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#### **EDGEWOOD**

CHEMICAL BIOLOGICAL CENTER

U.S. ARMY SOLDIER AND BIOLOGICAL CHEMICAL COMMAND

ECBC-TR-294

# PHYSICAL PROPERTY DATA REVIEW OF SELECTED CHEMICAL AGENTS AND RELATED COMPOUNDS: UPDATING FIELD MANUAL 3-9 (FM 3-9)

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RESEARCH AND TECHNOLOGY DIRECTORATE

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The U.S. Army Chemical School, Doctrine Training Leadership Organization Materiel Soldier Division, is in the process of updating Field Manual 3-9 (FM 3-9), Potential Military Chemical/Biological Agents and Compounds. The manual will include the best available/most accurate physical properties and toxicological data along with their appropriate sources. The U.S. Army Edgewood Chemical Biological Center was tasked with critically reviewing the toxicological and physical property data for selected chemical agents and related compounds to be included in the update. This report contains the critically reviewed physical property data and the associated source references, where available.						
14. SUBJECT TERMS				15. NUMBER OF PAGES		
Physical Properties	Molecular Weight	Physical Stat				
Odor	Boiling Point	Freezing Poi Vapor Pressi		115		
Liquid Density	Vapor Density  Latent Heat of Vaporization	Flash Point	ui <del>C</del>			
Decomposition Temperature	Olumey					
Hydrolysis Products	Stability in Storage	Action on Me				
Chemical Agents	Choking Agents	Phosgene (C	(G)			
Diphosgene (DP)	Nerve Agents	Tabun (GA)				
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#### 14. SUBJECT TERMS (Continued).

Sarin (GB) Soman (GD) GF VX Vx **Blood Agents** Hydrogen Cyanide (AC) Cyanogen Chloride (CK) Arsine (SA) **Blister Agents** Levinstein Mustard (H) Distilled Mustard (HD) Nitrogen Mustard HN-1 HN-2 HN-3 HT Lewisite (L) HL Phenyldichloroarsine (PD) Ethyldichloroarsine (ED) Methyldichloroarsine (MD) Phosgene oxime (CX) Incapacitating Agent Quinuclidinyl benzilate (BZ) Respiratory Irritants Diphenylchloroarsine (DA) Diphenylcyanoarsine (DC) Adamsite (DM) Chlorine **Riot Control Agent** Capsaicin **Chemical Agent Precursors** DF QL OPA

Sulfur NE

Dimethylpolysulfides (NM)

#### **PREFACE**

The work described in this report was authorized under Sales Order No. 2RGD12. This work was started in February 2002 and completed in October 2002.

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This report has not been approved for public release.

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### PHYSICAL PROPERTY DATA REVIEW OF SELECTED CHEMICAL AGENTS AND RELATED COMPOUNDS: UPDATING FIELD MANUAL 3-9 (FM 3-9)

#### 1. INTRODUCTION

The U.S. Army Chemical School (CMLSC), Doctrine Training Leadership Organization Materiel Soldier (DTLOMS) Division has been tasked with revising Field Manual 3-9 (FM 3-9), Potential Military Chemical/Biological Agents and Compounds. As part of this effort, the Joint Requirements Office (JRO) formerly known as the Joint Service Integrations Group (JSIG) has funded the U.S. Army Soldier and Biological Chemical Command (SBCCOM)/ Edgewood Chemical Biological Center (ECBC) to critically review and assess selected toxicology and physical property data for the compounds to be included in the updated manual. This updated version of the Field Manual is being called Field Manual 3-11.9 (FM 3-11.9), Potential Military Chemical/Biological Agents and Compounds<sup>2</sup> and will supersede FM 3-9, 12 December 1990. A final coordinating draft of this manual (Final Coordinating Draft: Field Manual 3-11.9, Potential Military Chemical/Biological Agents and Compounds) is currently available on the U.S. Army Chemical School password protected AKO website.

One of the key features of the updated Field Manual will be the inclusion of data sources for relevant physical property data. This is pertinent information that the manual does not currently provide.

Results from this effort are being documented in two separate technical reports. The details from the toxicological review will be addressed in a technical report being prepared by the ECBC Toxicology Division, R&T Directorate.<sup>3</sup> The physical properties portion of the effort will be addressed in this report.

#### 2. OBJECTIVE

The purpose of this physical properties review is two-fold. It consists of identifying (1) the best physical property data available for the compounds of interest and (2) the sources for the data.

#### 2.1 Background.

Physical properties are essential tools used to predict the behavior of a given material. Measurement of these properties encompasses a wide variety of techniques and instrumentation. The prospective users of this physical property data will normally have a broad range of needs regarding how the data will be applied. Some applications of physical property

<sup>&</sup>lt;sup>1</sup> Potential Military Chemical/Biological Agents and Compounds; FM 3-9/NAVFAC P-467/AFR 355-7; Department of the Army, Navy, and Air Force: Washington, DC, 12 December 1990; UNCLASSIFIED Technical Manual.

<sup>&</sup>lt;sup>2</sup> Final Coordinating Draft: Potential Military Chemical/Biological Agents and Compounds; FM 3-11.9; Departments of the Army, Marine Corps, Navy, and Air Force: July 2003, unpublished data.

<sup>&</sup>lt;sup>3</sup> Reutter, S.; Miller, L. Jr.; Sommerville, D. *Review and Recommendations for Human Toxicity Estimates for FM 3-11.9*; ECBC-TR-349; U.S. Army Edgewood Chemical Biological Center: Aberdeen Proving Ground, MD, 2003; UNCLASSIFIED Report.

data are straightforward and require little knowledge about how the property was measured. For example, to determine whether or not a material is a liquid or solid at ambient temperature, the user does not need to know how the melting point was determined. However, other applications of property data may be more complex, requiring multiple properties and details regarding the specifics of the measurement. To properly address how much agent will remain on a given surface after 72 hr at ambient conditions would require knowledge of such properties as vapor pressure, volatility, surface tension, viscosity, wind speed, humidity, temperature fluctuations, initial purity of the agent, etc.

Physical property data provided without reference to the source can present problems. In the absence of a source, the user has no way of assessing the data to determine whether it is appropriate for the intended use. Important information such as data accuracy, sample purity, determining whether or not the value was measured or estimated, the experimental method, correct recording of the data, etc., are all vital pieces of information that the user can not obtain/verify if the source of the data is not identified. In many situations, physical property data can be used with little knowledge of how the data was generated, but proper application of some properties requires more detailed information.

Although the primary application of the FM 3-9 is to provide general information and technical data for planning, preparing, and conducting military operations, the wealth of information contained in the Field Manual makes it a valuable technical reference document for a variety of users with a wide range of data requirements. Inclusion of source references in the update increases the probability that the manual will meet the needs of a greater number of users. If the user simply needs to quickly locate the best value for a particular property, the updated Manual should contain that information. On the other hand, if the user needs the best value, but also requires some of the technical details such as method used, sample purity, etc., the updated Field Manual should provide the pathway to that information as well.

#### 2.2 <u>Compounds of Interest.</u>

This review encompasses many of the compounds currently provided in FM 3-9, 12 December 1990. These compounds include:

- Choking Agents
  - > Phosgene CG
  - > Diphosgene DP
- Nerve Agents
  - > Tabun GA
  - > Sarin GB
  - > Soman GD
  - ▶ GF
  - > VX
  - > Vx
- Blood Agents
  - > Hydrogen Cyanide AC
  - > Cyanogen Chloride CK
  - > Arsine SA

- Blister Agents
  - Distilled Mustard HD
  - Nitrogen Mustard HN-1
  - Nitrogen Mustard HN-2
  - Nitrogen Mustard HN-3
  - > HT (HD and Bis [2(2-chloroethylthio)ethyl]ether)
  - ➤ Lewisite L
  - Mustard-Lewisite Mixture HL
  - > Phenyldichloroarsine PD
  - > Ethyldichloroarsine ED
  - ➤ Methyldichloroarsine MD
  - ➤ Phosgene oxime (CX)
- Incapacitating Agent
  - Quinuclidinyl benzilate BZ
- Respiratory Irritants
  - > Diphenylchloroarsine DA
  - > Diphenylcyanoarsine DC
  - > Adamsite DM
  - > Chlorine
- Chemical Agent Precursors
  - > Methylphosphonic difluoride DF
  - > O-(2-Diisopropylaminoethyl)-O'-ethyl methylphosphonite QL
  - > Isopropylamine and Isopropyl Alcohol OPA
  - > Sulfur with a small amount of silica gel NE
  - > Dimethylpolysulfides (containing elemental sulfur) NM

In addition, the physical properties of the following two compounds have also been reviewed for inclusion in the updated Field Manual (FM 3-11.9).

- Blister Agent
  - Levinstein Mustard H
- Riot Control Agent
  - > Capsaicin

#### 2.3 Physical Properties of Interest.

The physical properties that have been requested for review in this task are the same properties listed in FM 3-9, December 1990. These physical properties are included below:

- Alternate Designations (for the agent)
- Chemical Name
- Synonyms
- CAS Registry Number
- RTECS Number
- Structural Formula

- Molecular Formula
- Molecular Weight
- Physical State
- Odor
- Boiling Point
- Freezing Point
- Liquid Density
- Vapor Density
- Vapor Pressure
- Volatility
- Latent Heat of Vaporization
- Flash Point
- Decomposition Temperature
- Solubility
- Rate of Hydrolysis
- Hydrolysis Products
- Stability in Storage
- Action on Metals or Other Materials

FM 3-9, 12 December 1990 includes detailed definitions of each physical property contained therein. A condensed version of these definitions along with several additional definitions and text are provided in Appendix A. Some of the property data being provided are in units different from those currently listed in FM 3-9, 12 December 1990. The unit conversions of these properties are given at the end of Appendix A.

#### 2.4 Approach.

The goal of this report was to provide the best value available for each compound of interest and to provide a source reference for the data (original source data, whenever possible). Although most of this data has been previously published in various compilations, generally these compilations do not include references. Therefore, compilations without references have not been cited as sources unless no other data source could be found.

Locating the references for this data was accomplished through numerous literature search strategies. The majority of these source documents are technical reports; however, articles from scientific journals, in-house laboratory notebooks, and peer-reviewed reference books were also used. A significant number of these source documents are quite old and are no longer in print or in some cases were improperly identified. As a result, many of these searches led to dead ends with source documents not being found.

Critical review of physical property data requires assessment of all the pertinent details associated with the measurement (sample purity, test method, instrumentation used, etc.). In many cases, all of these details were not available, so the assessment was made with the information available.

#### 3. RESULTS

#### 3.1 Organization of Data Tables.

The reviewed physical property data is presented in tables located in Appendixes B through I. Each table addresses one compound. Listed at the end of each table are the source references pertinent to the compound.

Because the tables contain such a large amount of physical property data, an effort was made to report the data in a consistent manner. Information contained in each table is provided in the same order that is presented in Section 2.3, Physical Properties of Interest. For properties that vary as a function of temperature, the data is provided at 25 and 0 °C, whenever possible. Any value reported outside the experimental range of the measurement is identified as "extrapolated." Reported values for properties such as volatility and latent heat of vaporization, which are calculated from vapor pressure equations, have been identified as "calculated." When information for a particular property cannot be located, it is identified as "data not available."

Since some of the properties being presented vary with temperature, the goal was to report these properties at both 25 and 0 °C for consistency. (Where low boiling points or high melting points preclude reporting certain properties at these specific temperatures, appropriate alternate temperatures were selected.) However, literature data was not always available at these specific temperatures. In order to report the property data for those compounds whose source references do not provide measured data at the selected temperatures, values had to be calculated using appropriate equations. For density, this was straightforward and simply involved fitting the available data to a linear equation.

However, for vapor pressure (and volatility and heat of vaporization which are calculated from vapor pressure), the process was somewhat more complicated. Typically vapor pressure data is expressed as a function of temperature using either the Clausius-Clapeyron or Antoine equation. The primary difference between the two equations involves the heat of vaporization of the compound (the slope of the vapor pressure curve). Derivation of the Clausius-Clapeyron equation assumes a constant heat of vaporization over the applicable temperature range (straight vapor pressure vs. temperature plot) while the Antoine equation assumes heat of vaporization changes with temperature (slight curvature of vapor pressure vs. temperature plot). For narrow temperature ranges, the slope of the vapor pressure curve is essentially straight and the Clausius-Clapeyron equation adequately reflects the vapor pressure/temperature relationship. However, experimental vapor pressure data covering a wide temperature range generally shows a slight curvature that is more accurately reflected by the Antoine equation. The Antoine equation is preferred for expressing vapor pressure as a function of temperature and extrapolating to temperatures beyond the experimental range.<sup>4</sup>

Vapor pressure date found in the literature is often reported in various formats that can range from a single boiling point to an extensive experimental data set with an accompanying equation. For purposes of this report, where only data points but no vapor pressure equation was reported in the literature, the data was fitted to an Antoine equation from which the vapor pressure at 0 and 25 °C as well as volatility and heat of vaporization were calculated. If a Clausius-Clapeyron equation was reported but the equation did not cover the

<sup>&</sup>lt;sup>4</sup> Thomson, G.W. The Antoine Equation for Vapor Pressure Data. Chem Rev. 1946, 38, pp 1-39.

desired temperature range (would require extrapolation), the values were refitted to an Antoine equation. Where a literature equation (either Clausius-Clapeyron or Antoine) was available that covered the desired temperature range, the equation was used as reported and no refit was necessary. For the heats of vaporization reported in these tables, a specific temperature is not listed where this property was calculated from a Clausius-Clapeyron equation but is specified where an Antoine fit had been used.

In terms of usage and application, vapor pressure data is critical for assessing agent persistency. This is a relative term describing the duration of effectiveness of a material that is useful for comparing the characteristics and behavior of different compounds. While vapor pressure is the primary physical property used for determining agent persistency, other parameters including humidity, wind speed, mode of dissemination, and stability are also taken into account. As a guide for ranking the persistency of each compound in a given category (i.e. Choking, Nerve, Blister, etc.), a plot of their vapor pressure is provided at the end of each appendix. The plots also include the vapor pressure as a relative comparison.

#### 3.2 Discussion.

Most of the data presented here as the best available is the same information published in FM 3-9, 12 December 1990. New data has been provided, where available, and corrections have been made, where necessary. In many cases, once fundamental physical property data was collected on some of these agents, no additional measurements or redeterminations were made. In general where new data is available, the additional measurements were made to supplement rather than replace the original data (i.e., to extend the experimental temperature range to predict agent behavior over a wider range of environmental conditions). Original property measurements are rarely repeated unless some conflict or inconsistency is identified.

With this in mind, the user is reminded that the data contained herein is presented as the best currently available. In some cases, updated instrumentation or improved techniques for sample characterization may improve the accuracy of some of these values. These situations are viewed as the exceptions rather than the rule. In most situations, a new measurement would increase the precision of the existing measured data (i.e., add more decimal places). In general, "vintage" data is considered accurate until proven otherwise.

#### CONCLUSION

The U.S. Army Chemical School (CMLSC), Doctrine Training Leadership Organization Materiel Soldier (DTLOMS) Division, is in the process of updating Field Manual 3-9 (FM 3-9), Potential Military Chemical/Biological Agents and Compounds to include the best available/most accurate physical properties and toxicological data along with their appropriate sources. The Edgewood Chemical Biological Center (ECBC) was tasked with critically reviewing the toxicological and physical property data for selected chemical agents and related compounds to be included in the update. This report contains the critically reviewed physical property data and the associated source references, where available.

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#### APPENDIX A

#### **DEFINITIONS OF SELECTED PHYSICAL PROPERTIES**

A. <u>Molecular Weight</u>. Molecular weight (MW) is the value represented by the sum of the atomic weights of all the atoms in the molecule.<sup>1</sup> For example, the MW of ethyldichloroarsine, C<sub>2</sub>H<sub>5</sub>AsCl<sub>2</sub>, is as follows:

C (atomic weight = 12.011) X 2 = 24.02 H (atomic weight = 1.0079) X 5 = 5.04 As (atomic weight = 74.9216) X 1 = 74.92 CI (atomic weight = 35.453) X 2 = 70.91 MW = 174.89

- B. <u>Physical State</u>. Chemical agents and military chemical compounds may exist as solids, liquids, or gases. To a certain extent the state in which an agent normally exists determines its use, duration of effectiveness, and physiological action. It also determines the type of munitions used for its dissemination.
- C. Odor. A detectable sensation that results from adequate stimulation of the olfactory gland .2
- D. <u>Boiling Point</u>. Boiling point is the temperature at which the transition from a liquid to the gaseous phase occurs in a pure substance at fixed pressure.<sup>3</sup>
- E. <u>Melting Point</u>. Melting point is the temperature at which a solid changes to a liquid.<sup>1</sup>
- F. <u>Freezing Point</u>. Freezing point is the temperature at which a liquid changes to a solid. It is generally equivalent to the melting point.<sup>1</sup>

**Note:** Some liquids can be cooled well below their freezing temperatures and still remain in a liquid state. This extended form of the liquid physical state is called supercooling. Supercooled liquids are unstable and can crystallize spontaneously. Constant agitation and/or the use of seed crystals can sometimes prevent or reduce the amount of supercooling that occurs. However, many chemical agents experience some degree of supercooling, especially the G –agents. Due to the potential for supercooling, freezing point values should be used with caution. Whenever possible, melting point values should be used because they are more thermodynamically reproducible than freezing point.<sup>4</sup>

G. <u>Density (Liquid/Solid)</u>. The density is the mass of unit volume of the substance. Because volume varies with temperature, a specific temperature should be given. Density of a liquid is the usually given as grams per milliliter or cubic centimeter (g/mL or g/cm³). 1

**Note:** Solid density can be further specified as bulk (or apparent) density or crystalline (or true) density. Both properties describe the mass per unit volume of a solid material. Bulk density includes the volume of the voids, pores or empty

spaces between particles whereas crystalline density includes only the volume occupied by the material itself.<sup>5</sup>

Linear Regression Equation:

 $d_t = a + bt$ 

where

 $d_t = density in (g/mL)$ 

a = y-intercept

b = slope

t = temperature in (°C)

- H. <u>Vapor Density</u>. Vapor density is the ratio of the density of any gas or vapor to the density of air, under the same conditions of temperature and pressure. To calculate the vapor density, divide the MW of the compound of interest by 29 (the average MW of air). It is a measure of how heavy the vapor is in relation to the same volume of air.
- I. <u>Vapor Pressure</u>. Vapor pressure is the pressure exerted by a vapor when a state of equilibrium exists between the vapor and its liquid (or solid) state. It is the pressure in a closed space above a substance when no other gas is present. Vapor pressure varies with temperature so the temperature should be reported with the vapor pressure.

Antoine Equation:7

 $\log P_{torr} = A - B/(C+t)$ 

where

P = Vapor pressure in torr A.B.C = Antoine constants

t = Temperature in °C

J. <u>Volatility</u>. Volatility is the concentration of saturated vapor as calculated from the vapor pressure and the absolute temperature. Volatility is expressed as milligrams of vapor per cubic meter (mg/m³). It is calculated numerically by an equation derived from the perfect gas law.<sup>8</sup>

 $V = \frac{16034 \times MW \times VP}{T}$ 

where

V = Volatility

MW = Molecular weight

VP = Vapor pressure in torr at a specified temperature

 $T = Kelvin temperature = (^{\circ}C + 273.15)$ 

K. <u>Latent Heat of Vaporization</u>. The latent heat of vaporization is the heat required to change 1 g of liquid into vapor without a change in temperature. That is, it is the total heat in calories that disappears at any given temperature when 1 g of liquid evaporates under an external pressure of one atmosphere.<sup>4</sup>

Latent Heat of Vaporization Equation:8

$$\Delta H_v = \frac{\log_e 10 \text{ RBT}^2}{(C + t)^2}$$

where

 $\Delta H_v$  = Enthalpy of vaporization

T = Kelvin temperature = ( $^{\circ}$ C + 273.15)

R = Ideal gas law constant (1.987 cal K<sup>-1</sup> mol<sup>-1</sup>)

B,C = Vapor pressure constants (from Antoine or Clausius-

Clapeyron fit)

t = Temperature in °C

L. <u>Flash Point</u>. The flash point is the lowest temperature at which vapors from a liquid or volatile solid will ignite upon application of an ignition source under specified conditions; test conditions can be either open or closed cup.<sup>3</sup>

- M. <u>Decomposition Temperature</u>. The decomposition temperature is that at which a chemical breaks down into two or more substances.<sup>4</sup>
- N. <u>Solubility</u>. The solubility of a solute is the quantity that will dissolve in a given amount of solvent to produce a saturated solution.<sup>1</sup>
- O. <u>Hydrolysis</u>. Hydrolysis is the reaction of a compound with water whereby decomposition of the substance occurs.<sup>1</sup> New substances (hydrolysis products) form when a compound reacts with water.
- P. Half –Life of a Reaction  $(t_{1/2})$ . The time required for half of the original concentration of the limiting reactant to be consumed.<sup>4</sup>
- Q. <u>Stability in Storage</u>. Stability in storage determines the practical usefulness of a compound. If a compound decomposes in storage, it will have little military operational value. The addition of stabilizers will typically slow down decomposition and polymerization in storage.
- R. <u>Action on Metals, Plastics, Fabrics, and Paint</u>. The action between a given compound and different materials. Depending on their activity, some chemicals can react with and degrade materials they contact. Chemical agent-resistant coatings can minimize this effect.

#### **CONVERSION TABLE**

- 1. Liquid Density --- 1 gram per milliliter (g/mL) is equivalent to 1 gram per cubic centimeter (g/cc or g/cm³)
- 2. Vapor Pressure --- 1 torr is equivalent to 1 millimeter of mercury (mm Hg)
- 3. Latent Heat of Vaporization --- To convert from kcal/mol to cal/g, multiply by 1000 and divide by the molecular weight

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#### **APPENDIX B**

#### **CHOKING AGENTS**

#### Table B-1: Phosgene (CG)

Alternate Designations: Collongite (French); Zusatz (German); Green Cross (German); D –gas (German); Fosgeen (Dutch); Fosgen (Polish); Fosgene (Italian); Phosgen (German); NCI-C60219

Chemical Name: Carbonyl chloride

Synonyms: Carbon oxychloride; Carbon dichloride oxide; Carbone (oxychlorure de) (French); Carbonic chloride; Carbonio (ossiclorurodi) (Italian); Carbonylchlorid (German); Carbonyl dichloride; Chloroformy chloride; Koolstofoxychloride (Dutch)

Chemical Abstract Service Registry Number: 75-44-5

Registry of Toxic Effects of Chemical Substances No.: SY5600000

#### **Physical and Chemical Properties**

Structural Formula:

o=c\_c

Molecular Formula: COCl<sub>2</sub>
Molecular Weight: 98 92

Molecular Weight: 98.92	
Physical State	Colorless gas that is readily liquefied (1)
Odor	Musty hay, or rotting fruit (2)
Boiling Point	7.8 °C (3,4)
Freezing Point	-128 °C (melting point) (5)
Liquid Density (g/mL)	Liquefied phosgene 1.360 @ 25 °C; 1.402 @ 7.8 °C; 1.420 @ 0 °C (6)
Vapor Density (relative to air)	3.4 (calculated)
Vapor Pressure (torr)	$1.40 \times 10^3$ @ 25 °C; $7.60 \times 10^2$ @ $7.8$ °C; $5.60 \times 10^2$ @ 0 °C (3,4)
Volatility (mg/m³)	$7.46 \times 10^{6}$ @ $25$ °C; $4.29 \times 10^{6}$ @ $7.8$ °C; $3.53 \times 10^{6}$ @ $0$ °C; (calculated from vapor pressure) (3,4)
Latent Heat of Vaporization (kcal/mol)	5.92 @ 25 °C; 5.95 @ 7.8 °C; 5.96 @ 0 °C (calculated from vapor pressure) (3,4)
Flash Point	Nonflammable (1)
Decomposition Temperature	Complete @ 800 °C (7)
Solubility	Limited in water; (8) Miscible with common organic solvents, petroleum, and lubricating oil (9,10)
Rate of Hydrolysis	t $_{1/2}$ = 0.25 sec. @ 13 °C; Does not react quickly with water vapor but it immediately reacts with liquid water to yield carbon dioxide and hydrochloric acid. (8,11)
Hydrolysis Products	Hydrochloric acid and carbon dioxide (9)
Stability in Storage	Stable in steel containers @ ambient temperatures for at least one year if CG is dry. Stability decreases at elevated temperatures. (12)
Action on Metals or Other Materials	None when CG is dry; acidic and corrosive when moist. (13)

## Table B-1: Phosgene (CG) (Continued)

<sup>&</sup>lt;sup>1</sup> Matheson Gas Data Book, 4th ed., The Matheson Company, Inc.: New Jersey, 1966; p 411.

<sup>&</sup>lt;sup>2</sup> Franke, S. *Manual of Military Chemistry Volume I- Chemistry of Chemical Warfare Agents*; ACSI-J-3890; Chemie der Kampfstoffe, East Berlin, 1968, UNCLASSIFIED Technical Manual (AD-849866).

<sup>&</sup>lt;sup>3</sup> Abercrombie, P., Edgewood Chemical Biological Center Notebook # NB 98-0079 p 7 (U).

<sup>&</sup>lt;sup>4</sup> Germann, A.F.O.; Taylor, Q.W. The Critical Constants and Vapor Tension of Phosgene. *J. Amer. Chem. Soc.* **1928**, *48*(5), pp. 1154 -1159.

<sup>&</sup>lt;sup>5</sup> Giauque, W. F.; Jones, W.M. Carbonyl Chloride. Entropy. Heat Capacity. Vapor Pressure. Heats of Fusion and Vaporization. Comments on Solid Sulfur Dioxide Structures. *J. Amer. Chem. Soc.* **1948**, *70*, p. 120.

<sup>&</sup>lt;sup>6</sup> Davies, C. N. The Density and Thermal Expansion of Liquid Phosgene. J. Chem. Phys. 1946, 14, p. 48.

<sup>&</sup>lt;sup>7</sup> Bodenstein, M.; Durant, G. Die Dissociation des Kohlenoxychlorids. Z. Physik. Chem. 1908, 61, p. 437.

<sup>&</sup>lt;sup>8</sup> Hall, R.W. An Investigation on the Solubility and Rate of Hydrolysis of Phosgene in Water; Porton Report 2663; Chemical Defence Experimental Establishment: Porton, England, 1944, UNCLASSIFIED Report (AD-E482245).

<sup>&</sup>lt;sup>9</sup> Atkinson, R.H.; Heycock, C.T.; Pope, W.J. The Preparation and Physical Properties of Carbonyl Chloride. *J. Chem. Soc.* **1920**, *117*, pp 1410-1426.

<sup>&</sup>lt;sup>10</sup> Baskerville, C.; Cohen, P.W. Solvents for Phosgene. J. Ind. Eng. Chem. 1921, 13, p 333.

<sup>&</sup>lt;sup>11</sup> Properties of War Gases Volume III: Vomiting & Choking Gases & Lacrimators (U); ETF 100-41/Vol-3; Chemical Corps Board: Army Chemical Center, MD, 1944, CONFIDENTIAL Report (AD-108458).

<sup>&</sup>lt;sup>12</sup> Henley, F.M. Surveillance Tests on 75 mm Steel Gas Shell Extending Over a Period of One Year; EACD 11; Chemical Warfare Service: Edgewood Arsenal, MD, 1920, UNCLASSIFIED Report (AD-B959731).

<sup>&</sup>lt;sup>13</sup> Patten, H.E.; Bouder, N.M. *Chemical Properties of Phosgene*; EACD 124; Chemical Warfare Service: Edgewood Arsenal, MD, 1923, UNCLASSIFIED Report (AD-B955133).

## Table B-2: Diphosgene (DP)

Alternate Designations: Difosgene; Superpalite (British); Perstoff (German); Surpalite(French); Green Cross (German)

Chemical Name: Trichloromethyl chloroformate

Synonyms: Trichloromethyl chlorocarbonic acid ester; Chloroformic acid trichloromethyl ester; Trichloromethyl chlorocarbonate; Trichloromethyl carbonochloridate; Formic acid, chloro-, trichloromethyl

ester; Carboncohloridic acid trichloromethyl ester

Chemical Abstract Service Registry Number: 503-38-8

Registry of Toxic Effects of Chemical Substances Number: LQ7350000

### **Physical and Chemical Properties**

#### Structural Formula:

Molecular Formula: C<sub>2</sub>Cl<sub>4</sub>O<sub>2</sub> Molecular Weight: 197.83

Wickerdia Weight. 107.00	
Physical State	Colorless oily liquid (1)
Odor	Musty hay (2)
Boiling Point	127 °C (3,4)
Freezing Point	-57 °C (melting point) (2)
Liquid Density (g/mL)	Munitions grade: 1.656 @ 20 °C; 1.687@ 0 °C (2)
Vapor Density (relative to air)	6.8 (calculated)
Vapor Pressure (torr)	4.41 @ 20 °C; 9.14 x 10 <sup>-1</sup> @ 0 °C (3,4)
Volatility (mg/m³)	4.77 x 10 <sup>4</sup> @ 20 °C; 1.06 x 10 <sup>4</sup> @ 0 °C (calculated from vapor pressure) (3,4)
Latent Heat of Vaporization (kcal/mol)	12.2 @ 20 °C; 12.8 @ 0 °C (calculated from vapor pressure) (3,4)
Flash Point	None (5)
Decomposition Temperature	300 °C to 350 °C (yields two molecules of CG) (1)
Solubility	Solubility in water is 44.6 g DP/L @ 20 °C (6); Readily soluble in common organic solvents (2)
Rate of Hydrolysis	Slow @ ambient temperature and fairly rapid @ 100 °C (1)
Hydrolysis Products	Hydrogen chloride (HCl) and carbon dioxide (1)
Stability in Storage	Unstable; converts to CG (1)
Action on Metals or Other Materials	Metals act as catalyzers in conversion to CG. (1,2) Also attacks rubber, cork, (2,4) and cement (2)

# Table B-2: Diphosgene (DP) (Continued)

<sup>&</sup>lt;sup>1</sup> Hood, H.P.; Murdock, H.R. Superpalite. J. Phys. Chem. 1919, 23, p 498.

<sup>&</sup>lt;sup>2</sup> Potts, A.M. *The Physical and Chemical Properties of Phosgene and Diphosgene*; OEMCMR-114; 1945, UNCLASSIFIED Report (AD-E477810).

<sup>&</sup>lt;sup>3</sup> Abercrombie, P., Edgewood Chemical Biological Center Notebook # NB 98-0079 p 34 (U).

<sup>&</sup>lt;sup>4</sup> Herbst, V.H. Uber die Fluchtigkeit und Vernebelung einer Reihe organischer Stoffe. Kolloid Beihefte 1927, 23, p 330.

<sup>&</sup>lt;sup>5</sup> Military Chemistry and Chemical Agents; TM 3-215/AFM 355-7; Departments of the Army and the Air Force: Washington, DC, December 1963; UNCLASSIFIED Technical Manual (AD-A292141).

<sup>&</sup>lt;sup>6</sup> Carter, R.H.; Knight, H.C. Fundamental Study of Toxicity: Solubility of Certain Toxics in Water and in Olive Oil; EACD 445; Chemical Warfare Service: Edgewood Arsenal, MD, 1928, UNCLASSIFIED Report (AD-B955216).

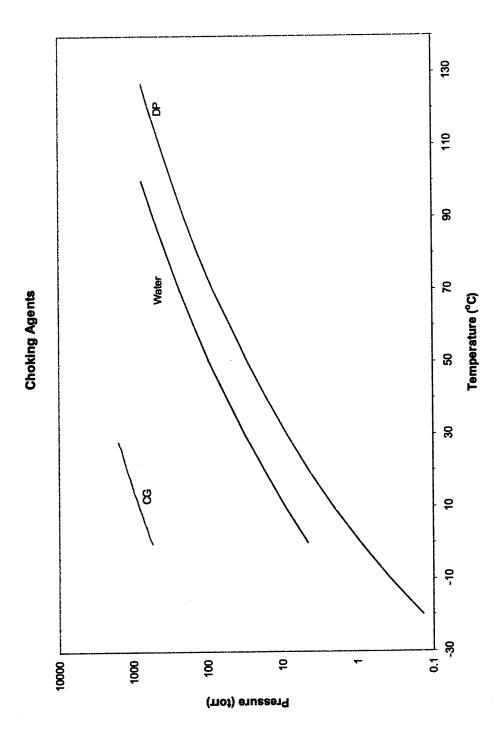


Figure B: Vapor Pressure of Choking Agents

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#### APPENDIX C

#### **NERVE AGENTS**

### Table C-1: Tabun (GA)

Alternate Designations: EA 1205; Le-100 (German), T-83 (German); MCE; FM-511; T-2104 (British); TL-1578 (UCTL); Trilon 83 (German); T 83 (German); Gelan I (German); Taboon A

Chemical Name: Ethyl N, N-dimethylphosphoroamidocyanidate

Synonyms: Ethyl dimethylamidocyanophosphate; Dimethylaminoethoxyphosphoryl cyanide; Dimethylaminocyanophosphoric acid ethyl ester; Cyanodimethylaminoethoxyphosphine; Dmethylaminocyanoethoxyphosphine oxide; Ethyl dimethylaminocyanophosphonate

Phosphoramidocyanidic acid, dimethyl-, ethyl ester; Dimethylamidoethoxyphosphoryl cyanide;

Dimethylaminocyanphosphorsaeureaethylester (German); Dimethylphosphoramidocyanidic acid, ethyl ester; Ethyl dimethylphosphoramidocyanidate; Ethylester-dimethylamid kyseliny kyanfosfonove (Czech)

Chemical Abstract Service Registry Number: 77-81-6

Registry of Toxic Effects of Chemical Substances Number: TB4550000

## **Physical and Chemical Properties**

#### Structural Formula:

Molecular Formula: C<sub>5</sub>H<sub>11</sub>N<sub>2</sub>O<sub>2</sub>P Molecular Weight: 162.13

Molecular VVelgrit. 102.13	
Physical State	Colorless to brown liquid (1)
Odor	Faintly fruity; none when pure (2)
Boiling Point	248 °C (extrapolated) (3-7)
Freezing Point	-50 °C <b>(5)</b>
Liquid Density (g/mL)	1.0756 @ 25 °C; 1.0999 @ 0 °C (3)
Vapor Density (relative to air)	5.6 (calculated)
Vapor Pressure (torr)	5.70 x 10 <sup>-2</sup> @ 25 °C; 4.75 x 10 <sup>-3</sup> @ 0 °C (extrapolated) (3-7)
Volatility (mg/m³)	4.97 x 10 <sup>2</sup> @ 25 °C; 4.52 x 10 <sup>1</sup> @ 0 °C (calculated from vapor pressure) (3-7)
Latent Heat of Vaporization (kcal/mol)	15.5 @ 25 °C; 16.7 @ 0 °C (calculated from vapor pressure) (3-7)
Flash Point	78 °C (closed cup) (8)
Decomposition Temperature	Decomposes completely @ 150 °C after about 3 to 3 1/4 hr (9)
Solubility	Solubility in water is approximately 7.2 g GA/100 g @ 20 °C and 9.8 g GA/100 g @ 0 °C (3); Readily soluble in common organic solvents (2)
Rate of Hydrolysis	$t_{1/2}$ = 8.5 hr @ 20 °C and pH 7 (10) Slow in water but fairly rapid with strong acids and alkalis with self-buffering @ pH 4 to 5 (1); autocatalytic below pH 4 (11)
Hydrolysis Products	Hydrogen cyanide, dimethylaminocyanophosphonic acid, and other products (10)

## Table C-1: Tabun (GA) (Continued)

Stability in Storage	When stabilized with 5% chlorobenzene, GA can be stored in steel containers for several years @ ambient temperatures. The degree of stability decreases @ elevated temperatures with decomposition occurring within 6 months @ 50 °C and 3 months @ 65 °C. (12)
Action on Metals or Other Materials	Corrosion rate of steel on crude GA with 5 to 20% chlorobenzene is 0.000034 in./month @ 65 °C (12)

<sup>&</sup>lt;sup>1</sup>Witten, B. *The Hydrolysis of MCE;* Technical Division Memorandum Report 1121 (TDMR 1121); U.S. Army Chemical Research and Development Laboratories: Army Chemical Center, MD, 1945, UNCLASSIFIED Report (AD-B964102).

<sup>&</sup>lt;sup>2</sup>Welchman, R.M.A. *Preliminary Report on the Potential Value of Nerve Gases as C.W. Agents;* Porton Report No. 2747 (PR 2747); Chemical Defence Experimental Establishment: Porton, England, 1947, UNCLASSIFIED Report (AD-E470188).

<sup>&</sup>lt;sup>3</sup> Samuel, J.B.; Penski, E.C.; Callahan, J.J. *Physical Properties of Standard Agents, Candidate Agents, and Related Compounds at Several Temperatures (U);* ARCSL-SP-83015; U.S. Army Armament Research and Development Command: Aberdeen Proving Ground, MD, 1983, UNCLASSIFIED Report (AD-C033491).

<sup>&</sup>lt;sup>4</sup> Abercrombie, P., Edgewood Chemical Biological Center Notebook # NB 98-0079 p 36 (U).

<sup>&</sup>lt;sup>5</sup> Harris, B.L. *Physical Constants of MCE;* Technical Division Memorandum Report 1094; U.S. Army Chemical Research and Development Laboratories: Army Chemical Center, MD, 1945, UNCLASSIFIED Report (AD-B964103).

<sup>&</sup>lt;sup>6</sup> Balson, E.W. *Determination of the Vapour Pressure of T.2104*; A.3804/3; Military Intelligence Division, Chemical Defence Experimental Establishment: Porton, England, April 1945, UNCLASSIFIED Report.

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<sup>&</sup>lt;sup>8</sup>Walpole, J.L. Determination of the Flash Points of GA and GB; Porton Technical Paper No. 45 (PTP 45); Chemical Defence Experimental Establishment: Porton, England, 1948, UNCLASSIFIED Report (AD-E481350).

<sup>&</sup>lt;sup>9</sup> Miller, C.E. *Thermal Studies on MCE;* Technical Division Memorandum Report 1132; U.S. Army Chemical Research and Development Laboratories; Army Chemical Center, MD, 1945, UNCLASSIFIED Report (AD-B964104).

<sup>&</sup>lt;sup>10</sup> Marsh, D.J.; Williams, L.T.D.; Liddell, H.F. *Kinetics of the Hydrolysis of Ethyl Dimethylamino Cyanophosphonate (and certain other related compounds) in Water*; Proton Technical Paper No. 85 (PTP-85); Chemical Defense Experimental Establishment: Porton, England, 1948, UNCLASSIFIED Report (AD-E481381).

<sup>&</sup>lt;sup>11</sup>Clark, D.N. Review of Reactions of Chemical Agents in Water, Final Report to U.S. Army Biomedical Research and Development Laboratory; Battelle: Columbus, OH, 1989, UNCLASSIFIED Report (AD-A213287).

<sup>&</sup>lt;sup>12</sup> Harris, B.L.; Macy, R. Storage Stability of German GA in Uncoated and Lacquered 75mm Shell at 50 °C and 65 °C. Corrosion Rate of Steel by GA at 65 °C; Technical Division Memorandum Report 1299; U.S. Army Chemical Research and Development Laboratories: Army Chemical Center, MD, 1946, UNCLASSIFIED Report (AD-B964902).

### Table C-2: Sarin (GB)

Alternate Designations: EA 1208; T-144 (German); Trilon 144 (German); Trilon 46 (German); T 46 German); TL-1618 (UCTL); T-2106 (British); MFI; IMPF; Sarin II

Chemical Name: Isopropyl methylphosphonofluoridate

Synonyms: Fluorisoproopoxymethylphosphine oxide; Isopropyl methylfluorophosphate; Isopropyl methanefluorophosphonate; Isopropoxymethylphosphoryl fluoride; Propoxyl-(2)-methylphosphoryl fluoride; Phosphonofluoridic acid, methyl-, isopropyl ester; Isopropylester kyseliny methylfluorfosfonove (Czech); O-Isopropyl methylphosphonofluoridate; Isopropyl-methylphosphoryl fluoride; Methylphosphonofluoridic acid isopropyl ester; Methylphosphonofluoridic acid 1-methylethyl ester; Phosphine oxide, fluoroisopropoxymethyl-; Phosphoric acid, methylfluoro-, isopropyl ester; Methylfluorphosphorsaeureisopropylester (German)

Chemical Abstract Service Registry Number: 107-44-8

Registry of Toxic Effects of Chemical Substances Number: TA8400000

#### **Physical and Chemical Properties**

Structural Formula:

Molecular Formula: C<sub>4</sub>H<sub>10</sub>FO<sub>2</sub>P

Molecular Weight: 140.09	
Physical State	Colorless liquid (1)
Odor	None when pure (2)
Boiling Point	150°C (extrapolated) (3)
Freezing Point	-56°C ( <b>3-5</b> )
Liquid Density (g/mL)	Pure: 1.0887 @ 25 °C; 1.1182 @ 0 °C (extrapolated) (6)
	Munitions grade: 1.0964 @ 25 °C; 1.1255 @ 0 °C (extrapolated) (6)
Vapor Density (relative to air)	4.8 (calculated)
Vapor Pressure (torr)	2.48 x 10° @ 25 °C; 4.10 x 10 <sup>-1</sup> @ 0 °C (3)
Volatility (mg/m³)	1.87 x 10 <sup>4</sup> @ 25 °C; 3.37 x 10 <sup>3</sup> @ 0 °C (calculated from vapor pressure) (3)
Latent Heat of Vaporization (kcal/mol)	11.6 @ 25 °C; 11.7 @ 0 °C (calculated from vapor pressure) (3)
Flash Point	Nonflammable (7)
Decomposition Temperature	Complete decomposition occurs within 2 1/2 hr @ 150 °C (8)
Solubility	Completely miscible with water and common organic solvents (1,2)
Rate of Hydrolysis	Varies with pH and temperature; At 20 °C t <sub>1/2</sub> = 27 min @ pH 1;
	$t_{1/2}$ = 3 1/2 hr @ pH 2; $t_{1/2}$ = 80 hr @ pH 7; $t_{1/2}$ = 5.4 min @ pH 10; and $t_{1/2}$ = 0.6 min @ pH 11 (9)
Hydrolysis Products	Under acidic conditions, hydrogen fluoride (HF) and isopropyl methylphosphonic acid (IMPA) are formed which further hydrolyze to produce methylphosphonic acid (MPA) and isopropanol. Under alkaline conditions, methylfluorophosphonic acid (MFPA) and isopropyl alcohol are initially formed which further hydrolyze to produce (MPA) and HF. (10)

## Table C-2: Sarin (GB) (Continued)

Stability in Storage	GB stabilized with tributylamine can be stored in steel containers for at least 5 to 10 years @ ambient temperature. At elevated temperatures up to 71 °C storage life decreases slightly. (11)
Action on Metals or Other Materials	At 71 °C, slightly corrosive on steel, copper, brass, inconel, K-monel, and lead as well as slight to severe amounts of corrosion on aluminum, depending on the type. (12)

<sup>&</sup>lt;sup>1</sup> Franke, S. *Manual of Military Chemistry Volume I- Chemistry of Chemical Warfare Agents;* ACSI-J-3890; Chemie der Kampfstoffe, East Berlin, 1968, UNCLASSIFIED Technical Manual (AD-849866).

<sup>&</sup>lt;sup>2</sup>Welchman, R.M.A. *Preliminary Report on the Potential Value of Nerve Gases as C.W. Agents;* Porton Report No. 2747 (PR 2747); Chemical Defence Experimental Establishment: Porton, England, 1947, UNCLASSIFIED Report (AD-E470188).

<sup>&</sup>lt;sup>3</sup> Penski, Elwin C. *The Properties of 2-Propyl Methylfluorophosphonate (GB) I. Vapor Pressure Data Review and Analysis;* ERDEC-TR-166; U.S. Army Chemical and Biological Defense Command: Aberdeen Proving Ground, MD, 1994, UNCLASSIED Report (AD-B187225).

<sup>&</sup>lt;sup>4</sup> Zeffert, B.M.; Tannenbaum, H.; Coulter, P.B. Slow Fractional Crystallization of GB; CRLR 2; U.S. Army Chemical and Radiological Laboratories; Army Chemical Center, MD, 1951, UNCLASSIFIED Report (AD-498968).

<sup>&</sup>lt;sup>5</sup> Tannenbaum, H.; Zeffert, B.M. *Crystallization of GB;* TCIR-513; U.S. Army Chemical and Radiological Laboratories; Army Chemical Center, MD, 1949, UNCLASSIFIED Report (AD-E471275).

<sup>&</sup>lt;sup>6</sup>Wardrop, A.W.H.; Bryant, P.J.R. *Physico-Chemical Properties of Phosphorus Esters Part II: Some Constants of Isopropyl methylfluorophosphinate (GB)*; Porton Technical Paper No. 278 (PTP-278); Chemical Warfare Laboratories: Army Chemical Center, MD, 1952, UNCLASSIFIED Report (AD-E481544).

<sup>&</sup>lt;sup>7</sup>Walpole, J.L. *Determination of the Flash Points of GA and GB;* Porton Technical Paper No. 45 (PTP 45); Chemical Defence Experimental Establishment: Porton, England, 1948, UNCLASSIFIED Report (AD-E481350).

<sup>&</sup>lt;sup>8</sup> Perry, B.J.; Thomas, L.C. *The Chemistry of the Alkylfluorophosphonites and Related Compounds;* Porton Technical Paper No. 258; Chemical Defense Experimental Establishment: Porton, England, 1951, UNCLASSIFIED Report (AD-E481528).

<sup>&</sup>lt;sup>9</sup> Epstein, J.; Bauer, V.E.; Somers, L.M. Studies on Hydrolysis of GB I. Effect of pH and Temperature on Hydrolysis Rates. II. Observations on Hydrolysis of GB in Sodium Bicarbonate Buffered Waters; MDR-132; Chemical Warfare Laboratories: Army Chemical Center, MD, 1948, UNCLASSIFIED Report (AD-E471762).

<sup>&</sup>lt;sup>10</sup> Clark, D.N. Review of Reactions of Chemical Agents in Water, Final Report to U.S. Army Biomedical Research and Development Laboratory; Battelle: Columbus, OH, 1989, UNCLASSIFIED Report (AD-A213287).

<sup>&</sup>lt;sup>11</sup> Comparison of GA and GB as Chemical Warfare Agents (U); CWL-SP-1; U.S. Army Chemical Warfare Laboratories: Army Chemical Center, MD, 1957, UNCLASSIFIED Report (AD-E471076).

<sup>&</sup>lt;sup>12</sup> Hutchcraft, A. S. Jr.; Mochel, V.D.; Buckles, L.C. *Special Report: Corrosion Resistance of Metals Toward Isopropyl Methylphosphonofluoridate (GB)*; CRLR 510; U.S. Army Chemical and Radiological Laboratories: Army Chemical Center, MD. 1955. UNCLASSIFIED Report (AD-474404).

Table C-3: Soman (GD)

Alternate Designations: EA 1210 (US); Zoman (USSR); T-2107 (British, UK); Trilon (German); PMFP

Chemical Name: Pinacolyl methyl phosphonofluoridate

Synonyms: 3,3-Dimethyl-n-but-2-yl methylphosphonofluoridate; 3,3-Dimethyl-2-butyl methylphosphonofluoridate; 2-Butanol, 3,3-dimethyl-, methylphosphonofluoridate; Methylphosphonofluoridic acid, 3,3-dimethyl-2-butyl ester; 1,2,2-Trimethylpropyl methyphosphonofluoridate; 1,2,2-Trimethylpropylester kyseliny methylfluorfosfonove (Czech); Methylphosphonofluoridic acid 1,2,2-trimethylpropyl ester; Phosphonofluoridic acid, methyl-, 1,2,2-trimethylpropyl ester; Phosphine oxide, fluoromethyl (1,2,2-trimethylpropoxy)-; Methyl pinacolyl phosphonofluoridate; Pinacolyl methylfluorophosphonate; Fluoromethylpinacolyloxyphosphine oxide; Methyl pinacolyloxyfluorophosphone oxide; Pinacolyl methane fluorophosphorsaeurepinakolylester (German); Methyl pinacolyloxy phosphorylfluoride; Methyl pinacolyl phosphonofluoridate; Pinacoloxymethylphosphoryl fluoride; Pinacolyl methylphosphonofluoride; Pinacolyl methylphosphonofluoride; Pinacolyl methylphosphonofluoride; Pinacolyl methylphosphonate

Chemical Abstract Service Registry Number: 96-64-0

Registry of Toxic Effects of Chemical Substances Registry Number: TA8750000

## **Physical and Chemical Properties**

Structural Formula:

Molecular Formula: C<sub>7</sub>H<sub>16</sub>FO<sub>2</sub>P

Molecular Weight: 182.17	
Physical State	Colorless liquid when pure (1)
Odor	Fruity; impurities give it the odor of camphor (2,3)
Boiling Point	198 °C (extrapolated) decomposes (4)
Melting Point	-42 °C (5,6); Generally solidifies to a noncrystalline, glasslike material (7)
Liquid Density (g/mL)	1.0222 @ 25 °C; 1.0456 @ 0 °C (extrapolated) (7)
Vapor Density (relative to air)	6.3 (calculated)
Vapor Pressure (torr)	4.01 x 10 <sup>-1</sup> @ 25 °C; 4.96 x 10 <sup>-2</sup> @ 0 °C (4)
Volatility (mg/m³)	3.93 x 10 <sup>3</sup> @ 25 °C; 5.31 x 10 <sup>2</sup> @ 0 °C (calculated from vapor pressure) <b>(4)</b>
Latent Heat of Vaporization (kcal/mol)	13.2 @ 25 °C; 13.8 @ 0 °C (calculated from vapor pressure) (4)
Flash Point	121 °C (open cup) (5,8)
Decomposition Temperature	Above 150 °C (1) Stabilized GD decomposes in 200 hr @ 130 °C; unstabilized GD decomposes in 4 hr @ 130 °C (9)
Solubility	Solubility of GD in water is 2.1 g GD/100 g @ 20 °C (9,10); 3.4 g GD/100 g @ 0 °C (9); very soluble in organic solvents (1)
Rate of Hydrolysis	Varies with pH; using a 0.003 M solution of GD @ 25 °C,
	t <sub>1/2</sub> =3 hr @ pH 2; t <sub>1/2</sub> = 45 hr @ pH 6.65; t <sub>1/2</sub> =60hr @ pH 10; complete hydrolysis occurs in less than 5 min in a 5% NaOH solution (11)
Hydrolysis Products	Essentially pinacolyl methylphosphonic acid (PMPA) and hydrogen fluoride (HF) (11)

## Table C-3: Soman (GD) (Continued)

Stability in Storage	Relatively stable in glass for 5-1/2 months @ ambient temperature with or without a stabilizer. (12) Stabilized GD can be stored for at least 6 months @ elevated temperatures (71 °C) in glass, steel, and aluminum containers. (13)
Action on Metals or Other Materials	Corrosion rate on steel is 0.00001 in./month @ 65 °C (14)

<sup>&</sup>lt;sup>1</sup> Franke, S. Manual of Military Chemistry Volume I- Chemistry of Chemical Warfare Agents; ACSI-J-3890; Chemie der Kampfstoffe, East Berlin, 1968, UNCLASSIFIED Technical Manual (AD-849866).

<sup>&</sup>lt;sup>2</sup> Welchman, R.M.A. *Preliminary Report on the Potential Value of Nerve Gases as C.W. Agents;* Porton Report No. 2747 (PR 2747); Chemical Defence Experimental Establishment: Porton, England, 1947, UNCLASSIFIED Report (AD-E470188).

<sup>&</sup>lt;sup>3</sup> Military Chemistry and Chemical Agents; TM 3-215/AFM 355-7; Departments of the Army and the Air Force: Washington, DC, December 1963; UNCLASSIFIED Technical Manual (AD-A292141).

<sup>&</sup>lt;sup>4</sup> Savage, J. J.; Fielder, D. *The Vapor Pressure of Chemical Agents GD, VX, EA2223, EA 3547, EA 3580, EA 5365, and EA 5533*; EC-TR-76058; Aberdeen Proving Ground, MD, 1976, UNCLASSIFIED Report (AD-B013164).

<sup>&</sup>lt;sup>5</sup> Samuel, J.B.; Penski, E.C.; Callahan, J,J. *Physical Properties of Standard Agents, Candidate Agents, and Related Compounds at Several Temperatures (U);* ARCSL-SP-83015; U.S. Army Armament Research and Development Command: Aberdeen Proving Ground, MD, 1983, UNCLASSIFIED Report (AD-C033491).

<sup>&</sup>lt;sup>6</sup> Stern, R.A., U.S. Army Chemical Research and Development Laboratories Notebook # NB 7265 p 45 (C).

<sup>&</sup>lt;sup>7</sup> Zeffert, B.M.; Coulter, P.B. *Physical Constants of G-Series Compounds: EA1210, EA1211, EA1212, EA1213, EA1214;* Technical Division Memorandum Report 1292; U.S. Army Chemical Research and Development Laboratories: Army Chemical Center, MD, 1947, UNCLASSIFIED Report (AD-B964904).

<sup>&</sup>lt;sup>8</sup> Fielder, D, U.S. Army Chemical Warfare Laboratories Notebook # NB 6695 p 72 (C).

<sup>&</sup>lt;sup>9</sup> Chemical Agent Data Sheets Volume I; Edgewood Arsenal Special Report EO-SR-74001; U.S. Army Armament Command: Edgewood Arsenal, Aberdeen Proving Ground, MD, 1974, UNCLASSIFIED Report (AD-B028222).

<sup>&</sup>lt;sup>10</sup> Witten, B. *The Search for Toxic Chemical Agents (U);* EATR 4210; Edgewood Arsenal Research Laboratories: Edgewood Arsenal, MD, 1969, UNCLASSIFIED Report (AD-507852).

<sup>&</sup>lt;sup>11</sup> Buckles, L.C. *The Hydrolysis Rate of GD;* TCIR 373; Chemical Corps Technical Command: Army Chemical Center, MD, 1947, UNCLASSIFIED Report (AD-B966291).

<sup>&</sup>lt;sup>12</sup> Newman, J.H.; Callahan, J.J. *A Thickener for GD (U)*; EC-TR-77016; U.S. Armament Command: Edgewood Arsenal: Aberdeen Proving Ground, MD, 1977, CONFIDENTIAL Report (AD-C009719).

<sup>&</sup>lt;sup>13</sup> Grula, R.S.; Callahan, J.J.; Stern, R.A. *Storage Stability of GD, GF and EA 1356 (U);* CRDLR 3342; U.S. Army Chemical Research and Development Laboratories: Edgewood Arsenal, MD, 1965, CONFIDENTIAL Report (AD-369299).

<sup>&</sup>lt;sup>14</sup> Hormats, S.; Miller C.E. Storage Stability in Steel at 65 °C of Pure GD. Corrosion Rate of Steel at 65 °C; TDMR 1346; Chemical Corps Technical Command: Army Chemical Center, MD, 1948, UNCLASSIFIED Report (AD-B964759).

Table C-4: GF

	Alternate Designations:	EA 1212 (US); T-2139 (British); C	MPF
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Chemical Name: Cyclohexyl methylphosphonofluoridate

Synonyms: Cyclohexyloxyfluoromethylphosphine oxide; Cyclohexyl methylfluorophosphate; Phosphonofluoridic acid, methyl-, cyclohexyl ester; Methyl cyclohexylfluorophosphonate

Chemical Abstract Service Registry Number: 329-99-7

Registry of Toxic Effects of Chemical Substances Number: TA 8225000

## **Physical and Chemical Properties**

Structural Formula:

Molecular Formula: C<sub>7</sub>H<sub>14</sub>FO<sub>2</sub>P Molecular Weight: 180.16

Wolcould Weight: 100:10	
Physical State	Colorless liquid (1)
Odor	None if pure (2)
Boiling Point	228 °C (extrapolated) (3)
Freezing Point	-30 to -50 °C (freezing point) (4); -12 °C (melting point); Below — 30 °C, a metastable crystalline form of GF is produced which slowly converts into a stable form that melts @ -12 °C (5)
Liquid Density (g/mL)	1.1276 @ 25 °C; 1.1525 @ 0 °C (extrapolated) (4)
Vapor Density (relative to air)	6.2 (calculated)
Vapor Pressure (torr)	9.27 x 10 <sup>-2</sup> @ 25 °C; 9.78 x 10 <sup>-3</sup> @ 0 °C (3)
Volatility (mg/m³)	8.98 x 10 <sup>2</sup> @ 25 °C; 1.03 x 10 <sup>2</sup> @ 0 °C (calculated from vapor pressure) (3)
Latent Heat of Vaporization (kcal/mol)	14.3 @ 25 °C; 14.8 @ 0 °C (calculated from vapor pressure) (3)
Flash Point	94 °C (6)
Decomposition Temperature	Completely decomposes within 2 hr @ 150 °C (7)
Solubility	Solubility in water is 3.7 g GF/100g @ 20 °C
	5.1 g GF/100 g @ 0 °C (6)
Rate of Hydrolysis	t <sub>1/2</sub> = 42 hr @ 25 °C using a 0.003 M solution of GF in distilled water (8)
Hydrolysis Products	Hydrogen fluoride and cyclohexyl methylphosphonic acid (5)
Stability in Storage	Stabilized GF can be stored @ 71 °C for at least 6 months in glass containers and at least one year in steel and aluminum containers. (9)
Action on Metals or Other Materials	Corrosion rate on steel is 0.000053 in./month @ 65 °C (10)

### Table C-4: GF (Continued)

- <sup>1</sup> Eakle, B.F. Chemical Agent GF (U); Technical Study 69-C4; U.S. Army Deseret Test Center. Fort Douglas, Utah, 1969, UNCLASSIFIED Report (AD-509689).
- <sup>2</sup> Chemical Agent Data Sheets Volume II; Edgewood Arsenal Special Report EO-SR-74002; U.S. Army Armament Command: Edgewood Arsenal, Aberdeen Proving Ground, MD, 1974, CONFIDENTIAL Report (AD-000020).
- <sup>3</sup> Tevault, D.E.; Buchanan, J.H.; Buettner, L.C. *Vapor Pressure of GF;* TR-304S; U.S. Army Edgewood Chemical Biological Center: Aberdeen Proving Ground, MD, submitted for publication May 2003, UNCLASSIFIED Report.
- <sup>4</sup> Zeffert, B.M.; Coulter, P.B. *Physical Constants of G-Series Compounds: EA1210, EA1211, EA1212, EA1213, EA1214;* Technical Division Memorandum Report 1292; U.S. Army Chemical Research and Development Laboratories: Army Chemical Center, MD, 1947, UNCLASSIFIED Report (AD-B964904).
- <sup>5</sup> Chinn, Kenneth, S. K. Joint CB Technical Data Source Book, Volume III, G Nerve Agents, Part Three: Agents GD and GF (U); DPG-TR-82-004; U.S. Army Dugway Proving Ground, Utah, 1983, SECRET Report (AD-C032927).
- <sup>6</sup> Samuel, J.B.; Penski, E.C.; Callahan, J,J. *Physical Properties of Standard Agents, Candidate Agents, and Related Compounds at Several Temperatures (U);* ARCSL-SP-83015; U.S. Army Armament Research and Development Command: Aberdeen Proving Ground, MD, 1983, UNCLASSIFIED Report (AD-C033491).
- <sup>7</sup> Perry, B.J.; Thomas, L.C. *The Chemistry of the Alkytfluorophosphonites and Related Compounds;* Porton Technical Paper No. 258; Chemical Defense Experimental Establishment: Porton, England, 1951, UNCLASSIFIED Report (AD-E481528).
- <sup>8</sup> Buckles, L.C. *The Hydrolysis Rate of G Agents;* TCIR 393; U.S. Army Chemical Research and Development Laboratories: Army Chemical Center, MD, 1947, UNCLASSIFIED Report (AD-B966236).
- <sup>9</sup> Grula, R.S.; Callahan, J.J.; Stern, R.A. *Storage Stability of GD, GF and EA 1356 (U);* CRDLR 3342; U.S. Army Chemical Research and Development Laboratories: Edgewood Arsenal, MD, 1965, CONFIDENTIAL Report (AD-369299).
- <sup>10</sup> Kaiser, W.A. Summary of Information on Agent GF; CRLR 164; U.S. Army Chemical Research and Development Laboratories: Army Chemical Center, MD, 1954, UNCLASSIFIED Report (AD-B969120).

Table C-5: VX

Alternate Designations: EA 1701; TX60

Chemical Name: O-Ethyl-S-(2-diisopropylaminoethyl) methyl phosphonothiolate

Synonyms: S-(2-Diisopropylaminoethyl) O-ethyl methyl phosphonothiolate; Ethyl-S-dimethylaminoethyl methylphosphonothiolate; Phosphonothioic acid, methyl-, S-(2-(diisopropylamino)ethyl) O-ethyl ester; Ethyl S-2-diisopropylaminoethyl methylphosphonothiolate; Ethyl-S-diisopropylaminoethyl methylphosphonothioic acid S-(2- (bis(methylethyl)amino)ethyl) O-ethyl ester; O-Ethyl-S-2-diisopropylaminoethylester kyseliny methylthiofosfonove (Czech)

Chemical Abstract Service Registry Number: 50782-69-9

Registry of Toxic Effects of Chemical Substances Number: TB1090000

### **Physical and Chemical Properties**

#### Structural Formula:

$$\begin{array}{c} \text{CH}_{3}\text{CH}_{2}\text{--O-P-S-CH}_{2}\text{CH}_{2}\text{--N} \\ \text{CH}_{3}\text{CH}_{3} \\ \end{array} \\ \begin{array}{c} \text{CH}(\text{CH}_{3})_{2} \\ \text{CH}(\text{CH}_{3})_{2} \\ \end{array}$$

Molecular Formula: C<sub>11</sub>H<sub>26</sub>NO<sub>2</sub>PS

Molecular Weight: 267.37

Physical State	Colorless liquid when pure (1)
Odor	Odorless when pure (1)
Boiling Point	292 °C (extrapolated) (2)
Freezing Point	Below -51 °C and -39 to -60 °C (3-5)
Liquid Density (g/mL)	1.0083 @ 25 °C; 1.0209 @ 0 °C (extrapolated) (4)
Vapor Density (relative to air)	9.2 (calculated)
Vapor Pressure (torr)	8.78 x 10 <sup>-4</sup> @ 25 °C; 4.22 x 10 <sup>-5</sup> @ 0 °C (extrapolated) (2)
Volatility (mg/m³)	1.26 x 10 <sup>1</sup> @ 25 °C; 6.62 x 10 <sup>-1</sup> @ 0 °C (calculated from vapor pressure) (2)
Latent Heat of Vaporization (kcal/mol)	19.2 @ 25 °C; 20.1 @ 0 °C; (calculated from vapor pressure) (6,2)
Flash Point	127 °C (continuously closed cup method) (7)
Decomposition Temperature	$t_{1/2}$ = 502 days @ 71 °C; $t_{1/2}$ = 41 days @ 100 °C; $t_{1/2}$ = 34.5 hr @ 150 °C; $t_{1/2}$ = 10 hr @ 170 °C (8); $t_{1/2}$ = 1.6 hr @ 200 °C; $t_{1/2}$ = 4 min @ 250 °C; $t_{1/2}$ = 36 sec. @ 295 °C (5)
Solubility	Water solubility of VX is 5% @ 21.5 °C (4); Miscible with water @ 9.4 °C (4); soluble in common organic solvents (5)
Rate of Hydrolysis	Hydrolysis rate of VX varies with temperature and concentration. At 22 °C $t_{1/2}$ = 1.8 min [1.25M NaOH]; $t_{1/2}$ = 10.8 min [0.25M NaOH]; $t_{1/2}$ = 31 min [0.10M NaOH]; $t_{1/2}$ = 3.3 hr [0.01M NaOH]; $t_{1/2}$ = 20.8 hr [0.001M NaOH]; and $t_{1/2}$ = 60 hr [pure H <sub>2</sub> O] (9)
Hydrolysis Products	VX hydrolyzes via three different pathways (P-S, P-O, and C-S), which vary significantly with temperature and pH. At pH below 12, the P-O bond cleavage path produces ethyl methylphosphonate (EMPA) and the toxic S-[2-diisopropylaminoethyl] methylphosphonothiolate ion (EA 2192) At room temperature EA 2192 reacts very slowly with OH <sup>-</sup> [EA 2192, t <sub>1/2</sub> = 7.4 days (1.0M NaOH)] eventually producing less toxic products. (9,10) Using an equimolar ratio of VX and water at elevated temperatures appears to reduce the persistency of EA 2192. (11)

### Table C-5: VX (Continued)

Stability in Storage	Relatively stable @ ambient temperature; unstabilized VX of 95% purity decomposes at a rate of 5% a month @ 71 °C (13) Highly purified VX is stable in both glass and steel. (1)
Action on Metals or Other Materials	Negligible on brass, steel, and aluminum. Slight corrosion with copper (12)

<sup>&</sup>lt;sup>1</sup>Witten, B. *The Search for Toxic Chemical Agents (U);* EATR 4210; Edgewood Arsenal Research Laboratories: Edgewood Arsenal, MD, 1969, UNCLASSIFIED Report (AD-507852).

<sup>&</sup>lt;sup>2</sup> Buchanan, J.H., et al., <u>Vapor Pressure of VX</u>, ECBC-TR-068, U.S. Army Soldier and Biological Chemical Command, Aberdeen Proving Ground, MD, November 1999, UNCLASSIFIED Report (AD-A371297).

<sup>&</sup>lt;sup>3</sup> Samuel, J.B.; Penski, E.C.; Callahan, J,J. *Physical Properties of Standard Agents, Candidate Agents, and Related Compounds at Several Temperatures (U);* ARCSL-SP-83015; U.S. Army Armament Research and Development Command: Aberdeen Proving Ground, MD, 1983, UNCLASSIFIED Report (AD-C033491).

<sup>&</sup>lt;sup>4</sup> Coulter, P.B.; Callahan, J.J.; Link, R.S. *Physical Constants of Thirteen V Agents;* CWLR 2346; U.S. Army Chemical Warfare Laboratories: Army Chemical Center, MD, 1959, UNCLASSIFIED Report (AD-314520).

<sup>&</sup>lt;sup>5</sup> Chemical Agent Data Sheets Volume I; Edgewood Arsenal Special Report EO-SR-74001; U.S. Army Amament Command: Edgewood Arsenal, Aberdeen Proving Ground, MD, 1974, UNCLASSIFIED Report (AD-B028222).

<sup>&</sup>lt;sup>6</sup> Abercrombie, P., Edgewood Chemical Biological Center Notebook # NB 98-0079 p 11 (U).

<sup>&</sup>lt;sup>7</sup> Butrow, B., Edgewood Chemical Biological Center Notebook # NB 97-0109 (C).

<sup>&</sup>lt;sup>8</sup> Rohrbaugh, D.K.; Grula, R.J.; Buchanan, J.H.; Samuel, .B.; Szafraniec, L.L. Studies in Support of SUPLECAM (Surveillance Program for Lethal Chemical Agents and Munitions) II, 1. Thermal Decomposition of VX; CRDEC-TR-88056; U.S. Army Chemical Research, Development and Engineering Center: Aberdeen Proving Ground, MD, 1988, UNCLASSIFIED Report (AD-B124301)..

<sup>&</sup>lt;sup>9</sup> Yang, Y.; Szafraniec, L.L.; Beaudry, W.T.; Samuel, J.B.; Rohrbaugh, D.K. Hydrolysis of VX: Activation Energies and Autocatalysis. *In Proceedings of the 1994 ERDEC Scientific Conference on Chemical Biological Defense Research*, 15-18 November1994; ERDEC-SP-036; Berg, D.A., Compiler; U.S. Army Edgewood Research, Development and Engineering Center: Aberdeen Proving Ground, MD, 1996; pp. 375-382; UNCLASSIFIED Report (AD-A313080).

<sup>&</sup>lt;sup>10</sup> Yang, Y.; Szafraniec, L.L.; Beaudry, W.T. Perhydrolysis of Nerve Agent VX. J. Org. Chem, 1993, 58, p 6965.

<sup>&</sup>lt;sup>11</sup> Szafraniec, L.L.; Beaudry, W.T.; Samuel, J.B.; Rohrbaugh, D.K.; Yang, Y. Hydrolysis of VX with Equimolar Water at Elevated Temperatures: Activation Parameters of VX, CV and EA 2192. *In Proceedings of the 1996 ERDEC Scientific Conference on Chemical Biological Defense Research*, 19-22 November1996; ERDEC-SP-048; Berg D.A., Compiler; U.S. Army Edgewood Research, Development and Engineering Center: Aberdeen Proving Ground, MD, 1997; pp. 599-605; UNCLASSIFIED Report (AD-A334105).

<sup>&</sup>lt;sup>12</sup> Eckhaus, S.R.; Gress, E.A.; Johnson, H.F. Resistance of Various Materials of Construction in Contact with Transester Process; CWL Technical Memorandum 31-73; U.S. Army Chemical Research and Development Laboratories: Army Chemical Center, MD, 1959, UNCLASSIFIED Report (AD-B963125).

<sup>&</sup>lt;sup>13</sup> Salamon, M.K. *Agent VX*; CWL Special Publication 4-10; U.S. Army Chemical Warfare Laboratories: Army Chemical Center, MD, 1959, UNCLASSIFIED Report (AD-E471109).

Table C-6: Vx

Alternate Designations: EA 1699; EDM	
Chemical Name: O-ethyl S-(2-dimethyl	aminoethyl) methylphosphonothiolate
dimethylaminoaethyl)-methylphosphono methylthiofosfonove (Czech); O-Ethyl-S	nyl-, S-[2-(dimethylamino)ethyl] O-ethyl ester; O-Aethyl-S-(2- othioate (German); S-2- Dimethylaminoethyl-O-ethylester kyseliny i-(dimethylaminoethyl)-methylphosphonothioate
Chemical Abstract Service Registry No:	
Registry of Toxic Effects of Chemical Si	ubstances No: 51366-09-7
Phy	sical and Chemical Properties
Structural Formula:	
CH <sub>2</sub> CH <sub>2</sub> —O-	O II -P—S—CH <sub>2</sub> CH <sub>2</sub> —N CH <sub>3</sub>
31.301.12	CH <sub>3</sub>
Molecular Formula: C <sub>7</sub> H <sub>18</sub> NO <sub>2</sub> PS	
Molecular Weight: 211.26	
Physical State	Liquid (1)
Odor	Odoriess (2)
Boiling Point	256 °C (extrapolated) (3,4)
Freezing Point	Data not available
Liquid Density (g/mL)	1.060 @ 25 °C; 1.0820 @ 0 °C (extrapolated) (1)
Vapor Density (relative to air)	7.3 (calculated)
Vapor Pressure (torr)	6.73 x 10 <sup>-3</sup> @ 25 °C; 5.7 x 10 <sup>-4</sup> @ 0 °C (extrapolated) (3,4)
Volatility (mg/m³)	7.64 x 10 <sup>1</sup> @ 25 °C; 7.02 @ 0 °C (calculated from vapor pressure) (3,4)
Latent Heat of Vaporization (kcal/mol)	16.0 @ 25 °C; 16.1 @ 0 °C (calculated from vapor pressure) (3,4)
Flash Point	Data not available
Decomposition Temperature	Data not available
Solubility	Soluble in organic solvents; slightly soluble in water (Source unidentified)
Rate of Hydrolysis	The rate coefficient for 7.8 x 10 <sup>-3</sup> hr <sup>-1</sup> (based on a nonlinear least square fit) (5)
Hydrolysis Products	Ethanol and the toxic product compound S-(2-dialkylamino-ethyl) methylphosphonothioic acid that is very stable in neutral water. (5)
Stability in Storage	Data not available
Action on Metals or Other Materials	Data not available

## Table C-6: Vx (Continued)

<sup>&</sup>lt;sup>1</sup> Coulter, P.B.; Callahan, J.J.; Link, R.S. *Physical Constants of Thirteen V Agents*; CWLR 2346; U.S. Army Chemical Warfare Laboratories: Army Chemical Center, MD, 1959, UNCLASSIFIED Report (AD-314520).

<sup>&</sup>lt;sup>2</sup>Military Chemistry and Chemical Agents; TM 3-215/AFM 355-7; Departments of the Army and the Air Force: Washington, DC, December 1963; UNCLASSIFIED Technical Manual (AD-A292141).

<sup>&</sup>lt;sup>3</sup> Samuel, J.B.; Penski, E.C.; Callahan, J.J. Physical Properties of Standard Agents, Candidate Agents, and Related Compounds at Several Temperatures (U); ARCSL-SP-83015; U.S. Army Armament Research and Development Command: Aberdeen Proving Ground, MD, 1983, UNCLASSIFIED Report (AD-C033491).

<sup>&</sup>lt;sup>4</sup> Newman, J.H., Edgewood Arsenal Notebook # NB 9298, p. 64 (U).

<sup>&</sup>lt;sup>5</sup> Szafraniec, L.J.; Szafraniec, L.L.; Beaudry, W.T.; Ward, J.R. *On the Stoichiometry of Phosphonothiolate Ester Hydrolysis*; CRDEC-TR-212; U.S. Army Chemical Research, Development & Engineering Center: Aberdeen Proving Ground, MD, 1990, UNCLASSIFIED Report (AD-A225952).

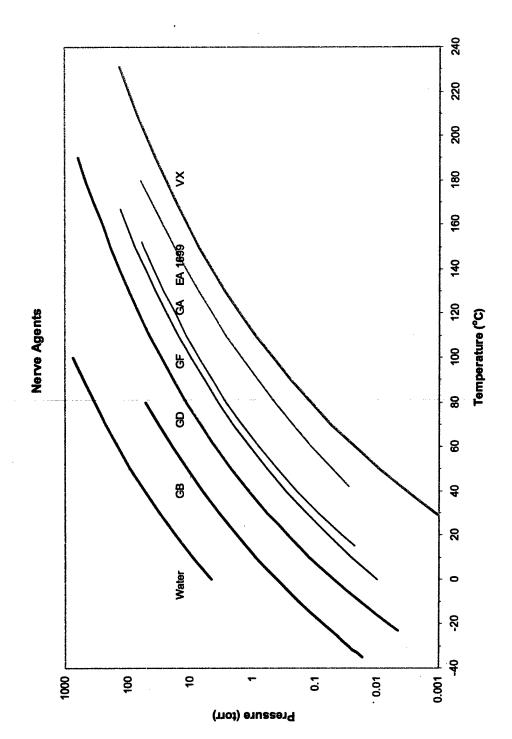


Figure C: Vapor Pressure of Nerve Agents

Blank

### **APPENDIX D**

#### **BLOOD AGENTS**

## Table D-1: Hydrogen Cyanide (AC)

Alternate Designations: Cyclone (Russian); Cyclone B; Cyclon; Prussic acid, Forestite (French); Aero Liquid HCN;

Chemical Name: Hydrogen cyanide

Synonyms: Hydrocyanic acid; Acide cyanhydrique (French); Acido cianidrico (Italian); Blausaeure (German); Blauwzuur (Dutch); Carbon hydride nitride (chn); Cyanwaterstof (Dutch); Cyanwasserstoff (German); Cyjanowodor (Polish); Evercyn; Formic anammonide; Formonitrile

Chemical Abstract Service Registry Number: 74-90-8

Registry of Toxic Effects of Chemical Substances Number: MW6825000

**Physical and Chemical Properties** 

Structural Formula:

H-C≡N

Molecular Formula: HCN Molecular Weight: 27.03

Wolecular Weight. 27.03	
Physical State	Colorless liquid (1)
Odor	Bitter almonds or peach kernels (2,3)
Boiling Point	25.5 °C (4,1)
Freezing Point	-13.3 °C (melting point) (1)
Liquid Density (g/mL)	0.6797 @ 25 °C; 0.7162 @ 0 °C (5)
Vapor Density (relative to air)	0.93 (calculated)
Vapor Pressure (torr)	$7.60 \times 10^{2}$ @ $25.5$ °C; $7.46 \times 10^{2}$ @ $25.0$ °C; $2.65 \times 10^{2}$ @ $0$ °C (4,1)
Volatility (mg/m³)	1.10 x 10 <sup>6</sup> @ 25.5 °C; 1.08 x 10 <sup>6</sup> @ 25.0 °C; 4.20 x 10 <sup>5</sup> @ 0 °C (calculated from vapor pressure) <b>(4,1)</b>
Latent Heat of Vaporization (kcal/mol)	6.72 @ 25.5 °C; 6.72 @ 25.0 °C; 6.71 @ 0 °C (calculated from vapor pressure) (4,1)
Flash Point	-18 °C (closed cup) (3); Frequently ignites when explosively disseminated (6)
Decomposition Temperature	Above 65.5 °C when stabilized (6); forms explosive polymer on standing (2,3); stabilized material can be stored up to 65 °C (6)
Solubility	Miscible w/ water and common organic solvents including alcohol and ether (7)
Rate of Hydrolysis	Slow under acidic conditions; rapid with traces of base or basic salts (8)
Hydrolysis Products	Ammonia, formic acid (HCOOH), and amorphous brown solids (9)
Stability in Storage	Pure AC is unstable on storage; forms explosive polymer on long standing (2,6); with the use of a stabilizer such as phosphoric acid, sulfur dioxide, or powdered copper, AC may be stored in metal containers for long periods of time @ temperatures up to 65 °C. (2,3,6)
Action on Metals or Other Materials	Corrodes iron, cast iron, chromium steel, and lead (2)

## Table D-1: Hydrogen Cyanide (AC) (Continued)

<sup>&</sup>lt;sup>1</sup> Giauque, W.F.; Ruehrwein, R.A. The Entropy of Hydrogen Cyanide. Heat Capacity, Heat of Vaporization and Vapor Pressure. Hydrogen Bond Polymerization of the Gas in Chains of Indefinite Length. *J. Am. Chem. Soc.* **1939**, *61* p. 2626.

<sup>&</sup>lt;sup>2</sup> Franke, S. *Manual of Military Chemistry Volume I- Chemistry of Chemical Warfare Agents;* ACSI-J-3890; Chemie der Kampfstoffe, East Berlin, 1968, UNCLASSIFIED Technical Manual (AD-849866).

<sup>&</sup>lt;sup>3</sup> Sax's Dangerous Properties of Industrial Materials; 10<sup>th</sup> ed.; Lewis, R.J., Ed.; Volume 3; John Wiley & Sons, Inc.: New York, 2001; p.1992.

<sup>&</sup>lt;sup>4</sup> Abercrombie, P., Edgewood Chemical Biological Center Notebook # NB 98-0079 p 16 (U).

<sup>&</sup>lt;sup>5</sup> Coates, J.E.; Davies, R.H. Studies on Hydrogen Cyanide. Part XVIII. Some Physical Properties of Anhydrous Hydrogen Cyanide. *J. Chem. Soc.* **1950**, p. 1194.

<sup>&</sup>lt;sup>6</sup> Kirner, W.R. Chemical Warfare Agents, and Related Chemical Problems Part I-II, Summary Technical Report of Division 9, NDRC Volume 1; Chapter 2, NDRC-DIV-9-VOL-1-PT1-2; Office of Scientific Research and Development: Washington, DC, 1946, UNCLASSIFIED Report (AD-234270).

<sup>&</sup>lt;sup>7</sup> The Merck Index: An Encyclopedia of Chemicals, Drugs, and Biologicals; 13<sup>th</sup> ed.; O'Neil, M.J., Ed.; Merck & Company, Inc.: New Jersey, 2001; p 857.

<sup>&</sup>lt;sup>8</sup> Properties of War Gases Volume II: Blood and Nettle Gases (U); ETF 100-41/Vol-2; Chemical Corps Board: Army Chemical Center, MD, 1956, CONFIDENTIAL Report (AD-108457).

<sup>&</sup>lt;sup>9</sup> Clark, D.N. Review of Reactions of Chemical Agents in Water, Final Report to U.S. Army Biomedical Research and Development Laboratory; Battelle: Columbus, OH, 1989, UNCLASSIFIED Report (AD-A213287).

Table D-2: Cyanogen Chloride (CK)

Alternate Designations: Mauguinite (French); CC; Klortsian		
Chemical Name: Cyanogen chloride		
Synonyms: Chlorcyan; Chlorine cyanide; Chlorocyan; Chlorocyanide; Chlorocyanogen; Chlorure de cyanogene (French)		
Chemical Abstract Service Registry Number: 506-77-4		
Registry of Toxic Effects of Chemical S	ubstances Number: GT2275000	
Phy	sical and Chemical Properties	
Structural Formula:		
CI—C≡≡N		
Molecular Formula: CNCI Molecular Weight: 61.47		
Physical State	Coloriess gas (1)	
Odor	Lacrimatory and irritating (2)	
Boiling Point	12.8 °C (calculated) (3-5)	
Freezing Point	-6.9 °C <b>(5)</b>	
Liquid Density (g/mL)	1.202 @ 10 °C; 1.222 @ 0 °C (4)	
Vapor Density (relative to air)	2.1 (calculated)	
Vapor Pressure (torr)	$7.60 \times 10^{2}$ @ 12.8 °C; $6.80 \times 10^{2}$ @ 10 °C; $4.48 \times 10^{2}$ @ 0 °C (3-5)	
Volatility (mg/m³)	2.62 x 10 <sup>6</sup> @ 12.8 °C; 2.37 x 10 <sup>6</sup> @ 10 °C; 1.62 x 10 <sup>6</sup> @ 0 °C (calculated from vapor pressure) <b>(3-5)</b>	
Latent Heat of Vaporization (kcal/mol)	6.40 @ 12.8°C; 6.41 @ 10 °C; 6.44 @ 0°C (calculated from vapor pressure) (3-5)	
Flash Point	Nonflammable (2)	
Decomposition Temperature	Approximately 149 °C (6)	
Solubility	Solubility of liquefied CK in water is 71.4 g/L @ 20 °C (7), Soluble in common organic solvents, sulfur mustard, and hydrogen cyanide (1)	
Rate of Hydrolysis	The hydrolysis rate of CK with tap water is $t_{1/2}$ = 180hr @ ambient temperature and pH 7 (8)	
Hydrolysis Products	Hydrogen chloride and cyanic acid (CNOH) (9)	
Stability in Storage	CK is stable in glass containers for long periods of time even @ elevated temperatures. Stable in steel containers for at least one year @ ambient temperature, but only about 9 weeks @ 60 °C, after which time the gas begins to polymerize with formation of the corrosive solid, cyanuric chloride. Impurities have a tendency to promote explosive polymerization. (10,2) When stabilized using 5% anhydrous, powdered sodium pyrophosphate, munitions grade CK with a water content of less than 0.5% can be stored in most common metals for extended periods of time @ temperatures up to 100 °C. (2)	
Action on Metals or Other Materials	None if CK is dry; slowly polymerizes when stored unstabilized in steel and other common metals @ elevated temperatures (see stability in storage section) (2)	

## Table D-2: Cyanogen Chloride (CK) (Continued)

<sup>&</sup>lt;sup>1</sup> Franke, S. *Manual of Military Chemistry Volume I- Chemistry of Chemical Warfare Agents;* ACSI-J-3890; Chemie der Kampfstoffe, East Berlin, 1968, UNCLASSIFIED Technical Manual (AD-849866).

<sup>&</sup>lt;sup>2</sup> Kirner, W.R. Chemical Warfare Agents, and Related Chemical Problems Part I-II, Summary Technical Report of Division 9, NDRC Volume 1; Chapter 2; NDRC-DIV-9-VOL-1-PT1-2; Office of Scientific Research and Development: Washington, DC, 1946, UNCLASSIFIED Report (AD-234270).

<sup>&</sup>lt;sup>3</sup> Abercrombie, P., Edgewood Chemical Biological Center Notebook # NB 98-0079 p 16 (U).

<sup>&</sup>lt;sup>4</sup> Cook, R.P.; Robinson, P.L. Certain Physical Properties of Cyanogen and its Halides. J. Chem. Soc. 1935, p. 1001.

<sup>&</sup>lt;sup>5</sup> Douglas, D.E.; Winkler, C.A. The Preparation, Purification, Physical Properties and Hydrolysis of Cyanogen Chloride. *Ca. J. Research* **1947**, *25B*, p. 381.

<sup>&</sup>lt;sup>6</sup> Brooks, M.E.; Parker, G.A. *Incineration/Pyrolysis of Several Agents and Related Chemical Materials Contained in Identification Sets;* ARCSL-TR-79040; U.S. Army Armament Research and Development Command: Aberdeen Proving Ground, MD, 1979, UNCLASSIFIED Report (AD-B042888).

<sup>&</sup>lt;sup>7</sup> Carter, R.H.; Knight, H.C. Fundamental Study of Toxicity: Solubility of Certain Toxics in Water and in Olive Oil; EACD 445; Chemical Warfare Service: Edgewood Arsenal, MD, 1928, UNCLASSIFIED Report (AD-B955216).

<sup>&</sup>lt;sup>8</sup> Price, C.C.; Larson, T.E.; Beck, K.M.; Harrington, F.C.; Smith, L.C.; Stephanoff, I. Hydrolysis and Chlorinolysis of Cyanogen Chloride. *J. Amer. Chem. Soc.* **1947**, *69*, p. 1640.

<sup>&</sup>lt;sup>9</sup> Edwards, J.O.; Sauer, M. Chemical Reactivity of Cyanogen Chloride in Aqueous Solution, Quarterly Status Report (March through May 1972); Report No. III; DAAA15-71-C-0478-QSR 3; U.S. Army Chemical Laboratories: Edgewood Arsenal, MD, 1973, UNCLASSIFIED Report (AD-A090556).

<sup>&</sup>lt;sup>10</sup> Henley, F.M. Surveillance Tests on 75 mm Steel Gas Shell Extending Over a Period of One Year, EACD 11; Chemical Warfare Service: Edgewood Arsenal, MD, 1920, UNCLASSIFIED Report (AD-B959731).

Table D-3: Arsine (SA)

Alternate Designations: Arthur

Chemical Name: Arsenic trihydride

Synonyms: Hydrogen arsenide, Arseniuretted hydrogen; Arsenic hydride; Arsenous hydride; Arsenowodor

(Polish); Aresenwasserstoff (German)

Chemical Abstract Service Registry Number: 7784-42-1

Registry of Toxic Effects of Chemical Substances Number: CG6475000

**Physical and Chemical Properties** 

Structural Formula:

Molecular Formula: AsH<sub>3</sub>
Molecular Weight: 77.95

Molecular vveignt: 77.95	
Physical State	Colorless gas (1)
Odor	Disagreeable, garlic-like (1)
Boiling Point	-62.2 °C (extrapolated) (2)
Freezing Point	-116 °C (melting point) (2)
Liquid Density (g/mL)	1.667 @ -75 °C; 1.734 @ -100 °C (2)
Vapor Density (relative to air)	2.7 (calculated)
Vapor Pressure (torr)	4.00 x 10 <sup>2</sup> @ -75 °C and 8.69 x 10 <sup>1</sup> @ -100 °C (2)
Volatility (mg/m³)	$2.55 \times 10^6$ @ -75 °C and $6.27 \times 10^5$ @ -100 °C (calculated from vapor pressure) (2)
Latent Heat of Vaporization (kcal/mol)	4.17 (calculated from Clausius Clapeyron equation which assumes constant heat of vaporization as a function of temperature) (2)
Flash Point	Flammable; forms explosive mixtures with air (3)
Decomposition Temperature	300 °C (1)
Solubility	Solubility of SA in water is 0.028 g/100 g @ 20 °C (4); soluble in alkalis, halogen alkanes, hydrocarbons, and benzene (3,4)
Rate of Hydrolysis	Rapid in the presence of light (1) Slow, in the absence of light and air @ 15.5 °C and pH ~ 7; 32% of SA is hydrolyzed within 5 hr and about 66% within 24 hr (5)
Hydrolysis Products	SA hydrolyzes to produces shiny black arsenic, which is also very toxic. (1)
Stability in Storage	Unstable in most metal containers; metals catalyze decomposition. (6); On exposure to light, moist arsine decomposes quickly depositing shiny black arsenic (1)
Action on Metals or Other Materials	Corrosive to most metals (6)

### Table D-3: Arsine (SA) (Continued)

<sup>&</sup>lt;sup>1</sup> The Merck Index: An Encyclopedia of Chemicals, Drugs, and Biologicals; 13<sup>th</sup> ed.; O'Neil, M.J., Ed.; Merck & Company, Inc.: New Jersey, 2001; p 138.

<sup>&</sup>lt;sup>2</sup> Johnson, W. and Pechukas, A. Hydrogen Compounds of Arsenic. I. Preparation of Arsine in Liquid Ammonia Some Physical Properties of Arsine. *J. Am. Chem. Soc.* **1937**, *59*, p. 2065.

<sup>&</sup>lt;sup>3</sup> Franke, S. *Manual of Military Chemistry Volume I- Chemistry of Chemical Warfare Agents;* ACSI-J-3890; Chemie der Kampfstoffe, East Berlin, 1968, UNCLASSIFIED Technical Manual (AD-849866).

<sup>&</sup>lt;sup>4</sup> Sax's Dangerous Properties of Industrial Materials; 10<sup>th</sup> ed.; Lewis, R.J., Ed.; Volume 2; John Wiley & Sons, Inc.: New York, 2001; p 309.

<sup>&</sup>lt;sup>5</sup> Properties of War Gases Volume II: Blood and Nettle Gases (U); ETF 100-41/Vol-2; Chemical Corps Board: Army Chemical Center, MD, 1956, CONFIDENTIAL Report (AD-108457).

<sup>&</sup>lt;sup>6</sup> Military Chemistry and Chemical Agents; TM 3-215/AFM 355-7; Departments of the Army and the Air Force: Washington, DC, December 1963; UNCLASSIFIED Technical Manual (AD-A292141).

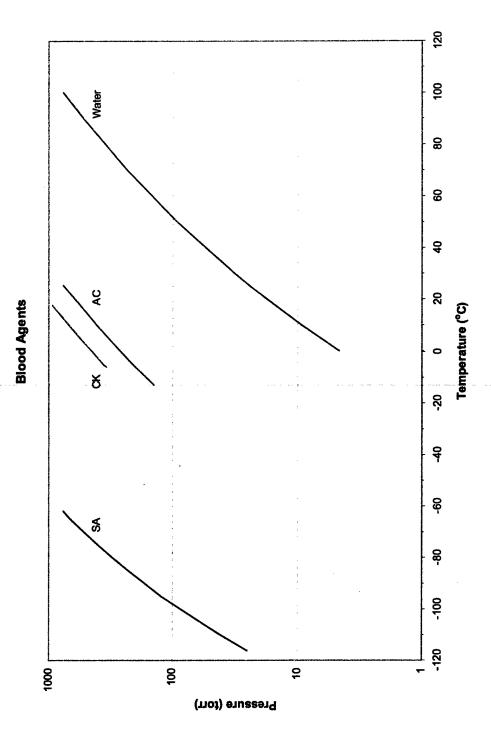


Figure D: Vapor Pressure of Blood Agents

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#### APPENDIX E

#### **BLISTER AGENTS**

## Table E-1: Levinstein Mustard (H)

Alternate Designations: Levinstein H

Volatility (mg/m<sup>3</sup>)

Chemical Name: 70% Bis (2-chloroethyl) sulfide + 30% impurities		
Synonyms: N/A		
Chemical Abstract Service Registry Number: Data not available		
Registry of Toxic Effects of Chemical So	ubstances Number: Data not available	
Physical and Chemical Properties		
Structural Formula:		
70 wt% CICH <sub>2</sub> CH <sub>2</sub> SCH <sub>2</sub> CH <sub>2</sub> CI		
30 wt% Impurities		
Molecular Formula: Since H is not a pure compound; there is no clearly defined formula.  Molecular Weight: This value varies w/ purity, but is normally higher than distilled mustard (HD)159.07		
Physical State	Pale yellow to colorless liquid (1)	
Odor	Garlic-like (2)	
Boiling Point	217 °C (2)	
Freezing Point	0.5 °C (melting point based on 70% purity; calculated from HD purity equation) (3)	
Liquid Density (g/mL)	1.27 @ 25 °C (2)	
Vapor Density (relative to air)	Higher than 5.5 based on vapor density of HD	
Vapor Pressure (torr)	Generally vapor pressure decreases with increasing molecular weight, thus, Levinstein mustard will probably have a lower vapor pressure than HD since its molecular weight will generally be higher. (1)	

Data not available

Table E-1: Levinstein Mustard (H) (Continued)

Stability in Storage	Relatively stable for at least 20 years when stored in steel ton containers @ ambient temperature. Sulfur deposits are formed but they do not seem to react with H; there is however, a purity increase of the remaining liquid with formation of the sulfur deposits. (5)
Action on Metals or Other Materials	No appreciable amount of corrosion or pressure occurs @ temperatures up to 55 °C. The corrosion rate on steel is 15.0 to 40.0 x 10 <sup>-5</sup> in./month @ 60 °C (5) At 65 °C, the corrosion rate on steel when H is stabilized with hexamine is 26.8 x 10 <sup>-5</sup> in./month; this rate can be reduced with the use of chromium plated steel. Cast iron and stainless steel corrodes H 10 times as fast as steel. Also at 65 °C, H rapidly corrodes brass, while aluminum corrosion rate of 0.00006 in./month. (6)

<sup>&</sup>lt;sup>1</sup> Properties of War Gases Volume IV: Vesicants (U); ETF 100-41/Vol-4; Chemical Corps Board: Army Chemical Center, MD, 1956, CONFIDENTIAL Report (AD-108459).

<sup>&</sup>lt;sup>2</sup> Kirner, W.R. Chemical Warfare Agents, and Related Chemical Problems Part I-II, Summary Technical Report of Division 9, NDRC Volume 1; Chapter 5; NDRC-DIV-9-VOL-1-PT1-2; Office of Scientific Research and Development: Washington, DC, 1946, UNCLASSIFIED Report (AD-234270).

<sup>&</sup>lt;sup>3</sup> Abercrombie, P.L.; Butrow, A.B. Selected Physical Properties of Ton Container HD (Mustard) and VX; ERDEC-TR-450; U.S. Army Edgewood Research, Development, and Engineering Center: Aberdeen Proving Ground, MD, 1998; UNCLASSIFIED Report (AD-A350462).

<sup>&</sup>lt;sup>4</sup> Kirner, W.R. Chemical Warfare Agents, and Related Chemical Problems Part I-II, Summary Technical Report of Division 9, NDRC Volume 1; Chapter 6; NDRC-DIV-9-VOL-1-PT1-2; Office of Scientific Research and Development: Washington, DC, 1946, UNCLASSIFIED Report (AD-234270)...

<sup>&</sup>lt;sup>5</sup> Rouiller, C.A. Levinstein Mustard: Composition, Purification, Stabilization; TDMR 612; U.S. Army Chemical Research and Development Laboratories: Army Chemical Center, MD, 1943, UNCLASSIFIED Report (AD-B969803).

<sup>&</sup>lt;sup>6</sup> Harris, B.L.; Macy, R. Corrosion by Vesicants: Rate of Corrosion of Steel and Other Metals by H, HQ, HN-3, HN-1, and L, Mostly at 65 °C; Technical Division Memorandum Report 1031 (TDMR 1031); U.S. Army Chemical Research and Development Laboratories: Army Chemical Center, MD, 1945, UNCLASSIFIED Report (AD-B963161).

## Table E-2: Distilled Mustard (HD)

Alternate Designations: EA 1033; HS; G.34; M.O; Kampstoff "Lost"; Mustard HD; Mustard gas; Mustard Sulfur; Mustard vapor; S-Lost; Schewefel-lost; S mustard; Sulfur mustard gas; Sulfur mustard; Sulphur mustard gas; Yellow Cross liquid; Y; Yperite (French & German)

Chemical Name: Bis (2-chloroethyl) sulfide

Synonyms: 2, 2'-dichloroethyl sulfide; 1, 1'-Thiobis(2-chloroethane);  $\beta-\beta$ '-dichlorodiethyl sulphide;  $\beta,\beta$ '-dichloroethylsulfide ; di – (2-chloro-ethyl) sulfide; Sulfide, bis (2-chloroethyl); Bis (beta-chloroethyl)sulfide; Bis (2-chloroethyl) sulphide; 1-Chloro-2-(beta-chloroethylthio)ethane; 2,2'-Dichlorodiethyl sulfide; Di-2-chloroethyl sulfide; beta,beta'-Dichloroethyl sulfide; beta,beta-Dichlor-ethyl-sulphide; 2,2'-Dichloroethyl sulphide; Gelbkreuz (Czech); 1,1'-Thiobis(2-chloroethane)

Chemical Abstract Service Registry Number: 505-60-2

Registry of Toxic Effects of Chemical Substances Number: WQ0900000

### **Physical and Chemical Properties**

Structural Formula:

## CICH2CH2SCH2CH2CI

Molecular Formula: C<sub>4</sub>H<sub>8</sub>Cl<sub>2</sub>S Molecular Weight: 159.07

Molecular vveight: 159.07	
Pale yellow to dark brown oily liquid (1); colorless when pure (1,2)	
Garlic-like (1,3) or horseradish (3)	
218 °C (extrapolated); at atmospheric pressure HD starts to decompose below the boiling point (4)	
14.45 °C (2)	
1.372 @ 0 °C; 1.333 @ 10 °C (5)	
1.2685 @ 25 °C (6)	
5.5 (calculated)	
1.06 x 10 <sup>-1</sup> @ 25 °C (4)	
9.06 x 10 <sup>2</sup> @ 25 °C (calculated from vapor pressure) (4)	
15.0 @ 25 °C (calculated from vapor pressure) (4)	
105 °C (5)	
180 °C (7)	
HD is practically insoluble in water; solubility of HD in distilled water is only 0.92 g HD/100 g solution @ 22 °C. HD is freely soluble in fats and oils, gasoline, kerosene, most organic solvents, and chemical warfare agents. (5)	
t <sub>1/2</sub> = 5 min @ 25 °C via a S <sub>n</sub> 1 mechanism (8); t <sub>1/2</sub> = 60 min @	
25 °C in salt water (9). HD on or under water undergoes hydrolysis only if dissolved. The rate of HD hydrolysis is controlled by the rate of mass transfer and is very slow (10)	
Hydrogen chloride, thiodiglycol, and sulfonium ion aggregates one of which is also very toxic. (10)	
A small amount of degradation occurs when stored in steel ton containers for over 50 years. (11) This degradation appears to be caused by the formation of solid deposits "heels" comprised of a six-membered ring cyclic sulfonium ion {1-(2-chloroethyl) -1,4-dithianium chloride}, HD, and Fe, which were detected at the bottom of the containers. (12)	
Very little when pure. (3) The corrosion rate of HD on steel is 0.0001 in./month @ 65 °C using munitions grade HD (13)	

## Table E-2: Distilled Mustard (HD) (Continued)

<sup>&</sup>lt;sup>1</sup> Franke, S. *Manual of Military Chemistry Volume I- Chemistry of Chemical Warfare Agents;* ACSI-J-3890; Chemie der Kampfstoffe, East Berlin, 1968, UNCLASSIFIED Technical Manual (AD-849866).

<sup>&</sup>lt;sup>2</sup> Felsing, W.A.; Hunting, C.A.; Fell, S.D. The Melting Point of Mustard Gas. J. Amer. Chem. Soc. 1948, 70, p 1966.

<sup>&</sup>lt;sup>3</sup> Kibler, A.L. *Data on Chemical Warfare;* Technical Division Memorandum Report 456; Chemical Warfare Center: Edgewood Arsenal, MD, 1942, UNCLASSIFIED Report (AD-B969725).

<sup>&</sup>lt;sup>4</sup> Penski, E.C. *Properties of Di-(2-Chloroethyl) Sulfide I. Vapor Pressure Data Review and Analysis;* ERDEC-TR-043; U.S. Army Edgewood Research, Development and Engineering Center: Aberdeen Proving Ground, MD, 1993, UNCLASSIFIED Report (AD-A267059).

<sup>&</sup>lt;sup>5</sup> Buckles, M.F. *CW Vesicants: Selected Values for the Physical Properties of H, T, and Q (U);* Special Report CRLR 542; Chemical Corps Chemical and Radiological Laboratories: Army Chemical Center; MD, 1956, UNCLASSIFIED Report (AD-108272).

<sup>&</sup>lt;sup>6</sup> Moelwyn-Hughes, E.A.; Owens, R. *The Surface Tension, The Molecular Surface Energy and the Parachor of Toxic Compounds and of Certain Chlorides Used in Their Manufacture, Part XV of The Thermal Decomposition of the Secondary Alkylflurophosphonites*; Sutton Oak Report 544; Sutton Oak, England, 1941, UNCLASSIFIED Report (AD-E486435

<sup>&</sup>lt;sup>7</sup> Williams, A.H. The Thermal Decomposition of 2:2'-Dichlorodiethyl Sulphide. J. Chem. Soc. 1947, p. 318.

<sup>&</sup>lt;sup>8</sup> Bartlett, P.D.; Swain, C.G. Kinetics of Hydrolysis and Displacement Reactions of  $\beta$ , β'-Dichlorodiethyl Sulfide (Mustard Gas) and of  $\beta$ -Chloro-β'-hydroxydiethyl Sulfide (Mustard Chlorohydrin). *J.Am. Chem.* Soc. **1949**, *71*, pp 1406-1415.

<sup>&</sup>lt;sup>9</sup> Brookfield, K.J.; Woodward, F.N.; Owens, R. *The Kinetics of the Hydrolysis of Vesicants Part II.*–2:2'-Dichlorodiethylsulphide (H); SO/R/576; Military Intelligence Division: Great Britain, 1942, UNCLASSIFIED Report (AD-E486460)..

<sup>&</sup>lt;sup>10</sup> Yang, Y.; Baker, J.A.; Ward, J.R. Decontamination of Chemical Warfare Agents. Chem. Rev. 1992, 92, p 1729.

<sup>&</sup>lt;sup>11</sup> Abercrombie, P.L.; Butrow, A.B. Selected Physical Properties of Ton Container HD (Mustard) and VX; ERDEC-TR-450; U.S. Army Edgewood Research, Development, and Engineering Center: Aberdeen Proving Ground, MD, 1998; UNCLASSIFIED Report (AD-A350462).

<sup>&</sup>lt;sup>12</sup> Yang, Y.; Szafraniec, L.L.; Beaudry, W.T.; Rohrbaugh, D.K. Characterization of HD Heels and the Degradation of HD in Ton Containers. *In Proceedings of the 1996 ERDEC Scientific Conference on Chemical and Biological Defense Research*, 19-22 November 1996; ERDEC-SP-048; Berg, D.A., Compiler; U.S. Army Edgewood Research, Development and Engineering Center: Aberdeen Proving Ground, MD, 1997; pp 353-360; UNCLASSIFIED Report (AD-A334105).

<sup>&</sup>lt;sup>13</sup> Harris, B.L.; Macy, R. Corrosion by Vesicants: Rate of Corrosion of Steel and Other Metals by H, HQ, HN-3, HN-1, and L, Mostfy at 65 °C; Technical Division Memorandum Report 1031 (TDMR 1031); U.S. Army Chemical Research and Development Laboratories: Army Chemical Center, MD, 1945, UNCLASSIFIED Report (AD-B963161).

### Table E-3: Nitrogen Mustard (HN-1)

Alternate Designations: Ethyl S; NH-Lost; NOR nitrogen mustard; Nitrogen mustard gas -1; NSC 10873; TL 329; TL 1149 Chemical Name: 2,2'-Dichlorotriethylamine Synonyms: Bis (2-chloroethyl)ethylamine; Ethylbis(2-chloroethyl)amine; N-ethyl, bis (β-chloroethyl)amine Ethylbis (beta-chloroethyl)amine Chemical Abstract Service Registry Number: 538-07-8 Registry of Toxic Effects of Chemical Substances Number: YE1225000 **Physical and Chemical Properties** Structural Formula: CH<sub>2</sub>CH<sub>2</sub>CI CH<sub>3</sub>CH<sub>2</sub>—N CH<sub>2</sub>CH<sub>2</sub>CI Molecular Formula: C<sub>6</sub>H<sub>13</sub>Cl<sub>2</sub>N Molecular Weight: 170.08 Dark oily liquid (1); colorless when pure (1,2) **Physical State** Faint, fishy or soapy (3) Odor 192 °C (extrapolated) (4,2); at atmospheric pressure HN-1 **Boiling Point** decomposes below the boiling point (5) -34.2 °C (melting point) (2) Freezing Point 1.086 @ 25 °C; 1.110 @ 0 °C (extrapolated) (2) Liquid Density (g/mL) 5.9 (calculated) Vapor Density (relative to air) 2.44 x 10<sup>-1</sup> @ 25 °C; 3.32 x 10<sup>-2</sup> @ 0 °C (extrapolated) (4,2) Vapor Pressure (torr) 2.23 x 10<sup>3</sup> @ 25 °C; 3.31 x 10<sup>2</sup> @ 0 °C (calculated from vapor Volatility (mg/m<sup>3</sup>) pressure) (4,2) 13.0 @ 25 °C; 12.9 @ 0 °C (calculated from vapor pressure) (4,2) Latent Heat of Vaporization (kcal/mol) Data not available; flashing has occurred on static detonation (3) Flash Point For HN-1+ HCl, 12.7% is destroyed @ 149 °C and @ 426 °C >99% **Decomposition Temperature** is destroyed (5) Solubility in water is approximately 4g HN1/L @ ambient Solubility temperature. Miscible with common organic solvents (3)  $t_{1/2} = 1.3 \text{ min } @ 25 ^{\circ}\text{C} \text{ in aqueous solution (3)}$ Rate of Hydrolysis Complete hydrolysis yields the following: hydrochloric acid and **Hydrolysis Products** ethyl diethanolamine (EtDEA), CH<sub>3</sub>CH<sub>2</sub>N(CH<sub>2</sub>CH<sub>2</sub>OH)<sub>2</sub>. (1) The process involves a complex series of reactions, with formation of the hydrochloride, cyclic imonium salts, a dimer, etc. (6) Polymerizes with the formation of solid deposits, when stored in Stability in Storage steel containers; this amount is slight @ ambient temperature, but increases @ temperatures above 50°C (7) Corrosion of HN-1 on steel @ 65 °C is 1 x 10<sup>-5</sup> to 5 x 10<sup>-5</sup> in./month Action on Metals or Other Materials

(8)

## Table E-3: Nitrogen Mustard (HN-1) (Continued)

- <sup>1</sup> Cheicante, R.L.; Durst, D.H.; Stuff, J.R.; Albro, T.G. Investigation for the Determination of Nitrogen Mustard and Related Compounds in Air by Gas Chromatography Using Solid Sorbent Collection and Thermal Desorption. *In Proceedings of the 1998 ERDEC Scientific Conference on Chemical and Biological Defense Research*, 17-20 November 1998; ERDEC-SP-004; Berg, D.A., Compiler; U.S. Army Edgewood Chemical Biological Center: Aberdeen Proving Ground, MD, 1999; pp 781-792; UNCLASSIFIED Report (AD-A375171).
- <sup>2</sup> Dawson, T.P. A Memorandum Report: New Compounds Bis(B-Chloroethylthioethyl) Ether (T) and its Mixtures with Mustard (HT); TDMR 534; U.S. Army Chemical Research and Development Laboratories: Army Chemical Center, MD, 1943, UNCLASSIFIED Report (AD-B960651).
- <sup>3</sup> Kirner, W.R. Chemical Warfare Agents, and Related Chemical Problems Part I-II, Summary Technical Report of Division 9, NDRC Volume 1; Chapter 6; NDRC-DIV-9-VOL-1-PT1-2; Office of Scientific Research and Development: Washington, DC, 1946, UNCLASSIFIED Report (AD-234270).
- <sup>4</sup> Abercrombie, P., Edgewood Chemical Biological Center Notebook # NB 98-0079 p 24 (U).
- <sup>5</sup> Brooks, M.E.; Parker, G.A. *Incineration/Pyrolysis of Several Agents and Related Chemical Materials Contained in Identification Sets*; ARCSL-TR-79040; U.S. Army Armament Research and Development Command: Aberdeen Proving Ground, MD, 1979, UNCLASSIFIED Report (AD-B042888).
- <sup>6</sup> Kirner, W.R. Chemical Warfare Agents, and Related Chemical Problems Parts III-VI, Summary Technical Report of Division 9, NDRC Volume 1; Chapter 19; NDRC-DIV-9-VOL-1-PT3-6, Office of Scientific Research and Development: Washington, DC, 1946, UNCLASSIFIED Report (AD-234249).
- <sup>7</sup> Harris, B.L.; Bull, W.C.; Macy, R. *Thickened Vesicants: Storage Stability of Unthickened and Thickened Nitrogen Mustards and Their Mixtures with Levinstein Mustard;* Technical Division Memorandum Report 706; U.S. Army Chemical Research and Development Laboratories: Army Chemical Center, MD, 1943, UNCLASSIFIED Report (AD-B962153).
- <sup>8</sup> Harris, B.L.; Macy, R. *Corrosion by Vesicants: Rate of Corrosion of Steel and Other Metals by H, HQ, HN-3, HN-1, and L, Mostly at 65 °C*; Technical Division Memorandum Report 1031 (TDMR 1031); U.S. Army Chemical Research and Development Laboratories: Army Chemical Center, MD, 1945, UNCLASSIFIED Report (AD-B963161).

## Table E-4: Nitrogen Mustard (HN-2)

Alternate Designations: Dichloren; N-methyl-Lost (German); Mustine; Mustargen; Mutagen; Nitrogen mustard; NSC 762; S; TL 146; T-1024; ENT-25294; MBA

Chemical Name: Bis-(2-chloroethyl)methylamine

Synonyms: 2,2'-Dichloro-N-methyldiethylamine; N, N-bis(2-chloroethyl)methylamine, N-methyl, bis(βchloroethyl)amine; Bis(beta-chloroethyl)methylamine; Chloramine; Chlorethazine; Chlormethine; 2-Chloro-N-(2-chloroethyl)-N-methylethanamine; beta, beta'-Dichlorodiethyl-N-methylamine; 2,2'-Dichlorodiethyl-methylamine; Di(2-chloroethyl)methylamine; N,N-Di(chloroethyl)methylamine; Ethanamine, 2-chloro-N-(2-chloroethyl)-N-methyl-; Mechlorethamine; Mecloretamina (Italian); Methylbis(beta-chloroethyl)amine; N-Methyl-bis-chloraethylamin (German); N-Methyl-bis(beta-chloroethyl)amine; N-Methyl-bis(2-chloroethyl)amine; N-Methyl-2,2'-dichlorodiethylamine; Methyldi(2-chloroethyl)amine

Chemical Abstract Service Registry Number: 51-75-2

Registry of Toxic Effects of Chemical Substances Number: IA750000

#### **Physical and Chemical Properties**

Structural Formula:

$$\begin{array}{c} \text{CH}_2\text{CH}_2\text{CI} \\ \text{CH}_2\text{CH}_2\text{CI} \end{array}$$

Molecular Formula: C<sub>5</sub>H<sub>11</sub>Cl<sub>2</sub>N Molecular Weight: 156.05

Molecular Weight: 156.05	
Physical State	Colorless liquid when pure (1)
Odor	Fishy or soapy (2)
Boiling Point	177 °C (extrapolated) (3,2,4); at atmospheric pressure HN-2 decomposes below its boiling point (5)
Freezing Point	-70 °C (2)
Liquid Density (g/mL)	1.118 @ 25 °C; 1.1425 @ 0 °C (extrapolated) (3,4)
Vapor Density (relative to air)	5.4 (calculated)
Vapor Pressure (torr)	4.16 x 10 <sup>-1</sup> @ 25 °C; 5.70 x 10 <sup>-2</sup> @ 0 °C (extrapolated) (3,2,4)
Volatility (mg/m³)	3.49 x 10 <sup>3</sup> @ 25 °C; 5.22 x 10 <sup>2</sup> @ 0 °C (calculated from vapor pressure) (3,2,4)
Latent Heat of Vaporization (kcal/mol)	12.9 @ 25 °C; 12.8 @ 0 °C (calculated from vapor pressure) (3,2,4)
Flash Point	Data not available
Decomposition Temperature	Decomposes before boiling point is reached; instability of HN-2 is associated with its tendency to polymerize or condense; the reactions involved could generate enough heat to cause an explosion (5)
Solubility	Solubility in water is approximately 13 g HN-2/L @ ambient temperature. Miscible with common organic solvents (2)
Rate of Hydrolysis	t <sub>1/2</sub> = 4 min @ 25 °C in an aqueous solution. Slow except where alkali is present; dimerizes fairly rapidly in water <b>(2)</b>
Hydrolysis Products	The process involves a complex series of reactions, with formation of the hydrochloride, cyclic imonium salts, a dimer, etc. (6)
Stability in Storage	Not stable, dimerizes on storage and deposits crystalline dimers (2)
Action on Metals or Other Materials	None on steel and brass (2)
	<u> </u>

# Table E-4: Nitrogen Mustard (HN-2) (Continued)

<sup>&</sup>lt;sup>1</sup>Witten, B. *The Search for Toxic Chemical Agents (U);* EATR 4210; Edgewood Arsenal Research Laboratories: Edgewood Arsenal, MD, 1969, UNCLASSIFIED Report (AD-507852).

<sup>&</sup>lt;sup>2</sup> Kirner, W.R. Chemical Warfare Agents, and Related Chemical Problems Part I-II, Summary Technical Report of Division 9, NDRC Volume 1;Chapter 6; NDRC-DIV-9-VOL-1-PT1-2; Office of Scientific Research and Development: Washington, DC, 1946, UNCLASSIFIED Report (AD-234270).

<sup>&</sup>lt;sup>3</sup> Abercrombie, P., Edgewood Chemical Biological Center Notebook # NB 98-0079 p 26 (U).

<sup>&</sup>lt;sup>4</sup> Dawson, T.P.; Witten, B. *Bis (2-chloroethyl) methylamine, Preparation, Decontamination, and Stability*; Technical Division Memorandum Report 442; Chemical Warfare Center: Edgewood Arsenal, MD, 1942, UNCLASSIFIED Report (AD-B960331).

<sup>&</sup>lt;sup>5</sup> Military Chemistry and Chemical Agents; TM 3-215/AFM 355-7; Departments of the Army and the Air Force: Washington, DC, December 1963; UNCLASSIFIED Technical Manual (AD-A292141).

<sup>&</sup>lt;sup>6</sup> Kirner, W.R. Chemical Warfare Agents, and Related Chemical Problems Parts III-VI, Summary Technical Report of Division 9, NDRC Volume 1; Chapter 19; NDRC-DIV-9-VOL-1-PT3-6, Office of Scientific Research and Development: Washington, DC, 1946, UNCLASSIFIED Report (AD-234249).

Table E-5: Nitrogen Mustard (HN-3)

	1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1		
Alternate Designations: EA 1053; Nitro			
Chemical Name: 2, 2', 2"-Trichlorotriethylamine			
	ris (2-chloroethyl)amine; Tris (β-chloroethyl)amine		
Chemical Abstract Service Registry Nur			
Registry of Toxic Effects of Chemical S			
Ph	Physical and Chemical Properties		
Structural Formula:			
	CH <sub>2</sub> CH <sub>2</sub> CI -N CH <sub>2</sub> CH <sub>2</sub> CI		
CICH <sub>2</sub> CH <sub>2</sub> —	-N		
	CH <sub>2</sub> CH <sub>2</sub> CI		
Molecular Formula: C <sub>6</sub> H <sub>12</sub> Cl <sub>3</sub> N			
Molecular Weight: 204.53			
Physical State	Oily dark liquid; colorless when pure (1)		
Odor	Geranium-like; none when pure (2)		
Boiling Point	257 °C (extrapolated) (3); at atmospheric pressure HN-3 decomposes below the boiling point (4)		
Freezing Point	-3.74 °C (melting point) (3)		
Liquid Density (g/mL)	1.2352 @ 25 °C; 1. 2596 @ 0 °C (extrapolated) (3)		
Vapor Density (relative to air)	7.1 (calculated)		
Vapor Pressure (torr)	1.1 x 10 <sup>-2</sup> @ 25 °C; 9.2 x 10 <sup>-4</sup> @ 0 °C (extrapolated) (3)		
Volatility (mg/m³)	1.2 x 10 <sup>2</sup> @ 25 °C; 1.1 x 10 <sup>1</sup> @ 0 °C (calculated from vapor pressure) (3)		
Latent Heat of Vaporization (kcal/mol)	15.8 @ 25 °C; 16.0 @ 0 °C (calculated from vapor pressure) (3)		
Flash Point	Data not available		
Decomposition Temperature	Above 150 °C (4); remains stable when explosively disseminated (2)		
Solubility	Solubility in water is approximately 0.08 g HN-3/L @ ambient temperature. Miscible with common organic solvents (2)		
Rate of Hydrolysis	Very slow; hydrolysis is not complete even after several days unless alkali is present. (5)		
Hydrolysis Products	Complete hydrolysis gives the following products: Hydrochloric acid and triethanolamine (TEA), N(CH <sub>2</sub> CH <sub>2</sub> OH) <sub>3</sub> , (1) The process involves a complex series of reactions, with formation of the hydrochloride, cyclic imonium salts, a dimer, etc. (6)		
Stability in Storage	In storage HN-3 darkens and forms crystalline deposits. (4) Relatively stable in steel containers, if dry. (2)		
Action on Metals or Other Materials	No attack on iron if dry. (4) Corrodes steel @ a rate of 1 x $10^{-5}$ to $5 \times 10^{-5}$ in./month @ 65 °C (7)		

## Table E-5: Nitrogen Mustard (HN-3) (Continued)

- <sup>1</sup> Cheicante, R.L.; Durst, D.H.; Stuff, J.R.; Albro, T.G. Investigation for the Determination of Nitrogen Mustard and Related Compounds in Air by Gas Chromatography Using Solid Sorbent Collection and Thermal Desorption. *In Proceedings of the 1998 ERDEC Scientific Conference on Chemical and Biological Defense Research*, 17-20 November 1998; ERDEC-SP-004; Berg, D.A., Compiler; U.S. Army Edgewood Chemical Biological Center: Aberdeen Proving Ground, MD, 1999; pp 781-792; UNCLASSIFIED Report (AD-A375171).
- <sup>2</sup> Kirner, W.R. Chemical Warfare Agents, and Related Chemical Problems Part I-II, Summary Technical Report of Division 9, NDRC Volume 1; Chapter 6; NDRC-DIV-9-VOL-1-PT1-2; Office of Scientific Research and Development: Washington, DC, 1946, UNCLASSIFIED Report (AD-234270).
- <sup>3</sup> Samuel, J.B.; Penski, E.C.; Callahan, J,J. *Physical Properties of Standard Agents, Candidate Agents, and Related Compounds at Several Temperatures (U);* ARCSL-SP-83015; U.S. Army Armament Research and Development Command: Aberdeen Proving Ground, MD, 1983, UNCLASSIFIED Report (AD-C033491).
- <sup>4</sup> Kibler, A.L. *Data on Chemical Warfare;* Technical Division Memorandum Report 456; Chemical Warfare Center: Edgewood Arsenal, MD, 1942, UNCLASSIFIED Report (AD-B969725).
- <sup>5</sup> Bartlett, P.D.; Ross, S.D; Swain, C.S. Kinetics and Mechanism of the Reactions of Tertiary β–Chloroethylamines in Solution. III. β-Chloroethylamine and tris-β-Chloroethylamine. *J. Am. Chem.* Soc. **1949**, *71*, p1415-419.
- <sup>6</sup> Kirner, W.R. Chemical Warfare Agents, and Related Chemical Problems Parts III-VI, Summary Technical Report of Division 9, NDRC Volume 1; Chapter 19; NDRC-DIV-9-VOL-1-PT3-6, Office of Scientific Research and Development: Washington, DC, 1946, UNCLASSIFIED Report (AD-234249).
- <sup>7</sup> Harris, B.L.; Macy, R. *Corrosion by Vesicants: Rate of Corrosion of Steel and Other Metals by H, HQ, HN-3, HN-1, and L, Mostly at 65 °C*; Technical Division Memorandum Report 1031 (TDMR 1031); U.S. Army Chemical Research and Development Laboratories: Army Chemical Center, MD, 1945, UNCLASSIFIED Report (AD-B963161).

Table E-6: Mustard-T Mixture (HT)

Alternate Designations: Distilled mustard and T mixture

Chemical Name: HD: Bis-(2-chloroethyl) sulfide; T: Bis {2(2-chloroethylthio)ethyl} ether

Synonyms: N/A

Chemical Abstract Service Registry Number: HD: 505-60-2; T: 63918-89-8

Registry of Toxic Effects of Chemical Substances Number: HD: WQ0900000; T: KN1400000

**Physical and Chemical Properties** 

Structural Formula:

 $60 \text{ wt\% } \text{HD: } \text{CICH}_2\text{CH}_2\text{SCH}_2\text{CH}_2\text{CI}$ 

40 wt% T: (CICH<sub>2</sub>CH<sub>2</sub>SCH<sub>2</sub>CH<sub>2</sub>)<sub>2</sub>O

 $\label{eq:molecular-formula: HD: C4H8Cl2S; T: C8H16Cl2OS2} Molecular Formula: HD: C4H8Cl2S; T: C8H16Cl2OS2$ 

Molecular Weight: HD: 159.07; T: 263.24; Average: 188.96 (based on 60:40 wt. %)

Wolecular Weight. 11D. 100.07, 1. 200.	24, 7 Welage: 100:00 (based 07:00:10 III. 75)
Physical State	Pale yellow to brown liquid (1)
Odor	Garlic-like; less pronounced than mustard (1)
Boiling Point	No constant boiling point (2)
Freezing Point	1.3 °C (melting point) (3)
Liquid Density (g/mL)	1.263 @ 20 °C ( <b>3</b> )
Vapor Density (relative to air)	6.5 (calculated based on 60:40 HT mixture)
Vapor Pressure (torr)	7.7 x 10 <sup>-2</sup> @ 25 °C (calculated based on Raoult's Law equation) (4)
Volatility (mg/m³)	7.83 x 10 <sup>2</sup> @ 25 °C (calculated from vapor pressure) (4)
Latent Heat of Vaporization (kcal/mol)	Data not available
Flash Point	Flash point range 109 to 115 °C (5)
Decomposition Temperature	165 °C to 180 °C (4)
Solubility	Slightly soluble in water; soluble in most organic solvents (2)
Rate of Hydrolysis	Hydrolyzed by prolonged boiling w/ water or treatment w/ caustic alkalis (4)
Hydrolysis Products	Hydrogen chloride, thiodiglycol, and sulfonium aggregates; based on HD (6)
Stability in Storage	Pressure develops in steel (2)
Action on Metals or Other Materials	Very little when pure. Canadian HT corrodes steel at a rate of 0.00007 in./ month @ 65 °C (7)

# Table E-6: Mustard-T Mixture (HT) (Continued)

<sup>&</sup>lt;sup>1</sup> Cone, N.M., Rouiller, C.A. *HQ & HT Review of British & U.S. Literature;* TDMR 575; U.S. Army Chemical Research and Development Laboratories: Army Chemical Center, MD, 1943, UNCLASSIFIED Report (AD-E471215).

<sup>&</sup>lt;sup>2</sup> Chemical Agent Data Sheets Volume II; Edgewood Arsenal Special Report EO-SR-74002; U.S. Army Armament Command: Edgewood Arsenal, Aberdeen Proving Ground, MD, 1974, CONFIDENTIAL Report (AD-000020).

<sup>&</sup>lt;sup>3</sup> Dawson, T.P. A Memorandum Report: New Compounds Bis(B-Chloroethylthioethyl) Ether (T) and its Mixtures with Mustard (HT); TDMR 534; U.S. Army Chemical Research and Development Laboratories: Army Chemical Center, MD, 1943, UNCLASSIFIED Report (AD-B960651).

<sup>&</sup>lt;sup>4</sup> Properties of War Gases Volume IV: Vesicants (U); ETF 100-41/Vol-4; Chemical Corps Board: Army Chemical Center, MD, 1956, CONFIDENTIAL Report (AD-108459).

<sup>&</sup>lt;sup>5</sup> Butrow, A.B., Edgewood Chemical Biological Center Notebook # NB 03-0025 p 50 (U).

<sup>&</sup>lt;sup>6</sup> Yang, Y.; Baker, J.A.; Ward, J.R. Decontamination of Chemical Warfare Agents. Chem. Rev. 1992, 92, p 1729.

<sup>&</sup>lt;sup>7</sup> Harris, B.L.; Macy, R. *Corrosion by Vesicants: Rate of Corrosion of Steel and Other Metals by H, HQ, HN-3, HN-1, and L, Mostly at 65 °C*; Technical Division Memorandum Report 1031 (TDMR 1031); U.S. Army Chemical Research and Development Laboratories: Army Chemical Center, MD, 1945, UNCLASSIFIED Report (AD-B963161).

## Table E-7: Lewisite (L)

Alternate Designations: EA 1034; Lyvizit; LI; M-1; Lewisite (arsenic compound)

Chemical Name: Dichloro(2-chlorovinyl)arsine

Synonyms: Arsonous dichloride, (2-chloroethenyl)-; Chlorovinylarsine dichloride; 2-Chlorovinyldichloroarsine; β-Chlorovinyldichloroarsine; (2-Chloroethenyl) arsonous dichloride; Arsine, dichloro (2-chlorovinyl)-

Chemical Abstract Service Registry Number: 541-25-3

Registry of Toxic Effects of Chemical Substances Number: CH2975000

**Physical and Chemical Properties** 

Structural Formula:

CICH=HC-As CI

Molecular Formula: C<sub>2</sub>H<sub>2</sub>AsCl<sub>3</sub>
Molecular Weight: 207 32

Molecular Weight: 207.32	
Physical State	Brown liquid; colorless when pure (1)
Odor	Geranium-like; odorless when pure (1)
Boiling Point	196 °C (extrapolated) (2,3); decomposes prior to boiling (4)
Freezing Point	- 44.7 to -1.8 °C (depending on purity and isomers present) (5)
Liquid Density (g/mL)	1.8793 @ 25 °C; 1.9210 @ 0 °C (extrapolated) (2)
Vapor Density (relative to air)	7.1 (calculated)
Vapor Pressure (torr)	3.46 x 10 <sup>1</sup> @ 25 °C (extrapolated); 2.71 x 10 <sup>-2</sup> @ 0 °C (extrapolated) (2,3)
Volatility (mg/m³)	3.86 x 10 <sup>3</sup> @ 25 °C; 3.30 x 10 <sup>2</sup> @ 0 °C (calculated from vapor pressure) (2,3)
Latent Heat of Vaporization (kcal/mol)	15.5 @ 25 °C; 17.5 @ 0 °C (calculated from vapor pressure) (2,3)
Flash Point	Nonflammable (6)
Decomposition Temperature	At 149 °C 0.5% of L is destroyed and @ 493 °C > 99.99% was destroyed (4)
Solubility	Lewisite on contact with water or moist surfaces immediately hydrolyzes to form lewisite oxide (solid), which dissolves very slowly in water. (1,7) Readily soluble in common organic solvents, oils and chemical warfare agents (8)
Rate of Hydrolysis	Rapid (1,7)
Hydrolysis Products	2-Chlorovinylarsonous acid (CVAA), 2-chlorovinylarsenious oxide (lewisite oxide), and hydrochloric acid. (9)
Stability in Storage	Fairly stable in glass and steel containers, but decomposes considerably upon denotation; alkalis decompose L @ ambient temperatures. (1)
Action on Metals or Other Materials	None if L is dry; corrosive penetration on steel is 1 x 10 <sup>-5</sup> to 5 x 10 <sup>-5</sup> in./month @ 65 °C (10) Extremely corrosive towards aluminum and aluminum alloys. (8)

### Table E-7: Lewisite (L) (Continued)

- <sup>1</sup> Kirner, W.R. Chemical Warfare Agents, and Related Chemical Problems Part I-II, Summary Technical Report of Division 9, NDRC Volume 1; Chapter 7; NDRC-DIV-9-VOL-1-PT1-2; Office of Scientific Research and Development: Washington, DC, 1946, UNCLASSIFIED Report (AD-234270).
- <sup>2</sup> Samuel, J.B.; Penski, E.C.; Callahan, J.J. *Physical Properties of Standard Agents, Candidate Agents, and Related Compounds at Several Temperatures (U)*; ARCSL-SP-83015; U.S. Army Armament Research and Development Command: Aberdeen Proving Ground, MD, 1983, UNCLASSIFIED Report (AD-C033491).
- <sup>3</sup> Sumner, J.F.; Woodward, F.N.; Owens, R. *The Vapour Pressure of Arsenious Chloride and of Lewisite* I; Sutton Oak Report 561(SO/R/561); Military Intelligence Division: Great Britain, 1941, UNCLASSIFIED Report.
- <sup>4</sup> Brooks, M.E.; Parker, G.A. *Incineration/Pyrolysis of Several Agents and Related Chemical Materials Contained in Identification Sets*; ARCSL-TR-79040; U.S. Army Armament Research and Development Command: Aberdeen Proving Ground, MD, 1979, UNCLASSIFIED Report (AD-B042888).
- <sup>5</sup> Macy, R. Constants and Physiological Action of Chemical Warfare Agents; EATR 78; Chemical Warfare Service: Edgewood Arsenal, MD, 1932, UNCLASSIFIED Report (AD-B956574).
- <sup>6</sup> Chemical Agent Data Sheets Volume I; Edgewood Arsenal Special Report EO-SR-74001; U.S. Army Armament Command: Edgewood Arsenal, Aberdeen Proving Ground, MD, 1974, UNCLASSIFIED Report (AD-B028222).
- <sup>7</sup> Buswell, A.M.; Price, C.C.; Roberts, R.M.; Smith, C.W.; Velzen, B.H. *The Chemistry of Certain Arsenical Chemical Warfare Agents as Water Contaminants*; OSRD 4193; Division 9 National Defense Research Committee of the Office of Scientific Research and Development: Washington, DC; 1944, UNCLASSIFIED Report (AD-E474136).
- <sup>8</sup> Franke, S. *Manual of Military Chemistry Volume I- Chemistry of Chemical Warfare Agents;* ACSI-J-3890; Chemie der Kampfstoffe, East Berlin, 1968, UNCLASSIFIED Technical Manual (AD-849866).
- <sup>9</sup> Bossle, P.C.; Ellzy, M.W.; Martin, J.J. Determination of Lewisite Contamination in Environmental Waters by High Performance Liquid Chromatography; CRDEC-TR-042; U.S. Army Chemical Research, Development and Engineering Center: Aberdeen Proving Ground, MD, 1989, UNCLASSIFIED Report (AD-A206000).
- <sup>10</sup> Harris, B.L.; Macy, R. Corrosion by Vesicants: Rate of Corrosion of Steel and Other Metals by H, HQ, HN-3, HN-1, and L, Mostly at 65 °C; Technical Division Memorandum Report 1031 (TDMR 1031); U.S. Army Chemical Research and Development Laboratories: Army Chemical Center, MD, 1945, UNCLASSIFIED Report (AD-B963161).

Table E-8: Mustard - Lewisite Mixture (HL)

Alternate Designations: Distilled musta			
Chemical Name: HD: Bis-(2-chloroethy	l) sulfide; L: Dichloro-(2-chlorovinly)arsine		
Synonyms: N/A			
Chemical Abstract Service Registry Nur			
	ubstances Number: HD: WQ0900000; L: CH2975000		
Phy	sical and Chemical Properties		
Structural Formula:			
<b>37 wt</b> % HD:	CICH <sub>2</sub> CH <sub>2</sub> SCH <sub>2</sub> CH <sub>2</sub> CI		
	63 wt% L: CICH—HC-As		
63 wt% L:	CICH=HC-As.		
<u> </u>	Cl		
Molecular Formula: HD: C₄H₅Cl₂S; L: C	CoHoAsClo		
	32; Average: 186.39 (based on 37:63 wt %)		
Physical State	Liquid (1)		
Odor	Garlic-like (HD) (2)		
Boiling Point	200 °C (extrapolated) (3,4)		
Freezing Point	-42 °C (munitions grade); -25.4 °C (pure) (4)		
Liquid Density (g/mL)	1.6383 @ 20 °C (calculated) (based on 67 wt% L) (1)		
Vapor Density (relative to air)	6.4 (calculated)		
Vapor Pressure (torr)	3.63 x 10 <sup>-1</sup> @ 25 °C; 4.93 x 10 <sup>-2</sup> @ 0 °C; (calculated based on Raoult's law; actual values are assumed to be somewhat lower than calculated values.) (3,4)		
Volatility (mg/m³)	3.64 x 10 <sup>3</sup> @ 25 °C, 5.39 x 10 <sup>2</sup> @ 0 °C (calculated based on Raoult's law; actual values are assumed to be somewhat lower than calculated values.) (3,4)		
Latent Heat of Vaporization (kcal/mol)	12.8 @ 25 °C; 13.1 @ 0 °C; (calculated from vapor pressure) (3,4)		
Flash Point	Data not available for the mixture; HD flashes @ 105 °C (5)		
Decomposition Temperature	Above 100 °C; based on data, which shows that HD decomposes @ 180 °C (6) and that L starts to decomposes @ 150 °C; (7) this might suggest that HL also decomposes in this temperature range.		
Solubility	Both HD and L are soluble in most organic solvents but only slightly soluble in water suggesting that HL has a similar degree of solubility towards organic solvents and water. (8)		
Rate of Hydrolysis	HD $t_{1/2}$ = 5 min @ 25 °C (9) HD on or under water undergoes hydrolysis only if dissolved. The rate of HD hydrolysis is controlled by the rate of mass transfer and is very slow (10) Lewisite on contact with water or moist surfaces immediately hydrolyzes to form lewisite oxide (solid), which dissolves very slowly in water. (11,12)		
Hydrolysis Products	Hydrogen chloride, thiodiglycol, sulfonium aggregates, (CVAA), and lewisite oxide based on HD and L (13,14)		
Stability in Storage	Stable in lacquered steel containers for approximately 3 months @ 65 °C, 6 months @ 50 °C, and for a year or more @ ambient temperature when using a 50:50 mixture of HD and L. Less stable in uncoated steel containers @ temperatures above 50 °C. Stable in glass @ 65 °C (15)		
Action on Metals or Other Materials	Little or none if dry (8)		

## Table E-8: Mustard - Lewisite Mixture (HL) (Continued)

- <sup>13</sup> Yang, Y.; Szafraniec, L.L.; Beaudry, W.T.; Rohrbaugh, D.K. Characterization of HD Heels and the Degradation of HD in Ton Containers. In Proceedings of the 1996 ERDEC Scientific Conference on Chemical and Biological Defense Research, 19-22 November 1996; ERDEC-SP-048; Berg, D.A., Compiler; U.S. Army Edgewood Research, Development and Engineering Center: Aberdeen Proving Ground, MD, 1997; pp 353-360; UNCLASSIFIED Report (AD-A334105).
- <sup>14</sup> Bossle, P.C.; Ellzy, M.W.; Martin, J.J. Determination of Lewisite Contamination in Environmental Waters by High Performance Liquid Chromatography; CRDEC-TR-042; U.S. Army Chemical Research, Development and Engineering Center: Aberdeen Proving Ground, MD, 1989, UNCLASSIFIED Report (AD-A206000).
- <sup>15</sup> Harris, B.L.; Macy,R. *Memorandum Report Storage Stability of HL, Mixtures of Mustard and Lewisite*; Technical Division Memorandum Report 1302; U.S. Army Chemical Research and Development Laboratories: Army Chemical Center, MD, 1947, UNCLASSIFIED Report (AD-B964981).

<sup>&</sup>lt;sup>1</sup> Mumford, S.A.; Parry, G.A. Report on Physical Properties of Mixtures of H and Lewisite I; PR-1342; U.S. Army Chemical Research and Development Laboratories: Army Chemical Center, MD, 1935, UNCLASSIFIED Report (AD-E481723).

<sup>&</sup>lt;sup>2</sup> Military Chemistry and Chemical Agents; TM 3-215/AFM 355-7; Departments of the Army and the Air Force: Washington, DC, December 1963; UNCLASSIFIED Technical Manual (AD-A292141).

<sup>&</sup>lt;sup>3</sup> Abercrombie, P., Edgewood Chemical Biological Center Notebook # NB 98-0079 p 29 (U).

<sup>&</sup>lt;sup>4</sup> Macy, R. Freezing Point and Volatilities of Mustard and Lewisite Mixtures; TCIR 512; U.S. Army Chemical Research and Development Laboratories: Army Chemical Center, MD, 1935, UNCLASSIFIED Report (AD-B967044).

<sup>&</sup>lt;sup>5</sup> Buckles, M.F. *CW Vesicants: Selected Values for the Physical Properties of H, T, and Q (U);* Special Report CRLR 542; Chemical Corps Chemical and Radiological Laboratories: Army Chemical Center; MD, 1956, UNCLASSIFIED Report (AD-108272).

<sup>&</sup>lt;sup>6</sup> Williams, A.H. The Thermal Decomposition of 2:2'-Dichlorodiethyl Sulphide. J. Chem. Soc. 1947, p. 318.

<sup>&</sup>lt;sup>7</sup> Brooks, M.E.; Parker, G.A. *Incineration/Pyrolysis of Several Agents and Related Chemical Materials Contained in Identification Sets*; ARCSL-TR-79040; U.S. Army Armament Research and Development Command: Aberdeen Proving Ground, MD, 1979, UNCLASSIFIED Report (AD-B042888).

<sup>&</sup>lt;sup>8</sup> Properties of War Gases Volume IV: Vesicants (U); ETF 100-41/Vol-4; Chemical Corps Board: Army Chemical Center, MD, 1956, CONFIDENTIAL Report (AD-108459).

<sup>&</sup>lt;sup>9</sup> Bartlett, P.D.; Swain, C.G. Kinetics of Hydrolysis and Displacement Reactions of β,β'-Dichlorodiethyl Sulfide (Mustard Gas) and of β-Chloro-β'-hydroxydiethyl Sulfide (Mustard Chlorohydrin). *J.Am. Chem. Soc.* **1949**, *71*, pp 1406-1415.

<sup>&</sup>lt;sup>10</sup> Yang, Y.; Baker, J.A.; Ward, J.R. Decontamination of Chemical Warfare Agents. Chem. Rev. 1992, 92, p 1729.

<sup>&</sup>lt;sup>11</sup> Kirner, W.R. Chemical Warfare Agents, and Related Chemical Problems Part I-II, Summary Technical Report of Division 9, NDRC Volume 1; Chapter 7; NDRC-DIV-9-VOL-1-PT1-2; Office of Scientific Research and Development: Washington, DC, 1946, UNCLASSIFIED Report (AD-234270).

<sup>&</sup>lt;sup>12</sup> Buswell, A.M.; Price, C.C.; Roberts, R.M.; Smith, C.W.; Velzen, B.H. *The Chemistry of Certain Arsenical Chemical Warfare Agents as Water Contaminants*; OSRD 4193; Division 9 National Defense Research Committee of the Office of Scientific Research and Development: Washington, DC; 1944, UNCLASSIFIED Report (AD-E474136).

# Table E-9 Phenyldichloroarsine (PD)

Alternate Designations: Pfiffikus; DJ; Sternite, M.A., TL 69; FDA

Chemical Name: Phenyldichloroarsine

Synonyms: Arsine, dichlorophenyl-; Arsonous dichloride, phenyl-; Dichlorophenylarsine; Phenylarsonous dichloride; Phenylarsinedichloride; Dichlor-fenylarsin (Czech); Fenildicloroarsina (Italian); Fenyldichlorarsin (Czech)

Chemical Abstract Service Registry Number: 696-28-6

Registry of Toxic Effects of Chemical Substances Number: CH5425000

**Physical and Chemical Properties** 

Structural Formula:

As C

Molecular Formula: C<sub>6</sub>H<sub>5</sub>AsCl<sub>2</sub> Molecular Weight: 222.93

Colorless to yellow liquid (1)
None (2)
233 °C (extrapolated) (3)
-22.5 °C (3)
1.645 @ 25 °C; 1.677@ 0 °C ( <b>3</b> )
7.7 (calculated)
2.2 x 10 <sup>-2</sup> @ 25 °C; 2.1 x 10 <sup>-3</sup> @ 0 °C (both values are extrapolated) <b>(3)</b>
2.64 x 10 <sup>2</sup> @ 25 °C; 2.3 x 10 <sup>1</sup> @ 0 °C (calculated from vapor pressure) <b>(3)</b>
15.1 (calculated from Clausius Clapeyron equation which assumes constant heat of vaporization as a function of temperature) (3)
Data not available
Stable to the normal boiling point (3)
Immediately hydrolyzes in the presence of water (4) Miscible with alcohol, benzene, ether, acetone (5,6) kerosene, petroleum, and olive oil (6)
Very Rapid (4)
Hydrochloric acid and phenylarsine oxide which is also very toxic (4)
Data not available
No serious affects on mild steel and cast iron (7)

## Table E-9: Phenyldichloroarsine (PD) (Continued)

<sup>&</sup>lt;sup>1</sup> Sax's Dangerous Properties of Industrial Materials; 10<sup>th</sup> ed.; Lewis, R.J., Ed.; Volume 2; John Wiley & Sons, Inc.: New York, 2001; p 1215.

<sup>&</sup>lt;sup>2</sup> Military Chemistry and Chemical Agents; TM 3-215/AFM 355-7; Departments of the Army and the Air Force: Washington, DC, December 1963; UNCLASSIFIED Technical Manual (AD-A292141).

<sup>&</sup>lt;sup>3</sup> Owens, R. Diphenylcyanoarsine: Part V – The Physical Properties of M.A., D.A. T.A., and D.C.; SO/R 492; Sutton Oak, England, 1940, UNCLASSIFIED Report (AD-E486397).

<sup>&</sup>lt;sup>4</sup> Buswell, A.M.; Price, C.C.; Roberts, R.M.; Smith, C.W.; Velzen, B.H. *The Chemistry of Certain Arsenical Chemical Warfare Agents as Water Contaminants;* OSRD 4193; Division 9 National Defense Research Committee of the Office of Scientific Research and Development: Washington, DC; 1944, UNCLASSIFIED Report (AD-E474136).

<sup>&</sup>lt;sup>5</sup> CRC Handbook of Chemistry and Physics; 82<sup>nd</sup> ed.; Lide, D.R., Ed.; Section 3; CRC Press: Washington, DC, 2001; p 15.

<sup>&</sup>lt;sup>6</sup> Chemical Agent Data Sheets Volume I; Edgewood Arsenal Special Report EO-SR-74001; U.S. Army Armament Command: Edgewood Arsenal, Aberdeen Proving Ground, MD, 1974, UNCLASSIFIED Report (AD-B028222).

<sup>&</sup>lt;sup>7</sup> Owens, R. *Diphenylcyanoarsine Part III – The Pope-Turner Process*; SO/R 488; Sutton Oak, England, 1940, UNCLASSIFIED Report (AD-E486396).

## Table E-10: Ethyldichloroarsine (ED)

Alternate Designations: DICK (German); TL 214; Green Cross 3; Yellow Cross 1

Chemical Name: Ethyldichloroarsine

Synonyms: Dichloroethylarsine; Arsine, dichloroethyl-; Arsenic dichloroethane; Ethylarsonous dichloride;

Arsonous dichloride, ethyl-

Chemical Abstract Service Registry Number: 598-14-1

Registry of Toxic Effects of Chemical Substances Number: CH3500000

**Physical and Chemical Properties** 

Structural Formula:

Molecular Formula: C<sub>2</sub>H<sub>5</sub>AsCl<sub>2</sub> Molecular Weight: 174.89

Molecular Weight. 174.09	
Physical State	Colorless liquid (1)
Odor	Fruity, biting, and irritating (1)
Boiling Point	156 °C (2); decomposes (3)
Melting Point	Below - 65 °C (2)
Liquid Density (g/mL)	1.742 @ 14 °C (2)
Vapor Density (relative to air)	6.0 (calculated)
Vapor Pressure (torr)	2.29 @ 21.5 °C (2)
Volatility (mg/m³)	2.19 x 10 <sup>4</sup> @ 20 °C (2)
Latent Heat of Vaporization (kcal/mol)	9.18 (3)
Flash Point	Data not available
Decomposition Temperature	Stable to boiling point (3)
Solubility	Immediately hydrolyzes in the presence of water. (4) Soluble in ethyl chloride, alcohol, ether, benzene, acetone, kerosene and cyclohexane (3)
Rate of Hydrolysis	Very Rapid (4)
Hydrolysis Products	Hydrochloric acid and ethylarsine oxide, which is also very toxic. (4)
Stability in Storage	Stable (3)
Action on Metals or Other Materials	None on steel when pure (2); noncorrosive towards iron @ temperatures up to 50 °C, when ED is dry (5); attacks brass @ 50 °C and is destructive to rubber and plastics (3)

# Table E-10: Ethyldichloroarsine (ED) (Continued)

<sup>&</sup>lt;sup>1</sup> Dangerous Properties of Industrial Materials, 3<sup>rd</sup> ed., Sax, N.I., Ed.; Reinhold Book Corporation: New York, 1968; p741.

<sup>&</sup>lt;sup>2</sup> Dawson, T.P. *Ethyldichloroarsine (ED): Preliminary Investigation (1939);* EATR 325; Chemical Warfare Service: Edgewood Arsenal, MD, 1941, UNCLASSIFIED Report (AD-B957078).

<sup>&</sup>lt;sup>3</sup> Military Chemistry and Chemical Agents; TM 3-215/AFM 355-7; Departments of the Army and the Air Force: Washington, DC, December 1963; UNCLASSIFIED Technical Manual (AD-A292141).

<sup>&</sup>lt;sup>4</sup> Buswell, A.M.; Price, C.C.; Roberts, R.M.; Smith, C.W.; Velzen, B.H. *The Chemistry of Certain Arsenical Chemical Warfare Agents as Water Contaminants*; OSRD 4193; Division 9 National Defense Research Committee of the Office of Scientific Research and Development: Washington, DC; 1944, UNCLASSIFIED Report (AD-E474136).

<sup>&</sup>lt;sup>5</sup> Kibler, A.L. *Data on Chemical Warfare;* Technical Division Memorandum Report 456; Chemical Warfare Center: Edgewood Arsenal, MD, 1942, UNCLASSIFIED Report (AD-B969725).

Table E-11: Methyldichloroarsine (MD)

Alternate Designations: TL 294; Methyl-dick; Medikus

Chemical Name: Methyldichloroarsine

Synonyms: Arsine, dichloromethyl-; Arsonous dichloride, methyl-; Dichloromethylarsine; Methylarsine

dichloride; Methylarsonous dichloride;

Chemical Abstract Service Registry Number: 593-89-5

Registry of Toxic Effects of Chemical Substances Number: CH4375000

Physical and Chemical Properties

Structural Formula:

Molecular Formula: CH<sub>3</sub>AsCl<sub>2</sub> Molecular Weight: 160.86

Colorless liquid (1)
Extremely irritating; none when pure (1)
132.6 °C (2)
-54.8 °C (3)
1.839 @ 20 °C; 1.875 @ 0 °C (4)
5.5 (calculated)
7.593 @ 20 °C; 2.063 @ 0 °C <b>(2)</b>
6.68 x 10 <sup>4</sup> @ 20 °C; 1.95 x 10 <sup>4</sup> @ 0 °C (calculated from vapor pressure) <b>(2)</b>
10.5 @ 20 °C; 10.2 @ 0 °C (calculated from vapor pressure) (2)
Data not available
Stable up to the boiling point (2)
Immediately hydrolyzes in the presence of water (5) Soluble in common organic solvents @ ambient temperatures (1)
Very rapid (5); Complete in less than 2 min @ 25 °C in dilute solution (6)
Hydrogen chloride and methylarsenic oxide (5)
Stable in steel containers @ 60 °C for a period of at least 15 weeks and for at least 1 year @ ambient temperatures. (7)
No appreciable amount of corrosion on steel when MD is pure and acid free. (8) Satisfactory with steel for at least 1year @ ambient temperature, but @ elevated temperatures (60 °C) crude pitting occurs within 15 weeks. (7)

## Table E-11: Methyldichloroarsine (MD) (Continued)

- <sup>1</sup> Macintire, B.G.; Smith, B.F.; Macy, R.; Scherr, H. *Methyldichloroarsine and Methyldifluoroarsine Field Tests;* EACD 410; Chemical Warfare Service: Edgewood Arsenal, MD, March 1931, UNCLASSIFIED Report (AD-B955243).
- <sup>2</sup>Watson, P.D. *Determination of the Vapor Pressure of Methyldichloroarsine*; EACD 176; Chemical Warfare Service: Edgewood Arsenal, MD, 1922, UNCLASSIFIED Report (AD-B959625).
- <sup>3</sup> Mead, W.P. Freezing Points of Mixtures of Methyldichloroarsine and Mustard Gas and of Lewisite and Mustard Gas; EACD 170; Chemical Warfare Service: Edgewood Arsenal, MD, 1922, UNCLASSIFIED Report (AD-B95011).
- <sup>4</sup> Klosky, S.; Stricker, P.F. *The Physico Chemical Properties of Methyldichloroarsine and Arsenic Trichloride;* EACD 63; Chemical Warfare Service: Edgewood Arsenal, MD, 1921, UNCLASSIFIED Report (AD-B955049).
- <sup>5</sup> Buswell, A.M.; Price, C.C.; Roberts, R.M.; Smith, C.W.; Velzen, B.H. *The Chemistry of Certain Arsenical Chemical Warfare Agents as Water Contaminants*; OSRD 4193; Division 9 National Defense Research Committee of the Office of Scientific Research and Development: Washington, DC; 1944, UNCLASSIFIED Report (AD-E474136).
- <sup>6</sup> Beebe, C.H. *Important Constants of Fourteen Common Chemical Warfare Agents;* EACD 328; Chemical Warfare Service: Edgewood Arsenal, MD, 1924, UNCLASSIFIED Report (AD-B958296).
- <sup>7</sup>Henley, F.M. Surveillance Tests on 75 mm Steel Gas Shell Extending Over a Period of One Year; EACD 11; Chemical Warfare Service: Edgewood Arsenal, MD, 1920, UNCLASSIFIED Report (AD-B959731).
- <sup>8</sup> Siegel, M. *The Corrosive Effect of War Gases on Metals and Materials;* EACD 113; Chemical Warfare Service: Edgewood Arsenal, MD, 1921, UNCLASSIFIED Report (AD-B955153).

Table E-12: Phosgene Oxime (CX)

Alternate Designations: Fosgen Oksim; Phosgen-oxime

Chemical Name: Dichloroformoxime

Synonyms: 1,2-Dichloroformoxime; Dichloroformaldoxime; Dichloroximinomethane; Dichlorformaldehydoxime; Kohlensaure-dichlorid-oxime; Dichlormethylen-hydroxylamine; Carbonyl chloride oxime

Chemical Abstract Service Registry No: 1794-86-1

Registry of Toxic Effects of Chemical Substances No: Data not available

### **Physical and Chemical Properties**

Structural Formula:

Molecular Formula: CHCl<sub>2</sub>NO Molecular Weight: 113.93

Wichecular Weight. 113.33	
Physical State	Colorless crystalline deliquescent solid, when pure (1)
Odor	Unpleasant and irritating (1); resembles new-mown hay at low concentrations (2)
Boiling Point	129 °C (3) (with decomposition unless highly pure)
Freezing Point	39 °C (melting point) (3)
Liquid Density (g/mL)	Data not available
Vapor Density (relative to air)	3.9 (calculated)
Vapor Pressure (torr)	2.43 x 10 <sup>1</sup> @ 50 °C (3)
Volatility (mg/m³)	1.37 x 10 <sup>5</sup> @ 50 °C (calculated from vapor pressure) (3)
Latent Heat of Vaporization (kcal/mol)	11.2 @ 50 °C (calculated from vapor pressure) (3)
Flash Point	Data not available
Decomposition Temperature	Below 129 °C (4)
Solubility	Very soluble in both water and common organic solvents (5)
Rate of Hydrolysis	Slow in water@ ambient temperature and pH 7; hydrolyzes 5% within six days @ ambient temperature; dilute acids slow down the hydrolysis rate even further; whereas basic solutions react very violently with CX (2)
Hydrolysis Products	Carbon dioxide, hydrogen chloride, and hydroxylamine (2)
Stability in Storage	Pure unstabilized CX, decomposes on storage @ ambient temperature. If stored @ -20 °C it can be kept indefinitely. (1) CX is extremely unstable in the presence of impurities such as metals; even trace amounts of iron chloride may cause explosive decomposition (2)
Action on Metals or Other Materials	Metals especially iron cause rapid decomposition of CX; trace amounts of iron chloride may cause explosive decomposition (2) Also attacks rubber, especially upon heating. (5)

# Table E-12: Phosgene Oxime (CX) (Continued)

<sup>&</sup>lt;sup>1</sup>Witten, B. *The Search for Toxic Chemical Agents (U);* EATR 4210; Edgewood Arsenal Research Laboratories: Edgewood Arsenal, MD, 1969, UNCLASSIFIED Report (AD-507852).

<sup>&</sup>lt;sup>2</sup> Petersen, T.G. *Agent CX (Phosgene Oxime) Summary Report (U);* CRDL Special Publication 7; U.S. Army Chemical Research and Development Laboratories: Edgewood Arsenal, MD, 1965, CONFIDENTIAL Report (AD-367890).

<sup>&</sup>lt;sup>3</sup> Penski, E, C. *Vapor Pressure Data Analysis of Dichloroformoxime;* ERDEC-TR-042; U.S. Army Chemical and Biological Defense Agency: Aberdeen Proving Ground, MD, 1993, UNCLASSIFIED Report (AD-A265873).

<sup>&</sup>lt;sup>4</sup> Properties of War Gases Volume II: Blood and Nettle Gases (U); ETF 100-41/Vol-2; Chemical Corps Board: Army Chemical Center, MD, 1956, CONFIDENTIAL Report (AD-108457).

<sup>&</sup>lt;sup>5</sup> Prandtl, W.; Sennewald, K. Trichloronitrosomethane, Dichloroformoxime (Phosgene Oxime) and Their Derivatives. *Chemische Berichte*. **1929**, **62**, p 1766.

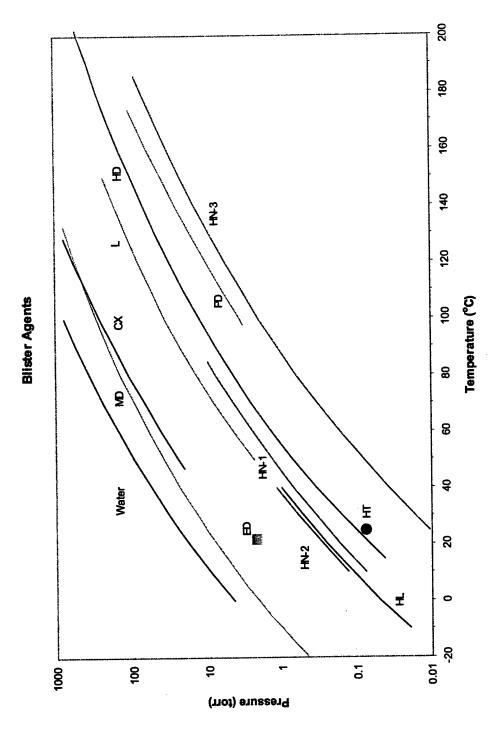


Figure E: Vapor Pressure of Blister Agents

Blank

#### APPENDIX F

### **INCAPACITATING AGENT**

## Table F: Quinuclidínyl Benzilate (BZ)

Alternate Designation: EA 2277; CS 4030; Oksilidin; QNB

Chemical Name: 3-Quinuclidinyl benzilate

Synonym: Benzilic acid, 3-quinuclidinyl ester; 1-Azabicyclo (2.2.2) octan-3-ol, benzilate; Benzeneacetic acid, alpha-hydroxy-alpha-phenyl-,1-azabicyclo (2.2.2)oct-3-yl ester; 3-Chinuclidylbenzilate; 3-(2,2-Diphenyl-2-hydroxyethanoyloxy)-quinuclidine; 3-Quinuclidinol benzilate; 3-Quinuclidyl benzilate

Chemical Abstract Service Registry Number: 6581-06-2

Registry of Toxic Effects of Chemical Substances Number: DD4638000

#### **Physical and Chemical Properties**

#### Structural Formula:

Molecular Formula: C<sub>21</sub>H<sub>23</sub>NO<sub>3</sub> Molecular Weight: 337.42

Molecular Weight: 337.42	
Physical State	White crystalline solid (1)
Odor	None (2)
Melting Point	167.5 °C (3)
Boiling Point	412 °C (extrapolated) (4)
Solid Density (g/cm³)	Bulk: 0.51(2)
	Crystal: 1.33 (2)
Vapor Density	11.6 (calculated)
Vapor Pressure (torr)	1.43 x 10 <sup>-10</sup> @ 25 °C (extrapolated); 4.74 x 10 <sup>-13</sup> @ 0 °C (extrapolated) (4)
Volatility (mg/m³)	2.60 x 10 <sup>-6</sup> @ 25 °C; 9.0 x 10 <sup>-9</sup> @ 0 °C (calculated from vapor pressure) <b>(4)</b>
Latent Heat of Vaporization (kcal/mol)	21.2 (calculated from Clausius Clapeyron equation which assumes constant heat of vaporization as a function of temperature) (4)
Flash Point	Pure: 246 °C (2)
	Munitions grade: 220 °C (2)
Decomposition Temperature	Stable up to the melting point. During prolonged heating at temperatures approximately 170 °C, BZ begins to decompose, producing carbon dioxide, benzophenone, benzhydrol, and other products. The rate of decomposition is both temperature and purity dependent. (1)

Table F: Quinuclidinyl Benzilate (BZ) (Continued)

Solubility	Solubility in water is approximately 1.18 g/L (5) Slightly soluble in water; soluble in dilute acids and common organic solvents such as alcohol and chloroform; insoluble in aqueous alkali. (1)
Rate of Hydrolysis	t <sub>1/2</sub> = 6.7 hr @ 25 °C and pH 9.8; <b>(6)</b>
,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	t <sub>1/2</sub> = 1.8 min @ 25 °C and pH 13+; <b>(6)</b>
	t <sub>1/2</sub> = 3 to 4 weeks @ 25 °C in moist air and pH 7 (6)
	t <sub>1/2</sub> = 12 min @ 37 °C and pH 12; <b>(5)</b>
	t <sub>1/2</sub> = 1.4 hr @ 50 °C and pH 8.5; <b>(5)</b>
	t <sub>1/2</sub> = 9.5 hr @ 100 °C and pH 0; <b>(5)</b>
Hydrolysis Products	3-Quinuclidinol and benzylic acid. (6)
Stability in Storage	Stable in aluminum and stainless steel @ 71 °C for at least 2 years. (7)
Action on Metals or Other Materials	Slight pitting of aluminum and stainless steel occurs after 2 years @ 71 °C (7)

<sup>&</sup>lt;sup>1</sup>Witten, B. *The Search for Toxic Chemical Agents (U);* EATR 4210; Edgewood Arsenal Research Laboratories: Edgewood Arsenal, MD, 1969, UNCLASSIFIED Report (AD-507852).

<sup>&</sup>lt;sup>2</sup> Chemical Agent Data Sheets Volume I; Edgewood Arsenal Special Report EO-SR-74001; U.S. Army Armament Command: Edgewood Arsenal, Aberdeen Proving Ground, MD, 1974, UNCLASSIFIED Report (AD-B028222).

<sup>&</sup>lt;sup>3</sup> Lochboehler, C.M. *The Physical Properties of the Glycolates (U)*; EASP-100-61; U.S. Army Munitions Command; Chemical Research Laboratory; Edgewood Arsenal, MD, 1970, CONFIDENTIAL Report, (AD-508308).

<sup>&</sup>lt;sup>4</sup> Cogliano, J.A.; Braude, G.L. *Corrosion, Compatibility and Other Physicochemical Studies (U), Final Report –Task II;* DA18-108-CML-6602; W.R. Grace and Company, Washington Research Center: Clarksville, MD, 1963, UNCLASSIFIED Report (AD-359603).

<sup>&</sup>lt;sup>5</sup> Rosenblatt, D.H.; Dacre, J.C.; Shiotsuka, R.N.; Rowlett, C.D. *Problem Definition Studies on Potential Environmental Pollutants VIII*; Chemistry and Toxicology of BZ (3-Quinuclidinyl Benzilate); USAMBRDL-TR 7710; U.S. Army Medical Bioengineering Research and Development Laboratory; Fort Detrick: Frederick, MD, 1977, UNCLASSIFIED Report (AD-B030349).

<sup>&</sup>lt;sup>6</sup> Sass, S.; Master, I. Basic Esters of Glycolic Acids (U): Part III Analysis and Chemical Properties of Microgram and Larger Quantities of EA 2277 and Related Compounds; CRDLR 3088; U.S. Army Chemical Research and Development Laboratories: Army Chemical Center, MD, 1961, UNCLASSIFIED Report (AD-325351).

<sup>&</sup>lt;sup>7</sup>Brooks, M.E.; Coglliano, J.A; Braude, G.L. *Corrosion, Compatibility and Other Physicochemical Studies (U)*, DA18-108-CML-6602 (A), Final Report – Task I; W.R. Grace and Company; Washington Research Center: Clarksville, MD, 1964, UNCLASSIFIED Report (AD-350755).

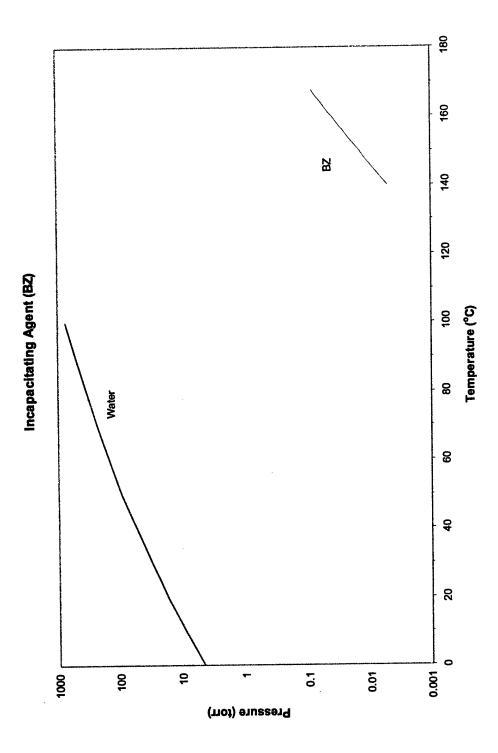


Figure F: Vapor Pressure of Incapacitating Agent (BZ)

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#### **APPENDIX G**

#### RESPIRATORY IRRITANTS

# Table G-1: Diphenylchloroarsine (DA)

Alternate Designations: Clark I (German); Blue Cross (German); Sternite (French); Sneezing gas; DIK;

Chemical Name: Diphenylchloroarsine

Synonyms: Arsine, chloro, diphenyl; Chlorodiphenylarsine; Diphenylarsenious chloride; Chlorodiphenylarsine; Arsinous chloride, diphenyl-; Diphenyl arsenic chloride; Chlor-difenylarsin (Czech); Chlorodiphenylarsine; Difenylchlorarsin (Czech); Diphenylarsinous chloride; Diphenylchlorarsine (Dutch)

Chemical Abstract Service Registry Number: 712-48-1

Registry of Toxic Effects of Chemical Substances Number: CG9900000

## **Physical and Chemical Properties**

Structural Formula:

Molecular Formula: C<sub>12</sub>H<sub>10</sub>AsCl Molecular Weight: 264.59

Molecular vveignt: 264.59	
Physical State	Colorless crystalline solid when pure (1)
Odor	None (1)
Boiling Point	383 °C (extrapolated) decomposes (2)
Freezing Point	37.3 °C (3); 39 to 44 °C (melting point) (2) DA also exists in an unstable modification which melts between 18.2 to 18.4 °C (3)
Liquid Density (g/mL)	1.3875 @ 50 °C (3)
Vapor Density (relative to air)	9.1 (calculated)
Vapor Pressure (torr)	1.79 x 10 <sup>-2</sup> @ 50 °C (extrapolated) (3)
Volatility (mg/m³)	2.36 x 10 <sup>2</sup> @ 50 °C (calculated from vapor pressure) (3)
Latent Heat Vaporization (kcal/mol)	15.1 (calculated from Clausius Clapeyron equation which assumes constant heat of vaporization as a function of temperature) (3)
Flash Point	350 °C (1)
Decomposition Temperature	300 to 350 °C (2)
Solubility	Solubility in water is 0.078 g/L @ 37 °C. (4) Soluble in acetone, ether (5) ethanol, benzene; carbon tetrachloride, ethylene chloride, chloroform, and dichloroethylene (2,5)
Rate of Hydrolysis	Slow in bulk but rapid when finely divided. (2)
Hydrolysis Products	Diphenylarsenious oxide and hydrogen chloride. (2)
Stability in Storage	Stable when pure. Stable in steel shells for almost 4 months @ 60 °C and for 1 year @ room temperature (2)
Action on Metals or Other Materials	None when dry (2)

# Table G-1: Diphenylchloroarsine (DA) (Continued)

<sup>&</sup>lt;sup>1</sup> Lau, T.M.K. *Brief Evaluation of the Possibilities of Using Arsenicals as Incapacitating Agents*; CRDEC-TR-87061; U.S. Army Chemical Research, Development and Engineering Center: Aberdeen Proving Ground, MD, 1987, UNCLASSIFIED Report (AD-B114319).

<sup>&</sup>lt;sup>2</sup> Macy, R. Constants and Physiological Action of Chemical Warfare Agents; EATR 78; Chemical Warfare Service: Edgewood Arsenal, MD, 1932, UNCLASSIFIED Report (AD-B956574).

<sup>&</sup>lt;sup>3</sup> Owens, R. Diphenylcyanoarsine: Part V – The Physical Properties of M.A., D.A. T.A., and D.C.; SO/R 492; Sutton Oak, England, 1940, UNCLASSIFIED Report (AD-E486397).

<sup>&</sup>lt;sup>4</sup>Carter, R.H.; Knight, H.C. Fundamental Study of Toxicity: Solubility of Certain Toxics in Water and in Olive Oil; EACD 445; Chemical Warfare Service: Edgewood Arsenal, MD, 1928, UNCLASSIFIED Report (AD-B955216).

<sup>&</sup>lt;sup>5</sup> CRC Handbook of Chemistry and Physics; 82<sup>nd</sup> ed.; Lide, D.R., Ed.; Section 3; CRC Press: Washington, DC, 2001; p

# Table G-2: Diphenylcyanoarsine (DC)

Alternate Designations: CLARK II (German); Clark 2 (German); Blue Cross (German), Sternite (French)

Chemical Name: Diphenylcyanoarsine

Synonyms: Diphenylarsinous cyanide; Diphenylarsinecarbonitrile; Arsinous cyanide, diphenyl-; Arsinecarbonitrile diphenyl-

Chemical Abstract Service Registry Number: 23525-22-6

Registry of Toxic Effects of Chemical Substances Number: Data not available

**Physical and Chemical Properties** 

Structural Formula:

Molecular Formula: C<sub>13</sub>H<sub>10</sub>AsN Molecular Weight: 255.15

Molecular Weight: 255.15	
Physical State	Colorless crystalline solid (1)
Odor	Similar to garlic and bitter almonds (1)
Boiling Point	341 °C (extrapolated) decomposes (2)
Freezing Point	31.2 °C (2)
Liquid Density (g/mL)	1.3338 @ 35 °C (2)
Vapor Density (relative to air)	8.8 (calculated)
Vapor Pressure (torr)	7.2 x 10 <sup>-4</sup> @ 35 °C (extrapolated) (2)
Volatility (mg/m³)	9.56 @ 35 °C (calculated from vapor pressure) (2)
Latent Heat of Vaporization (kcal/mol)	17.1 (calculated from Clausius Clapeyron equation which assumes constant heat of vaporization as a function of temperature) (2)
Flash Point	Low (1)
Decomposition Temperatures	Above 240 °C (2)
Solubility	Solubility in water is 0.021 g/L @ 37 °C (3); Soluble in chloroform and other organic solvents (4)
Rate of Hydrolysis	Very slow (1)
Hydrolysis Products	Hydrogen cyanide and diphenylarsenious oxide (1)
Stability in Storage	Stable at all ordinary temperatures (1)
Action on Metals or Other Material	None on metals (4)
t	<u>, , , , , , , , , , , , , , , , , , , </u>

# Table G-2 Diphenylcyanoarsine (DC) (Continued)

<sup>&</sup>lt;sup>1</sup> Lau, T.M.K. *Brief Evaluation of the Possibilities of Using Arsenicals as Incapacitating Agents;* CRDEC-TR-87061; U.S. Army Chemical Research, Development and Engineering Center: Aberdeen Proving Ground, MD, 1987, UNCLASSIFIED Report (AD-B114319).

<sup>&</sup>lt;sup>2</sup> Owens, R. *Diphenylcyanoarsine: Part V – The Physical Properties of M.A., D.A. T.A., and D.C.;* SO/R 492; Sutton Oak, England, 1940, UNCLASSIFIED Report (AD-E486397).

<sup>&</sup>lt;sup>3</sup> Carter, R.H.; Knight, H.C. Fundamental Study of Toxicity: Solubility of Certain Toxics in Water and in Olive Oil; EACD 445; Chemical Warfare Service: Edgewood Arsenal, MD, 1928, UNCLASSIFIED Report (AD-B955216).

<sup>&</sup>lt;sup>4</sup> Franke, S. *Manual of Military Chemistry Volume I- Chemistry of Chemical Warfare Agents*; ACSI-J-3890; Chemie der Kampfstoffe, East Berlin, 1968, UNCLASSIFIED Technical Manual (AD-849866).

## Table G-3: Adamsite (DM)

Alternate Designations: Azine; RI5

Chemical Name: 10-Chloro-5,10-dihydrophenarsazine

Synonyms: Diphenylamine chloroarsine; Diphenylamine arsenious chloride; Phenarsazine chloride; 1-Chloro-1,6-dihydrophenarsazine; 10-Chlorophenarsazine; 6-Chlorophenarsazine, Phenarsazine, 10-chloro-5,10-dihydro-; 5-Aza-10-arsenaanthracene chloride; 10-Chloro-5,10-dihydroarsacridine; Diphenylaminechlorarsine; Fenarsazinchlorid (Czech); Phenazsarine chloride; 10-chloro-9,10-dihydro-phenarsazine

Chemical Abstract Service Registry Number: 578-94-9

Registry of Toxic Effects of Chemical Substances Number: SG0680000

#### **Physical and Chemical Properties**

#### Structural Formula:

Molecular Formula: C<sub>12</sub>H<sub>9</sub>AsClN

Wiolcodia Formala. O 12. Is to all	
Molecular Weight: 277.58	
Physical State	Light yellow to green crystals (1)
Odor	No pronounced odor, but irritating (2)
Boiling Point	410 °C (extrapolated) decomposes (3)
Freezing Point	195 °C (melting point) with slight decomposition (3)
Solid Density (g/cm³)	1.648 @ 20 °C; 1.672 @ 0 °C (4)
Vapor density (relative to air)	9.6 (calculated)
Vapor Pressure (torr)	Negligible @ ambient temperature (5,6)
Volatility (mg/m³)	Negligible @ ambient temperature (5,6)
Latent Heat of Vaporization (kcal/mol)	14.2 @ 410 °C (calculated from vapor pressure) (5)
Flash Point	Nonflammable (2)
Decomposition Temperatures	Slight decomposition @ 195 °C; (3) 0.02% per min @ 200 °C; and 0.15% per min @ 250 °C (5)
Solubility	Solubility in water is 0.044 g/L @ 37 °C. (7) Slightly soluble in benzene xylene, carbon tetrachloride (8,9) acetone, alcohols, tetrachlorethane (9)
Rate of Hydrolysis.	When solid DM is covered with water it slowly hydrolyzes and a protective oxide coating forms that hinders further hydrolysis. Finely divided DM hydrolyzes rapidly. (4) Acidic solutions prevent hydrolysis. 0.5% HCI @ room temperature and 0.8% at temperatures between 70-80 °C (4)
Hydrolysis Products.	Diphenylaminearsenious oxide and hydrochloric acid (4)
Stability in Storage.	At room temperature, DM is stable for at least 1 year when pure and 6 months with munitions grade material. (10) Stable in aluminum and stainless steel for at least 2 years @ 71 °C when pure, but the containers are severely pitted (10)
Action on Metals or Other Material.	After 3 months causes extensive corrosion on aluminum and stainless steel @ 71 °C. (10); Also corrodes iron, bronze and brass (8)

## Table G-3: Adamsite (DM) (Continued)

- <sup>1</sup> Sax's Dangerous Properties of Industrial Materials; 10<sup>th</sup> ed.; Lewis, R.J., Ed.; Volume 3; John Wiley & Sons, Inc.: New York, 2001; p 2875.
- <sup>2</sup> Lau, T.M.K. Brief Evaluation of the Possibilities of Using Arsenicals as Incapacitating Agents; CRDEC-TR-87061; U.S. Army Chemical Research, Development and Engineering Center: Aberdeen Proving Ground, MD, 1987, UNCLASSIFIED Report (AD-B114319).
- <sup>3</sup> Klosky, S.; Stricker, P.F. *Physico Chemical Constants of Diphenylaminochlorarsine;* EATR 58; Chemical Warfare Service: Edgewood Arsenal, MD, July 1921, UNCLASSIFIED Report (AD-B955024).
- <sup>4</sup>Macy, R. Constants and Physiological Action of Chemical Warfare Agents; EATR 78; Chemical Warfare Service: Edgewood Arsenal, MD, 1932, UNCLASSIFIED Report (AD-B956574).
- <sup>5</sup> Parker, D.H. *Vapor Pressure of D.M. (Diphenylaminechloroarsine);* EATR 46; Chemical Warfare Service: Edgewood Arsenal, MD, 1921, UNCLASSIFIED Report (AD-B955053).
- <sup>6</sup> Properties of War Gases Volume III: Vomiting & Choking Gases & Lacrimators (U); ETF 100-41/Vol-3; Chemical Corps Board: Army Chemical Center, MD, 1944, CONFIDENTIAL Report (AD-108458).
- <sup>7</sup> Carter, R.H.; Knight, H.C. Fundamental Study of Toxicity: Solubility of Certain Toxics in Water and in Olive Oil; EACD 445; Chemical Warfare Service: Edgewood Arsenal, MD, 1928, UNCLASSIFIED Report (AD-B955216).
- <sup>8</sup> The Merck Index: An Encyclopedia of Chemicals, Drugs, and Biologicals; 13<sup>th</sup> ed.; O'Neil, M.J., Ed.; Merck & Company, Inc.: New Jersey, 2001; p 1294.
- <sup>9</sup> Kibler, A.L. Fundamental Study of Toxicity Miscellaneous Data; EACD 456; Chemical Warfare Service: Edgewood Arsenal, MD, 1928, UNCLASSIFIED Report (AD-B955210).
- <sup>10</sup> Brooks, M.E.; Coglliano, J.A; Braude, G.L. Corrosion, Compatibility and Other Physicochemical Studies (U), DA18-108-CML-6602 (A), Final Report Task I; W.R. Grace and Company; Washington Research Center: Clarksville, MD, 1964, UNCLASSIFIED Report (AD-350755).

Table G-4: Chlorine

Alternate Designations: Bertholite		
Chemical Name: Chlorine		
Synonyms: Chloor (Dutch); Chlor (German); Chlore (French); Chlorine mol.; Cloro (Italian); Molecular chlorine		
Chemical Abstract Service Registry Number: 7782-50-5		
Registry of Toxic Effects of Chemical Substances Number: FO2100000		
Physical and Chemical Properties		
Structural Formula:		
	CI—CI	
Molecular Formula: Cl <sub>2</sub>		
Molecular Weight: 70.91		
Physical State	Greenish-yellow diatomic gas (1)	
Odor	Disagreeable and suffocating; irritating to the nose and throat (2)	
Boiling Point	-34.7 °C (3,4)	
Freezing Point	-101.6 °C <b>(5)</b>	
Liquid Density (g/mL)	Liquified chlorine: 1.393 @ 25 °C; 1.468 @ 0 °C (4)	
Vapor Density (relative to air)	2.4 (calculated)	
Vapor Pressure (torr)	5.75 x 10 <sup>3</sup> @ 25 °C; 2.73 x 10 <sup>3</sup> @ 0 °C (3,4)	
Volatility (mg/m³)	2.19 x 10 <sup>7</sup> @ 25 °C; 1.14 x 10 <sup>7</sup> @ 0 °C (calculated from vapor pressure) (3,4)	
Latent Heat of Vaporization (kcal/mol)	4.86 @ 25 °C; 4.80 @ 0 °C; (calculated from vapor pressure) (3,4)	
Flash Point	Nonflammable (2)	
Decomposition Temperature	Above 600 °C (5)	
Solubility	Solubility in water is 0.63 g/100g water @ 25 °C. Solubility in carbon tetrachloride is 3.5% @ ambient temperature (5)	
Rate of Hydrolysis	Slow (6)	
Hydrolysis Products	HCI and HOCI (5)	
Stability in Storage	Stable when dry (5)	
Action on Metals or Other Materials	None if chlorine is dry. Vigorous action with metals when chlorine is moist due to the presence of hypochlorous acid. (5)	

## **Table G-4: Chlorine (Continued)**

<sup>&</sup>lt;sup>1</sup> The Merck Index: An Encyclopedia of Chemicals, Drugs, and Biologicals; 13<sup>th</sup> ed.; O'Neil, M.J., Ed.; Merck & Company, Inc.: New Jersey, 2001; p. 361.

<sup>&</sup>lt;sup>2</sup> Matheson Gas Data Book, 7<sup>th</sup> ed.; Yaws, C.L. Ed.; McGraw-Hill Companies: New York, 2001; p 162.

<sup>&</sup>lt;sup>3</sup> Abercrombie, P., Edgewood Chemical Biological Center Notebook # NB 98-0079 p 32 (U).

<sup>&</sup>lt;sup>4</sup> Beebe, C.H. *Important Constants of Fourteen Common Chemical Warfare Agents*; EACD 328; Chemical Warfare Service: Edgewood Arsenal, MD, 1924, UNCLASSIFIED Report (AD-B958296).

<sup>&</sup>lt;sup>5</sup> Macy, R. *Constants and Physiological Action of Chemical Warfare Agents*; EATR 78; Chemical Warfare Service: Edgewood Arsenal, MD, 1932, UNCLASSIFIED Report (AD-B956574).

<sup>&</sup>lt;sup>6</sup> Military Chemistry and Chemical Agents; TM 3-215/AFM 355-7; Departments of the Army and the Air Force: Washington, DC, December 1963; UNCLASSIFIED Technical Manual (AD-A292141).

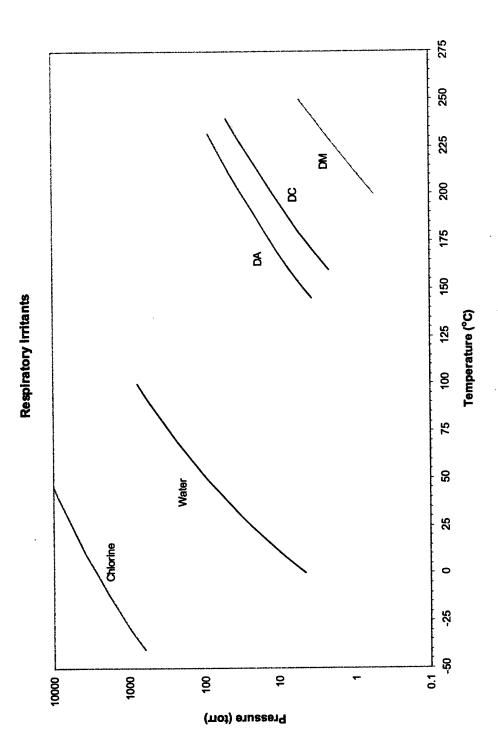


Figure G: Vapor Pressure of Respiratory Irritants

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### APPENDIX H

#### **RIOT CONTROL AGENTS**

## Table H: Capsaicin (Pepper Spray)\*

Alternate Designations: D.C.; Pepper Spray.

Chemical Name: Trans-8-methyl-N-vanillyl-6-nonenamide

Synonym: Vanillyl decenamide; 8-Methyl non-6-enoyl vanillylamide; 8 Methyl nonen-6-oxyl-vanillyl amide;

N-(4-Hydroxy-3-methoxybenzyl)-8-methylnon-trans-6-enamide; (E)-N-[(4-Hydroxy-3-methoxyphenyl)methyl]-8-methyl-6-nonenamide; Trans-8-methyl-N-vanillyl-6-nonenamide; 6-Nonenamide, N-((4-Hydroxyl-3-methoxyphenyl)methyl)-8-methyl-, (E)-; 6-Nonenamide, 8-methyl-N-vanillyl-, (E)

Chemical Abstract Service Registry Number: 404-86-4

Registry of Toxic Effects of Chemical Substances Number: RA8530000

#### **Physical and Chemical Properties**

Structural Formula:

Molecular Formula: C<sub>18</sub>H<sub>27</sub>NO<sub>3</sub> Molecular Weight: 305.42

Wolesdan Weight: See: 12	
Physical State	Colorless monoclinic plates (1,2)
Odor	Pungent, irritating (1)
Boiling Point	340.4 °C (extrapolated) (3)
Freezing Point	65 °C (2,4)
Liquid density (g/mL)	Data not available
Vapor Density (relative to air)	10.5 (calculated)
Vapor Pressure (torr)	1.5 x 10 <sup>-7</sup> @ 65 °C (extrapolated) (3)
Volatility (mg/m³)	2.2 x 10 <sup>-3</sup> @ 65 °C (calculated from vapor pressure) (3)
Latent Heat of Vaporization (kcal/mol)	33.4 (calculated from Clausius Clapeyron equation which assumes constant heat of vaporization as a function of temperature) (3)
Flash Point	Capsaicin in the form of pepper spray may be flammable or nonflammable depending on the type of delivery (carrier) system used. (5)
Decomposition Temperature	Above 150 °C (3)
Solubility	Solubility in water is 0.090 g/ L @ 37 °C (6) Soluble in alcohol, ether, chloroform, carbon disulfide, conc. HCl, aromatic solvents, hydrocarbons, ketones, and aqueous alkali (1,2,7)
Rate of Hydrolysis	Data not available

## Table H: Capsaicin (Pepper Spray)\* (continued)

Hydrolysis Products	Alkaline hydrolysis yields vanillylamine and isomeric decenoic acid (7)
Stability in Storage	Data not available
Action on Metals or Other Materials	Data not available

<sup>\*</sup>Capsaicin is the principal capsaicinoid compound present in oleoresin capsicum (OC). Oleoresin capsicum (OC) is commonly known as pepper spray. When pepper spray is combined with various carrier systems, (i.e., isopropyl alcohol, methylene chloride, water, etc.) it has the potential of being an effective riot control agent

<sup>&</sup>lt;sup>1</sup> Sherrill, M.L. *Investigation of the Synthesis of Capsaicin and Related Compounds;* EACD 307; U.S. Army Chemical Research Laboratories: Edgewood Arsenal, MD, 1924, UNCLASSIFIED Report (AD-B955292).

<sup>&</sup>lt;sup>2</sup> Steadman, A. *Isolation of Capsaicin from Capsicum;* EACD 188; U.S. Army Chemical Research Laboratories: Edgewood Arsenal, MD, 1922, UNCLASSIFIED Report (AD-B955131).

<sup>&</sup>lt;sup>3</sup>Watson, P.D. Determination of the Vapor Pressure of D.C.; EACD 79; Chemical Warfare Service: Edgewood Arsenal, MD, 1921, UNCLASSIFIED Report (AD-B959611).

<sup>&</sup>lt;sup>4</sup> Nelson, E.K.; Dawson, L.E. The Constitution of Capsaicin, The Pungent Principle of Capsicum. III. *J. Am. Chem. Soc.* **1923**, *45*, p 2179.

<sup>&</sup>lt;sup>5</sup> Daroff, P.M.; Metz, D.; Roberts, A.; Adams, J.A.; Jenkins, W. *Oleoresin Capsicum: An Effective Less-Than Lethal Riot Control Agent;* DPG/JCP-097-002; Chemical Biological Defense; U.S. Army Dugway Proving Ground, UT, 1997, UNCLASSIFIED Report (AD-B225032).

<sup>&</sup>lt;sup>6</sup> Carter, R.H.; Knight, H.C. Fundamental Study of Toxicity: Solubility of Certain Toxics in Water and in Olive Oil; EACD 445; Chemical Warfare Service: Edgewood Arsenal, MD, 1928, UNCLASSIFIED Report (AD-B955216).

<sup>&</sup>lt;sup>7</sup>Rosenberg, H.R.; Sharp, S.S. *Evaluation and Synthesis of Chemical Compounds Volume II, Final Comprehensive Report November 1961 – February 1965;* Contract No. DA-18-108-CML-6673 (A); E.I. Du Pont De Nemours and Company Industrial and Biochemicals Department: Wilmington, DE, 1965, UNCLASSIFIED Report (AD-B253543).

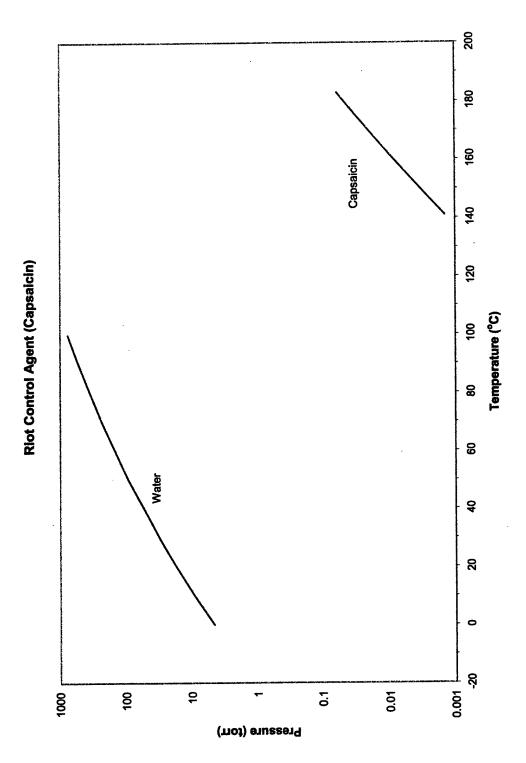


Figure H: Vapor Pressure of Riot Control Agent (Capsaicin)

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#### APPENDIX I

#### CHEMICAL AGENT PRECURSORS

## Table I-1: Methylphosphonic Difluoride (DF)

Alternate Designations: Difluoro; EA 1251

Chemical Name: Methylphosphonic Difluoride

Synonyms: Phosphonic difluoride, methyl-; Difluoromethyl phosphonate; Difluoromethylphosphine oxide; Methyl difluorophosphite; Methylphosphonyldifluoride; Phosphonodifluoridic acid, methyl-

Chemical Abstract Service Registry Number: 676-99-3

Registry of Toxic Effects of Chemical Substances Number: TA1840700

**Physical and Chemical Properties** 

Structural Formula:

O || CH<sub>3</sub>---P---F

Molecular Formula: CH<sub>3</sub>F<sub>2</sub>PO

Molecular vveignt: 100.00	
Physical State	Liquid (1)
Odor	Pungent, acid like (1)
Boiling Point	99.7 °C <b>(2)</b>
Freezing Point	- 36.9 °C (3)
Liquid Density (g/mL)	1.3595 @ 25 °C; 1.4060 @ 0 °C (extrapolated) (2)
Vapor Density (relative to air)	3.4 (calculated)
Vapor Pressure (torr)	3.6 x 10 <sup>1</sup> @ 25 °C; 8.5 @ 0 °C (extrapolated) (2)
Volatility (mg/m³)	$1.9 \times 10^5$ @ 25 °C; $5.0 \times 10^4$ @ 0 °C (calculated from vapor pressure) (2)
Latent Heat of Vaporization (kcal/mol)	9.2 @ 25 °C; 9.5 @ 0 °C (calculated from vapor pressure) (2)
Flash Point	Nonflammable (4)
Decomposition Temperature	Data not available
Solubility	Immediately decomposes with the addition of water (5)
Rate of Hydrolysis	Virtually instantaneous to produce methylphosphonofluoridic acid (MF) and hydrogen fluoride (HF) which are also toxic. Further hydrolysis is a slow reaction that produces methylphosphonic acid (MPA); MF $t_{1/2}$ = 162 days @ pH 7, $t_{1/2}$ = 90 days @ pH 4, and $t_{1/2}$ = 47 days @ pH 3. <b>(5)</b>
Hydrolysis Products	Hydrolyzes to give toxic products, MF and HF. Further hydrolysis of MF results in MPA and a second mole of HF (5)
Stability in Storage	Remains stable for at least 20 years, when stored in high-density polyethylene containers enclosed in steel. (6) Avoid contact with water mist or sprays, metals, alkaline materials, and some organics. (1) Never store DF with alcohols; DF will react with alcohols to form a lethal chemical, such as crude GB. (7)

#### Table I-1: Methylphosphonic Difluoride (DF) (Continued)

Action on Metals or Other Materials	Incompatible with water, glass, concrete (8), most metals, natural rubber (9), and organic materials like glycols, which is mainly due to the acidic corrosive nature of the hydrolysis products. (1,10-12) HF may react with some metals, to give off hydrogen gas, a potential fire and explosive hazard. (10,13)
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<sup>&</sup>lt;sup>1</sup> Buchi, K.M. *Environmental Overview of Intermediates, By-Products, and Products in the Production of QL, DC, and DF;* CRDEC-TR-076; U.S. Army Chemical Research, Development and Engineering Center: Aberdeen Proving Ground, MD, 1991, UNCLASSIFIED Report (AD-B155651).

- <sup>5</sup> Dahl, A.R.; Bechtold, W.E.; Cheng, Y.S.; Hahn, F.F.; Marshall, T.C. Acute Toxicity of Methylphosphonic Difluoride (DF) Methylphosphonic Dichloride (DC) and their Hydrolysis Products by Inhalation and other Routes in Mice, Rats and Guinea Pigs; CRDEC-CR-86049; U.S. Army Chemical Research, Development and Engineering Center: Aberdeen Proving Ground, MD, 1986, UNCLASSIFIED Report (AD-B105158).
- <sup>6</sup> Jackson, A.M.; Semiatin, W.J. Long-Term Storability of the M20 DF Canister Used in the M687 Binary Projectile; CRDC-TR-84104; U.S. Army Chemical Research, Development and Engineering Center: Aberdeen Proving Ground, MD, 1985, UNCLASSIFIED Report (AD-B092563).
- <sup>7</sup> Hyttinen, L.J.; Dagostin, F.A.; Sze, J.M.; Sakay, G.G.; Szafraniec, L.L. *Mixed Binary Agents New Approach Toward Meeting Expanded Chemical Munitions Effectiveness Requirements;* ARCSL-TR-83080; U.S. Army Armament Research and Development Command: Aberdeen Proving Ground, MD, 1983, CONFIDENTIAL Report (AD-C033576).
- <sup>8</sup> Ellzy, M.; Piffath, R.J.; Bouck, J.B. *Difluor (DF) Flooring Compatibility Studies;* CRDEC-TR-229; U.S. Army Chemical Research, Development and Engineering Center: Aberdeen Proving Ground, MD, 1991, UNCLASSIFIED Report (AD-B154752).
- <sup>®</sup> Corrosion Resistance Tables: Metals, Plastics, Nonmetallics, and Rubbers; 2<sup>nd</sup> ed.; Schweitzer, P.A.. Ed.; Marcel Dekker, Inc.: New York, 1986; pp 572-573.
- <sup>10</sup> Buchi, K.M. *Environmental Overview of Common Industrial Chemicals with Potential Application in the Binary Munitions Program;* CRDEC-TR-87041; U.S. Army Chemical Research, Development and Engineering Center: Aberdeen Proving Ground, MD, 1987, UNCLASSIFIED Report (AD-A186083).
- <sup>11</sup> Thomas, M.T. Research and Development for Candidate Materials for Use as a DF Containment Vessel; CRDC-CR-85058; U.S. Army Chemical Research, Development and Engineering Center: Aberdeen Proving Ground, MD, 1985, UNCLASSIFIED Report (AD-B096058).
- <sup>12</sup> Kay Lau, Tony Man. Glass or Polymer Etching Due to the Reaction of Methylphosphonic Difluoride (DF) with Water (U); CRDEC-TR-86074; U.S. Army Chemical Research, Development and Engineering Center: Aberdeen Proving Ground, MD, 1986, CONFIDENTIAL Report (AD-C039896).
- <sup>13</sup> Tarantino, P.A. *Electrochemical Corrosion Study of Miscellaneous Metals/Alloys with Methylphosphonic Difluoride;* CRDEC-TR-88032; U.S. Army Chemical Research, Development and Engineering Center: Aberdeen Proving Ground, MD, 1987, UNCLASSIFIED Report (AD-B117574).

<sup>&</sup>lt;sup>2</sup> Zeffert, B.M.; Coulter, P.B.; Tannenbaum, H. Properties, Interaction and Esterification of Methylphosphonic Dihalides. *J. Am. Chem. Soc.* **1960**, *82*, p 3843.

³ Furukawa, G.T.; Reilly, M.L.; Piccirelli, J.H.; Tenenbaum, M. Thermodynamic Properties of Some Methylphosphonyl Dihalides From 15 to 335°K, *J. Rsch. NBS Phy. & Chem.* **1964**, *68A*, *No. 4*, p 367.

<sup>&</sup>lt;sup>4</sup> Allan, C.R. *The Relationship Between Oxygen Index and the Flashing Propensity of Explosively Disseminated Liquids; ARCSL-TR-77061;* U.S. Army Armament Research and Development Command, Chemical Systems Laboratory: Aberdeen Proving Ground, MD, 1977; UNCLASSIFIED Report (AD-A045976).

Table I-2: O-(2-Diisopropylaminoethyl)-O'-Ethyl Methylphosphonite (QL)

All	
Alternate Designations: EA 1724; EDMP Chemical Name: O-(2-Diisopropylamino	
	ninoethyl) methylphosphonite; Phosphonous acid, methyl-, 2-[bis(1-
methylethyl)amino]ethyl ethyl ester	
Chemical Abstract Service Registry Nun	
Registry of Toxic Effects of Chemical Su	
Phy	sical and Chemical Properties
Structural Formula:	
CH <sub>3</sub>	
P—(	$O-CH_2CH_2N[CH(CH_3)_2]_2$
CH <sub>3</sub> CH <sub>2</sub> O	
Molecular Formula: C <sub>11</sub> H <sub>26</sub> NO <sub>2</sub> P	
Molecular Weight: 235.31	
Physical State	Liquid (1)
Odor	Strong, fishy (1)
Boiling Point	244.8 °C (extrapolated) (2)
Freezing Point	Data not available
Liquid Density (g/mL)	0.9080 @ 25 °C; 0.9307 @ 0 °C (2)
Vapor Density (relative to air)	8.1 (calculated)
Vapor Pressure (torr)	1.8 x 10 <sup>-2</sup> @ 25 °C (extrapolated); 7.1 x 10 <sup>-4</sup> @ 0 °C (extrapolated) <b>(2)</b>
Volatility (mg/m³)	2.3 x 10 <sup>2</sup> @ 25 °C; 9.8 @ 0 °C (calculated from vapor pressure) (2)
Latent Heat of Vaporization (kcal/mol)	19.4 @ 25 °C; 22.3 @ 0 °C (calculated from vapor pressure) (2)
Flash Point	89 °C (closed cup) (3) In addition, QL has an autoignition temperature of 129 °C. (2) A hydrolysis product, O,O'-diethylmethylphosphonite (TR), has a flash point of 28 °C (4) and an autoignition temperature of 40 °C. (1)
Decomposition Temperature	Data not available
Solubility	Slightly soluble in water. Soluble in methanol, 2-propanol, acetone, and benzene. (5)
Rate of Hydrolysis	Rapid. QL can be completely hydrolyzed within 5hr (6)
Hydrolysis Products	With excess of water by weight, QL primarily forms O-ethyl methylphosphonic acid (YL) and 2-diisopropylaminoethanol (KB), but also forms O-(2-diisopropylaminoethyl) methylphosphonic acid (QA) and ethanol (ZS) as secondary products. With traces of water or other proton donors, QL will produce O,O'-diethyl methylphosphonite (TR) and O,O'-bis-(2-diisopropylaminoethyl) methylphosphonite (LT). (1) TR has a boiling point of 120 °C (4), a vapor pressure of 10 mm Hg @ 20 °C (1) and is flammable. (4)
Stability in Storage	Stable in aluminum, steel and stainless steel containers for at least 6 months @ 71 °C, if kept dry and pure. (5) Always store QL away from heat or ignition sources and sulfur compounds because of the potential to form highly toxic V-agents. (7)
Action on Metals or Other Materials	Satisfactory against aluminum, steel and stainless steel, but not glass unless a stabilizer is used. (5) Reacts with sulfur and sulfur compounds to produce highly toxic VX or VX-like compounds. (7) It is incompatible with calcium hypochlorite (HTH), many chlorinated hydrocarbons, selenium, selenium compounds, moisture, oxidants, and carbon tetrachloride. (1)

### Table I-2: O-(2-Diisopropylaminoethyl)-O'-Ethyl Methylphosphonite QL (Continued)

<sup>&</sup>lt;sup>1</sup> Buchi, K.M. Environmental Overview of Intermediates, By-Products, and Products in the Production of QL, DC, and DF; CRDEC-TR-076; U.S. Army Chemical Research, Development and Engineering Center: Aberdeen Proving Ground, MD, 1991, UNCLASSIFIED Report (AD-B155651).

<sup>&</sup>lt;sup>2</sup> Samuel, J.B.; Penski, E.C.; Callahan, J,J. *Physical Properties of Standard Agents, Candidate Agents, and Related Compounds at Several Temperatures (U);* ARCSL-SP-83015; U.S. Army Armament Research and Development Command: Aberdeen Proving Ground, MD, 1983, UNCLASSIFIED Report (AD-C033491).

<sup>&</sup>lt;sup>3</sup> Butrow, A., Chemical Research and Development Center Notebook #NB 83-0155 p 45 (U).

<sup>&</sup>lt;sup>4</sup> Kinkead, E.R. Evaluation of the Acute Toxicity of Four Compounds Associated with the Manufacture of O-Ethyl-O'- (2-Diisopropyaminoethyl) Methylphosphonite; CRDEC-CR-87077; U.S. Army Chemical Research, Development & Engineering Center: Aberdeen Proving Ground, MD, 1987, UNCLASSIFIED Report (AD-B113969).

<sup>&</sup>lt;sup>5</sup> Brooks, M.E.; Cogliano, J.A.; Braude, G.L. *Final Report – Task VII, Contract DA18-108-CML-6602 (A), Corrosion, Compatibility and Other Physicochemical Studies (U)*, Final Report – Task VII RES-64-86; W. R. Grace & Co.; Washington Research Center; Clarksville, Maryland, 1964, UNCLASSIFIED Report (AD-352753).

<sup>&</sup>lt;sup>6</sup> Rohrbaugh, D.K. Detection and Identification of QL Impurities by Electron and Chemical Ionization Gas Chromatography/ Mass Spectrometry; CRDEC-TR-097; U. S. Army Chemical Research, Development, & Engineering Center: Aberdeen Proving Ground, MD, 1989, UNCLASSIFIED Report (AD-B136428).

<sup>&</sup>lt;sup>7</sup> Nowlin, T.E.; Grula. R.J.; Samuel, J.B.; Callahan, J.J.; Zeffert, B.M. *A New Binary VX Reaction-Two-Liquid System (U);* EATR 4700; U.S. Army Munitions Command: Edgewood Arsenal, MD, 1972, UNCLASSIFIED Report (AD-524088).

Table I-3: Isopropylamine and Isopropyl Alcohol (OPA)

Alternate Designations: N/A

Chemical Name: 2-Propanol (isopropyl alcohol) and Isopropyl amine mixture

Synonyms: N/A

Chemical Abstract Service Registry Number: 2-Propanol: 67-63-0; Isopropyl amine: 75-31-0

Registry of Toxic Effects of Chemical Substances Number: 2-Propanol: NT8050000; Isopropyl amine:

NT8400000

#### **Physical and Chemical Properties**

#### Structural Formula:

72 wt% 2-Propanol

28 wt% Isopropylamine

Molecular Formula: C<sub>3</sub>H<sub>8</sub>O and C<sub>3</sub>H<sub>9</sub>N

Molecular Weight: 2-Propanol: 60.10; Isopropyl amine: 59.11; Average: 59.81 (based on 72:28 wt. %)

Physical State	Colorless liquid (1)
Odor	Alcohol and ammonia (based on the two components) (2)
Boiling Point	60.8 °C (based on Raoult's law calculation) (3)
Freezing Point	Less than - 88 °C (1)
Liquid Density (g/mL)	0.7520 @ 25 °C (1,4); 0.7759 @ 0 °C (extrapolated) (4)
Vapor Density (relative to air)	2.1 (calculated)
Vapor Pressure (torr)	$1.955 \times 10^2$ @ $25$ °C; $6.128 \times 10^1$ @ $0$ °C (based on Raoult's law calculation) (3)
Volatility (mg/m³)	6.288 x $10^5$ @ 25 °C; 2.152 x $10^5$ @ 0 °C (calculated from vapor pressure) (3)
Latent Heat of Vaporization (kcal/mol)	7.51 (calculated from Clausius Clapeyron equation which assumes constant heat of vaporization as a function of temperature) (3)
Flash Point	Less than 0 °C (5)
Decomposition Temperature	Data not available
Solubility	Both 2- propanol and isopropyl amine are miscible in water, alcohol, ether and soluble in acetone, benzene, and chloroform suggesting that OPA has a similar degree of solubility (2,6)
Rate of Hydrolysis	Data not available
Hydrolysis Products	Data not available
Stability in Storage	Relatively stable for at least 5 years at temperatures between ambient and 71 °C, if stored in carbon steel containers lined with an ethylenebutylene copolymer. (7) Store OPA away from heat, open flame, and DF because they react to form highly toxic compounds such as crude GB. (1)
Action on Metals or Other Materials	Reacts readily with oxidizing materials and organophosphorus halides, such as DF. Contact with DF can produce extremely toxic compounds such as crude GB (1)

#### Table I-3: Isopropylamine and Isopropyl Alcohol (OPA) (Continued)

<sup>&</sup>lt;sup>1</sup> Hyttinen, L.J.; Dagostin, F.A.; Sze, J.M.; Sakay, G.G.; Szafraniec, L.L. *Mixed Binary Agents New Approach Toward Meeting Expanded Chemical Munitions Effectiveness Requirements*; ARCSL-TR-83080; U.S. Army Armament Research and Development Command: Aberdeen Proving Ground, MD, 1983, CONFIDENTIAL Report (AD-C033576).

<sup>&</sup>lt;sup>2</sup> The Merck Index: An Encyclopedia of Chemicals, Drugs, and Biologicals; 13<sup>th</sup> ed.; O'Neil, M.J., Ed.; Merck & Company, Inc.: New Jersey, 2001; p 932.

<sup>&</sup>lt;sup>3</sup> Abercrombie, P., Edgewood Chemical Biological Center Notebook #NB 98-0079 p 45 (U).

<sup>&</sup>lt;sup>4</sup> Fielder, D., Chemical Systems Laboratories Notebook #NB-CSL-82-0213 p 13 (U).

<sup>&</sup>lt;sup>5</sup> Allan, C.R. *The Relationship Between Oxygen Index and the Flashing Propensity of Explosively Disseminated Liquids; ARCSL-TR-77061;* U.S. Army Armament Research and Development Command, Chemical Systems Laboratory: Aberdeen Proving Ground, MD, 1977; UNCLASSIFIED Report (AD-A045976).

<sup>&</sup>lt;sup>6</sup> CRC Handbook of Chemistry and Physics; 50<sup>th</sup> ed.; Weast, R.C., Ed.; Section C; The Chemical Rubber Company: Ohio, 1969; pp 440, 453.

<sup>&</sup>lt;sup>7</sup> Sze, J.M.; Simak, R.S. *Binary GB: A Compilation of Relevant Data;* ARCSL-TR-82019; U.S. Army Armament Research and Development Command: Aberdeen Proving Ground, MD, 1983, CONFIDENTIAL Report (AD-C030931).

Table I-4: Sulfur w/ small amounts of Silica Gel (NE)

Alternate Designation: Brimstone

Chemical Name: Sulfur (with small amount of silica aerogel)

Synonyms: Alpha sulfur; Beta sulfur; Atomic sulfur; Bensulfoid; Brimstone; Colloidal sulfur; Collokit; Colsul; Cosan; Crystex; Elemental sulfur; Flowers of sulfur; Flour sulfur; Ground vocle sulphur; Hexasul; Kocide; Kolofog; Kolospray; Kumulus; Microflotox; Orthorhombic sulfur; Precipitated sulfur; Rhombic sulfur; Sofril; Sperlox-s; Spersul; Spersul thiovit; Sublimed sulfur; Sulfidal; Sulforon; Sulfur flower; Sulkol; Super cosan; Sulphur; Sulsol; Sulfur atom; Sulfur ointment; Sulfur vapor; Tesuloii; Thiolux; Thiovit

Chemical Abstract Service Registry Number: Sulfur: 7704-34-9 and 10544-50-0

Registry of Toxic Effects of Chemical Substances Number: Data not available

#### **Physical and Chemical Properties**

Structural Formula:

Molecular Formula: S<sub>8</sub>
Molecular Weight: 256.48

Molecular Weight: 256.48	
Physical State	Rhombic, yellow crystals (1)
Odor	Odorless when pure (2), but many sulfur compounds tend to be vile-smelling
Boiling Point	444.6 °C (1)
Freezing Point	The rhombic form of sulfur transforms into the monoclinic form @ 95.3 °C. The melting point of monoclinic sulfur is 115.21 °C (1)
Solid Density (g/cm³)	2.07 @ 20 °C (2)
Vapor Density (relative to air)	8.8 (calculated)
Vapor Pressure (torr)	1 @ 183.8 °C (3)
Volatility (mg/m³)	9.0 x 10 <sup>3</sup> @ 184 °C (calculated from vapor pressure) (3)
Latent Heat of Vaporization (kcal/mol)	2.21 (4)
Flash Point	207 °C (closed cup) (3)
Decomposition Temperature	Data not available
Solubility	Insoluble in water; slightly soluble in alcohol, ether; soluble in carbon disulfide, benzene (1,2) toluene, liquid NH <sub>3</sub> , acetone, methylene iodide and chloroform (1)
Rate of Hydrolysis	Data not available
Stability in Storage	Always store NE away from heat or ignition sources and QL because of the potential to form highly toxic VX. (5)
Action on Metals or Other Materials	Reacts with QL to produce extremely toxic VX. (5)

#### Table I-4: Sulfur w/ small amounts of Silica Gel (NE) (Continued)

<sup>&</sup>lt;sup>1</sup> The Merck Index: An Encyclopedia of Chemicals, Drugs, and Biologicals; 13<sup>th</sup> ed.; O'Neil, M.J., Ed.; Merck & Company, Inc.: New Jersey, 2001; p 1599.

<sup>&</sup>lt;sup>2</sup> CRC Handbook of Chemistry and Physics; 82<sup>nd</sup> ed.; Lide, D.R., Ed.; CRC Press: Washington, DC, 2001.

<sup>&</sup>lt;sup>3</sup> Sax's Dangerous Properties of Industrial Materials; 10<sup>th</sup> ed.; Lewis, R.J., Ed.; Volume 3; John Wiley & Sons, Inc.: New York, 2001; p 3328.

<sup>&</sup>lt;sup>4</sup> Buchi, K.M. Environmental Overview of Common Industrial Chemicals with Potential Application in the Binary Munitions Program; CRDEC-TR-87041; U.S. Army Chemical Research, Development and Engineering Center: Aberdeen Proving Ground, MD, 1987, UNCLASSIFIED Report (AD-A186083).

<sup>&</sup>lt;sup>5</sup> Nowlin, T.E.; Grula. R.J.; Samuel, J.B.; Callahan, J.J.; Zeffert, B.M. *A New Binary VX Reaction-Two-Liquid System (U)*; EATR 4700; U.S. Army Munitions Command: Edgewood Arsenal, MD, 1972, UNCLASSIFIED Report (AD-524088).

Table I-5: Dimethyl Polysulfides (containing Elemental Sulfur) (NM)

Alternate Designation: NM5	A TOTAL OF THE PROPERTY OF THE	
Chemical Name: Dimethyl polysulfide mixture [powdered sulfur + dimethyl disulfide (DMDS)]		
Synonyms: Dimethyl disulfide: 2,3-Dithiabutane; Methyl disulfide; (Methyldithio) methane; Disulfide, dimethyl		
Chemical Abstract Service Registry Number: Dimethyl disulfide: 624-92-0		
Registry of Toxic Effects of Chemical S		
Physical and Chemical Properties		
Structural Formula:		
$CH_3$ — $S$ — $S$ — $S$ — $S$ — $CH_3$		
Molecular Formula: C₂H₅S₅	•	
Molecular Weight: 190.37		
Physical State	Liquid (1)	
Odor	Very noxious (2)	
Boiling Point	117 °C (3)	
Freezing Point	<-40 °C (1); DMDS: -84.72 °C (4)	
Liquid Density (g/mL)	1.3895 @ 25 °C (1)	
Vapor Density (relative to air)	6.6 (calculated)	
Vapor Pressure (torr)	DMDS: 2.864 x 10 <sup>1</sup> @ 25 °C (4); Generally vapor pressure decreases with increasing molecular weight (5), thus, NM will probably have a lower vapor pressure than DMDS since its molecular weight will generally be higher.	
Volatility (mg/m³)	DMDS: 1.45 x 10 <sup>5</sup> @ 25 °C (calculated from vapor pressure) (4)	
Latent Heat of Vaporization (kcal/mol)	DMDS: 9.21 @ 25 °C (4); Generally latent heat of vaporization increases with molecular weight of similar compounds (5), thus,	
	the latent heat of vaporization for NM will probably be above	
	9.21 kcal/mol based on DMDS	
Flash Point	105 to 108 °C (6)	
Decomposition Temperature	Data not available	
Solubility	Dimethyl disulfide is soluble in alcohols but insoluble in water. (7,8)	
Rate of Hydrolysis	Data not available	
Hydrolysis Products	Data not available	
Stability in Storage	Satisfactory in storage for at least 1 year at temperatures between - 40 to 71 °C. (1) Always store NM away from heat or ignition sources and QL because of the potential to form highly toxic VX. (6)	
Action on Metals or Other Materials	Stains the surface of steel, and various metal-plated steels when stored in glass vessels for 4 months @ 71 °C. (3) Reacts with QL to produce extremely toxic VX. (6)	

#### Table I-5: Dimethyl Polysulfides (containing Elemental Sulfur) (NM) (Continued)

<sup>&</sup>lt;sup>1</sup> Brown, H.A., Jr.; Newman, J.H.; Armelie, D.; Grula, R.J. *Modified NM: An Improved Liquid Binary VX Reactant (U);* ECTR-76075; U.S. Army Armament Command: Edgewood Arsenal; Aberdeen Proving Ground, MD, 1976, UNCLASSIFIED Report (AD-C008561).

<sup>&</sup>lt;sup>2</sup> Riordan, M.B. *Pilot-Scale Operations of Process for Manufacture of VX Binary Intermediate NM (U);* EM-TR-76055; U.S. Army Armament Command: Edgewood Arsenal, Aberdeen Proving Ground, MD, November 1976, CONFIDENTIAL Report (AD-C008383).

<sup>&</sup>lt;sup>3</sup> Grula, R.J., Armelie, D.; Schenk, W.N. *Compatibility Studies with Candidate Binary VX2 Components;* EC-TM-76009; U.S. Army Armament Command: Edgewood Arsenal; Aberdeen Proving Ground, MD, 1976, UNCLASSIFIED Report (AD-E470951).

<sup>&</sup>lt;sup>4</sup> Scott, D.W.; Finke, H.L.; Gross, M.E.; Guthrie, G.B.; Huffman, H.M. 2,3-Dithiabutane: Low Temperature Heat Capacity, Heat of Fusion, Heat of Vaporization, Vapor Pressure, Entropy and Thermodynamic Functions. *J. Amer. Chem. Soc.*, **1950**, *72*, p. 2424.

<sup>&</sup>lt;sup>5</sup> Properties of War Gases Volume IV: Vesicants (U); ETF 100-41/Vol-4; Chemical Corps Board: Army Chemical Center, MD, 1956, CONFIDENTIAL Report (AD-108459).

<sup>&</sup>lt;sup>6</sup> Nowlin, T.E.; Grula. R.J.; Samuel, J.B.; Callahan, J.J.; Zeffert, B.M. *A New Binary VX Reaction-Two-Liquid System (U);* EATR 4700; U.S. Army Munitions Command: Edgewood Arsenal, MD, 1972, UNCLASSIFIED Report (AD-524088).

<sup>&</sup>lt;sup>7</sup> Buchi, K.M. Environmental Overview of Common Industrial Chemicals with Potential Application in the Binary Munitions Program; CRDEC-TR-87041; U.S. Army Chemical Research, Development and Engineering Center: Aberdeen Proving Ground, MD, 1987, UNCLASSIFIED Report (AD-A186083).

<sup>&</sup>lt;sup>8</sup> CRC Handbook of Chemistry and Physics; 82<sup>nd</sup> ed.; Lide, D.R., Ed.; Section 3; CRC Press: Washington, DC, 2001; p 146.

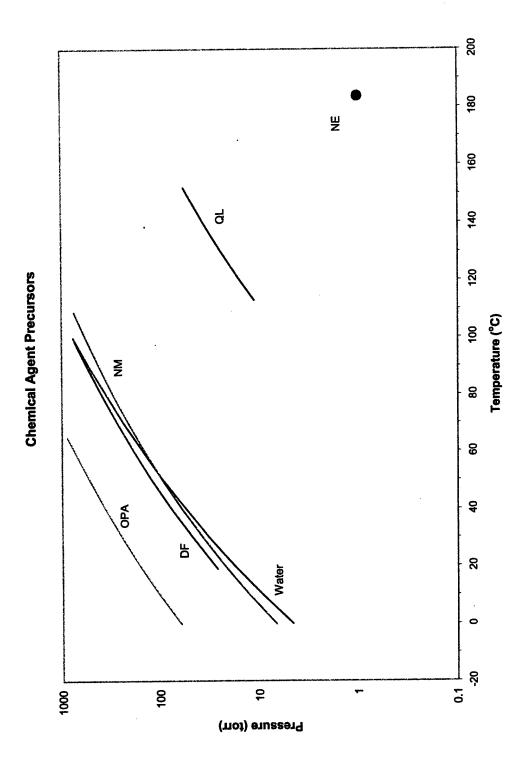


Figure I: Vapor Pressure of Chemical Agent Precursors

# REPLY TO ATTENTION OF

## DEPARTMENT OF THE ARMY US ARMY RESEARCH, DEVELOPMENT AND ENGINEERING COMMAND EDGEWOOD CHEMICAL BIOLOGICAL CENTER 5183 BLACKHAWK ROAD

ABERDEEN PROVING GROUND, MD 21010-5424

RDCB-DPC-RS

FEB 18 2016

MEMORANDUM THRU Director, Edgewood Chemical Biological Center, (RDCB-D/Dr. Joseph L. Corriveau), 5183 Blackhawk Road, Aberdeen Proving Ground, Maryland 21010-3424

FOR Defense Technical Information Center (DTIC), 8725 John J. Kingman Road, Ft Belvoir, VA 22060-6218

SUBJECT: Request for Change in Distribution

- 1. This action is in response to an Edgewood Chemical Biological Center (ECBC) internal request for a Change in Distribution for the attached listed documents.
- 2. The listed documents have current distribution statements or classifications which limit their release. ECBC Subject Matter Experts have reviewed the documents and deem them all suitable for the change in distribution to read "Distribution A: Approved for public release; distribution unlimited."
- 3. The point of contact is Adana Eilo, ECBC Security Specialist, (410) 436-2063 or adana.l.eilo.civ@mail.mil.

Encl

Security Manager

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- 2. Rueggeberg, W. H. C.; Ginsburg, A. *The Synthesis of MCE, Cyano (Dimethylamino) Ethoxyphosphine Oxide*, Chemical Warfare Service Technical Data Memorandum Report 1138, **1945** (ADB968799) Dist. "D"
- 3. Doyle, W. L., et al. *Informal Monthly Progress Report on Toxicity and Irritancy of Chemical Agents, No. N.S.* 3, The University of Chicago Toxicity Laboratory in cooperation with The Medical Division, Chemical Warfare Service, U.S. Army and the Bureau of Medicine and Surgery, U.S. Navy, **1945**. (CBRNIAC-CB-068173) Dist. "E"
- 4. Panariello, V. Monthly Intelligence Report, 40<sup>th</sup> Chemical Laboratory Company, April **1945**. (HDIAC-2075468) Dist. "E"
- 5. Snyder, Jr., H. L.; Hudgin, D. E.; Schlesinger, A. Captured Material Technical Report #60, New German Chemical Warfare Agent, A Cyano Phosphate, 44<sup>th</sup> Chemical Laboratory Company, APO 298, US Army, **1945**. (HDIAC-2075719) Dist. "E"
- 6. Reuggeberg, W.H.C. German Agent MCE, Letter Report of Visit to University of Chicago and University of Illinois, Chemical Division, Edgewood Arsenal, MD, **1945**. (CBRNIAC-CB-114805) Dist. "E"
- 7. Samuel, J. B.; Penski, E. C.; Callahan, J. J. Physical Properties of Standard Agents, Candidate Agents, and Related Compounds at Several Temperatures, UNCLASSIFIED Special Publication ARCSL-SP-83015, U.S. Army Chemical Systems Laboratory, Aberdeen Proving Ground, MD, 1983, (ADC033491) Dist. "E"
- 8. Abercrombie, P.L. Physical Property Data Review of Selected Chemical Agents and Related Compounds: Updating Field Manual 3-9 (FM 3-9); ECBC TR-294; U.S. Army Edgewood Chemical Biological Center: Aberdeen Proving Ground, MD, 2003; Report (ADB294480) Dist. "D"
- 9. Chemical Agent Data Sheets, Volume 1, EO-SR-74001, Department of the Army, Headquarters, Edgewood Arsenal, Aberdeen Proving Ground, Maryland, 1974. (CBRNIAC-CB-007206) Dist. C (export controlled)
- 10. War Department Memorandum, Subject: New German Gas, MCE, Preliminary Report, 19 June **1945**. (CBRNIAC-CB-093876)