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THEORETICAL INVESTIGATION OF PLASMA INDUCED DEGRADATION OF CHLORPYRIFOS

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Chlorpyrifos (O,O-diethyl O-3,5,6-trichloro-2-pyridyl phosphorothioate) is one of the harmful pesticide that persist long time in the environment and effect human health [1]. As a result of its accumulation in the environment and the effect it causes on human health its degradation into non-harmful substances is of high importance. In recent days, Plasma assisted degradation that involves highly energetic species such as radicals, ions to induce molecular fragmentation is emerging as an effective method for their removal.

In this work, Potential energy surface (PES) scans were performed to identify the most stable conformer of chlorpyrifos by systematically varying key dihedral angles [2]. Then, degradation mechanisms were identified by modelling the reaction pathways of atomic oxygen and nitrogen radicals with chlorpyrifos. Degradation studies revealed that, under radical attack chlorpyrifos gets converted into reactive intermediates and fragmentation into less harmful products. Further, potential protonation sites were identified by the calculation of proton affinities, relevant for charge transfer reactions identified in positive corona discharge. In addition to radical attack and protonation, attachment of water clusters to chlorpyrifos has also been studied to understand the structural stability and also to explore other possible degradation pathways.

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