Surface chemical properties of interstellar grains. Insights from quantum chemical simulations

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There is clear evidence that dust grain particles are central players contributing to the chemical inventory of the Universe. However, the exact role played by the grains is still not well understood and hard to unveil in a "rule-of-thumb" fashion: with the research progress made, the role of grains appears to be case-dependent. Grains are usually referred to as catalysts, a concept attributed in a generic sense, meaning that their presence allows the reactions to evolve, which is not the case in their absence. However, by dissecting this general idea of catalysis, for the case of ices, one can realize that, rather than being actual chemical catalysts (i.e., bodies that activate the reactants and provide alternative routes with lower energy requirements) they are more like reactant concentrators/suppliers [1,2,3,4] and/or third bodies that absorb the large extra energies released in chemical reactions (hence stabilizing the newly formed products) [5,6]. Thus, for a paradox, the capability of water ices to act as chemical catalysts is limited due to their relatively chemical inertness. In contrast, chemical catalytic properties can be found in interstellar refractory materials (e.g., silicates, iron sulfides, metallic grains…) due to the presence of transitions metals (e.g., Fe, Ni) that can activate the reactants [7,8]. In this contribution, different paradigmatic roles exerted by grains (ices and refractories) in different chemical reactions of astrochemical interest will be shown, which have been discerned thanks to the unique capabilities of quantum chemical simulations at providing exclusive atomic-scale information.

References

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