4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

Information regarding the chemical identity of chlorine is located in Table 4-1. This information includes synonyms, chemical formula and structure, and identification numbers.

4.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of chlorine is located in Table 4-2.

Chlorine (Cl_2) is a heavier-than-air, greenish-yellow gas with a pungent, irritating odor (HSDB 2007). The odor threshold for chlorine is 0.002 ppm in air and 0.31 ppm in water (EPA 1994b, 1999). Perceivable sensory irritation occurs at 1.0 ppm in air (EPA 1999). Chlorine is a nonflammable gas; however, it is a very strong oxidizing agent, reacting explosively or forming explosive compounds or mixtures with many common chemicals (O'Neil et al. 2001). Chlorine reacts directly with nearly all of the elements to form chlorides (Lide 2005; O'Neil et al. 2001). Chlorine is stored and transported as a liquid in pressurized containers (EPA 1999).

Chlorine hydrolyzes rapidly and almost completely in water to form hypochlorous acid and hypochlorite as follows:

$$Cl_2 + H_2O \rightleftharpoons HOCl + H^+ + Cl^-$$

$$HOCl \rightleftharpoons H^+ + OCl^-$$

The equilibrium constants for these reactions are represented by:

$$K_1 = \frac{[HOCl][H^+][Cl^-]}{[Cl_2]} \quad (1)$$

$$K_2 = \frac{[H^+][OCl^-]}{[HOCl]} \quad (2)$$

Table 4-1. Chemical Identity of Chlorine[a]

Characteristic	Information
Chemical name	Chlorine
Synonyms/trade names	Chlorine gas[b], Bertholite, molecular chlorine, chlorine mol
Chemical formula	Cl_2
Chemical structure	Cl—Cl
Identification numbers:	
CAS registry	7782-50-5
NIOSH RTECS	FO2100000[c]
EPA hazardous waste	No data
DOT/UN/NA/IMCO shipping	UN1017; IMO 2.0
HSDB	206
EINECS	231-959-5[d]
NCI	No data

[a]All information obtained from HSDB 2007 except where noted.
[b]EPA 1999
[c]RTECS 2007
[d]IPCS 2006

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; RTECS = Registry of Toxic Effects of Chemical Substances

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

Property	Information
Molecular weight	70.906
Color	Greenish-yellow
Physical state	Gas
Melting point	-105.5 °C
Boiling point	-34.04 °C
Density in air	2.482 (air=1)[b]
Density, as liquid	
20 °C, 6.864 atm	1.4085 g/mL[c]
-35 °C, 0.9949 atm	1.5648 g/mL[c]
Odor	Pungent, irritating
Odor threshold:	
Water	0.002 ppm[c,d]
Air	0.31 ppm[c,d]
Solubility:	
Water	14.6 g/L at 0 °C; 7.3 g/L at 20 °C[c,d]
Other solvents	Glacial acetic acid, dimethylformamide, nitrobenzene, phosphoryl chloride, carbon tetrachloride, tetrachloroethane, pentachloroethane, hexachlorobutadiene, and chlorobenzene[e]
Partition coefficients:	
Log K_{ow}	Not applicable
Log K_{oc}	Not applicable
Vapor pressure at 20 °C	5,830 mm Hg
Henry's law constant	1.17×10^{-2} atm-m^3/mol[f]
Autoignition temperature	Not applicable
Flashpoint	Not applicable
Reactivity	Strong oxidizer; reacts explosively with many materials
Conversion factors	1 ppm=2.9 mg/m^3; 1 mg/m^3=0.344 ppm[c]

[a]All information obtained from HSDB 2007, except where noted.
[b]O'Neil et al. 2001
[c]EPA 1999
[d]EPA 1994b
[e]Schmittinger et al. 1996
[f]Staudinger and Roberts 1996

The relative percentage of Cl_2, HOCl, and OCl^- at some fixed concentration of Cl^- can be expressed as:

$$\%Cl_2 = \frac{[Cl_2]}{[Cl_2]+[HOCl]+[OCl^-]} \quad (3)$$

$$\%HOCl = \frac{[HOCl]}{[Cl_2]+[HOCl]+[OCl^-]} \quad (4)$$

$$\%OCl^- = \frac{[OCl^-]}{[Cl_2]+[HOCl]+[OCl^-]} \quad (5)$$

Using the expressions for the equilibrium constants in Equations 1 and 2 and the relationship that pH is equivalent to the negative logarithm of the hydronium ion concentration, Equations 3–5 can be re-written as:

$$\%Cl_2 = \frac{1}{1+\frac{K_1}{[Cl^-]}10^{pH}+\frac{K_1K_2}{[Cl^-]}10^{2pH}} \quad (6)$$

$$\%HOCl = \frac{1}{1+\frac{[Cl^-]}{K_1 10^{pH}}+K_2 10^{pH}} \quad (7)$$

$$\%OCl^- = \frac{1}{1+\frac{[Cl^-]}{K_1K_2 10^{2pH}}+\frac{1}{K_2 10^{pH}}} \quad (8)$$

Figure 4-1 illustrates the speciation as a function of pH using values for $K_1 = 3.9\text{x}10^{-4}$ M^2 (Cotton et al. 1999; Farr et al. 2003) and $K_2 = 2.9\text{x}10^{-8}$ M (Farr et al. 2003) at 25 °C.

Figure 4-1. Speciation of Cl_2, HOCl, and OCl^- as a Function of pH