

## CHAPTER 4. CHEMICAL AND PHYSICAL INFORMATION

### 4.1 CHEMICAL IDENTITY

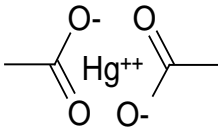

Information regarding the chemical identity of mercury compounds is located in Table 4-1. For this profile, mercury compounds are classified into three general categories: (1) elemental mercury; (2) inorganic mercury compounds (e.g., mercuric chloride); and (3) organic mercury compounds (e.g., methylmercury). An inorganic mercury compound is a compound of mercury that does not contain a chemical bond between mercury and carbon. Inorganic mercury salts are inorganic mercury compounds that can dissociate into a mercury cation (e.g., mercuric chloride, mercuric sulfide). Inorganic mercury compounds that are not salts include mercury oxides (e.g., mercuric oxide). Organic mercury compounds contain bonds between mercury and carbon (e.g., methylmercuric chloride, phenylmercuric acetate). 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 4-1. Chemical Identity of Selected Inorganic and Organic Mercury Compounds<sup>a</sup>**

Characteristic	Elemental	Inorganic	Inorganic
Chemical name	Mercury	Mercuric (II) chloride	Mercuric (II) sulfide
Synonym(s) and registered trade name(s)	Colloidal mercury; liquid silver; mercury, metallic; quicksilver; metallic mercury <sup>b</sup> ; hydrargyrum	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; Calochlor; Fungchex; TL 898	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>
Chemical formula	Hg <sup>c</sup>	HgCl <sub>2</sub> <sup>c</sup>	HgS <sup>c</sup>
Chemical structure	Hg	Hg <sup>++</sup> Cl <sup>-</sup> Cl <sup>-</sup>	Hg=S
CAS Registry Number	7439-97-6 <sup>c</sup>	7487-94-7 <sup>c</sup>	1344-48-5 <sup>c</sup>

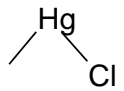

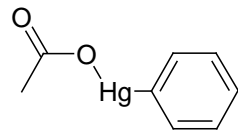
## 4. CHEMICAL AND PHYSICAL INFORMATION

**Table 4-1. Chemical Identity of Selected Inorganic and Organic Mercury Compounds<sup>a</sup>**

Characteristic	Inorganic	Inorganic	Organic
Chemical name	Mercurous (I) chloride	Mercuric (II) acetate <sup>e</sup>	Methylmercury
Synonym(s) and registered trade name(s)	Calomel; mild mercury chloride; mercury monochloride; mercury protochloride; mercury subchloride; calogree; cyclosan <sup>c</sup> ; mercury chloride <sup>d</sup> ; Calogreen; Calomel Calotab; Cylosan	Acetic acid, mercury (2+ salt); bis(acetyloxy) mercury; diacetocymcury; mercury diacetate; mercury (II) acetate; mercury (2+) acetate; mercury acetate <sup>d</sup>	Methylmercury cation; methylmercury II; mercury(1+), methyl; methylmercury ion; methylmercury(II) cation; monomethylmercury cation
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> Hg
Chemical structure	Cl–Hg–Hg–Cl		
CAS Registry Number	10112-91-1	1600-27-7	22967-92-6

## 4. CHEMICAL AND PHYSICAL INFORMATION

**Table 4-1. Chemical Identity of Selected Inorganic and Organic Mercury Compounds<sup>a</sup>**

Characteristic	Organic	Organic	Organic
Chemical name	Methylmercuric chloride	Dimethyl mercury	Phenylmercuric acetate
Synonym(s) and registered trade name(s)	Chloromethylmercury; monomethyl mercury chloride; methylmercury chloride; methylmercury monochloride <sup>b</sup> ; Caspan	Mercury, dimethyl; methyl mercury <sup>c</sup>	(Acetato)phenylmercury; acetoxyphenylmercury; phenylmercury acetate <sup>c</sup> ; acetophenylmercury; mercury (II) acetate, phenyl-; mercury, (acetato)phenyl-; phenylmercury acetate; phenylmercuriactetate; PMA; PMAC; Pmacetate; Cerasan Slaked Lime; Gollitox; liquiphene; Mersolite; Tag Fungicide; Tag HL-331; Nylmerate; Scutl; Riogen; PMAS
Chemical formula	CH <sub>3</sub> HgCl <sup>f</sup>	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			
CAS Registry Number	115-09-3	593-74-8 <sup>c</sup>	62-38-4 <sup>c</sup>

<sup>a</sup>All information obtained from NLM (2020), except where noted.

<sup>b</sup>RTECS 1997.

<sup>c</sup>Budavari 1989.

<sup>d</sup>Lewis 1993.

<sup>e</sup>Although organic moieties are associated with the mercury atom, the mercury-carbon bonds are ionic, not covalent, in nature; in aqueous solution, Hg<sup>2+</sup> is released. Therefore, based on chemical properties, mercuric acetate is classified as an inorganic compound for this profile. Due to the presence of carbon in the acetate moiety, mercuric acetate could also be classified as an organic compound.

<sup>f</sup>ASTER 1997.

CAS = Chemical Abstracts Service

## 4.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of mercury compounds is located in Table 4-2. Mercury has seven naturally occurring isotopes, with the most common being mercury-202 (Gonzalez-Raymat et al. 2017). The fate and properties of mercury are greatly dependent upon its oxidation state which are mainly: elemental mercury Hg<sup>0</sup>, mercurous Hg<sup>+</sup> (I), and mercuric Hg<sup>2+</sup> (II).

## 4. CHEMICAL AND PHYSICAL INFORMATION

**Table 4-2. Physical and Chemical Properties of Selected Inorganic and Organic Mercury Compounds<sup>a</sup>**

Property	Elemental	Inorganic		
	Mercury	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 (mercury sulfide, red)	White
Physical state	Heavy, mobile, liquid metal; solid mercury is a ductile, malleable mass that may be cut with a knife	Crystals, granules, or powder; rhombic crystalline solid <sup>b</sup>	Heavy amorphous powder, also occurs as black cubic crystals (mercury sulfide, black); powder, lumps, hexagonal crystals (mercury sulfide, red)	Heavy powder; rhombic crystals or crystalline powder <sup>c</sup>
Melting point	-38.87°C	277°C	Transition temperature (red to black) 386°C; sublimes at 446°C (mercuric sulfide, black) <sup>c</sup> ; sublimes at 583°C (mercuric sulfide, red)	Sublimes at 400–500°C without melting; 302°C <sup>c</sup>
Boiling point	357.72°C	302°C	502°C (predicted) <sup>d</sup>	384°C <sup>c</sup>
Density (g/cm <sup>3</sup> )	13.534 at 25°C	5.4 at 25°C	7.55–7.70 (mercuric sulfide, black); 8.06–8.12 g/cc (mercuric sulfide, red) <sup>c</sup>	7.15 g/cc; 6.993 g/cc <sup>c</sup>
Odor	Odorless <sup>b</sup>	Odorless <sup>c</sup>	Odorless	Odorless
Odor threshold:				
Water	No data	No data	No data	No data
Air	No data	No data	No data	No data

## 4. CHEMICAL AND PHYSICAL INFORMATION

**Table 4-2. Physical and Chemical Properties of Selected Inorganic and Organic Mercury Compounds<sup>a</sup>**

Property	Elemental	Inorganic		
	Mercury	Mercuric (II) chloride	Mercuric (II) sulfide	Mercurous (I) chloride
Solubility:				
Water	0.28 µmoles/L at 25°C	69 g/L at 20°C <sup>e</sup>	Insoluble (mercuric sulfide, black), soluble in aqua regia with separation of sulfur, in warm hydriodic acid with evolution of hydrogen sulfide (mercuric sulfide, red)	2x10 <sup>-4</sup> g/100 mL at 25°C
Organic solvents	Soluble in H <sub>2</sub> SO <sub>4</sub> upon boiling in lipids; readily soluble in HCl <sup>c</sup> ; soluble in 2.7 mg/L pentane <sup>b</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>b</sup>	Insoluble in alcohol, dilute mineral acids	Insoluble in alcohol, ether
Partition coefficients:				
Log K <sub>ow</sub>	5.95 <sup>f</sup>	No data	1.53 (predicted) <sup>d</sup>	-0.550 (predicted) <sup>d</sup>
Log K <sub>oc</sub>	No data	No data	No data	No data
Vapor pressure	2x10 <sup>3</sup> mmHg at 25°C	1 mmHg at 136.2°C	No data	No data
Henry's law constant	No data	No data	No data	No data
Autoignition temperature	Not flammable <sup>b</sup>	No data	No data	No data
Flashpoint	Not flammable <sup>b</sup>	Not flammable <sup>b</sup>	No data	No data
Flammability limits	Not flammable <sup>b</sup>	Not flammable <sup>b</sup>	No data	No data
Conversion factors	1 ppm=8.18 mg/m <sup>3</sup> 1 mg/m <sup>3</sup> =0.122 ppm	No data	No data	No data
Explosive limits	Non-combustible <sup>b</sup>	Non-combustible <sup>b</sup>	No data	No data
Valence states	+1, +2	+2	+2	+2

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**Table 4-2. Physical and Chemical Properties of Selected Inorganic and Organic Mercury Compounds<sup>a</sup>**

Property	Inorganic		Organic		
	Mercuric (II) acetate	Methylmercury	Methylmercuric chloride <sup>g</sup>	Dimethyl mercury	Phenylmercuric acetate
Molecular weight	318.70	216.63	251.1 <sup>h</sup>	230.66	366.75
Color	White <sup>c</sup>	White (chloride salt) <sup>e</sup>	White <sup>i</sup>	Colorless	White to cream <sup>c</sup>
Physical state	Crystals or crystalline powder; solid at 25°C and 1 atm <sup>b</sup>	Crystalline solid (chloride salt) <sup>e</sup>	Crystals <sup>i</sup>	Liquid	Small lustrous prisms; crystalline powder, small prisms or leaflets <sup>b</sup>
Melting point	178–180°C	-60.5°C (predicted) <sup>d</sup>	170°C <sup>h</sup>	-56.6°C (predicted) <sup>d</sup>	149°C; 148–150°C <sup>c</sup>
Boiling point	118°C (predicted) <sup>d</sup>	83.0°C (predicted) <sup>d</sup>	117°C (predicted) <sup>d</sup>	92°C	291°C (predicted) <sup>d</sup>
Density (g/cm <sup>3</sup> )	3.28	4.06 g/mL at 25°C (chloride salt) <sup>e</sup>	4.06 g/mL at 25°C <sup>i</sup>	3.1874 g/mL at 20°C	No data
Odor	Slight acetic odor	Disagreeable odor <sup>e</sup>	No data	No data	Odorless <sup>j</sup>
Odor threshold:					
Water	No data	No data	No data	No data	No data
Air	No data	No data	No data	No data	No data
Solubility:					
Water	1 g in 2.5 mL cold; 1 mL boiling water; 25 g/100 mL at 10°C, 100 g/100 mL at 100°C <sup>b</sup>	0.145 mol/L (predicted) <sup>d</sup>	<0.1 mg/mL at 21°C <sup>i</sup>	Insoluble 1.00x10 <sup>3</sup> mg/L <sup>h</sup>	Soluble in about 600 parts water; 1 g/180 mL <sup>b</sup>
Organic solvents	Soluble in alcohol, acetic acid <sup>b</sup>	No data	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>i</sup>	Easily soluble in ether, alcohol	Soluble in alcohol, benzene, acetone; 6.8 mL CHCl <sub>3</sub> , 200 mL ether <sup>b</sup>
Partition coefficients:					
Log K <sub>ow</sub>	-0.662 (predicted) <sup>d</sup>	0.08 (predicted) <sup>d</sup>	0.390 (predicted) <sup>d</sup>	2.28 <sup>b</sup>	0.71 <sup>b</sup>
Log K <sub>oc</sub>	No data	No data	No data	2.73 <sup>h</sup>	1.72 <sup>h</sup>

## 4. CHEMICAL AND PHYSICAL INFORMATION

**Table 4-2. Physical and Chemical Properties of Selected Inorganic and Organic Mercury Compounds<sup>a</sup>**

Property	Inorganic		Organic		
	Mercuric (II) acetate	Methylmercury	Methylmercuric chloride <sup>g</sup>	Dimethyl mercury	Phenylmercuric acetate
Vapor pressure	13.9–15.6 mmHg at 25°C (predicted) <sup>d</sup>	0.0085 mmHg at 25°C (chloride salt) <sup>e</sup>	0.0085 mmHg at 25°C <sup>i</sup>	62.3 mmHg at 25°C <sup>i</sup>	1.20x10 <sup>-4</sup> mmHg at 25°C <sup>b</sup>
Henry's law constant at 25°C	1.00x10 <sup>-7</sup> (predicted) <sup>d</sup>	No data	No data	No data	1.22x10 <sup>-8</sup> atm m <sup>3</sup> /mol <sup>b</sup>
Autoignition temperature	No data	No data	Probably nonflammable <sup>i</sup>	Easily inflammable	No data
Flashpoint	Not flammable <sup>b</sup>	No data	Probably nonflammable <sup>i</sup>	Easily inflammable	No data
Flammability limits	Not flammable <sup>b</sup>	No data	Probably nonflammable <sup>i</sup>	Easily inflammable	No data
Conversion factors	No data	No data	1 ppm=10.27 mg/m <sup>3</sup> 1 mg/m <sup>3</sup> =0.097413 ppm	1 ppm=9.43 mg/m <sup>3</sup> 1 mg/m <sup>3</sup> =0.106 ppm	No data
Explosive limits	Noncombustible <sup>b</sup>	No data	No data	No data	Probably combustible <sup>i</sup>
Valence state	+2	+2	+2	+2	+2

<sup>a</sup>All information obtained from Budavari (1989) except where noted.

<sup>b</sup>NLM 2020.

<sup>c</sup>Lewis 1993.

<sup>d</sup>EPA 2021a, 2021b, 2021c, 2021d, 2021e.

<sup>e</sup>Grandjean and Yorifuji 2012.

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

<sup>g</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>h</sup>ASTER 1997.

<sup>i</sup>NTP 1997.

<sup>j</sup>Long and Cattanach 1961.