# CHAPTER 4. CHEMICAL AND PHYSICAL INFORMATION

## 4.1 CHEMICAL IDENTITY

Information regarding the chemical identity of mercury compounds is presented 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[a]**

| 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[b]; hydrargyrum | Bichloride of mercury; mercury bichloride[c]; mercury chloride[c]; mercury dichloride; mercury perchloride; mercury (II) chloride; perchloride of mercury; corrosive sublimate[c]; corrosive mercury chloride; dichloromercury; Calochlor; Fungchex; TL 898 | Etiops mineral[d]; mercury sulfide, black[c]; vermillion; Chinese red; C.I. Pigment Red 106; C.I. 77766[d]; quicksilver vermillion; Chinese vermillion; red mercury sulfide; artificial cinnabar; red mercury sulfuret[d] |
| SMILES | [Hg] | Cl[Hg]Cl | S=[Hg] |
| Chemical formula | Hg[d] | $HgCl_2$[d] | HgS[d] |
| Chemical structure | Hg | $Hg^{++}$ $Cl^-$ $Cl^-$ | Hg=S |
| CAS Registry Number | 7439-97-6[d] | 7487-94-7[d] | 1344-48-5[d] |

**Table 4-1. Chemical Identity of Selected Inorganic and Organic Mercury Compounds[a]**

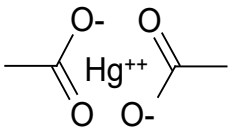
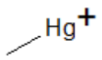
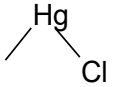
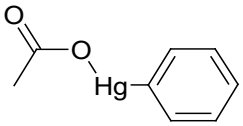
| Characteristic | Inorganic | Inorganic | Organic |
|---|---|---|---|
| Chemical name | Mercurous (I) chloride | Mercuric (II) acetate[e] | Methylmercury |
| Synonym(s) and registered trade name(s) | Calomel; mild mercury chloride; mercury monochloride; mercury protochloride; mercury subchloride; calogree; cyclosan[d]; mercury chloride[c]; Calogreen; Calomel Calotab; Cylosan | Acetic acid, mercury (2+ salt); bis(acetyloxy) mercury; diacetocymercury; mercury diacetate; mercury (II) acetate; mercury (2+) acetate; mercury acetate[d] | Methylmercury cation; methylmercury II; mercury(1+), methyl; methylmercury ion; methylmercury(II) cation; monomethylmercury cation |
| SMILES | Cl[Hg]Cl | CC(=O)[O-].CC(=O)[O-].[Hg+2] | C[Hg] |
| Chemical formula | $Hg_2Cl_2$[b] | $HgC_4H_6O_4$[b] | $CH_3Hg$ |
| Chemical structure | Cl–Hg–Hg–Cl |   |   |
| CAS Registry Number | 10112-91-1 | 1600-27-7 | 22967-92-6 |

**Table 4-1. Chemical Identity of Selected Inorganic and Organic Mercury Compounds[a]**

| 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[b]; Caspan | Mercury, dimethyl; methyl mercury[d] | (Acetato)phenylmercury; acetoxyphenylmercury; phenylmercury acetate[d]; acetophenylmercucy; 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 |
| SMILES | C[Hg]Cl | C[Hg]C | CC(=O)O[Hg]C1=CC=CC=C1 |
| Chemical formula | $CH_3HgCl$[f] | $C_2H_6Hg$[d] | $C_8H_8HgO_2$[d] |
| Chemical structure |  |  |  |
| CAS Registry Number | 115-09-3 | 593-74-8[d] | 62-38-4[d] |

[a]All information obtained from NLM (2020), except where noted.
[b]RTECS 1997.
[c]Lewis 1993.
[d]Budavari 1989.
[e]Although organic moieties are associated with the mercury atom, the mercury-carbon bonds are ionic, not covalent, in nature; in aqueous solution, $Hg^{2+}$ 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.
[f]ASTER 1997.

CAS = Chemical Abstracts Service; SMILES = simplified molecular-input line-entry system

## 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 $Hg^0$, mercurous $Hg^+$ (I), and mercuric $Hg^{2+}$ (II).

**Table 4-2. Physical and Chemical Properties of Selected Inorganic and Organic Mercury Compounds[a]**

| | Elemental | Inorganic | | |
|---|---|---|---|---|
| Property | 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[b] | 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[c] |
| Melting point | -38.87°C | 277°C | Transition temperature (red to black) 386°C; sublimes at 446°C (mercuric sulfide, black)[c]; sublimes at 583°C (mercuric sulfide, red) | Sublimes at 400–500°C without melting; 302°C[c] |
| Boiling point | 357.72°C | 302°C | 502°C (predicted)[d] | 384°C[c] |
| Density ($g/cm^3$) | 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)[c] | 7.15 g/cc; 6.993 g/cc[c] |
| Odor | Odorless[b] | Odorless[c] | Odorless | Odorless |
| Odor threshold: | | | | |
| Water | No data | No data | No data | No data |
| Air | No data | No data | No data | No data |

**Table 4-2. Physical and Chemical Properties of Selected Inorganic and Organic Mercury Compounds[a]**

| | Elemental | Inorganic | | |
|---|---|---|---|---|
| Property | 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[e] | Insoluble (mercuric sulfide, black), soluble in aqua regia with separation of sulfur, in warm hydriodic acid with evolution of hydrogen sulfide (mercuric sulfide, red) | $2x10^{-4}$ g/100 mL at 25°C |
| Organic solvents | Soluble in $H_2SO_4$ upon boiling in lipids; readily soluble in HCl[c]; soluble in 2.7 mg/L pentane[b] | 1 g/3.8 mL alcohol, 1 g/200 mL $C_6H_6$, 22 mL ether, 12 mL glycerol, 40 mL $CH_3COOH$, acetone, $CH_3OH$, ethyl acetate; 33 g/100 cc alcohol at 25°C, slightly soluble in carbon disulfide, pyridine[b] | Insoluble in alcohol, dilute mineral acids | Insoluble in alcohol, ether |
| Partition coefficients: | | | | |
| Log $K_{ow}$ | 5.95[f] | No data | 1.53 (predicted)[d] | -0.550 (predicted)[d] |
| Log $K_{oc}$ | No data | No data | No data | No data |
| Vapor pressure | $2x10^3$ 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[b] | No data | No data | No data |
| Flashpoint | Not flammable[b] | Not flammable[b] | No data | No data |
| Flammability limits | Not flammable[b] | Not flammable[b] | No data | No data |
| Conversion factors | 1 ppm=8.18 mg/m$^3$<br>1 mg/m$^3$=0.122 ppm | 1 ppm=11.1 mg/m$^3$;<br>1 mg/m$^3$=0.09 ppm | 1 ppm=9.5 mg/m$^3$;<br>1 mg/m$^3$=0.11 ppm | 1 ppm=19.3 mg/m$^3$;<br>1 mg/m$^3$=0.052 ppm |
| Explosive limits | Non-combustible[b] | Non-combustible[b] | No data | No data |
| Valence states | +1, +2 | +2 | +2 | +2 |

**Table 4-2. Physical and Chemical Properties of Selected Inorganic and Organic Mercury Compounds[a]**

| | Inorganic | Organic | | | |
|---|---|---|---|---|---|
| Property | Mercuric (II) acetate | Methylmercury | Methylmercuric chloride[g] | Dimethyl mercury | Phenylmercuric acetate |
| Molecular weight | 318.70 | 216.63 | 251.1[h] | 230.66 | 366.75 |
| Color | White[c] | White (chloride salt)[e] | White[i] | Colorless | White to cream[c] |
| Physical state | Crystals or crystalline powder; solid at 25°C and 1 atm[b] | Crystalline solid (chloride salt)[e] | Crystals[i] | Liquid | Small lustrous prisms; crystalline powder, small prisms or leaflets[b] |
| Melting point | 178–180°C | -60.5°C (predicted)[d] | 170°C[h] | -56.6°C (predicted)[d] | 149°C; 148–150°C[c] |
| Boiling point | 118°C (predicted)[d] | 83.0°C (predicted)[d] | 117°C (predicted)[d] | 92°C | 291°C (predicted)[d] |
| Density ($g/cm^3$) | 3.28 | 4.06 g/mL at 25°C (chloride salt)[e] | 4.06 g/mL at 25°C[i] | 3.1874 g/mL at 20°C | No data |
| Odor | Slight acetic odor | Disagreeable odor[e] | No data | No data | Odorless[j] |
| 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[b] | 0.145 mol/L (predicted)[d] | <0.1 mg/mL at 21°C[i] | Insoluble $1.00x10^3$ mg/L[h] | Soluble in about 600 parts water; 1 g/180 mL[b] |
| Organic solvents | Soluble in alcohol, acetic acid[b] | No data | DMSO ≥100 mg/mL at 27°C, 95% $C_2H_5OH$ 10–50 mg/mL at 27°C; acetone ≥100 mg/mL at 27°C[i] | Easily soluble in ether, alcohol | Soluble in alcohol, benzene, acetone; 6.8 mL $CHCl_3$, 200 mL ether[b] |
| Partition coefficients: | | | | | |
| Log $K_{ow}$ | -0.662 (predicted)[d] | 0.08 (predicted)[d] | 0.390 (predicted)[d] | 2.28[b] | 0.71[b] |
| Log $K_{oc}$ | No data | No data | No data | 2.73[h] | 1.72[h] |

## Table 4-2. Physical and Chemical Properties of Selected Inorganic and Organic Mercury Compounds[a]

| | Inorganic | Organic | | | |
|---|---|---|---|---|---|
| Property | Mercuric (II) acetate | Methylmercury | Methylmercuric chloride[g] | Dimethyl mercury | Phenylmercuric acetate |
| Vapor pressure | 13.9–15.6 mmHg at 25°C (predicted)[d] | 0.0085 mmHg at 25°C (chloride salt)[e] | 0.0085 mmHg at 25°C[i] | 62.3 mmHg at 25°C[j] | $1.20 \times 10^{-4}$ mmHg at 25°C[b] |
| Henry's law constant at 25°C | $1.00 \times 10^{-7}$ atm $m^3$/mol (predicted)[d] | No data | No data | No data | $1.22 \times 10^{-8}$ atm $m^3$/mol[b] |
| Autoignition temperature | No data | No data | Probably nonflammable[i] | Easily inflammable | No data |
| Flashpoint | Not flammable[b] | No data | Probably nonflammable[i] | Easily inflammable | No data |
| Flammability limits | Not flammable[b] | No data | Probably nonflammable[i] | Easily inflammable | No data |
| Conversion factors | No data | No data | 1 ppm=10.27 mg/$m^3$<br>1 mg/$m^3$=0.097413 ppm | 1 ppm=9.43 mg/$m^3$<br>1 mg/$m^3$=0.106 ppm | No data |
| Explosive limits | Noncombustible[b] | No data | No data | No data | Probably combustible[i] |
| Valence state | +2 | +2 | +2 | +2 | +2 |

[a]All information obtained from Budavari (1989) except where noted.
[b]NLM 2020.
[c]Lewis 1993.
[d]EPA 2021a, 2021b, 2021c, 2021d, 2021e.
[e]Grandjean and Yorifuji 2012.
[f]Stein et al. 1996.
[g]Commonly occurring form of methylmercury; proprietary names include bis-methylmercuric sulfate (cerewet), methylmercury cyanoguianidine or methylmercury dicyanodiamide (agrosol, morsodren, panogen, panospray), methylmercury nitrile (chipcote), and methylmercury proprionate (metasol MP).
[h]ASTER 1997.
[i]NTP 1997.
[j]Long and Cattanach 1961.