# Formation of phosphorus monoxide (PO) in the interstellar medium: insights from quantum-chemical and kinetic calculations

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In recent years, phosphorus monoxide (PO) –an important molecule for prebiotic chemistry– has been detected in star-forming regions and in the comet 67P/Churyumov-Gerasimenko [1]. These studies have revealed that, in the interstellar medium, PO is systematically the most abundant P-bearing species, with abundances that are ∼1-3 times greater than those derived for phosphorus nitride (PN), the second most abundant P-containing molecule. The reason why PO is more abundant than PN remains still unclear. Experimental studies with phosphorus in the gas phase are not available. Therefore, the reactivity of atomic phosphorus needs to be investigated using reliable computational tools. To this end, state-of-the-art quantum-chemical computations have been employed to evaluate accurate reaction rates and branching ratios for the P + OH → PO + H and P + $H_2O$ → PO + $H_2$ reactions in the framework of a master equation approach based on ab-initio transition state theory. While the reaction of atomic phosphorus in its ground state with water is not a relevant source of PO because of emerged energy barriers, the P + OH reaction represents an important formation route of PO in the interstellar medium[2].

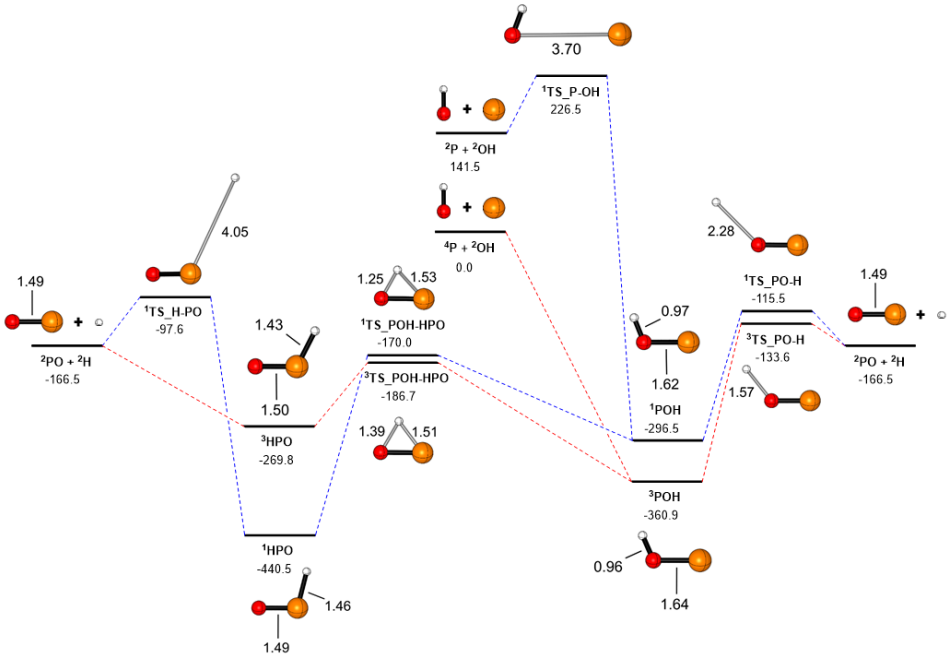


Figure 1. Singlet (blue profile) and triplet (red profile) potential energy surfaces (ZPE-corrected energies) for the formation of PO from OH + P

## References

[1] K. Altwegg et al. 2016, Sci Adv, 2:e1600285.

[2] J. García de la Concepción, C. Puzzarini, V. Barone, I. Jiménez-Serra & O. Roncero. 2021, ApJ, arXiv:2108.08530 [astro-ph.GA].