CHAPTER 4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

Information regarding the chemical identities of the most common compounds containing cyanide is presented 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 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.

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

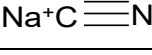
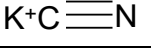
Characteristic	Information		
Chemical name	Hydrogen cyanide	Sodium cyanide	Potassium cyanide
Synonym(s) and registered trade name(s)	Formonitrile; hydrocyanic acid; prussic acid; Cyclone B; Cyclon[b]	Cyanide of sodium; hydrocyanic acid; sodium salt; Cyanogran[c]	Cyanide of potassium; hydrocyanic acid; potassium salt
Chemical formula	HCN	NaCN	KCN
SMILES	C#N	[C-]#N.[Na+]	[C-]#N.[K+]
Chemical structure			
CAS Registry Number	74-90-8	143-33-9	151-50-8
Chemical name	Calcium cyanide	Copper(I) cyanide	Potassium silver cyanide
Synonym(s) and registered trade name(s)	Calcid; calcyan; cyanide of calcium; Caswell No. 142; Cyanogas[c]	Cuprous cyanide[c]; cupricin[c]; AI3–28745	Potassium argentocyanide; potassium dicyanoargentate
Chemical formula	$Ca(CN)_2$	CuCN	$KAg(CN)_2$
SMILES	[Ca+2].[C-]#N.[C-]#N	[C-]#N.[Cu+]	[C-]#N.[C-]#N.[K+].[Ag+].

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

Characteristic	Information		
Chemical structure	$^{-}N\equiv C\ Ca^{+2}C\equiv N^{-}$	$Cu^{+}C\equiv N^{-}$	$K^{+}[Ag(CN)_2]^{-}$
CAS Registry Number	592-01-8	544-92-3	506-61-6
Chemical name	Cyanogen	Cyanogen chloride	Ammonium thiocyanate
Synonym(s) and registered trade name(s)	Carbon nitride; dicyanogen; ethanedinitrile	Chlorine cyanide; chlorocyan; Caswell No. 267	Thiocyanic acid, ammonium salt; ammonium rhodanide; ammonium sulfocyanate[c]; Trans-Aid[b]
Chemical formula	$(CN)_2$	CNCl	NH_4SCN
SMILES	N#CC#N	ClC#N	[S-]C#N.[NH4+]
Chemical structure	$N\equiv C-C\equiv N$	$Cl-C\equiv N$	$NH_4{}^{+}S-C\equiv N^{-}$
CAS Registry Number	460-19-5	506-77-4	1762-95-4

[a]All data are from HSDB 2004 unless otherwise noted.
[b]NLM 2024a, 2024b.
[c]Budavari 1989.

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

4.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding physical and chemical properties of cyanide is presented 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 1978) 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 then hydrolyzes prunasin to form hydrogen cyanide, glucose, and benzaldehyde.

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

Property	Information	
Chemical name	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
Taste threshold	No data	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 (calculated)[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	Information	
Chemical name	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
Taste threshold	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	Information	
Chemical name	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]
Taste threshold	No data	No data
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	Information	
Chemical name	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
Taste threshold	No data	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	Information
Chemical name	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
Taste threshold	No data
Solubility:	
Water	128 g/100 cc at 0°C[a]; Very soluble in hot water[a]; 181 g/100 cc at 25°C[p]
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

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

Property	Information
Explosive limits	No data

[a]Lide 1990.
[b]Budavari 1989.
[c]Jenks 1979.
[d]Hawley 1981.
[e]Amoore and Hautala 1983.
[f]HSDB 2004.
[g]EPA 1984.
[h]Verschueren 1983.
[i]Yoo et al. 1986; value at 25°C and saturation pressure.
[j]NLM 2024a, 2024c, 2024d, 2024e, 2024f.
[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 1985b.
[n]Hansch et al. 1995.
[o]EPA 1978.
[p]Lide 2005.

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 1976); therefore, solutions of cyanide compounds in water (such as from sodium cyanide and potassium cyanide) can form hydrogen cyanide and acid at slightly lower than 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.