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Rotational excitation of the CP($X^2\Sigma^+$) open shell molecule due to Collision with He(^1S)

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Phosphorus bearing molecules have been discovered in the circumstellar and interstellar media. Modeling their abundance accurately requires computations of rate coefficients induced by collision with He and H_2 (i.e., the most abundant gaseous components). Without these data along with radiative transitions, astrophysicists would assume the Local Thermodynamic Equilibrium (LTE) which is rarely verified in space. Rate coefficients may be computed by first determining highly accurate Potential Energy Surface (PES) and cross sections. Here, we present the first PES of the CP($X^2\Sigma^+$)-He(^1S) Van Der Waals collisional complex. The ab initio interaction potential was performed using the explicitly correlated restricted coupled cluster approach with simple, double, and perturbative triple excitation (RCCSD(T)-F12) in connection with the augmented correlation consistent polarized valence triple-ζ Gaussian basis set (aug-cc-pVTZ), as implemented in the Molpro program. The potential presents two minima of -18.62 cm^{-1} and -18.72 cm^{-1}. From the PES obtained, we have computed state-to-state excitation cross sections of CP due to collision with He for energies up to 500 cm^{-1}. Rotational transitions involving the fine-structure levels of the CP molecule were treated with a Recoupling Technique based on the scattering matrix calculated with the exact quantum mechanical close coupling method implemented in the Molscat code. Discussions on the propensity rules between the fine-structure levels were made and we found that the $\Delta j=\Delta N$ transitions are favored with respect to the $\Delta j\neq\Delta N$ ones. The data presented here may have a great impact on the accurate determination of the CP abundance in space. This would yield a better understanding of the phosphorous interstellar chemistry. Indeed, carbon phosphorus is expected to originate from HCP photo-dissociation and it is thought to be the main precursor of CCP formation.

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