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# **Neutralization and Disposal of Laboratory Scale Toxic Chemicals**

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## ABSTRACT

This report provides guidance on the neutralization, destruction, and disposal of small quantities of chemicals designated in the Chemical Weapons Convention (CWC) Schedules 1, 2, and 3 [1]. It provides a review of commonly used methods and techniques for chemical neutralization that involve hydrolysis, oxidation, and pH adjustment reactions. For any given hazardous chemical discussed, the aim is to produce non-toxic products that can be disposed of by conventional wastewater treatment processes or in some cases completely mineralized through secondary oxidation. The outlined processes were designed to be used under the following conditions and circumstances:

- 1) Complete adherence to all international, national, and local laws and/or regulations
- 2) Used only for small quantities of the chemicals (i.e., < 100 grams)
- 3) Laboratory personnel and all who share a common space with these materials must be properly trained and protected from exposure

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## **EXECUTIVE SUMMARY**

This report is designed to give guidance for the treatment and subsequent disposal of small volumes of CWC scheduled chemicals and related precursors. The report also includes several admonitions and conditions that must be considered before action is taken to destroy these chemicals. Chemical treatment in this report specifically refers to the detoxification of chemicals through neutralization, hydrolysis, or oxidation leading to disposal in conventional biological or enhanced oxidative wastewater treatment. The objective is to provide guidance on the removal and disposal options of small quantities of these sensitive chemicals from academic and government laboratories to reduce the security risks of those institutions. Techniques in this report can be used to enhance the Chemical Management System (CMS©) and Chemical Asset Tracker (CAT©) software developed by Sandia National Laboratories.

## ACRONYMS AND DEFINITIONS

Abbreviation	Definition
CWC	Chemical Weapons Convention
CAS#	Chemical Abstract Services Number (Unique Chemical Identifier)
WISER	Wireless Information System for Emergency Responders
HD	Sulfur Mustard
HN-1-HN2-HN-3	Nitrogen Mustard Agents (listed in text)
L1-L2-L3	Lewisite Agents (listed in text)
GA-GB-GC-GF-VX	Nerve Agents (specific agents listed in text)
UV	Ultraviolet (light)
BZ	3-Quinuclidinyl benzilate (incapacitating agent)
DF	Methylphosphonyl difluoride (precursor)
QL	O- Ethyl-O-2-diisopropylaminoethyl methylphosphonite (precursor)
MPA	Methylphosphonic acid
IMPA	Isopropyl methylphosphonic acid
EMPA	Ethyl methylphosphonic acid
DMMP	Dimethyl methyl phosphonate
i-PrOH	Isopropyl alcohol
t-BuOH	Tertiary butyl alcohol
PBFIB	Perfluoroisobutene
GCMS	Gas Chromatography / Mass Spectrometry
HF, NaOH, H <sub>2</sub> O <sub>2</sub> ...	Specific chemicals are identified by their formula (not as abbreviations)



## 1. INTRODUCTION

This report gives guidance for laboratory-based chemical treatment and disposal of CWC scheduled chemicals. The report will be incorporated into the Chemical Management System (CMS©) and Chemical Asset Tracker (CAT©) software programs provided by Sandia National Laboratories to international partners to assist them in reducing the risks related to the storage and disposal of these types of chemicals. This report is only meant to provide a review of feasible chemical treatment and disposal options for small quantities of CWC scheduled chemicals and is limited in scope to 1) the destruction of specific chemicals listed in the Annex of Chemicals [1] from the Convention on the Prohibition of the Development, Production, Stockpiling and Use of Chemical Weapons [2] (summarized in Table 1 below), and 2) small chemical quantities no greater than 1g for Schedule 1, 100 g for Schedule 2, and 1000 g for Schedule 3 designations.

The procedures for the treatment and disposal of CWC scheduled chemicals (even small quantities) can be complicated and problematic due to a variety of issues. First, and most importantly, these chemicals pose an extreme safety risk to those who handle them due to their hazardous nature, and typical treatment methods to reduce their hazards are inherently dangerous. From a purely technical point of view, these chemicals can often be readily neutralized through one of the following:

- a) hydrolysis with a large quantity of water
- b) caustic hydrolytic treatment
- c) oxidation using readily available oxidants, or
- d) a combination of the above methods.

The difficulty of disposal, however, is twofold. First, it is imperative to know that the original chemical has been consumed by the treatment method. This is usually confirmed by the disappearance of the agent in question and can be measured by some type of analytical test (test strip, GCMS, etc.). The second concern is to ensure that the products of the neutralization are not themselves toxic or otherwise hazardous. This includes knowing if the products of neutralization are compatible with conventional waste disposal methods (such as sewage treatment or landfill). For this report, we assume the volumes being treated are relatively minor, and the waste effluents can be disposed of in an environmentally safe manner.

**Table 1.1 CWC Schedules**

Schedule	Description from the CWC, Annex on Chemicals [1]
1	A chemical “developed, produced, stockpiled or used as a chemical weapon,” “possesses such lethal or incapacitating toxicity as well as other properties that would enable it to be used as a chemical weapon,” or “used as a precursor in the final single technological stage of production of a toxic chemical listed in Schedule 1.”
2	A chemical that “may be used as a precursor” in the “final stage of formation of a chemical listed in Schedule 1,” “possesses such lethal or incapacitating toxicity as well as other properties that could enable it to be used as a chemical weapon,” and “not produced in large commercial quantities.”
3	A chemical that “has been produced, stockpiled or used as a chemical weapon” or as precursors for them, “possesses such lethal or incapacitating toxicity as well as other properties that might enable it to be used as a chemical weapon,” and “may be produced in large commercial quantities.”

### **1.1. Structure of this Report**

The subsequent sections of this report consist of two parts. The first part provides the Chemical Abstract Services (CAS) numbers and descriptions of the CWC scheduled chemicals. The second part, in table form, delineates: 1) the treatment and/or decontamination reactions necessary to destroy or decompose the chemicals, and 2) recommended procedures for the safe disposal of the reaction products of treatment and/or decontamination. The reactions usually include neutralization, hydrolysis, and oxidation (or a combination of these reactions). Waste disposal recommendations are made on the assumption that the CWC reactant has been completely neutralized (no residual toxicity), and that the quantity of waste is low; this should be verified using a reliable chemical test procedure.

### **1.2. Compliance with International, National, and Local Laws and Regulations**

The methods and techniques provided in this report are not exempt from international or national laws and regulations. It is imperative that the reader review international and national laws that may be relevant to the neutralization and disposal of chemicals. International guidance that may be important to review includes a) the Organization for the Prohibition of Chemical Weapons, Convention on the Prohibition of the Development, Production, Stockpiling and Use of Chemical Weapons and Their Destruction [2] available at <http://www.opcw.org> and b) Basel Convention on the Control of Transboundary Movements of Hazardous Wastes and their Disposal available at <http://www.basel.int/>. National and local laws vary greatly depending on the geographic location of the reader. It is strongly encouraged that the reader reviews all laws that govern hazardous chemical storage, transportation, and disposal before conducting the chemical treatment recommendations described herein.

### **1.3. Safety and Security Considerations**

This report is a review of techniques and methods for chemical neutralization and disposal. The recommendations do NOT include safety or security practices related to the handling, storage, or transport of these chemicals. It is essential that an experimental plan be developed and reviewed by all staff or laboratory personnel who will be involved in the destruction and disposal of these chemicals, and that the plan include appropriate safety and security practices. This should include an in-depth knowledge of the potential hazards as well as use of appropriate procedures, engineering controls, and personal protective equipment. The lab must be adequately prepared for emergencies and have procedures for evacuation and medical treatment in case of unforeseen or accidental releases. Since many of the compounds have been used for malevolent purposes, the lab should also have procedures (such as access control and inventory management) in place to prevent the theft or misuse of these chemicals, and verification procedures for their destruction and disposal.

### **1.4. Practical Considerations**

Laboratory chemicals are often packaged in non-uniform, non-standard plastic or glass containers. Sometimes there is little or no history for the chemicals, and some have been aging in the laboratory for an indeterminate amount of time. It is essential to understand how this will affect the decontamination procedures. One very important consideration is the miscibility of a chemical in various solvents. Sulfur mustard (HD) and VX are not very soluble in water, and so treatment techniques often involve an organic solvent (e.g., various alcohols).

Another consideration is the production of toxic or hazardous gases during chemical treatment. Several of the described methods include the production of toxic gas (such as  $\text{H}_2\text{S}$ ). Appropriate precautions must be taken to collect and neutralize the gas in order to prevent exposure to the staff and environment. It is also important to know about and control exothermic reactions that may cause effervescence and loss of containment. Finally, laboratory personnel engaged in decontamination of these compounds must never work alone, but be accompanied by a competent and well-trained assistant.

### **1.5. Chemical Treatment/Decontamination**

The chemical treatment reactions listed in this report have been covered in various academic and applied chemistry articles. References have been provided; some of the recent applied chemistry articles use readily available household chemicals. These techniques and the underlying chemistry of decomposition are meant to impart a measure of irreversibility to the reactions. The products of treatment may therefore be disposed of as laboratory hazardous waste or as a treatable waste in a sanitary sewer (if appropriate conditions are met). Many of the treatment reactions listed in this report come from decontamination studies with trace amounts of material, so scaling up to 100 g quantities will require calculating reaction mixtures and required decontamination solutions with enough excess to ensure complete destruction. This may actually increase the volume of waste produced and therefore require appropriate considerations for waste disposal. Additionally, scaling up reactions can also result in exothermic conditions or pressure increases and should therefore only be done by an experienced laboratory professional and under strict observation to control the reaction.

### **1.6. Waste Disposal**

Waste disposal recommendations are made on the assumption that 1) the CWC reactant has been completely neutralized (no residual toxicity) and the quantity of waste is small, and 2) landfill or incinerator disposal and sanitary sewer waste facilities utilize modern techniques and methods. The reader should review any national laws or guidelines on appropriate disposal facilities to ensure that there are no ill effects on the facilities handling the wastes. Liquid wastes may be collected along with other compatible wastes for landfill or incinerator disposal using appropriate waste facilities, to include licensed hazardous waste facilities in the reader's country or local territory. Some liquid wastes may be suitable for waste disposal in a sanitary sewer if quantities are not significant and they are amenable to the biological oxidation processes in the modern sanitary treatment facility. In some cases, the pH of the products must be adjusted to a non-corrosive range (pH 5.5–9.5). Solid waste can be collected and sent for landfill disposal, with special attention given to heavy metal types and quantity.

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## 2. CWC SCHEDULE 1 CHEMICALS

The CWC Schedule 1 chemicals are generally the most hazardous and toxic chemicals addressed in this report. Therefore, the safety and security requirements should be addressed at the highest level. Special care must be taken to ensure that complete destruction is achieved and that the products of decontamination are non-toxic (see especially the note on VX).

### 2.1. Sulfur Mustards

Sulfur mustard agents include CAS registry numbers: 505-60-2 (HD); 3563-36-8; 63905-10-2; 142868-93-7; 142868-94-8; 63869-13-6; 2625-76-5; 63918-89-8; and 63918-90-1. These chemicals are not very soluble in water, and therefore oxidation is the preferred form of treatment over hydrolysis.

**Table 2.1 Sulfur Mustards Treatment/Decontamination and Waste Disposal**

Treatment Method(s) Type	Techniques/Methods	Products	Waste Disposal
Oxidation	<p>Activated Peroxidation: HD + 0.1 M NaHCO<sub>3</sub> + 50 wt% H<sub>2</sub>O<sub>2</sub> (ethanol solvent) – <math>t_{1/2}</math> = 1.8 min. Essentially only very low-toxicity sulfoxides formed [3].</p> <p>HD + 50 vol% H<sub>2</sub>O<sub>2</sub> (3 wt%) + NaHCO<sub>3</sub> (5 wt%) + 50 vol% <i>i</i>-PrOH (70%) [4].</p> <p>H<sub>2</sub>O<sub>2</sub>: HD + H<sub>2</sub>O<sub>2</sub> – <math>t_{1/2}</math> = 133 min. Essentially only sulfoxides formed [5].</p> <p>UV light + 10<sup>-4</sup> M H<sub>2</sub>O<sub>2</sub> – <math>t_{1/2}</math> = ~3 min [6].</p> <p>Bleach: HD + NaOCl (~5 wt%, household, full strength) – <math>t_{1/2}</math> = 8 min vinyl-2-chloroethyl sulfone and "slight" mustard sulfone and toxic divinyl sulfone products [5].</p>	The main product includes mustard sulfoxide (Bis(2-chloroethyl) sulfoxide) with some additional oxidation to produce mustard sulfone (Bis(2-chloroethyl) sulfone).	Waste collection and disposal as hazardous waste or diluted for sanitary sewer disposal with a (large excess of water [7].

### 2.2. Nitrogen Mustards

Nitrogen mustard agents include CAS registry numbers: 538-07-8 (HN1); 51-75-2 (HN2); and 555-77-1 (HN3). These agents are soluble in water, and hydrolysis is the most efficient means of neutralization.

**Table 2.2 Nitrogen Mustards Treatment/Decontamination and Waste Disposal**

Treatment Method(s) Type	Techniques/Methods	Products	Waste Disposal
Hydrolysis	Hydrolysis: HN(1, 2, 3) + water + slightly basic conditions, rate increases with temperature and pH [7]	HN1 products—very low toxicity, mostly mild irritants. Some specific products include: Ethyldiethanolamine and diethanolamine.	Products from HN1 and HN3 may be disposed as hazardous waste or diluted for sanitary sewer disposal with a (large excess of water).

Treatment Method(s) Type	Techniques/Methods	Products	Waste Disposal
		<p>HN2 products—more toxic than HN1 products. Some specific products include: N-methyl-2-hydroxy-2-chloro diethyl ammonium chloride, 2-(2-chloroethyl)methylamino ethanol hydrochloride, N,N'-dimethyl-N,N'-bis(2-chloroethyl) piperazinium, N-methyldiethanolamine.</p> <p>HN3 products—low toxicity. Some specific products include: Bis(2-chloroethyl)-2-hydroxyethyl ammonium chloride, 2-chloroethyl-bis(2-hydroxyethyl) ammonium chloride, triethanolamine chloride.</p>	Products from HN2 should be disposed by hazardous waste collection and processed through an approved hazardous waste disposal facility.

### 2.3. Lewisites

Lewisites include CAS registry numbers: 541-25-3 (L1); 40334-69-8 (L2); and 40334-70-1 (L3).

**Table 2.3 Lewisites Treatment/Decontamination and Waste Disposal**

Treatment Method(s) Type	Techniques/Methods	Products	Waste Disposal
Oxidation	Oxidation: L(1, 2, 3) + NaOCl (5 wt%) OR H <sub>2</sub> O <sub>2</sub> (3 wt%)—not detected after 30 min [8].	2-chlorovinylarsonic acid (C <sub>2</sub> H <sub>4</sub> AsClO <sub>3</sub> ) is the main product. Additional products may include 2-chlorovinyl arsenous acid if hydrolysis occurs or if 2-chlorovinyl arsenous acid isn't fully oxidized to 2-chlorovinylarsonic acid.	2-chlorovinylarsonic acid can be converted to sodium arsenate salts, then to ferric arsenic salts for disposal in a licensed hazardous waste facility [9].

## 2.4. Nerve Agents

Nerve agents are generally subdivided into classes (G-series, V-series, Carbamates, and Insecticides). For the purpose of this report, the nerve agents are those listed in the CWC Schedule 1 chemicals, which include CAS registry numbers: 77-81-6 (GA); 107-44-8 (GB); 96-64-0 (GD); and 50782-69-9 (VX).

**Table 2.4 Nerve Agents Treatment/Decontamination and Waste Disposal**

Treatment Method(s) Type	Techniques/Methods	Products	Waste Disposal
Oxidation	<p>Activated Peroxidation: GB + 0.037 M NaHCO<sub>3</sub> + 30% H<sub>2</sub>O<sub>2</sub> + <i>t</i>-BuOH (cosolvent) – <math>t_{1/2}</math> &lt; 1 min [3].</p> <p>GD + 50 vol% H<sub>2</sub>O<sub>2</sub> (3 wt%) – ND (not detectable) after 4 min [4].</p> <p>VX + 50 vol% H<sub>2</sub>O<sub>2</sub> (3 wt%) + 1 wt% Na<sub>2</sub>CO<sub>3</sub> – ND after 4 min [4]. More reactions for VX are also listed in Table 1 [3]. Sodium perborate can be used as an alternative to H<sub>2</sub>O<sub>2</sub>.</p>	<p>IMPA, MPA (main), and possibly HF</p> <p>Pinacolyl methylphosphonic acid or MPA (main) and possibly HF</p> <p>EMPA, MPA, and ethyl diisopropylamino compound [9]</p>	<p>Alkyl methylphosphonic acids can be oxidized to H<sub>3</sub>PO<sub>4</sub>, CO<sub>2</sub>, and H<sub>2</sub>O using excess H<sub>2</sub>O<sub>2</sub>, O<sub>2</sub>, and UV light [12].</p> <p>If any organic products form (possibly <i>i</i>-PrOH, and alkanes), they will likely separate from the acidic aqueous solution. Acidic solution can be neutralized, and organic waste can be combined with like organic wastes for hazardous waste disposal (see section 3.1.2 for HF waste).</p>
	<p>Hydrogen peroxide and bleach: Very similar to reactions listed above for activated peroxidation, but much the reaction times are slower. Additionally, oxidation of VX cannot occur without basic conditions [9] and the presence of water [10] unless molybdate is present [3]. VX is not very miscible in water, forming a separate organic phase. Light mixing is necessary for rapid reactions.</p>	<p>Same as noted above</p>	
Hydrolysis	<p>GA/GB/GD + H<sub>2</sub>O + pH~10-11 (NaOH)</p>	<p>GA—end product is phosphoric acid (H<sub>3</sub>PO<sub>4</sub>) [9]. Acidic conditions produce dimethylamine as an intermediate byproduct. Basic conditions produce the CN anion as an intermediate byproduct [9].</p> <p>GB/GD—reduced to respective, non-toxic monophosphonic acids IMPA (GB), Pinacolyl MPA (GD), and HF within</p>	

Treatment Method(s) Type	Techniques/Methods	Products	Waste Disposal
		a few minutes [7] [10]. Acetate ions were also found to significantly accelerate hydrolysis of GB and GD [11].	

## 2.5. Schedule 1 B: Precursors

“Precursors” are defined in Schedule 1 Section B in the Annex of Chemicals and include CAS registry numbers: 1445-76-7 (Chlorosarin); 7040-57-5 (Chlorosoman); 676-99-3 (DF); and 57856-11-8 (QL).

**Table 2.5 Scheduled 1B Precursors Treatment/Decontamination and Waste Disposal**

Treatment Method(s) Type	Techniques/Methods	Products	Waste Disposal
Oxidation/Hydrolysis	Chlorosarin, Chlorosoman, and DF all have very similar structures to GB/GD and are expected to respond similarly to the reactions listed in the tables above.  QL has a structure similar to VX (used as a simulant), and it is expected the ester and amino groups will be susceptible to oxidation [12] [13].	R-MPAs, HCl (for chloro-GB/GD), HF (for DF)  EMPA is the main product. Trialkyl amines and dialkyl amines are possible products.	UV and advanced oxidation treatment (UV-H <sub>2</sub> O <sub>2</sub> ) can be performed for the generated wastes followed by disposal in sanitary sewer with a large excess of water. (See HF recommendations in section 3.1.2. below).

## 2.6. Ricin

Ricin has the CAS registry number: 9009-86-3.

**Table 2.6 Ricin Treatment/Decontamination and Waste Disposal**

Treatment Method(s) Type	Techniques/Methods	Products	Waste Disposal
Oxidation	Bleach: Deactivated after 15 min treatment with NaOCl (household concentrations) [14]. Lowest concentration for deactivation of cytotoxicity is 3 mM NaOCl [15].	Denatured ricin protein	Neutralization of caustic solution followed by disposal in sanitary sewer with a large excess of water.



## 2.7. Saxitoxin

Saxitoxin has the CAS registry numbers: 35523-89-8.

**Table 2.7 Saxitoxin Treatment/Decontamination and Waste Disposal**

<b>Treatment Method(s) Type</b>	<b>Techniques/Methods</b>	<b>Products</b>	<b>Waste Disposal</b>
Oxidation	Bleach: Deactivated after 30 min treatment with >0.1% NaOCl or 0.25% NaOCl + 0.25N NaOH [14].	Denatured saxitoxin protein	Neutralization of caustic solution followed by disposal in sanitary sewer with a large excess of water.

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### 3. CWC SCHEDULE 2 CHEMICALS

The CWC Schedule 2 chemicals include those that possess a lethal or incapacitating toxicity as well as other properties that could enable them to be used as chemical weapon precursors. This section is divided into 2A: Toxic Chemicals and 2B: Precursors. The destruction of these compounds may not elicit the same safety concerns as the chemicals in CWC Schedule 1 or require elaborate efforts to reduce their toxicity. The approach to destruction may need to be modified to allow straightforward techniques including dilution and disposal or mixing with other compatible hazardous waste streams for disposal. The guiding principle is to reach irreversibility, so that the chemical cannot be readily reconstituted.

#### 3.1. Schedule 2A: Toxic Chemicals

This section includes specific toxic chemicals listed in CWC Schedule 2, Section A with CAS registry numbers: 78-53-5, 382-21-8, and 6581-06-2.

**Table 3.1 Schedule 2A Toxic Chemicals Treatment/Decontamination and Waste Disposal**

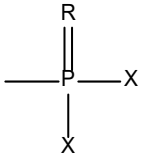
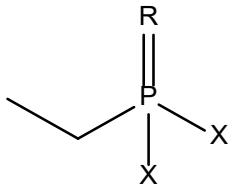
Chemical Name (CAS #)	Treatment Method(s) Type	Techniques/Methods	Products	Waste Disposal/Treatment
Amiton: O,O-Diethyl S-[2-(diethylamino) ethyl] phosphorothiolate (78-53-5)	Oxidation	Activated peroxidation [16] [17]	Alkyl methyl phosphonic acids	Alkyl methyl phosphonic acids can be oxidized to H <sub>3</sub> PO <sub>4</sub> , CO <sub>2</sub> , and H <sub>2</sub> O using excess H <sub>2</sub> O <sub>2</sub> , O <sub>2</sub> , and UV light [12].
PFIB: 1,1,3,3,3- Pentafluoro-2- (trifluoromethyl)-1- propene (382-21-8)	Hydrolysis	Decomposes rapidly in water, forming multiple Intermediates including fluorophosgene	Ultimately decomposes to the CO <sub>2</sub> radical anion and HF [18]	If fluorine is not a concern, HF can be neutralized with NaOH soln. If fluorine is a concern, then CaCO <sub>3</sub> can be used to form CaF <sub>2</sub> , a non-toxic precipitate that is disposed of as solid waste [19].
BZ: 3-Quinuclidinyl benzilate (6581-06-2)	Hydrolysis	BZ + water + acidic conditions (pH~13) – t <sub>1/2</sub> = 1.8 min. Rate of hydrolysis decreases as pH decreases and/or temperature increases [20].	3-quinuclidinol and benzilic acid	Neutralization and sanitary sewer disposal with a large excess of water. See additional treatment option for benzylic acid in Section 3.2.

### 3.2. Schedule 2B: Precursors

The chemicals listed under CWC Schedule 2B are those that may be used as a precursor or are of importance in the production for Schedule 1 or Schedule 2A chemicals. This section includes grouped dialkylated chemicals, followed by a list of alkyl groups in parentheses. For grouped chemicals the recommendations will include specific CAS numbers that meet those specific requirements and are listed in the Australia Group Export Control List: Chemical Weapons Precursors [16] as CWC Schedule 2B chemicals. The recommendation includes only chemicals for which treatment, decontamination, and/or waste disposal recommendations can be found.

**Table 3.2 Schedule 2B Precursors Treatment/Decontamination and Waste Disposal**

Chemical Name Chemical Group	CAS Number	Treatment Methods	Techniques/Methods	Products	Waste Disposal/Treatment
Methylphosphonyl dichloride	676-97-1	Hydrolysis/ Oxidation	Reacts violently with water. Further oxidation is likely.	HCl and methylphosphite, further oxidation to create phosphate/phosphoric acid	Alkyl methyl phosphonic acids can be oxidized to H <sub>3</sub> PO <sub>4</sub> , CO <sub>2</sub> , and H <sub>2</sub> O using excess H <sub>2</sub> O <sub>2</sub> , O <sub>2</sub> , and UV light [12].
Dimethyl methylphosphonate (DMMP)	756-79-6	Oxidation	Oxidized by OH radicals [17]	Phosphate/phosphoric acid	Neutralization and sanitary sewer disposal with a large excess of water
Dimethyl ethylphosphonate (DMEP)	6163-75-3	Oxidation	Oxidized by OH radicals [14]	Phosphate/phosphoric acid	Neutralization and sanitary sewer disposal with a large excess of water
Methylphosphinyl difluoride	753-59-3	Hydrolysis	Reacts with water [15]	HF and methyl phosphonic acid [15]	Neutralization and sanitary sewer disposal with a large excess of water  (See also methyl phosphonic acid below)
	993-13-5, 676-83-5, 676-97-1, 676-98-2	Hydrolysis/ Oxidation	Oxidized under supercritical conditions [21] [20]	Mineralized products [20]	Disposal after precipitation of calcium salts and evaporation of the water for recycle and burn [20]

Chemical Name Chemical Group	CAS Number	Treatment Methods	Techniques/Methods	Products	Waste Disposal/Treatment
 <p>To include:</p> <p>Methylphosphonic acid</p> <p>Methylphosphinyl dichloride</p> <p>Methylphosphonyl dichloride</p> <p>Methylphosphonothioic dichloride</p>			<p>Alkyl methyl phosphonic acids can be oxidized to H<sub>3</sub>PO<sub>4</sub>, CO<sub>2</sub>, and H<sub>2</sub>O using excess H<sub>2</sub>O<sub>2</sub>, O<sub>2</sub>, and UV light [12].</p> <p>Reacts violently with water. Further oxidation is likely [22].</p>	<p>H<sub>3</sub>PO<sub>4</sub>, CO<sub>2</sub>, and H<sub>2</sub>O [12].</p> <p>HCl and methylphosphite, further oxidation to create phosphate/phosphoric acid</p>	Neutralization and sanitary sewer disposal with a large excess of water
Methylphosphonyl difluoride	676-99-3	Hydrolysis/ Oxidation	Reacts with water and expected to react with oxidizing agents [23].	HF and methyl phosphonic acid [23]	
 <p>To Include:</p> <p>Ethylphosphinyl dichloride</p> <p>Ethylphosphonyl dichloride</p>	<p>1498-40-4</p> <p>1066-50-8</p>	Hydrolysis/ Oxidation	<p>Reacts violently with water. Further oxidation is likely.</p> <p>Acid chlorides react rapidly with potassium hydroxide [24]</p>	<p>HCl and ethylphosphite, further oxidation to create phosphate/phosphoric acid</p> <p>Mineralized products</p>	<p>Neutralization and sanitary sewer disposal with a large excess of water</p> <p>Disposal of salts after evaporation of the water for recycle.</p>
Diethyl methylphosphonite	15715-41-0	Hydrolysis/	Reacts with water [23] [25]	ethyl hydrogen methylphosphinate for 1:1 mole	

Chemical Name Chemical Group	CAS Number	Treatment Methods	Techniques/Methods	Products	Waste Disposal/Treatment
		Oxidation		ration and dihydrogen methylphosphinate and ethanol for 2:1 mole ratio [25]	(See alkyl methyl phosphonate above)
			Expected to react with oxidizing agents [23]		
Diethyl methylphosphonate (DEMP) Diethyl ethylphosphonate (DEEP)	683-08-9 78-38-6	Oxidation	Oxidized by OH radicals [14]	Phosphate/phosphoric acid	Neutralization and sanitary sewer disposal with a large excess of water
Arsenous Trichloride	7784-34-1	Hydrolysis	Reacts violently with water to form As(OH) <sub>3</sub> and HCl [25].	As(OH) <sub>3</sub> and HCl	Dissolve in acidified boiling water (1g As/100mL H <sub>2</sub> O with 6 drops conc. HCl). Add 0.2 g thioacetamide in 20 mL H <sub>2</sub> O per 1 g As. Boil for 20 min. and basify with 2M NaOH (8g NaOH(s) in 100mL H <sub>2</sub> O). As <sub>2</sub> S <sub>3</sub> precipitates and can be dried and packaged for disposal [26].
Benzilic Acid: 2,2-Diphenyl-2-hydroxyacetic acid	76-93-7	Acid-Based Neutralization or Electrophilic Substitution	Addition of a base to form ionic salt (i.e. NaHCO <sub>3</sub> or NH <sub>3</sub> ) or substitution of the hydrogen on the hydroxyl group with NaOH and an electrophile (i.e., RCOOH + NaOH + CH <sub>3</sub> I --> RCOOCH <sub>3</sub> + H <sub>2</sub> O + NaI, CH <sub>3</sub> <sup>+</sup> would be the electrophile) [21]	RCOOH + NaOH + CH <sub>3</sub> I --> RCOOCH <sub>3</sub> + H <sub>2</sub> O + NaI, CH <sub>3</sub> <sup>+</sup>	Neutralization and sanitary sewer disposal with a large excess of water.
Quinuclidin-3-ol	1619-34-7	Dehydration	Dehydration of alcohol (excess H <sub>2</sub> SO <sub>4</sub> & heat) [14]		UV and advanced oxidation treatment (UV-H <sub>2</sub> O <sub>2</sub> ), then disposed in sanitary sewer with a

Chemical Name Chemical Group	CAS Number	Treatment Methods	Techniques/Methods	Products	Waste Disposal/Treatment
					large excess of water. Quinuclidin-3-ol can be treated directly by modern sewage plant if dilute enough.
		Oxidation	Oxidation of alcohol to ketone ( $K_2Cr_2O_7$ + acidic conditions) [14]		
N,N-Dialkyl (Me, Et, n-Pr or i-Pr) aminoethyl-2-chlorides and corresponding protonated salts	41480-75-5, 4261-68-1	Oxidation	Reacts with strong acids, strong bases, strong oxidizing agents [27]	Hydrogen chloride, nitrogen oxides, carbon monoxide, carbon dioxide	Neutralization and sanitary sewer disposal with a large excess of water
N,N-Dialkyl (Me, Et, n-Pr or i-Pr) aminoethane-2-ols and corresponding protonated salts	(96-80-0)	Acid-Based Neutralization	Neutralizes acids in exothermic reactions to form salts plus water [19]		Disposal of salts after evaporation of the water for recycle.
N,N-Dimethylaminophosphoryl dichloride	(677-43-0)	Hydrolysis	Reacts with water [28]	Hydrochloride acid [28]	
Thiodiglycol (Bis(2-hydroxyethyl)sulfide)	111-48-8	Oxidation	Decontamination product of sulfur mustard (see sulfur mustard in section 2.1).	Oxidation to produce mustard sulfone (Bis(2-chloroethyl) sulfone) [5] [6].	Sanitary sewer disposal with a large excess of water [7].
		Biodegradation	Biodegradation reactor containing ordinary sewage sludge [7]	Carbon dioxide, water, and sulfate [7]	
Pinacolyl alcohol: 3,3-Dimethylbutan-2-ol	464-07-3	Dehydration	Dehydration of alcohol (excess $H_2SO_4$ & heat) [14]		UV and advanced oxidation treatment (UV- $H_2O_2$ ), then disposed in sanitary sewer with a large excess of water. Pinacolyl alcohol can be treated directly by

Chemical Name Chemical Group	CAS Number	Treatment Methods	Techniques/Methods	Products	Waste Disposal/Treatment
					modern sewage plant if dilute enough.
		Oxidation	Oxidation of alcohol to ketone ( $\text{K}_2\text{Cr}_2\text{O}_7$ + acidic conditions) [14]		



## 4. CWC SCHEDULE 3 CHEMICALS

The CWC Schedule 3 chemicals are often dual use chemicals that are readily available in the chemical industry. It is assumed that the decomposition and disposal reactions listed in this section still apply to small laboratory quantities. If large amounts of these chemicals are present, a different approach may be required (professional hazardous waste removal and treatment). This section is divided into 3A: Toxic Chemicals and 3B: Precursors.

### 4.1. Schedule 3A: Toxic Chemicals

The chemicals listed under CWC Schedule 3A possesses lethal, incapacitating toxicity, or other properties that might enable them to be used as a chemical weapon.

**Table 4.1 Schedule 3A Toxic Chemicals Treatment/Decontamination and Waste Disposal**

Chemical Name (CAS Number)	Treatment Method(s) Type	Techniques/Methods	Products	Waste Disposal/Treatment
Phosgene: Carbonyl dichloride (75-44-5)	Oxidation	Bubble phosgene gas through 10-20% NaOH concentration [26] [29].	Chloride salt and some CO <sub>2</sub>	Chloride salt solution can then be neutralized and disposed in sanitary sewer with a large excess of water
Cyanogen chloride (506-77-4)	Oxidation	CN-compounds can be oxidized to form cyanate. Examples: NaOCN, H <sub>2</sub> O <sub>2</sub> [30].	Cyanates	Disposed in sanitary sewer with a large excess of water. (~50:1 ratio) [26]
Hydrogen cyanide (74-90-8)	Oxidation	CN-compounds can be oxidized by H <sub>2</sub> O <sub>2</sub> [30]	Cyanates	Disposed in sanitary sewer with a large excess of water. (~50:1 ratio) [26]
	Oxidation/ Hydrolysis	NaOCl, oxidizes HCN to HOCN and forming CICH. CICH can then be hydrolyzed with NaOH solution, forming NaOCN (sodium cyanate)	Sodium cyanate	Disposed in sanitary sewer with a large excess of water. (~50:1 ratio) [26]
Chloropicrin: Trichloronitromethane (76-06-2)		Reacts steadily with alcoholic sodium sulfite solution	Methanetri- sulfonic acid	
		Ammonia [15]	Guanidine	Guanidine decomposes to CO <sub>2</sub> and Urea above 160 °C [21]—open burning may be a possible solution

## 4.2. Schedule 3B: Precursors

The chemicals listed under CWC Schedule 3B are those that may be used as precursors, are of importance in the production for CWC Schedule chemicals, or possess lethal, incapacitating toxicity or other properties that might enable them to be used as a chemical weapon.

**Table 4.2 Schedule 3B Precursors Treatment/Decontamination and Waste Disposal**

Chemical Name (CAS No.)	Treatment Method(s) Type	Techniques/Methods	Products	Waste Disposal/Treatment
Phosphorus oxychloride (10025-87-3)		Useful for reducing primary, secondary and tertiary alcohols to alkenes with pyridine and synthesizing alkylated phosphoric acids [31]		Small quantities: see Phosphorus pentachloride (10026-13-8)
	Hydrolysis	Hydrolyzes violently in water [32]	Phosphoric acid and HCl gas	Neutralization and sanitary sewer disposal with a large excess of water
Phosphorus trichloride		Reacts with primary alcohols forming phosphorous acid and alkyl chloride [33].	Phosphorous acid, alkyl chloride, and possibly HCl gas	Small quantities: see Phosphorus pentachloride (10026-13-8)
Phosphorus pentachloride (10026-13-8)		Reacts violently with water, carboxylic acids, and alcohols [33]	Phosphoric acid (in water), $\text{POCl}_3$ (carboxylic acids and alcohols) and HCl gas	Small quantities: In fume hood, cover with excess $\text{Na}_2\text{CO}_3$ or $\text{CaCO}_3$ add very slowly to a pail/bucket of cold water. Let stand for 24 hours, test pH, neutralize if necessary, and pour down drain with excess water ~50:1 ratio. $(\text{PCl}_5 + 4\text{H}_2\text{O} \rightarrow \text{NaOH} \rightarrow \text{H}_3\text{PO}_4 + 5\text{HCl} \rightarrow \text{Na}_3\text{PO}_4 + 5\text{NaCl})$ [14].
Trialkyl phosphites (121-45-9 and 122-52-1)	Oxidation	Trialkyl phosphites react with hydroperoxides [34]	Alcohol from hydroperoxide and a trialkyl phosphate	UV and advanced oxidation treatment ( $\text{UV-H}_2\text{O}_2$ ), then dispose in sanitary sewer with a large excess of water
		Hydrogen peroxide	Water and trialkyl phosphates	
Dialkyl phosphites (868-85-9 and 762-04-9)	Amines	Reactions of DMP with amines produce N-alkylammonium O-methylphosphites [35].	N-alkylammonium O-alkylphosphites	Dispose in sanitary sewer with a large excess of water
	Pudovik reaction	Pudovik reaction produces $\alpha$ -hydroxy phosphonates [36].	$\alpha$ -hydroxy phosphonates	
Sulfur monochloride (10025-67-9)	Hydrolysis	Hydrolysis: forms a variety of products,	HCl, $\text{H}_2\text{S}_2\text{O}_2$ , $\text{H}_2\text{S}_2\text{O}_3$ , and $\text{H}_2\text{S}$	Neutralize if necessary and dispose in sanitary

Chemical Name (CAS No.)	Treatment Method(s) Type	Techniques/Methods	Products	Waste Disposal/Treatment
		including HCl, H <sub>2</sub> S <sub>2</sub> O <sub>2</sub> , H <sub>2</sub> S <sub>2</sub> O <sub>3</sub> , and H <sub>2</sub> S [37] [38]		sewer with a large excess of water
Sulfur dichloride (10545-99-0)	Oxidation	Oxidized using SO <sub>3</sub> to form SO <sub>2</sub> and SOCl <sub>2</sub> [39]	SO <sub>2</sub> and SOCl <sub>2</sub>	Disposed in sanitary sewer with a large excess of water
Thionyl chloride (7719-09-7)		Reaction with 2° alcohols (Chlorinates) [40]	SO <sub>2</sub> and HCl	Dilute HCl can be neutralized with Na <sub>2</sub> CO <sub>3</sub> , CaCO <sub>3</sub> , or dilute NaOH soln disposed in sanitary sewer with a large excess of water [26].
Tertiary amines (139-87-7, 105-59-9, and 102-71-6)		Tertiary amines can be oxidized by H <sub>2</sub> O <sub>2</sub> (R <sub>3</sub> N + H <sub>2</sub> O <sub>2</sub> -> R <sub>3</sub> N <sup>(+)</sup> -O <sup>(-)</sup> + H <sub>2</sub> O) [41].	R <sub>3</sub> N <sup>(+)</sup> -O <sup>(-)</sup> + H <sub>2</sub> O	Disposed in sanitary sewer with a large excess of water

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## **5. CONCLUSIONS AND SUMMARY**

This report addresses the treatment and disposal of small quantities of hazardous chemicals related to the CWC. The report to assist them in reducing the risks related to the storage and disposal of these types of chemicals. Many of the reactions involve hydrolysis, oxidation, and neutralization. These techniques often produce other compounds that may need further treatment for disposal. The approach used in this report assumes that the nontoxic products of decomposition may be treated and diluted for acceptance into a modern sanitary sewer plant. There are of course products that could still be considered “hazardous waste,” and these should be collected with compatible wastes for appropriate disposal according to local and national regulations. The main objective for this report is to reduce the risks related to the storage and disposal of these types of chemicals. The lab should also have procedures for access control and inventory management in place to prevent the theft or misuse of these chemicals, and verification procedures for their destruction and disposal.

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