



K37 Chemical Warfare Agent Decontamination Reactions in Ionic Liquids (I): Decontamination of Diisopropylfluorophosphate (Simulant for Sarin) and Bis(2-ethylhexyl) Phosphite (Simulant for VX) in DMPITf₂N

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After attending this presentation, attendees will obtain an understanding of some of the basic research being conducted on decontaminating chemical warfare agents on buildings, vehicles, equipment, and personnel. The attendee will gain a better understanding of the role of ionic liquids as solvents, reactants, and catalysts in organic chemical reactions.

This presentation will impact the forensic sciences by acquainting first responders, medical examiners, coroners, investigators, and morgue attendants with some of the research efforts currently underway to neutralize facilities/equipment that may be exposed to various nerve agents. The impact of this paper is to instill confidence in all personnel that research is being conducted to establish protocols that minimize personal risks of exposure and rapidly return exposed equipment to use.

Because of 9/11, the vulnerability of America to attack became apparent and the threat of chemical attacks from within became real. Shortly after 9/11, major efforts were initiated to prepare for a chemical attack. The efforts involved establishing rapid and reliable decontamination processes for chemical warfare agents. In order for a decontamination process to be effective, it must be rapid, generate non-toxic reaction products, and be compatible with the environment. In studying decontaminating processes of chemical warfare agents, "simulants", in lieu of the actual chemical warfare agent itself, are used. Simulants are chemical compounds that are similar in chemical composition and physical properties to the actual agents, but considerably less toxic. For this study, the simulants, diisopropylfluorophosphate (DFP) and bis(2-ethylhexyl)phosphite (BEHP), were chosen which simulate the nerve agents Sarin and VX, respectively. The ionic liquid selected for study was 1,2-dimethyl-3-propyl imidazolium bistrifluoromethylsulfonamide (DMPITf₂N). DMPITf₂N was selected because of its favorable hydrophilic/hydrophobic properties.

The objective of studying decontamination reactions in DMPITf₂N as the ionic liquid is threefold: (1) identify those chemical compounds that are reactive with simulants in DMPITf₂N, (2) determine the composition of the reaction products, and (3) develop a reaction matrix that isolates the reactants and products from the environment. In this report we describe the results of the reactions between DFP and BEHP with tetraalkylammonium hydroxide/methanol in DMPITf₂N ionic liquid and the reaction between DFP and ethanolamine in DMPITf₂N. The reactions with tetraalkylammonium hydroxide/methanol were extremely rapid and produced both hydrolysis and alcoholysis reaction products. The reaction between DFP and ethanolamine resulted in nucleophilic substitution of the P-F bond with formation of isomeric phosphate esters and phosphoramides. A ¹H NMR Mercury 300 NMR was used to monitor the reaction between ethanolamine and DFP.

A liquid chromatograph coupled to an exact mass time-of-flight mass spectrometer (LC/MS-TOF) was used to identify the reaction products. A polar and aromatic reversed phase selectivity ether-linked phenyl with polar endcapping LC column (Synergi[™] Polar-RP[®]) was used. A mobile phase gradient elution with methanol and 5mM ammonium formate from 30–95% over 12 minutes at 0.3 mL/minute flow provided good retention and resolution. Electrospray ionization was used as the ionization source. A discussion of the TOF fragmentation patterns of the reaction products is presented. The data presented here are results of ongoing research.

Chemical Warfare Agents, VX, Sarin