Ab initio prebiotic chemistry: Miller-like experiments and beyond

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The celebrated Miller experiments [1] reported on the spontaneous formation of amino-acids from a mixture of simple molecules reacting under an electric discharge, giving birth to the research field of prebiotic chemistry. However, the chemical reactions involved in those experiments have rarely been studied at the atomic level. Here we report on the first ab initio computer simulations of Miller-like experiments in the condensed phase. Our study [2], based on the recent method of treatment of aqueous systems under electric fields and on metadynamics analysis of chemical reactions, shows that glycine spontaneously forms from mixtures of simple molecules once an electric field is switched on and identifies formic acid and formamide [3] as key intermediate products of the early steps of the Miller reactions, and the crucible of formation of complex biological molecules. This work, which has received considerable attention both from the specialized scientific media and the mainstream large public press [4] might have a relevance in geochemistry. We show in fact that the electric fields naturally present at mineral surfaces, albeit short-ranged, are sufficiently strong to induce "Miller-like" prebiotic chemical reactions [5]. This study emphasizes that mineral surfaces, and not only those usually considered as having catalytic properties, may play an important role in the emergence of abiotic organic chemistry of both the primordial and the modern Earth.

[1] Miller (1953), *Science* 117, 528-529. [2] Saitta & Saija (2014), *PNAS* **111**, 13767-13773. [3] Saitta, Saija, Pietrucci & Guyot (2015), *PNAS* **112**, E343-E344. [4] http://www.impmc.upmc.fr/~saitta/press_Miller.html [5] Laporte et al. (2015), submitted for publication.