4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

Information regarding the chemical identity of the most common cyanides is located in Table 4-1. Hydrogen cyanide is a toxic gas that may enter the environment from both natural processes and human industrial activities. It may exist in polymeric forms. The cyanide compounds in which cyanide can be obtained as CN^- are classified as simple and complex cyanides. Some simple cyanides are soluble in water (sodium cyanide, NaCN; potassium cyanide, KCN; and calcium cyanide, $Ca(CN)_2$), while others are sparingly soluble or almost insoluble (copper (I) cyanide, CuCN). Cyanogen (NC-CN) and cyanogen chloride (CNCl) are a highly toxic gases that are soluble in water. At neutral pH, cyanogen undergoes a slow hydrolysis to form hydrogen cyanide, cyanic acid (HOCN), and other products. At alkaline pH, CNCl hydrolyzes to CNO^-, which has only limited toxicity. Alkaline chlorination of water containing cyanide produces cyanogen chloride. Thiocyanate (SCN^-) is an oxidation product of the cyanide anion (CN^-), produced in the presence of a sulfur donor.

4.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of cyanide is located in Table 4-2. Cyanides form strong complexes with many metals, particularly those of the transition series. One example of such complex formation is the reaction of cyanide with iron in the formation of ferrocyanide and ferricyanide complexes. Solutions of ferrocyanides and ferricyanides can form hydrogen cyanide and cyanide ions when exposed to sunlight or ultraviolet radiation. Cyanogenic glycosides are cyanide compounds produced naturally in many plants (Jones 1998). These glycosides produce hydrogen cyanide when hydrolyzed (EPA 1978c) or digested (Ellenhorn and Barceloux 1997; WHO 2004). For example, in the human gut, the cyanogenic glycoside amygdalin, which is found in bitter almonds and in apricot pits and is the active ingredient in the drug Laetrile, undergoes two enzymatically catalyzed hydrolysis steps (Ellenhorn and Barceloux 1997). The first step involves the removal of one of the two β-D-glucopyranosyl groups from amygdalin through the action of beta-glucosidase to form the cyanogenic glycoside, prunasin. The enzyme, emulsion, then hydrolyzes prunasin to form hydrogen cyanide, glucose, and benzaldehyde.

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

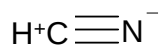
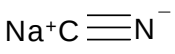
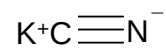
Characteristic	Hydrogen cyanide	Sodium cyanide	Potassium cyanide
Synonym(s)	Formonitrile; hydrocyanic acid; prussic acid	Cyanide of sodium; hydrocyanic acid; sodium salt	Cyanide of potassium; hydrocyanic acid; potassium salt
Registered trade name(s)	Cyclone B; Cyclon[b]	Cyanogran[c]	Carswell No. 688A
Chemical formula	HCN	NaCN	KCN
Chemical structure			
Identification numbers:			
CAS registry	74-90-8	143-33-9	151-50-8
NIOSH RTECS	MW6825000	VZ7530000	TS8750000
EPA hazardous waste	P063; D003	P106; D003	P098; D003
OHM/TADS	7216749	7216892	7216862
DOT/UN/NA/IMCO shipping	UN1051; IMO 6.1 UN1614; NA 1051	UN1689; IMO 6.1	UN1680; IMO 6.1
HSDB	165	734	1245
NCI	No data	No data	No data

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

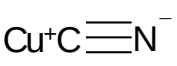
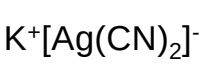
Characteristic	Calcium cyanide	Copper(I) cyanide	Potassium silver cyanide
Synonym(s)	Calcid; calcyan; cyanide of calcium	Cuprous cyanide[c]; cupricin[c]	Potassium argentocyanide; potassium dicyanoargentate
Registered trade name(s)	Caswell No. 142; Cyanogas[c]	AI3–28745	No data
Chemical formula	$Ca(CN)_2$	CuCN	$KAg(CN)_2$
Chemical structure			
Identification numbers:			
CAS registry	592-01-8	544-92-3	506-61-6
NIOSH RTECS	EW0700000	GL7150000	TT5775000
EPA hazardous waste	P021; D003	P029; D003	P099; D003; D011
OHM/TADS	7216626	No data	No data
DOT/UN/NA/IMCO shipping	UN1575; IMO 6.1	UN1587; IMO 6.1	No data
HSDB	242	1438	6053
NCI	No data	No data	No data

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

Characteristic	Cyanogen	Cyanogen chloride	Ammonium thiocyanate
Synonym(s)	Carbon nitride; dicyanogen; ethanedinitrile	Chlorine cyanide; chlorocyan	Thiocyanic acid, ammonium salt; ammonium rhodanide; ammonium sulfocyanate[c]
Registered trade name(s)	No data	Caswell No. 267	Trans-Aid[b]
Chemical formula	$(CN)_2$	CNCl	NH_4SCN
Chemical structure	$N\equiv C-C\equiv N$	$Cl-C\equiv N$	$NH_4^+S-C\equiv N^-$
Identification numbers:			
CAS registry	460-19-5	506-77-4	1762-95-4
NIOSH RTECS	GT1925000	GT2275000	XK7875000
EPA hazardous waste	P031; D003	P033; D003	No data
OHM/TADS	7216656	7216658	721218
DOT/UN/NA/IMCO shipping	UN1026; IMO 2.3	UN1589; IMO 2.3	NA9092
HSDB	2130	917	701
NCI	No data	No data	No data

[a]All data are from HSDB 2004 unless otherwise noted.
[b]Crop Protection Handbook 2004
[c]Budavari 1989

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

Table 4-2. Physical and Chemical Properties of Cyanide and Compounds

Property	Hydrogen cyanide	Sodium cyanide
Molecular weight	27.03[a]	49.01[a]
Color	Colorless[b]	White[b]; colorless[a]
Physical state	Gas or liquid[b]	Solid[b]
Melting point, °C	-13.4[b]	563.7[a]
Boiling point, °C	25.70[c]	1496[a]
Density, g/cm^3	0.6884 (liquid at 20 °C)[c]	1.60 (for cubic form)[c]
Odor	Faint bitter almond odor[d]	Odorless when dry, emits slight odor of HCN in damp air[b]
Odor threshold:		
Water	0.17 ppm (w/v)[e]	No data
Air	0.58 ppm (v/v)[e]; 0.8–4.4 ppm[f]	No data
Solubility:		
Water	Miscible[a]	48 g/100 mL at 10 °C[c]
Organic solvent(s)	Soluble in ethanol, ether[a]	Slightly soluble in ethanol[a] and formamide[c]
Partition coefficients:		
Log K_{ow}	0.66[g]; 1.07 (calc.)[h]	0.44[g]
Log K_{oc}	No data	No data
Vapor pressure, mm Hg	630 (at 20 °C)[f]	0.76 at 800 °C[c]
Henry's law constant	5.1x10^{-2} atm-m^3/mol[i]	No data
Autoignition temperature	538[c]	No data
Flashpoint, °C	-17.8 (closed cup)[c]	No data
Flammability limits	5.6–40%[j]	Not combustible[j]
Conversion factors:		
mg/m^3 to ppm in air, 20 °C	1 mg/m^3 = 0.890 ppm	NA[k]
ppm to mg/L in water	ppm (w/v) = mg/L = µg/mL	ppm (w/v) = mg/L = µg/mL
ppm to mg/kg in soluble samples	ppm (w/w) = mg/kg = µg/g	ppm (w/w) = mg/kg = µg/g
Explosive limits	Upper, 40%; lower, 5.6%[f]	No data

Table 4-2. Physical and Chemical Properties of Cyanide and Compounds

Property	Potassium cyanide	Calcium cyanide
Molecular weight	65.12[a]	92.12[a]
Color	White[b]; colorless[a]	White[a]
Physical state	Solid[b]	Solid[a]
Melting point, °C	634.5[a]	Decomposes at >350 °C[a]
Boiling point, °C	No data	No data
Density, g/cm^3	1.553 (for cubic form)[c]	1.8–1.9 (commercial product)[c]
Odor	Faint bitter almond odor[b]	Faint bitter almond odor[b]
Odor threshold:		
Water	No data	No data
Air	No data	No data
Solubility:		
Water	71.6 g/100 mL at 25 °C[c]	Soluble in water with gradual liberation of HCN[b]
Organic solvent(s)	Slightly soluble in ethanol[c] and methanol[b]	
Partition coefficients:		
Log K_{ow}	No data	No data
Log K_{oc}	3.0 (calculated)[l]	No data
Vapor pressure, mm Hg	No data	No data
Henry's law constant	No data	No data
Autoignition temperature	No data	No data
Flashpoint, °C	No data	No data
Flammability limits	Not combustible[j]	Not combustible[j]
Conversion factors:		
mg/m^3 to ppm in air, 20 °C	NA[k]	NA[k]
ppm to mg/L in water	ppm (w/v) = mg/L = µg/mL	ppm (w/v) = mg/L = µg/mL
ppm to mg/kg in soluble samples	ppm (w/w) = mg/kg = µg/g	
Explosive limits	No data	No data

Table 4-2. Physical and Chemical Properties of Cyanide and Compounds

Property	Potassium silver cyanide	Cyanogen
Molecular weight	199.01[b]	52.04[a]
Color	White[b]	Colorless[a]
Physical state	Solid[b]	Gas[a]
Melting point, °C	No data	-27.9[a]
Boiling point, °C	No data	-20.7[a]
Density, g/cm^3	2.36[a]	0.9577 at -21.17 °C[a]
Odor	No data	Almond-like odor[b]
Odor threshold:		
Water	No data	No data
Air	No data	230 ppm; irritating at 15 ppm[f]
Solubility:		
Water	Soluble[b]; 250 g/L (25 °C)[m]	450 cc/100 cc (20 °C)[a]
Organic solvent(s)	Slightly soluble in ethanol[a]	Soluble in ethanol and ethyl ether[a]
Partition coefficients:		
Log K_{ow}	No data	0.07[n]
Log K_{oc}	No data	No data
Vapor pressure, mm Hg	No data	3,800 at 20 °C[o]
Henry's law constant	No data	No data
Autoignition temperature	No data	No data
Flashpoint, °C	No data	No data
Flammability limits	No data	6.6–32% in air[j]
Conversion factors:		
mg/m^3 to ppm in air, 20 °C	NA[k]	1 mg/m^3 = 0.462 ppm
ppm to mg/L in water	ppm (w/v) = mg/L = µg/mL	ppm (w/v) = mg/L = µg/mL
ppm to mg/kg in soluble samples	ppm (w/w) = mg/kg = µg/g	ppm (w/w) = mg/kg = µg/g
Explosive limits	No data	No data

Table 4-2. Physical and Chemical Properties of Cyanide and Compounds

Property	Cyanogen chloride	Copper(I) cyanide
Molecular weight	61.47[a]	89.56[a]
Color	Colorless[d]	White to cream-colored[b]
Physical state	Gas[d]	Solid[a]
Melting point, °C	-6[a]	473 (in N_2)[a]
Boiling point, °C	13.8[b];12.7[a]	Decomposes[a]
Density, g/cm^3	1.186[b]	2.92[a]
Odor	Highly irritating[h]	No data
Odor threshold:		
Water	No data	No data
Air	1 ppm[f]	No data
Solubility:		
Water	Soluble[b]; 27.5 mg/L (25 °C)[m]	2.6 mg/L (25°C)[m]
Organic solvent(s)	Soluble in ethanol and ethyl ether[b]	Insoluble in alcohol[f]
Partition coefficients:		
Log K_{ow}	No data	No data
Log K_{oc}	No data	No data
Vapor pressure, mm Hg	760 at 13.8 °C	No data
Henry's law constant	3.2x10^{-3} atm-m^3/mol[m]	No data
Autoignition temperature	No data	No data
Flashpoint, °C	No data	No data
Flammability limits	Not combustible[f]	Does not readily ignite[f]
Conversion factors:		
mg/m^3 to ppm in air, 20 °C	1 mg/m^3 = 2.5 ppm	NA[k]
ppm to mg/L in water	ppm (w/v) = mg/L = µg/mL	ppm (w/v) = mg/L = µg/mL
ppm to mg/kg in soluble samples	ppm (w/w) = mg/kg = µg/g	ppm (w/w) = mg/kg = µg/g
Explosive limits	No data	No data

Table 4-2. Physical and Chemical Properties of Cyanide and Compounds

Property	Ammonium thiocyanate
Molecular weight	76.12[a]
Color	Colorless[a]
Physical state	Solid[a]
Melting point, °C	149.6[a]
Boiling point, °C	170 decomposes[a]
Density, g/cm^3	1.305[a]
Odor	Odorless[b]
Odor threshold:	
Water	No data
Air	No data
Solubility:	
Water	128 g/100 cc at 0 °C; Very soluble in hot water[a]
Organic solvent(s)	Very soluble in ethanol; soluble in acetone and methanol; insoluble in ethyl acetate and chloroform[b]
Partition coefficients:	
Log K_{ow}	No data
Log K_{oc}	No data
Vapor pressure, mm Hg	No data
Henry's law constant	No data
Autoignition temperature	No data
Flashpoint, °C	No data
Flammability limits	May be combustible[f]
Conversion factors:	
mg/m^3 to ppm in air, 20 °C	NA[k]
ppm to mg/L in water	ppm (w/v) = mg/L = µg/mL
ppm to mg/kg in soluble samples	ppm (w/w) = mg/kg = µg/g
Explosive limits	No data

[a]Lide 1993
[b]Budavari 1989
[c]Jenks 1979
[d]Hawley 1981
[e]Amoore and Hautala 1983
[f]HSDB 2004
[g]EPA 1984a
[h]Verschueren 1983
[i]Yoo et al. 1986; value at 25 °C and saturation pressure
[j]NFPA 1994
[k]Since these compounds do not exist in the atmosphere in the vapor phase, their concentrations are always expressed in weight by volume unit (e.g., mg/m^3).
[l]Kenaga 1980
[m]EPA 1985f
[n]Hansch et al. 1995
[o]EPA 1978c

EPA = Environmental Protection Agency; HCN = hydrogen cyanide; HSDB = Hazardous Substances Data Bank; NA = not applicable

Hydrogen cyanide has a pK_a of 9.2 (Smith and Martell 1989); therefore, solutions of cyanide compounds in water (such as from sodium cyanide and potassium cyanide) can form hydrogen cyanide at acid and neutral pHs. Alkaline solutions with pH >12 are practical for preventing significant outgassing of hydrogen cyanide.

Hydrogen cyanide is a fire hazard and may be explosive when an excess of a strong acid is added to confined hydrogen cyanide. Solutions of some cyanide compounds are not stable and may decompose upon exposure to air or light.