IN SEARCH OF PHOSPHORUS IN ASTRONOMICAL ENVIRONMENTS: THE REACTION BETWEEN THE CP RADICAL ($X^2\Sigma^+$) AND METHANIMINE

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Phosphorus belongs to the group of the so-called “main biogenic elements”, which includes the most abundant elements in living systems. Accordingly, when seeking to better understand the evolution of the universe -with a keen eye on abiogenesis- phosphorus and its compounds cannot be overlooked. However, the chemical evolution of such element in the interstellar medium (ISM) is still far from an accurate characterization.

To provide a contribution in this direction, a recent work investigated the reactivity beetween the CP radical ($X^2\Sigma^+$) and methanimine (CH_2NH), both detected in the carbon-rich circumstellar shell IRC+10216. This type of reaction is particularly promising because it fits into a peculiar reactivity of methanimine with different radicals, among which we find the isoelectronic CCH and CN radicals, the reactions with these latter being very well characterized. This supports the idea of a general mechanism for the formation of complex imines in the interstellar clouds.

An accurate investigation of the reactive CH_2NH + CP potential energy surface (PES) revealed the presence of submerged formation pathways for three main reaction products, namely E- and Z-2-phosphanylidyneethan-1-imine (HNCHCP) and N-(phosphaneylidynemethyl)methanimine (CH_2NCP).

Despite the proof of concept of their feasible formation in gas phase from an energetic point of view, the laboratory synthesis of species like HNCHCP and CH_2NCP is particularly complex. This could hamper the identification of their rotational transitions required in view of predicting and confirming their presence in the ISM.

In order to provide a useful support to experimental measurements, computed spectra represent a mandatory starting point. This talk will delve into the accurate spectroscopic characterization of these latter species with a methodology at the state of the art, which is able to predict rotational transitions with accuracy better than 0.2%.