A theoretical approach to the complex chemical evolution of phosphorus in the interstellar medium

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Phosphorus (P) chemistry in the Interstellar Medium (ISM) has become a topic of growing interest within the Astrobiology community [1]. P is present in many organic biomolecules such as phospholipids, nucleotides, and the energetic molecules ATP and GTP. On the other hand, many P-bearing species have been observed in astrophysical environments that cover a wide range of physical conditions, from cold molecular dark clouds to hot cores. Some of these molecules could have been introduced in the early Earth during the Late Heavy Bombardment that took place 4 billion years ago -inside asteroids or comets-, and importantly enriched prebiotic chemistry. This idea is supported by the recent discovery of certain P-bearing molecules in the comet 67P/Churyumov-Gerasimenko [2].

In particular, special attention has been recently paid to the abundances of PO and PN because, while most existing theoretical models lead to PO/PN$<$1, high-sensitivity observations have revealed that PO is substantially more abundant than PN in many different environments [3], a question that has been informally named as the *interstellar phosphorus problem*.

In order to shed light on the interstellar phosphorus problem, in this work [4] we introduce a mathematical model for the time evolution of the P chemistry in an interstellar molecular cloud and analyze its associated chemical network as a complex dynamical system composed of 17 ODEs and 14 different chemical species. We obtain explicit mathematical expressions that describe the abundance evolution of all the P-bearing species involved in the network, whose interactions are represented in the sub-network shown in Fig. 1. Despite the approximations applied, our mathematical solution of the system agrees with very high precision with the numerical results, for all different species and for all values of time (Fig. 2).

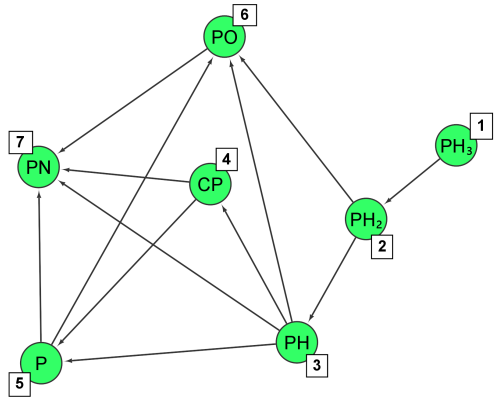

Fig. 1. Sub-network that sketches the theoretically solved system of the time evolution of P chemistry in an interstellar molecular cloud.

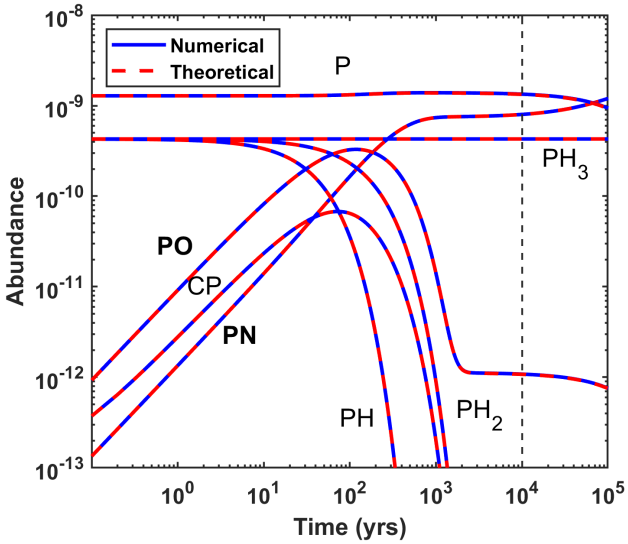

Fig. 2. Evolution of the abundances relative to H of the P-bearing molecules of a molecular cloud. A dashed vertical line remarks the typical cloud age, $t = 10^4 - 10^5$ yrs. This case represents a simulation at T=10 K.

Furthermore, our theoretical results allow much faster computation times than available numerical methods, being our model very powerful to analyze in detail the dependence of the chemical species abundances on the parameters. In particular, we focus on the rate coefficients of the chemical reactions involved in the model because most of them have not been calculated or measured and therefore their values are highly uncertain. Interestingly, we find that the formation of PO and PN is governed by a few critical reactions and we clearly show that the value of PO/PN is highly dependent on their rate coefficients, thus identifying a source that is significantly contributing to the PO/PN disagreement between models and real data. Next, we apply Bayesian inference to constrain the values of the most influential rate coefficients, obtaining results of PO/PN$>$1 that match the observations and suggesting a plausible solution for the interstellar phosphorus problem.

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[3] M. Sil *et al.*, The Astronomical Journal **162**, 119 (2021).

[4] M. Fernández-Ruz, I. Jiménez-Serra, and J. Aguirre, *A theoretical approach to the complex chemical evolution of phosphorus in the interstellar medium*, submitted.