

4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

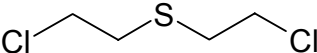
Information regarding the chemical identity of sulfur mustard is located in Table 4-1. Sulfur mustard has several synonyms; the most common are “mustard gas”, “H”, and “HD”. The term “mustard gas” may be used interchangeably to identify “sulfur mustard.” “H” refers to undistilled or raw sulfur mustard, which contains a large fraction of impurities (see Table 4-2). “HD” refers to a distilled or purified form of sulfur mustard (see Table 4-3). “HT” is often called sulfur mustard even though it is a mixture of 60% “HD”, <40% Agent T (bis[2-(2-chloroethylthio)ethyl]ether, CAS# 63918-89-8), and a variety of sulfur contaminants and impurities. Most studies on sulfur mustard are based on its distilled or purified form, “HD” (Munro et al. 1999). Other mustard agents, such as “HN” or nitrogen mustard (i.e., bis(2-chloroethyl)methylamine hydrochloride; CAS No. 55-86-7) and lewisite (i.e., 2-chlorovinyl dichloroarsine; CAS No. 541-25-3) are related to sulfur mustard. Information about “HN”, “HT”, and lewisite are not included in this document.

4.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of sulfur mustard (HD) is located in Table 4-4. Weapons-grade sulfur mustard can contain stabilizers, starting materials, or by-products formed during manufacturing, and products formed from slow reactions during storage (Munro et al. 1999). The typical compositions of HD and H are illustrated in Tables 4-3 and 4-4, respectively (NRC 1999; Rosenblatt et al. 1996). In general, a residual “heel” (i.e., a gel that will not flow) forms with the ageing of sulfur mustard. The heel can amount to more than 10% of the agent and usually contains 14–53% sulfur mustard, 42–86% cyclic sulfonium ions, and metals, such as iron sulfide (NRC 1999).

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Table 4-1. Chemical Identity of Sulfur Mustard

Characteristic	Information	Reference
Chemical name	Bis(2-chloroethyl) sulfide	HSDB 2002
Synonym(s)	β,β' -Dichloroethyl sulfide; β,β' -Dichloroethyl sulphide; 1-Chloro-2-(β -chloroethylthio)ethane; 1,1'-Thiobis-(2-chloroethane); 2,2'-Dichlorodiethyl sulfide; 2,2'-Dichlorodiethyl sulphide; 2,2'-Dichloroethyl sulphide; 2,2'-Dichloroethyl sulfide; Bis(β -chloroethyl)sulfide; Bis(β -chloroethyl)sulphide; Bis(2-chloroethyl)sulphide; Di-2-chloroethyl sulfide; Di-2-chloroethyl sulphide; Dichloro-diethyl-sulphide; Dichlorodiethyl sulfide; Dichloroethyl sulfide; Diethyl sulfide, 2,2'-dichloro; Distilled mustard; Ethane, 1,1'-thiobis(2-chloro-; Gelbkreuz; H; HD; Kampstoff "Lost"; Lost; Mustard, sulfur; Mustard vapor; Mustard gas; Mustard HD; S mustard; S-lost; S-Lost; S-yperite; Schwefel-Lost; Senfgas; Sulfide, bis(2-chloroethyl); Sulfur mustard gas; Sulfur mustard; Yellow Cross Liquid; Yellow Cross Gas	HSDB 2002
Registered trade name(s)	No data	
Chemical formula	C ₄ H ₈ Cl ₂ S	Budavari et al. 1996
Chemical structure		Budavari et al. 1996; IARC 1975
Identification numbers:		
CAS registry	505-60-2	HSDB 2002
NIOSH RTECS	WQ0900000	HSDB 2002
EPA hazardous waste	No data	
OHM/TADS	No data	
DOT/UN/NA/IMCO shipping	UN 2810	DOT 2002
HSDB	336	HSDB 2002
NCI	No data	

CAS = Chemical Abstracts Services; DOT/UN/NA/IMCO = Department of Transportation/United Nations/North America/International Maritime Dangerous Goods Code; EPA = Environmental Protection Agency; HSDB = Hazardous Substances Data Bank; NCI = National Cancer Institute; NIOSH = National Institute for Occupational Safety and Health; OHM/TADS = Oil and Hazardous Material/Technical Assistance Data system; RTECS = Registry of Toxic Effects of Chemical Substances

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Table 4-2. Typical Composition of Sulfur Mustard (H) from an Old Chemical Munition

Compound	CAS No.	GC/MS peak area percent
Sulfur mustard	505-60-2	62.2
Bis(2-chloroethyl) disulfide	1002-41-1	10.9
1,4-Dithiane	505-29-3	3.2
Bis(2-chloroethyl) trisulfide	19149-77-0	9.6
1,2-Bis(2-chloroethylthio)ethane	3563-36-8	2.6
1,2,3-Trithiolane	—	2.4
1,4-Thioxane	15980-15-1	0.1
1,2,5-Trithiepane	6576-93-8	0.9
1,2,3,4-Tetrathiane	—	1.4
1,2-Dichloroethane	107-06-2	3.2
HD tetrasulfide	—	0.6
Tetrachloroethene	127-18-4	0.3
Sulfur	7704-34-9	0.5
Other	—	1.3

GC/MS = gas chromatography/mass spectrometry

Source: Rosenblatt et al. 1996

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Table 4-3. Typical Composition of Sulfur Mustard (HD) in 1-Ton Storage Containers (Aberdeen, Maryland)

Compound	CAS No.	Mole percent
Sulfur mustard	505-60-2	91.38
Q sulfonium	30843-67-5	6.08
2-Chloroethyl 4-chlorobutyl sulfide	114811-35-7	0.86
1,4-Dithiane	505-29-3	0.81
1,2-Dichloroethane	107-06-2	0.35
Bis-3-chloropropyl sulfide	22535-54-2	0.18
2-Chloropropyl 3'-chloropropyl sulfide	—	0.18
2-Chloroethyl 3-chloropropyl sulfide	71784-01-5	0.14
1-Chloropropyl 2-chloroethyl sulfide	—	0.02
1,4-Thioxane	15980-15-1	<0.01

Source: NRC 1999

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Table 4-4. Physical and Chemical Properties of Sulfur Mustard

Property	Information	Reference
Molecular weight	159.08	Budavari et al. 1996
Color	Clear Pale yellow, black if impure	Budavari et al. 1996 Munro et al. 1999
Physical state	Oily liquid	Budavari et al. 1996
Melting point	13–14 °C	Budavari et al. 1996
Boiling point	217.5 °C	Budavari et al. 1996
Density:	1.338 at 13 °C 1.2685 at 25 °C	Budavari et al. 1996 Rosenblatt et al. 1996
Odor	Weak, sweet, agreeable odor	Budavari et al. 1996
Odor threshold:		
Water	No data	
Air	0.6 mg/m ³	Bowden 1943
Solubility:		
Water	920 mg/L at 22 °C 684 mg/L at 25 °C	Rosenblatt et al. 1996 Seidell 1941
Organic solvent(s)	Soluble in alcohol, ether, acetone, and benzene; miscible with petroleum ether Soluble in fat solvents and other common organic solvents	HSDB 2002 IARC 1975
Partition coefficients:		
Log K _{ow}	2.41 1.37	HSDB 2002 Rosenblatt et al. 1996
Log K _{oc}	2.43	HSDB 2002
Vapor pressure:		
at 22 °C	0.082 mmHg	Rosenblatt et al. 1996
at 25 °C	0.1059 mmHg	Rosenblatt et al. 1996
Henry's law constant	2.4x10 ⁻⁵ atm·m ³ /mol 1.87x10 ⁻⁵ atm·m ³ /mol	Opresko et al. 1998 Rosenblatt et al. 1996
Autoignition temperature	No data	
Flashpoint	221 °F	Sax 1989
Conversion factors:	No data	
Explosive limits	No data	

