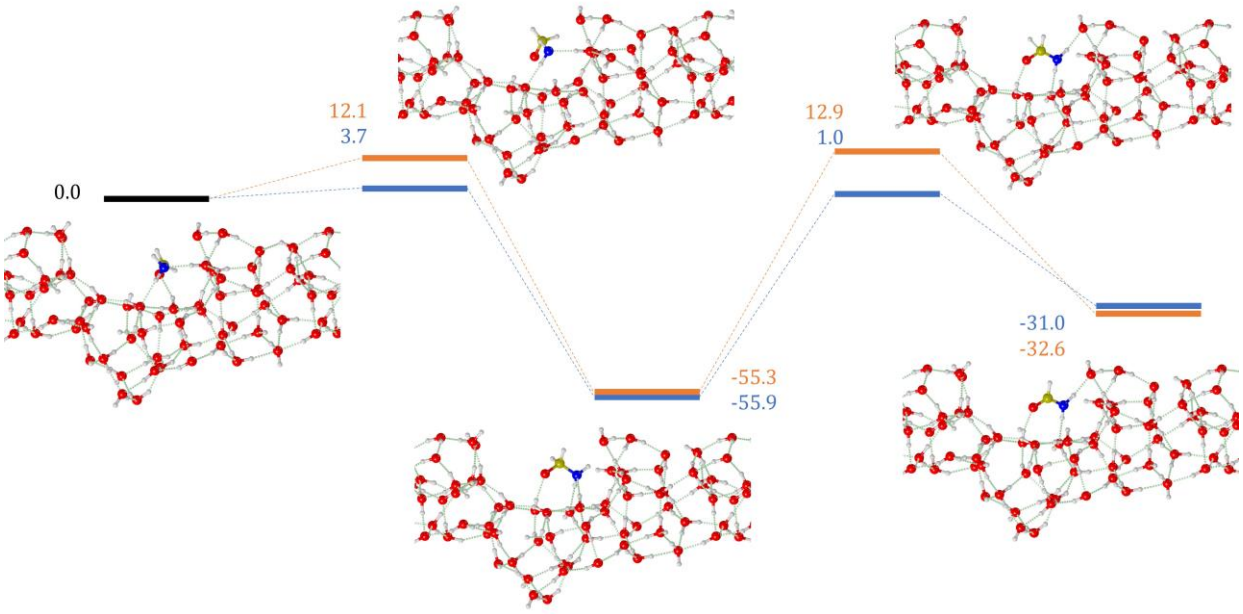

Figure 1: Potential Energy Surface and optimized structures of the stationary points of the studied reaction on the amorphous slab model. Values are in kJ/mol. Bare values correspond to those at B3LYP-D3(BJ), in brackets to those at PBE-D3(BJ) and in square brackets to those at M06-2X-D3. Atom color legend: red, O; blue, N; green, C white, H.

References

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[2] A. Rimola et al, 2018, ACS Earth Space Chem. 2, 7, 720.
[3] V. Barone et al., 2015, Mon. Not. R. Astron. Soc. Lett. 453, 1, L31.
[4] J. Enrique-Romero et al., 2019, ACS Earth Space Chem. 3, 10, 2158.