

### **3. CHEMICAL AND PHYSICAL INFORMATION**

#### **3.1 CHEMICAL IDENTITY**

Information regarding the chemical identity of mercury compounds is located in Table 3-1.

#### **3.2 PHYSICAL AND CHEMICAL PROPERTIES**

Information regarding the physical and chemical properties of mercury compounds is located in Table 3-2. Mercuric acetate has been included as an organic form of mercury. However, the bonds of the salt are not covalent and, in aqueous solution, the mercury behaves like an inorganic form.

Table 3-1. Chemical Identity of Selected Inorganic and Organic Mercury Compounds<sup>a</sup>

Characteristic	Mercury	Inorganic	
		Mercuric (II) chloride	Mercuric (II) sulfide
Chemical name	Mercury	Mercuric (II) chloride	Mercuric (II) sulfide
Synonym(s)	Colloidal mercury; liquid silver; mercury, metallic (DOT); quicksilver; metallic mercury <sup>b</sup> ; hydrargyrum <sup>c</sup>	Bichloride of mercury; mercury bichloride <sup>d</sup> ; mercury chloride <sup>d</sup> ; mercury dichloride; mercury perchloride; mercury (II) chloride; perchloride of mercury; corrosive sublimate <sup>d</sup> ; corrosive mercury chloride; dichloromercury	Etiops mineral <sup>c</sup> ; mercury sulfide, black <sup>d</sup> ; vermilion; chinese red; C.I. Pigment Red 106; C.I.77766 <sup>c</sup> ; quicksilver vermilion; chinese vermilion; red mercury sulfide; artificial cinnabar; red mercury sulfuret <sup>d</sup>
Registered trade name(s)	No data	Calochlor; Fungchex; TL 898	No data
Chemical formula	Hg <sup>c</sup>	HgCl <sub>2</sub> <sup>c</sup>	HgS <sup>c</sup>
Chemical structure	Hg <sup>c</sup>	Hg <sup>++</sup> Cl <sup>-</sup> Cl <sup>-</sup>	Hg = S
Identification numbers:			
CAS registry	7439-97-6 <sup>c</sup>	7487-94-7 <sup>c</sup>	1344-48-5 <sup>c</sup>
NIOSH RTECS	OVA4550000	OV9100000	No data
EPA hazardous waste	U151;D009	D009	No data
OHM/TADS	7216782	No data	No data
DOT/UN/NA/IMCO shipping	UN 2024 (mercury compounds, liquid); UN 2025 (mercury compounds, solid); IMO 6.1 (mercury compounds, liquid or solid); UN 2809 (DOT) <sup>b</sup>	UN 1624 (mercuric chloride) IMO 6.1 (mercuric chloride)	No data
HSDB	1208	33	No data
NCI	C60399 <sup>b</sup>	C60173	No data
STCC	49 232 69 (mercury compound, solid), 49 443 25 (mercury, metallic)	49 232 45 (mercuric chloride) 49 232 71 (mercuric chloride, solid)	No data

Table 3-1. Chemical Identity of Selected Inorganic and Organic Mercury Compounds<sup>a</sup> (continued)


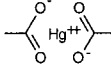
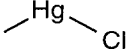
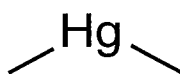
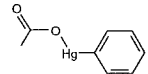
Characteristic	Inorganic (continued)		Organic	
	Mercurous (I) chloride	Mercuric (II) acetate <sup>f</sup>	Methylmercuric chloride	
Chemical name	Mercurous (I) chloride	Mercuric (II) acetate	Methylmercuric chloride	
Synonym(s)	Calomel; mild mercury chloride; mercury monochloride; mercury protochloride; mercury subchloride; calogreen; cyclosan <sup>c</sup> ; mercury chloride <sup>d</sup>	Acetic acid, mercury (2+) salt; bis(acetyloxy) mercury; diacetocymcury; mercury diacetate; mercuriacetate; mercury (II) acetate; mercury (2+) acetate; mercury acetate <sup>d</sup>	Chloromethylmercury; monomethyl mercury chloride; methylmercury chloride; methylmercury monochloride <sup>b</sup>	
Registered trade name(s)	Calogreen; Calomel Calotab; Cylcosan	No data	Caspan	
Chemical formula	Hg <sub>2</sub> Cl <sub>2</sub> <sup>b</sup>	HgC <sub>4</sub> H <sub>6</sub> O <sub>4</sub> <sup>b</sup>	CH <sub>3</sub> HgCl <sup>e</sup>	
Chemical structure				
Identification numbers:				
CAS registry	10112-91-1 <sup>c</sup>	1600-27-7	115-09-3 <sup>e</sup>	
NIOSH RTECS	OV8750000 <sup>b</sup>	A18575000	OW1225000	
EPA hazardous waste	No data	D009	No data	
OHM/TADS	No data	No data	No data	
DOT/UN/NA/IMCO shipping	No data	UN 1629 (mercury acetate); IMO 6.1 (mercury acetate)	No data	
HSDB	No data	1244	No data	
NCI	77764 <sup>b</sup>	No data	No data	
STCC	No data	49 232 41	No data	

Table 3-1. Chemical Identity of Selected Inorganic and Organic Mercury Compounds<sup>a</sup> (continued)

Characteristic	Organic (continued)	
	Dimethyl mercury	Phenylmercuric acetate
Chemical name	Dimethyl mercury	Phenylmercuric acetate
Synonym(s)	Mercury, dimethyl; methyl mercury <sup>c</sup>	(Acetato)phenylmercury; acetoxyphenylmercury; phenylmercury acetate <sup>c</sup> ; acetoxyphenylmercury; mercury (II) acetate, phenyl-; mercury, (acetato)phenyl-; phenylmercury acetate; phenylmercuriacetate
Registered trade name(s)	No data	PMA; PMAC; Pmacetate; Cerasan Slaked Lime; Gollitox; liquiphene; Mersolite; Tag Fungicide; Tag HL-331; Nylmerate; Scutl; Riogen; PMAS
Chemical formula	C <sub>2</sub> H <sub>6</sub> Hg <sup>c</sup>	C <sub>8</sub> H <sub>8</sub> HgO <sub>2</sub> <sup>c</sup>
Chemical structure		
Identification numbers:		
CAS registry	593-74-8 <sup>c</sup>	62-38-4 <sup>c</sup>
NIOSH RTECS	No data	OV6475000
EPA hazardous waste	No data	PO92
OHM/TADS	No data	7216544
DOT/UN/NA/IMO shipping	No data	UN 1674 (phenylmercuric acetate); IMO 6.1 (phenylmercuric acetate)
HSDB	No data	1670
NCI	No data	No data
STCC	No data	29 216 53

<sup>a</sup> All information obtained from HSDB 1997, except where noted. <sup>b</sup>RTECS 1997 <sup>c</sup>Merck 1989 <sup>d</sup>Lewis 1993 <sup>e</sup>ASTER 1997 <sup>f</sup> Although organic moieties are associated with the Hg atom, the mercury-carbon bonds are ionic, not covalent, in nature and in aqueous solution, Hg<sup>2+</sup> is released.

CAS = Chemical Abstracts Service; DOT/UN/NA/IMO = Dept. 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 Materials/Technical Assistance Data System; RTECS = Registry of Toxic Effects of Chemical Substances

Table 3-2. Physical and Chemical Properties of Selected Inorganic and Organic Mercury Compounds<sup>a</sup>

Property	Mercury	Inorganic		
		Mercuric (II) chloride	Mercuric (II) sulfide	Mercurous (I) chloride
Molecular weight	200.59	271.52	232.68	472.09
Color	Silver-white (liquid metal); tin-white (solid mercury)	White	Black or grayish-black (mercuric sulfide, black); bright scarlet-red blackens on exposure to light (mercuric sulfide, red)	White
Physical state	Heavy, mobile, liquid metal; Solid mercury is ductile, malleable mass which may be cut with a knife	Crystals, granules or powder; rhombic crystals, crystalline solid <sup>c</sup>	Heavy amorphous powder, also occurs as black cubic crystals (mercuric sulfide, black); powder, lumps, hexagonal crystals (mercuric sulfide, red)	Heavy powder; rhombic crystals or crystalline powder <sup>b</sup>
Melting point	-38.87 °C	277 °C	Transition temp (red to black) 386 °C; 583 °C, sublimes at 446 °C (mercuric sulfide, black) <sup>b</sup> ; sublimes at 583 °C (mercuric sulfide, red)	Sublimes at 400–500 °C without melting; 302 °C <sup>b</sup>
Boiling point	356.72 °C	302 °C	No data	384 °C <sup>b</sup>
Density at °C	13.534 g/cm <sup>3</sup> at 25 °C	5.4 g/cm <sup>3</sup> at 25 °C	7.55-7.70 (mercuric sulfide, black), 8.06-8.12 g/cc (mercuric sulfide, red) <sup>b</sup>	7.15 g/cc; 6.993 g/cc <sup>b</sup>
Odor	Odorless <sup>c</sup>	Odorless <sup>b</sup>	Odorless	Odorless
Odor threshold:				
Water	No data	No data	No data	No data
Air	No data	No data	No data	No data
Solubility:				
Water	0.28 µmoles/L at 25 °C	1 g/35 mL, 1 g/2.1 mL boiling H <sub>2</sub> O; 6.9 g/100 cc H <sub>2</sub> O at 20 °C <sup>c</sup> , 48 g/100 cc at 100 °C <sup>c</sup>	Insoluble (mercuric sulfide, black), soluble in aqua regia with separation of S, in warm hydriodic acid with evolution of H <sub>2</sub> S (mercuric sulfide, red)	2.0x10 <sup>-4</sup> g/100mL at 25 °C

Table 3-2. Physical and Chemical Properties of Selected Inorganic and Organic Mercury Compounds<sup>a</sup> (continued)

Property	Mercury	Inorganic		
		Mercuric (II) chloride	Mercuric (II) sulfide	Mercurous (I) chloride
Solubility:				
Organic solvents	Soluble in H <sub>2</sub> SO <sub>4</sub> upon boiling, in lipids, readily soluble in HNO <sub>3</sub> , insoluble in HCL <sup>b</sup> ; soluble in 2.7 mg/L pentane <sup>c</sup>	1 g/3.8 mL alcohol, 1 g/200 mL C <sub>6</sub> H <sub>6</sub> , 22 mL ether, 12 mL glycerol, 40 mL CH <sub>3</sub> COOH, acetone, CH <sub>3</sub> OH, ethyl acetate; 33 g/100 cc alcohol at 25 °C, slightly soluble in carbon disulfide, pyridine <sup>c</sup>	Insoluble in alcohol, dilute mineral acids	Insoluble in alcohol, ether
Partition coefficients:				
Log K <sub>ow</sub>	5.95 <sup>9</sup>	No data	No data	No data
Log K <sub>oc</sub>	No data	No data	No data	No data
Vapor pressure	2x10 <sup>-3</sup> mm Hg at 25 °C	1 mm Hg at 136.2 °C	No data	No data
Henry's law constant at 24.8 °C	No data	No data	No data	No data
Degradation reaction rate constant	Gas-phase reaction with O <sub>3</sub> = 1.7x10 <sup>-18</sup> cm <sup>3</sup> /mol/s <sup>j</sup> ; 8 x10 <sup>-19</sup> cm <sup>3</sup> /mol/s <sup>k</sup>	No data	No data	No data
Autoignition temperature	Not flammable <sup>c</sup>	No data	No data	No data
Flashpoint	Not flammable <sup>c</sup>	Not flammable <sup>c</sup>	No data	No data
Flammability limits in air	Not flammable <sup>c</sup>	Not flammable <sup>c</sup>	No data	No data
Conversion factors:				
ppm (v/v) to mg/m <sup>3</sup> in air at 25 °C	1 ppm = 8.18 mg/m <sup>3</sup>	No data	No data	No data
mg/m <sup>3</sup> to ppm (v/v) in air at 25 °C	1 mg/m <sup>3</sup> = 0.122 ppm	No data	No data	No data
Explosive limits	Non-combustible <sup>c</sup>	Non-combustible <sup>c</sup>	No data	No data
Valence states	+1, +2	+2	+2	+2

Table 3-2. Physical and Chemical Properties of Selected Inorganic and Organic Mercury Compounds<sup>a</sup> (continued)

Property	Organic			
	Mercuric (II) acetate	Methylmercuric chloride <sup>l</sup>	Dimethyl mercury	Phenylmercuric acetate
Molecular weight	318.70	251.1 <sup>d</sup>	230.66	336.75
Color	White <sup>b</sup>	White <sup>f</sup>	Colorless	White to cream <sup>b</sup>
Physical state	Crystals or crystalline powder; Solid at 25 °C and 1 atm <sup>c</sup>	Crystals <sup>f</sup>	Liquid	Small lustrous prisms; crystalline powder, small prisms or leaflets <sup>c</sup>
Melting point	178–180 °C	170 °C <sup>d</sup>	No data	149 °C; 148-150 °C <sup>b</sup>
Boiling point	No data	No data	92 °C	No data
Density at °C	3.28 g/cm <sup>3</sup>	4.06 g/mL at 25 °C <sup>f</sup>	3.1874 g/mL at 20 °C	No data
Odor	Slight acetic odor	No data	No data	Odorless <sup>e</sup>
Odor threshold:				
Water	No data	No data	No data	No data
Air	No data	No data	No data	No data
Solubility:				
Water at 25 °C	1 g in 2.5 mL cold, 1 mL boiling H <sub>2</sub> O; 25 g/100 mL at 10 °C, 100 g/100 mL at 100 °C <sup>c</sup>	<0.1 mg/mL at 21 °C <sup>f</sup>	Insoluble; 1.00x10 <sup>3</sup> mg/L <sup>d</sup>	Soluble in about 600 parts H <sub>2</sub> O; 1 g/180 mL <sup>c</sup>
Organic solvents	Soluble in alcohol; acetic acid <sup>c</sup>	DMSO ≥100 mg/mL at 27 °C, 95% C <sub>2</sub> H <sub>5</sub> OH 10–50 mg/mL at 27 °C; acetone ≥ 100 mg/mL at 27 °C <sup>f</sup>	Easily soluble in ether, alcohol	Soluble in alcohol, benzene, acetone; 6.8 mL CHCl <sub>3</sub> , 200 mL ether <sup>c</sup>
Partition coefficients:				
Log K <sub>ow</sub>	No data	No data	2.28 <sup>h</sup>	No data
Log K <sub>oc</sub>	No data	No data	2.73 <sup>d</sup>	1.72 <sup>d</sup>
Vapor pressure at 25 °C	No data	0.0085 mm Hg at 25 °C <sup>f</sup>	No data	9x10 <sup>-4</sup> mm Hg at 35 °C <sup>i</sup> ; 1.20x10 <sup>-4</sup> mm Hg at 25 °C <sup>c</sup> ; <1mm Hg at 35 °C <sup>e</sup>
Henry's law constant °C	No data	No data	No data	1.22x10 <sup>-8</sup> atm m <sup>3</sup> /mol <sup>c</sup>
Degradation reaction rate constant	No data	No data	Volatilizes to air where it photolyzes to CH <sub>4</sub> and Hg or is oxidized by the OH radical <sup>i</sup>	No data
Autoignition temperature	No data	probably nonflammable <sup>f</sup>	Easily inflammable	No data

**Table 3-2. Physical and Chemical Properties of Selected Inorganic and Organic Mercury Compounds<sup>a</sup> (continued)**

Property	Organic			
	Mercuric (II) acetate	Methylmercuric chloride <sup>l</sup>	Dimethyl mercury	Phenylmercuric acetate
Flashpoint	Not flammable <sup>c</sup>	probably nonflammable <sup>f</sup>	Easily inflammable	>38 °C <sup>e</sup>
Flammability limits in air	Not flammable <sup>c</sup>	probably nonflammable <sup>f</sup>	Easily inflammable	No data
Conversion factors: ppm (v/v) to mg/m <sup>3</sup> in air at 25 °C	No data	1 ppm = 10.27 mg/m <sup>3</sup>	1 ppm = 9.43 mg/m <sup>3</sup>	No data
mg/m <sup>3</sup> to ppm (v/v) in air at 25 °C	No data	1 mg/m <sup>3</sup> = 0.0974 ppm	1 mg/m <sup>3</sup> = 0.106 ppm	No data
Explosive limits	Non-combustible <sup>c</sup>	No data	No data	Probably combustible <sup>f</sup>
Valence state	+2	+2	+2	+2

<sup>a</sup> All information obtained from Merck 1989 except where noted.

<sup>b</sup> All information obtained from Lewis 1993

<sup>c</sup> HSDB 1997

<sup>d</sup> Aster 1997

<sup>e</sup> NFPA 1994

<sup>f</sup> NTP Chemical Repository 1997 (Radian Corporation)

<sup>g</sup> Stein et al. 1996

<sup>h</sup> Wasik 1978

<sup>i</sup> Bodek et al. 1988 (to be verified)

<sup>j</sup> Schroeder et al. 1991

<sup>k</sup> Signeur et al. 1994

<sup>l</sup> Commonly occurring form of methyl mercury; proprietary names include bis-methylmercuric sulfate (cerewet), methylmercury cyanoguanidine or methylmercury dicyanodiamide (agrosol, morsodren, panogen, panospray), methylmercury nitrile (chipcote) and methylmercury propionate (metasol MP)

<sup>m</sup> Iverfeldt and Lindquist 1984

<sup>n</sup> Although organic moieties are associated with the Hg atom, the bonds are ionic, not covalent, in nature. In aqueous solution, Hg<sup>2+</sup> is released.