

# Mechanism of Aqueous Hydroperoxidolysis of O,S-Dimethyl Methylphosphonothiolate

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O-ethyl S-(2-diisopropylamino)ethyl methylphosphonothioate (VX) is a V-series nerve agent used in chemical warfare which can cause convulsions and death by inhibiting acetylcholinesterase. To date, the United States Army has destroyed 88 percent of stockpiled agent, by first neutralizing it with sodium hydroxide followed by oxidation of the hydrolysate produced in the neutralization step. Previously, it has been shown that the hydroperoxide anion is a more effective nucleophile for the neutralization of VX, and the mechanism of hydroperoxidolysis has been thoroughly studied via gas-phase calculations and mass spectrometry. However, the precise mechanism of hydroperoxidolysis in aqueous solution remains unknown. The purpose of this experiment is to study the effects of the solvent during the hydroperoxidolysis of VX. Explicit solvent is represented by 200 effective fragment potential (EFP) water molecules surrounding the solute, and the entire system is embedded in an aqueous polarizable continuum model (PCM). In order to reduce computational time O,S-dimethyl methylphosphonothiolate (O,S-DMMP) is used as a simulant for VX. The M06-2X/6-31+G(d,p) level of theory has been used.