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Probing the Chemistry of P-Bearing Molecules in Interstellar Environments and other Extraterrestrial Environments

Luca Mancini[1], Marzio Rosi[2], Nadia Balucani[1,4,5], Dimitrios Skouteris[3], Claudio Codella[4], and Cecilia Ceccarelli[5]

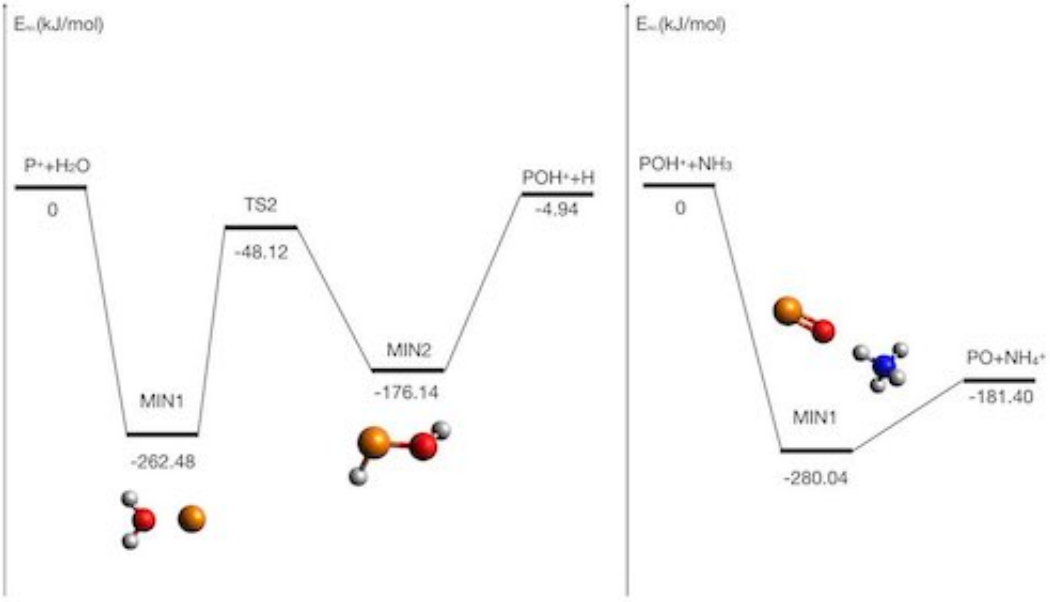
[1]Università degli Studi di Perugia, Department of Chemistry, Biology and Biotechnology, Italy (luca.mancini2@studenti.unipg.it)
[2]Università degli Studi di Perugia, Department of Civil and Environmental Engineering, Italy
[3]Master-Up, Perugia, Italy
[4]Osservatorio Astronomico di Arcetri, Firenze, Italy
[5]Université Grenoble Alpes, IPAG, Grenoble, France

Phosphorus is one of the most important elements in biochemistry together with carbon, oxygen, hydrogen and nitrogen. Therefore, P-bearing compounds with some prebiotic potential and their possible formation pathways in extraterrestrial environments are attracting a lot of interest.

In recent years, phosphorus has been clearly identified in the in the coma of comet 67P/Churyumov-Gerasimenko (1), while only a bunch of P-bearing molecules (namely PO, PN, CP, C_2P and HCP) have been observed in the gas phase of circumstellar envelopes around evolved stars (2-7) and only two simple species have been detected in star forming regions, that is, PO and PN (8-11). If we focus only on solar-type star forming regions, only two detections are available, that is PN and PO toward the shocked region L1157-B1 (12) and the Class I protostar B1-b (13). Phosphorus chemistry in the conditions of the interstellar medium is poorly understood and the interstellar reservoir of this element is strongly debated. Since the first experimental work on ion-molecule reactions by Anicich and coworkers (14), PO has been indicated as the main reservoir of phosphorus and HPO^+ as its major precursor. PO can also be transformed to PN by gas-phase chemistry (15). Thirty years ago, a series of theoretical investigation on ion-molecule reactions has been performed by Largo et al. (16-18) in order to explain the formation of P-O, P-N, P-C bonds. In spite of those efforts, the chemistry of interstellar phosphorus and its connections to the P-compounds detected in small bodies of the Solar System remains mostly unexplored and poorly characterized. For this reason, we have undertaken a systematic investigation of possible gas-phase formation routes of simple P-molecules by means of electronic structure and kinetic calculations. This approach is made necessary by the fact that P is a difficult species to deal with in laboratory experiments.

In this work we present a new theoretical analysis of the reaction $P^+ + H_2O$ and $P^+ + NH_3$ at a higher level of theory than those employed by Largo et al. in 1991. More specifically, we make use of DFT calculations for geometry optimization and frequency analysis coupled to a CCSD(T) reevaluation of the energy for each identified stationary point of the reaction potential energy surface. The data coming from electronic structure calculations will be used to perform a kinetic analysis using a Rice-Ramsperger-Kassel-Marcus (RRKM) code implemented for this purpose in order to derive the rate coefficients and branching ratios. A possible formation mechanism is proposed for the formation of both PO and PN. In the figure, the potential energy surface for the reaction of P^+ with a water

molecule is reported. This process leads to the formation of the POH^+ ion which can later transfer a proton to molecules like NH_3 which have a large proton affinity.



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