



HAL
open science

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

Luca Mancini, Marzio Rosi, Dimitrios Skouteris, Claudio Codella, Cecilia
Ceccarelli

► **To cite this version:**

Luca Mancini, Marzio Rosi, Dimitrios Skouteris, Claudio Codella, Cecilia Ceccarelli. Probing the Chemistry of P-Bearing Molecules in Interstellar Environments and other Extraterrestrial Environments. 14th Europlanet Science Congress 2020, 2020, à renseigner, Unknown Region. 10.5194/epsc2020-643 . insu-03705149

HAL Id: insu-03705149

<https://insu.hal.science/insu-03705149>

Submitted on 12 Jul 2022

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.



Distributed under a Creative Commons Attribution 4.0 International License



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

Luca Mancini¹, Marzio Rosi², Nadia Balucani^{1,4,5}, Dimitrios Skouteris³, Claudio Codella⁴, and Cecilia Ceccarelli⁵

¹Università degli Studi di Perugia, Department of Chemistry, Biology and Biotechnology, Italy (luca.mancini2@studenti.unipg.it)

²Università degli Studi di Perugia, Department of Civil and Environmental Engineering, Italy

³Master-Up, Perugia, Italy

⁴Osservatorio Astronomico di Arcetri, Firenze, Italy

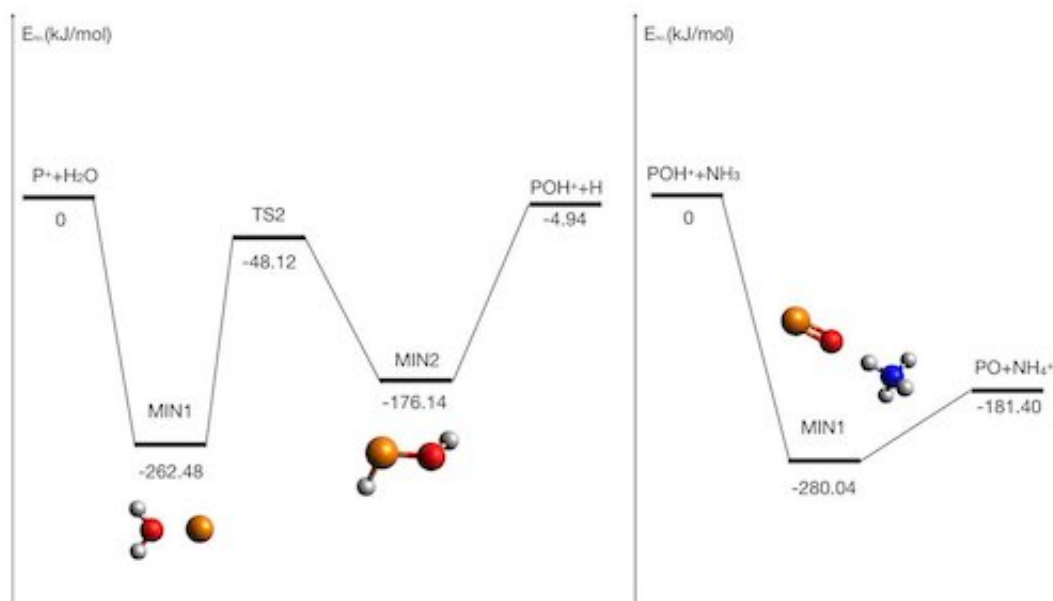
⁵Université Grenoble Alpes, IPAG, Grenoble, France

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 coma of comet 67P/Churyumov-Gerasimenko (1), while only a bunch of P-bearing molecules (namely PO, PN, CP, C₂P 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⁺ + H₂O and P⁺ + NH₃ 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.



[1] Altwegg K. et al., Prebiotic chemicals—amino acid and phosphorus—in the coma of comet 67P/Churyumov-Gerasimenko, *Sci. Adv.*, 2016, 2 : e1600285.

[2] Turner, B. E. & Bally, J., Detection of Interstellar PN: The First Identified Phosphorus Compound in the Interstellar Medium, 1987, *ApJL*, 321, L75.

[3] Ziurys L.M., Detection of Interstellar PN: The First Phosphorus-bearing Species Observed in Molecular Clouds, 1987, *ApJL*, 321, L81.

[4] Guelin M. et al., Free CP in IRC +10216, 1990, *ApJL*, 230, L9-L11.

[5] Agúndez M. et al., Discovery of Phosphaethyne (HCP) in Space: Phosphorus Chemistry in Circumstellar Envelopes, *ApJ*, 662, ApJ, 2, L91-L94.

[6] Tenenbaum E.D. et al., Identification of Phosphorus Monoxide (X2P^+) in VY Canis Majoris: Detection of the First PO Bond in Space, 2007, *ApJ*, 666, 1, L29-L32.

[7] Halfen D.T. et al., Detection of the CCP Radical (X2P^+) in IRC +10216: A New Interstellar Phosphorus-containing Species, 2008, *ApJL*, 667, 2, L101.

[8] Rivilla V.M. et al., Phosphorus-bearing molecules in the Galactic Center, 2018, *MNRAS*, 475, 1, L30-L34.

[9] Rivilla V.M. et al., ALMA and ROSINA detections of phosphorus-bearing molecules: the interstellar thread between star-forming regions and comets, 2020, *MNRAS*, 492, 1, 1180-1198.

[10] Rivilla V.M., The first detections of the key prebiotic molecule PO in star-forming regions, 2018, *IAU Symposium*, 332, 409-414.

[11] Rivilla V.M., The First Detections of the Key Prebiotic Molecule PO in Star-forming Regions, 2016, *ApJ*, 826, 2, 161.

- [12] Lefloch B. et al., Phosphorus-bearing molecules in solar-type star-forming regions: first PO detection, 2016, MNRAS 462, 3937–3944.
- [13] Bergner J.B. et al., Detection of Phosphorus-bearing Molecules toward a Solar-type Protostar, 2019, The ApJ Lett., 884, 2, L36.
- [14] Thorne L.R et al., The chemistry of Phosphorus in Dense Interstellar Clouds, 1984, ApJ, 280, 139-143.
- [15] Millar T.J. et al., An efficient gas phase synthesis for interstellar PN, 1987, Mon. Not. R. Aster. Soc., 229, 41-44.
- [16] Largo A. et al., Theoretical Studies of Possible Processes for the Interstellar Production of Phosphorus Compounds. Reaction of P^+ with Water, 1991, J. Phys. Chem., 95, 5443-5445.
- [17] Largo A. et al., Theoretical Studies of Possible Processes for the Interstellar Production of Phosphorus Compounds. Reaction of P^+ with Methane, 1991, J. Phys. Chem., 95, 6553-6557.
- [18] Largo A. et al., Theoretical Studies of Possible Processes for the Interstellar Production of Phosphorus Compounds. Reaction of P^+ with Ammonia, 1991, J. Phys. Chem., 95, 170-175.