Computational Studies on the Reduction of Chemical Warfare Agent Simulants

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The mechanism for the neutralization of chemical warfare agent simulants due to a one-electron reduction in aqueous solution has been studied using computational chemistry. Published experimental data concludes that the process through which this destruction occurs follows the same mechanism for a series of six simulants (Figure 1), which differ only in the identity of the leaving group (H, Cl, F, CN, CH_3, and CF_3). The goal of this project is to determine the exact means by which the reduction occurs for each simulant in an attempt to support or refute the previous work. Density functional theory (DFT) calculations, at the M052X/6-31+G(d,p) level of theory, were used to map a potential energy surface for each simulant after the addition of an electron. Afterwards, Atom-Centered Density Matrix Propagation (ADMP) calculations were used to map the molecular dynamics trajectories and give the molecule nuclear kinetic energy in order to better understand the reaction. So far, these ADMP results have led us to believe that most simulants will, in fact, follow the proposed mechanism, but the CH_3 leaving group appears to be doing something much different. This work will ultimately provide an accurate mechanism of the reduction process and allow for an enhanced understanding of the chemistry of chemical warfare agents.

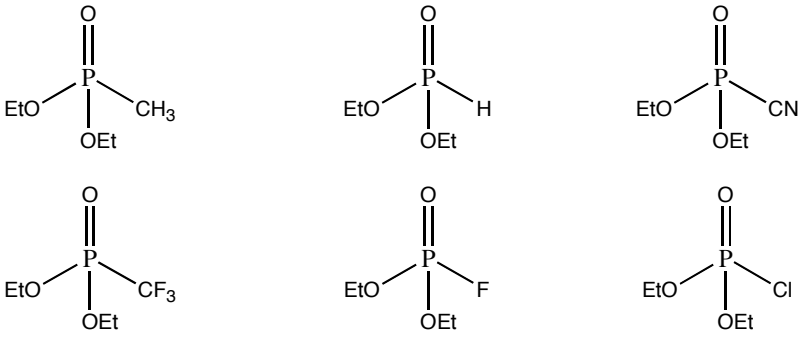

Figure 1: The six chemical warfare agent simulants included in this study