4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

Tin is a naturally occurring element that appears in group 14 (4A) of the periodic table at the boundary between the metals and nonmetals. Tin can form various compounds, both inorganic and organic. Inorganic tin compounds do not contain a tin-carbon bond, whereas organotin compounds contain at least one tin-carbon bond (Kroschwitz and Howe-Grant 1997; Lide 2000). The divalent and tetravalent oxidation states can be designated using the names stannous and stannic, respectively, in the name of the compound. Another commonly encountered nomenclature system, the Stock Oxidation-Number system, denotes the oxidation state in Roman numerals in parentheses following the metal's name: tin(II) and tin(IV) (Smith 1996). Table 4-1 lists common synonyms and other pertinent identification information for tin and representative inorganic and organic tin compounds.

4.2 PHYSICAL AND CHEMICAL PROPERTIES

Tin is a silver-white metal that is malleable and somewhat ductile. It has a highly crystalline structure and exists in two allotropic forms at normal pressures. Gray or α tin exists below 13.2 °C and has a cubic structure. At 13.2 °C, gray tin is converted to white or β tin, which has a tetragonal structure. In compounds, tin can exist in the +2 or +4 oxidation state. Industrially important organotin compounds include the dimethyltin, dibutyltin, tributyltin, dioctyltin, triphenyltin, and tricyclohexyltin families. Organotin compounds that are industrially important contain tin in the +4 oxidation state (Kroschwitz and Howe-Grant 1997; Lide 2000). Table 4-2 lists important physical and chemical properties of tin and representative inorganic and organic tin compounds.

Table 4-1. Chemical Identity of Tin and Tin Compounds[a]

Characteristic	Tin	Tin(II) chloride	Tin(IV) oxide
Synonyms	Metallic tin; silver matt powder; tin flake	Stannous chloride; tin dichloride; tin protochloride	Stannic oxide; tin oxide; stannic anhydride
Trade name	No data	No data	No data
Chemical formula	Sn	$SnCl_2$	SnO_2
Chemical structure	Sn	$SnCl_2$	SnO_2
Identification numbers:			
CAS registry	7440-31-5	7772-99-8	18282-10-5
NIOSH RTECS	XP7320000[b]	XP8700000[b]	XQ4000000[b]
EPA hazardous waste	No data	No data	No data
DOT/UN/NA/ IMCO shipping	No data	No data	No data
HSDB	5035	582	5064
NCI	No data	C02722	No data
EINECS	231-141-8	231-868-0	242-159-0

Table 4-1. Chemical Identity of Tin and Tin Compounds[a]

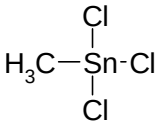
Characteristic	Tin(II) fluoroborate	Tin(II) fluoride	Monomethyltin trichloride
Synonyms	Tetraflurorborate(1-), tin(2+) (2:1); tin bis(tetrafluoroborate)	Stannous fluoride; easygel; fluoristan; Gel-Kam; Gel-Tin	Trichloromethyl stannane; methyltin trichloride
Trade name	No data	No data	No data
Chemical formula	SnB_2F_8	SnF_2	CH_3Cl_3Sn
Chemical structure	$Sn(BF_4)_2$	SnF_2	
Identification numbers:			
CAS registry	13814-97-6	7783-47-3	993-16-8
NIOSH RTECS	No data	XQ3450000[b]	WH8585500[b]
EPA hazardous waste	No data	No data	No data
DOT/UN/NA/ IMCO shipping	No data	No data	No data
HSDB	No data	783	No data
NCI	No data	No data	No data
EINECS	237-487-6	231-999-3	213-608-8

Table 4-1. Chemical Identity of Tin and Tin Compounds[a]

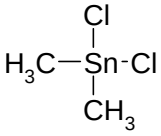
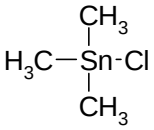
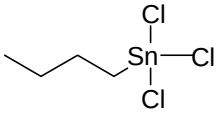
Characteristic	Dimethyltin dichloride	Trimethyltin chloride	Monobutyltin trichloride
Synonyms	Dichlorodimethyl stannane; Cotin 210	Chlorotrimethyl stannane; chlorotrimethyltin; trimethylchlorotin	Mono-n-butyltin trichloride; butyltrichloro stannane
Trade name	No data	No data	No data
Chemical formula	$C_2H_6Cl_2Sn$	C_3H_9ClSn	$C_4H_9Cl_3Sn$
Chemical structure			
Identification numbers:			
CAS registry	753-73-1	1066-45-1	1118-46-3
NIOSH RTECS	WH7245000[b]	WH6850000[b]	WH678000[b]
EPA hazardous waste	No data	No data	No data
DOT/UN/NA/ IMCO shipping	No data	No data	No data
HSDB	No data	6413	6073
NCI	No data	No data	No data
EINECS	212-039-2	213-917-8	214-263-6

Table 4-1. Chemical Identity of Tin and Tin Compounds[a]

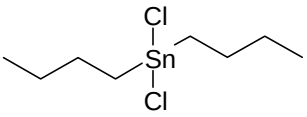
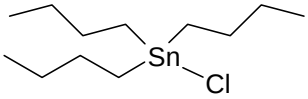
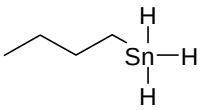
Characteristic	Dibutyltin dichloride	Tributyltin chloride	Monobutyltin hydride
Synonyms	Dibutyltin chloride; dichlorodibutyltin; dichlorodibutylstannane	Chlorotributylstannane; tri-n-butyltin chloride	n-Butyltin; butylstannane; butyltin trihydride
Trade name	No data	No data	No data
Chemical formula	$C_8H_{18}Cl_2Sn$	$C_{12}H_{27}ClSn$	$C_4H_{12}Sn$
Chemical structure			
Identification numbers:			
CAS registry	683-18-1	1461-22-9	2406-65-7
NIOSH RTECS	WH7100000[b]	WH6820000[b]	No data
EPA hazardous waste	No data	No data	No data
DOT/UN/NA/ IMCO shipping	No data	No data	No data
HSDB	6071	No data	No data
NCI	No data	No data	No data
EINECS	211-670-0	215-958-7	No data

Table 4-1. Chemical Identity of Tin and Tin Compounds[a]

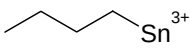
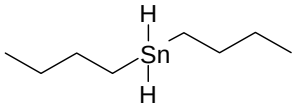
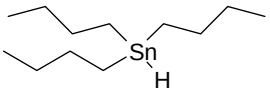
Characteristic	Monobutyltin ion	Dibutyltin hydride	Tributyltin hydride
Synonyms	No data	Di-n-butyltin; dibutylstannane; dibutyltin dihydride	Tributylstannane; tributyltin; Tributylstannic hydride
Trade name	No data	No data	No data
Chemical formula	C_4H_8Sn	$C_8H_{20}Sn$	$C_{12}H_{28}Sn$
Chemical structure			
Identification numbers:			
CAS registry	78763-54-9	1002-53-5	688-73-3
NIOSH RTECS	No data	WH6883600[b]	WH8675000[b]
EPA hazardous waste	No data	No data	No data
DOT/UN/NA/ IMCO shipping	No data	No data	No data
HSDB	No data	No data	6362
NCI	No data	No data	No data
EINECS	No data	No data	211-704-4

Table 4-1. Chemical Identity of Tin and Tin Compounds[a]

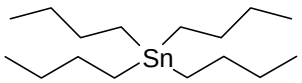
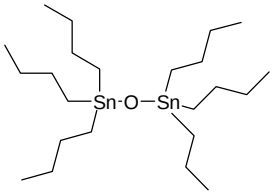
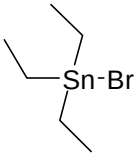
Characteristic	Tetrabutyltin	Bis(tributyltin) oxide	Triethyltin bromide
Synonyms	Tetrabutylstannane	Lastanox Q; Biomet TBTO; oxybis(tributyltin)	Bromotriethyl-stannane
Trade name	No data	TBTO[c]	No data
Chemical formula	$C_{16}H_{36}Sn$	$C_{24}H_{54}OSn_2$	$C_6H_{15}BrSn$
Chemical structure			
Identification numbers:			
CAS registry	1461-25-2	56-35-9	2767-54-6
NIOSH RTECS	WH8605000[b]	JN8750000[b]	WH6740000[b]
EPA hazardous waste	No data	No data	No data
DOT/UN/NA/IMCO shipping	No data	No data	No data
HSDB	6074	6505	No data
NCI	No data	No data	No data
EINECS	215-960-8	200-268-0	220-443-5

Table 4-1. Chemical Identity of Tin and Tin Compounds[a]

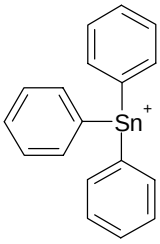
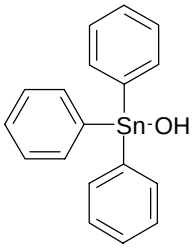
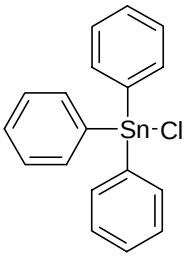
Characteristic	Triphenyltin	Triphenyltin hydroxide	Triphenyltin chloride
Synonyms	Fentin [ISO]; triphenylstannylium	Fentin hydroxide; hydroxytriphenyl stannane	Chlorotriphenyltin; triphenylchloro-stannane; Aquatin; fentin chloride
Trade name	No data	No data	No data
Chemical formula	$C_{18}H_{15}Sn$	$C_{18}H_{16}OSn$	$C_{18}H_{15}ClSn$
Chemical structure			
Identification numbers:			
CAS registry	668-34-8	76-87-9	639-58-7
NIOSH RTECS	No data	WH8575000[b]	WH6860000[b]
EPA hazardous waste	No data	No data	No data
DOT/UN/NA/ IMCO shipping	No data	No data	No data
HSDB	No data	1784	6404
NCI	No data	C00260	No data
EINECS	No data	200-990-6	211-358-4

Table 4-1. Chemical Identity of Tin and Tin Compounds[a]

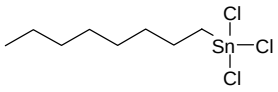
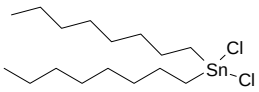
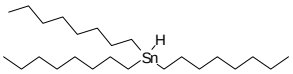
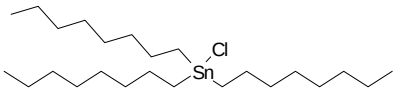
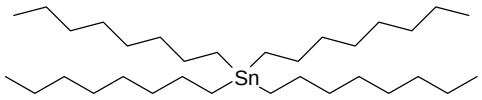
Characteristic	Mono-n-octyltin trichloride	Di-n-octyltin dichloride	Trioctyltin stannane
Synonyms	Trichlorooctylstannane; n-octyltin trichloride	Dichlorodioctyltin; DOTC; Stannane, dichlorodioctyl-	No data
Trade name	No data	No data	No data
Chemical formula	$C_8H_{17}Cl_3Sn$	$C_{16}H_{34}Cl_2Sn$	$C_{24}H_{52}Sn$
Chemical structure			
Identification numbers:			
CAS registry	3091-25-6	3542-36-7	869-59-0
NIOSH RTECS	WH8590000[b]	WH724700[b]	No data
EPA hazardous waste	No data	No data	No data
DOT/UN/NA/ IMCO shipping	No data	No data	No data
HSDB	No data	No data	No data
NCI	No data	No data	No data
EINECS	221-435-4	222-583-2	No data

Table 4-1. Chemical Identity of Tin and Tin Compounds[a]

Characteristic	Tri-n-octyltin chloride	Tetra-n-octylstannane
Synonyms	Chlorotrioctyl-stannane	Tetraoctylstannane
Trade name	No data	No data
Chemical formula	$C_{24}H_{51}ClSn$	$C_{32}H_{68}Sn$
Chemical structure		
Identification numbers:		
CAS registry	2587-76-0	3590-84-9
NIOSH RTECS	WH6855000[b]	WH8635500[b]
EPA hazardous waste	No data	No data
DOT/UN/NA/ IMCO shipping	No data	No data
HSDB	No data	No data
NCI	No data	No data
EINECS	219-969-8	222-733-7

[a]All information obtained from HSDB 2003 and ChemID 2003, except where noted.
[b]RTECS 2003
[c]Tomlin 1997

CAS = Chemical Abstracts Service; DOT/UN/NA/IMCO = Department of Transportation/United Nations/North America/International Maritime Dangerous Goods Code; EINECS = European Inventory of Existing Chemical Substances; EPA = Environmental Protection Agency; HSDB = Hazardous Substances Data Bank; NCI = National Cancer Institute; NIOSH = National Institute for Occupational Safety and Health; RTECS = Registry of Toxic Effects of Chemical Substances

Table 4-2. Physical and Chemical Properties of Tin and Tin Compounds[a]

Property	Tin	Tin(II) chloride	Tin(IV) oxide	Tin(II) fluoride
Molecular weight	118.69	189.60	150.71	156.71
Color	Silver-white	White	White	White
Physical state	Solid	Solid	Solid	Solid
Melting point	231.9 °C	246 °C	1,630 °C	213 °C
Boiling point	2,507 °C	623 °C	Sublimes 1,800–1,900 °C	850 °C
Density (g/cm^3)	7.265 (white tin) 5.769 (gray tin)	3.90	6.95	4.57 at 25 °C
Odor	Odorless	Odorless	No data	No data
Odor threshold:				
Water	No data	No data	No data	No data
Air	No data	No data	No data	No data
Solubility:				
Water	Insoluble	90 g/100 g water at 20 °C	Insoluble	30–39% in water at 20 °C
Other solvents	Soluble in hydrochloric acid, sulfuric acid, aqua regia, alkali, slightly soluble in dilute nitric acid	Very soluble in hydrochloric acid; soluble in alcohol, ethyl acetate, glacial acetic acid, sodium hydroxide solution	Insoluble in alcohol, cold acids; slowly soluble in hot concentrated potassium or sodium hydroxide solution	Practically insoluble in ethanol, ether, and chloroform
Partition coefficients:				
Log octanol/water	No data	No data	No data	No data
Log K_{oc}	No data	No data	No data	No data
Vapor pressure	$8x10^{-3}$ mm Hg at 1,224 °C	25 mm Hg at 427.9 °C	No data	No data
Henry's law constant	No data	No data	No data	No data
Autoignition temperature	No data	No data	No data	No data
Flashpoint	No data	No data	No data	No data
Flammability limits	No data	No data	No data	No data
Explosive limits	No data	No data	No data	No data

Table 4-2. Physical and Chemical Properties of Tin and Tin Compounds[a]

Property	Monomethyltin trichloride	Dimethyltin dichloride	Trimethyltin chloride	Monobutyltin trichloride
Molecular weight	240.08[b]	219.67[b]	199.26	282.17
Color	Colorless[b]	Colorless[b]	Colorless	Colorless
Physical state	Solid[b]	Solid[b]	Solid	Liquid
Melting point	43 °C[b]	90 °C (107 °C)[b]	37.5 °C	-63 °C
Boiling point	171 °C[b]	185–190 °C[b]	154–156 °C	102 °C at 12 mm Hg
Density (g/cm^3)	No data	No data	No data	1.71 at 25 °C
Odor	No data	No data	No data	No data
Odor threshold:				
Water	No data	No data	No data	No data
Air	No data	No data	No data	No data
Solubility:				
Water	Soluble in cold water[b]	Soluble in cold water[b]	Miscible with water	Sparingly soluble in water
Other solvents	Soluble in organic solvents[b]	Soluble in organic solvents[b]	Soluble in organic solvents	Soluble in organic solvents
Partition coefficients:				
Log octanol/water	No data	No data	No data	No data
Log K_{oc}	No data	No data	No data	No data
Vapor pressure	No data	No data	No data	No data
Henry's law constant	No data	No data	No data	No data
Autoignition temperature	No data	No data	No data	No data
Flashpoint	105 °F (40 °C)[c]	No data	207 °F (97 °C)[c]	No data
Flammability limits	No data	No data	No data	No data
Explosive limits	No data	No data	No data	No data

Table 4-2. Physical and Chemical Properties of Tin and Tin Compounds[a]

Property	Dibutyltin dichloride	Bis(tributyltin) oxide	Tributyltin chloride	Tributyltin hydride
Molecular weight	303.85	596.11	325.49[d]	291.09
Color	White	Slightly yellow	Colorless[d]	No data
Physical state	Solid	Liquid	Liquid[d]	Liquid
Melting point	43 °C	<-45 °C[e]	No data	No data
Boiling point	135 °C at 10mmHg	180°C at 2 mm Hg	145–147 °C at 5 mm Hg[e]	112.5-113.5 °C at 8 mm Hg
Density (g/cm^3)	1.36 at 24 °C	1.17 at 25 °C	1.20[e]	1.103 at 20 °C
Odor	No data	Weak odor	No data	No data
Odor threshold:				
Water	No data	No data	No data	No data
Air	No data	No data	No data	No data
Solubility:				
Water	Insoluble in cold water	4 mg/L at pH 7, 20 °C	Insoluble in cold water[d]	No data
Other solvents	Soluble in ether benzene, alcohol	Miscible with organic solvents	Soluble in oxygenated, chlorinated and aromatic solvents[d]	No data
Partition coefficients:				
Log octanol/water	0.97	No data	No data	No data
Log K_{oc}	No data	No data	No data	No data
Vapor pressure	2 mm Hg at 100 °C	7.5x10^{-6} mm Hg at 20 °C[f]	No data	No data
Henry's law constant	No data	No data	No data	No data
Autoignition temperature	No data	No data	No data	No data
Flashpoint	335 °F (168 °C)	>212 °F (100 °C)	>230 °F (110 °C)[c]	104 °F (40 °C)[c]
Flammability limits	No data	No data	No data	No data
Explosive limits	No data	No data	No data	No data

Table 4-2. Physical and Chemical Properties of Tin and Tin Compounds[a]

Property	Tetrabutyltin	Triethyltin bromide	Triphenyltin hydroxide	Triphenyltin chloride
Molecular weight	347.16	285.79[b]	367.03	385.48
Color	Colorless or slightly yellow	Colorless[b]	White	White
Physical state	Oily liquid	Liquid[b]	Solid	Solid
Melting point	-97 °C	-13.5 °C[b]	119 °C	103.5 °C
Boiling point	145 °C at 10 mm Hg	223–224 °C[b]	No data	240 °C at 13.5 mmHg
Density (g/cm^3)	1.054 at 20 °C	1.630 g/mL[b]	1.54 at 20 °C	No data
Odor	Distinct, characteristic	No data	Odorless	No data
Odor threshold:				
Water	No data	No data	No data	No data
Air	No data	No data	No data	No data
Solubility:				
Water	Insoluble in water	Very slightly soluble in cold water[b]	1.2 mg/L at 20 °C	40 mg/L at 20 °C
Other solvents	Soluble in organic solvents	Soluble in organic solvents[b]	Slightly soluble in toluene, alcohol	Moderately soluble in organic solvents
Partition coefficients:				
Log octanol/water	No data	No data	3.53	4.19
Log K_{oc}	No data	No data	No data	No data
Vapor pressure	No data	No data	$3.53x10^{-7}$ mm Hg at 25 °C	No data
Henry's law constant	No data	No data	No data	No data
Autoignition temperature	No data	No data	No data	No data
Flashpoint	225 °F (107 °C)[c]	211 °F (99 °C)[c]	211 °F (99 °C)[c]	No data
Flammability limits	No data	No data	No data	No data
Explosive limits	No data	No data	No data	No data

Table 4-2. Physical and Chemical Properties of Tin and Tin Compounds[a]

Property	Tetraoctylstannane
Molecular weight	571.59[b]
Color	No data
Physical state	No data
Melting point	No data
Boiling point	268 °C at 10 mm Hg[b]
Density (g/cm^3)	0.9605[b]
Odor	No data
Odor threshold:	
Water	No data
Air	No data
Solubility:	
Water	No data
Other solvents	No data
Partition coefficients:	
Log octanol/water	No data
Log K_{oc}	No data
Vapor pressure	No data
Henry's law constant	No data
Autoignition temperature	No data
Flashpoint	No data
Flammability limits	No data
Explosive limits	No data

[a]All information obtained from HSDB 2003, except where noted.
[b]Weast 1980
[c]Aldrich 2003-2004
[d]Ashford 1994
[e]Lewis 1997
[f]Blunden et al. 1984