MITIGATION - SCIENCE AND TECHNOLOGY ADVANCES FOR CHEMICAL AND BIOLOGICAL HAZARD MITIGATION

Decomposition Mechanism Of Organophosphate-based Nerve Agents In The Plasma-treated Water Environment: Theoretical Study Of Decomposition Reaction Under Acidic Condition

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Organophosphates (OPs) are used in various fields like herbicides, pesticides, and chemical warfare agents (CWAs). Despite their original uses, these compounds remained in natural environment make a lot of problems due to their toxicity. Especially for the cases of CWAs, a wide range of severe nerve agents are classified as OP. Therefore, in the environmental and military point of view, it is important and urgent to understand how these compounds are decomposed and detoxified. A lot of experiments report that various nerve agents are readily decomposed by alkaline hydrolysis. Newly emerged OPs are hard to be detoxified under alkaline media. Plasma-treated water (PTW) is emerging as an effective way of decontamination of advanced threat. PTW is generated by discharging water with plasma, thereby containing various reactive species with strong oxidation power. Also, those species make PTW to be acidic. Although previous studies are mainly focusing on elucidations of hydrolysis reaction mechanisms under alkaline environment, newly emerged OPs, on the contrary, show a possibility of efficient degradation under PTW condition. Thus, the decontamination mechanism of OPs under acidic environment have been investigated theoretically in this study. By using density functional theory (DFT) calculation, we tried to find the lowest energy barrier pathway among the possible routes of reactions and justified theoretically why newly emerged OPs are decomposed effectively under acidic condition. Furthermore, we investigated how solution environment effects to decomposition mechanism by implementing polarizable continuum model (PCM) calculations. We hope that this study contributes further understanding about degradation process of toxic OP compounds and to be helpful to design effective decontaminants.