

Characterizing the chemistry of phosphorus in the interstellar medium.

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Phosphorus plays a crucial role in the origin of life as we know it. Indeed, this element plays an important role in biochemistry (e.g., through P-O bonds in DNA and ATP molecules) and is part of the well-known CHNOPS. The key elements for life on Earth. Thus, understanding its interstellar journey from its initial carriers in the diffuse interstellar medium (ISM), through its depletion onto the dust grains, as well as its release in star- and planets-forming regions is important. However, phosphorus bearing molecules are poorly detected in star-forming regions, with only three different molecules detected: PN, PO and PO⁺. Up to now, phosphine (PH₃) is considered as the main phosphorus carrier according to chemical models. However, it has never been detected in protostellar systems but only in circumstellar media, which is not representative of the phosphorus chemistry in protostellar environments. In this work, we investigate alternative phosphorus reservoirs by reconstructing the chemical network of phosphorus in the ISM. We consider new reaction pathways that can occur in diffuse clouds (e.g., $P^+ + H_2 \rightarrow PH_2^+$ and $PH_2^+ + H_2 \rightarrow PH_4^+$) and on grain in dense clouds and protostars (e.g., $s\text{-P} + s\text{-CO} \rightarrow s\text{-PCO}$ and $s\text{-PCO} + s\text{-H} \rightarrow s\text{-HPCO}$, s- meaning on/in grains). These reactions are studied using CASSCF + MRCI and DFT computational methods. Our results suggest that the formation of PH₂⁺ and PH₄⁺ in the gas phase can happen in the ISM conditions, although not very effectively. The HPCO formation on the surface of the grains is likely to happen as well. These results give new insights on the possible phosphorus reservoirs in the ISM.