



### **K38 Chemical Warfare Agent Decontamination Reactions in Ionic Liquids (II): Decontamination of Chloroethylethyl Sulfide, Simulant for Sulfur Mustard (HD), in DMPITf2N**

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After attending this presentation, attendees will obtain a better understanding of some of the basic research associated with chemical warfare agent decontamination processes. The blister agent, chloroethylsulfide commonly referred to as mustard gas (HD), presents challenges to the scientific community in both its decontamination, if used as an offensive agent, as well as its disposal, as mandated by international agreements. The attendees will gain awareness of the chemistry being developed to convert this toxic material into non-toxic products by carrying out oxidation reactions in ionic liquids.

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 chemical warfare 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 at the same time will result in a rapid return of exposed equipment to use without fear of prolonged contamination or risk of exposure.

Many techniques currently exist, and more are being developed for the detection of toxins in chemical, biological and nuclear attacks. With the attacks of 9/11 and acts of terrorism abroad, the need has arisen for the scientific community to develop techniques centered upon a reactive posture. The end goal is to anticipate and mitigate the adverse effects of an actual chemical attack through a chemical process designed to be effective and rapid.

In this presentation we describe the results of some of the basic research being conducted in developing a reaction medium that: (a) will identify those chemical reagents that react with mustard gas stimulant (CEES) in an ionic liquid, (b) determine the composition of the reaction products, and finally (c) develop a reaction matrix that contains the reactants and products preventing them from entering the environment, i.e. Green Chemistry compatible. The ionic liquid selected for this study was 1,2-dimethyl-3-propylimidazolium bistrifluoromethylsulfonamide (DMPITf2N) because of its excellent hydrophilic and hydrophobic properties.

The copper II catalyzed oxidation of CEES with hydrogen peroxide in the DMPITf2N to the corresponding sulfoxide occurred with ease. Copper (II) bistrifluoromethylsulfonamide was selected as catalyst because of its compatibility and solubility in DMPITf2N. A Mercury 300 NMR (<sup>1</sup>H NMR) spectrometer provided a convenient method of monitoring the decrease in concentration of CEES in the ionic liquid. 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 column (Synergi<sup>imm</sup> Polar-RP<sup>R</sup>) 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 Thermo Electron Corporation PolarisQ ion trap GC/MS system was also used to determine the presence of remaining sulfide and sulfoxide and sulfone formation. 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, Mustard Gas Simulant, Ionic Liquids**