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Photoionization of phosphorous hydrides: experimental and theoretical comparison

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Phosphorous-bearing molecules have attracted increasing attention in astrochemistry due to their potential role in prebiotic chemistry and the growing number of detections in diverse astrophysical environments. However, the chemistry of phosphorous remains comparatively poorly understood.[a] In this contribution, we present a combined theoretical and experimental study of the photoionization of the phosphorous hydrides PH, PH_2 and PH_3.

The photoionization of several phosphorous, sulphur and oxygen-bearing molecules experiments were carried out at SOLEIL synchrotron. These data serve as a benchmark for theoretical simulations and allow us to assess the reliability of the underlying electronic structure description.

The theoretical calculations include high-level multireference Potential Energy Curves (PEC) and Surfaces (PES) for the relevant neutral and cationic species, explicitly accounting for spin-orbit coupling (SOC), effects. Photoionization spectra are simulated using the SHARC software and is use to interpret the experimental results, allowing us to gain further insight into which electronic states of the cationic species get populated. For PH, we been able to simulate rovibrationally resolved photoionization spectrum using the DUO software.[b]

This approach enables consistent treatment of the electronic states, spin-orbit interactions and the nuclear geometries of the system. Overall, this work provides a unified description of the photoionization behavior of phosphorous hydrides and delivers new data of relevance for astrochemical models of P-bearing species in irradiated environments.

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