3. CHEMICAL AND PHYSICAL INFORMATION

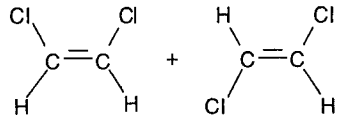
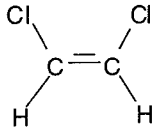
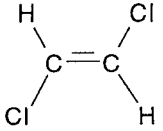
3.1 CHEMICAL IDENTITY

Information regarding the chemical identity of 1,2-dichloroethene is located in Table 3-l.

3.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of 1,2dichloroethene is located in Table 3-2. There are two isomers of 1,2-dichloroethene, the cis form and the trans form. Some important characteristics of the two forms are that they possess a high vapor pressure and the vapor is heavier than air (HSDB 1995). The trans form is sufficiently volatile that 50% evaporates from water in 22 minutes when stirred at 25 °C; the cis form is similarly volatile (HSDB 1995). Experiments have shown that the degradation of the trans form is relatively slow due to ultraviolet irradiation, unless lamps of approximately 15-20 watts are used (Guertler et al. 1994) to allow greater relative stability of the vapor form in the environment.

Table 3-1. Chemical Identity of 1,2-Dichloroethene

Characteristic	Information[a]		
	mixture	cis	trans
Chemical name	1,2,-Dichloroethene	cis-1,2-Dichloroethene	trans-1,2-Dichloroethene
Synonym(s)	Acetylene dichloride;[a,b] 1,2-dichloroethene;[a,c] 1,2-dichloroethylene; sym-1,2-dichloroethylene 1,2-DCE	(Z)-1,2-dichloroethene;[a,b] (Z)-1,2-dichloroethylene;[a,c] cis-acetylene dichloride; cis-1,2-dichloroethylene; cis-dichloroethylene	(E)-1,2-dichloroethene;[a,b] (E)-1,2-dichloroethylene; trans-acetylene dichloride; trans-1,2-dichloroethylene; trans-dichloroethylene
Registered trade name(s)	Dioform[d]	Not available	Not available
Chemical formula	$C_2H_2Cl_2$[a,e]	$C_2H_2Cl_2$[a,e]	$C_2H_2Cl_2$[a,e]
Chemical structure[f]			
Identification numbers:			
CAS registry	540-59-0[a,e]	156-59-2[a,e]	156-60-5[a,e]
NIOSH RTECS	KV9360000[a,g]	KV9420000[a,g]	KV9400000[a,g]
EPA hazardous waste	U079*	Not available	U079
OHM/TADS	8300194[h]	8300194[h]	8300194[h]
DOT/UN/NA/IMO shipping	UN 1150; dichloroethylene IMO 3.2; dichloroethylene	UN 1150; dichloroethylene IMO 3.2; dichloroethylene	UN 1150; 1,2-dichloroethylene IMO 3.2; 1,2-dichloroethylene
HSDB	149	5656	6361
NCI	C56031[a,c]	Not available	Not available

*This number, U079, applies to trans-1,2-dichloroethene and to the generic 1,2-dichloroethene; 1,2-dichloroethene is a mixture containing trans-1,2-dichloroethene (HSDB 1995). In effect, the hazardous waste number U079 refers to a mixture containing trans-1,2-dichloroethene.

[a]All information obtained from HSDB 1995, except where noted.
[b]SANSS 1994
[c]Chemline 1988
[d]Bennett 1981
[e]CAS 1994
[f]Merck 1989
[g]RTECS 1994
[h]OHM/TADS 1988

CAS = Chemical Abstracts Service; DOT/UN/NA/IMO = Dept. 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 3-2. Physical and Chemical Properties of cis- and trans-1,2-Dichloroethene

Property	Information		Reference
	cis	trans	
Molecular weight	96.95	96.95	Weast 1983; Merck 1989
Color	Colorless	Colorless	Hawley 1981; HSDB 1995
Physical state	Liquid	Liquid	Hawley 1981; HSDB 1995
Melting point	-81.5 °C -80.5 °C	-49.4 °C -50.0 °C	Weast 1983; Merck 1989 HSDB 1995
Boiling point	59.6 °C @ 745 mm Hg 60.3 °C @ 760 mm Hg	47.2 °C 745 mm Hg 48.0–48.5 °C @ 760 mm Hg	Weast 1983; Merck 1989
Density at 20/4 °C	1.2837	1.2565	Weast 1983; HSDB 1995
Odor	Ethereal, slightly acrid Sweet pleasant	Ethereal, slightly acrid Sweet pleasant	Merck 1989; HSDB 1995 HSDB 1995
Odor threshold:			
Water	No data	0.26 ppm	HSDB 1995
Air	No data	17 ppm v/v 0.084 ppm	Amoore and Hautala 1983 HSDB 1995
Solubility:			
Water at 25 °C	3.5 g/L	6.3 g/L	Horvath 1982; HSDB 1995
Organic solvents	Soluble in ether, alcohol, benzene, acetone, chloroform	Soluble in ether, alcohol, benzene, acetone, chloroform	Weast 1983; HSDB 1995
Partition coefficients:			
Log K_{ow}	1.86	2.09 (recommended value) 2.06	Hansch and Leo 1985; HSDB 1995
Log K_{oc}	1.69 (estimated)	1.56 (estimated)	HSDB 1995
Vapor pressure at 20 °C	180 mm Hg	265 mm Hg	Stevens 1979
Vapor pressure at 30 °C	273 mm Hg; 250 mm Hg	395 mm Hg; 410 mm Hg	HSDB 1995; Stevens 1979

TABLE 3-2. Physical and Chemical Properties of cis- and trans-1,2-Dichloroethene (continued)

Property	Information		Reference
	cis	trans	
Henry's law constant at 24.8 °C	4.08×10^{-3} atm-m^3/mol	9.38×10^{-3} atm-m^3/mol	Gossett 1987
	3.37×10^{-3} atm-m^3/mol	6.72×10^{-3} atm-m^3/mol	HSDB 1995
Autoignition temperature	460 °C	460 °C	Sax 1979
Flashpoint	6 °C	2–4 °C	Stevens 1979; HSDB 1995
Flammability limits in air	9.7–12.8 volume %	9.7–12.8 volume %	HSDB 1995
Conversion factors:			
ppm (v/v) to mg/m^3 in air at 25 °C	1 ppm (v/v) = 3.96 mg/m^3	1 ppm (v/v) = 3.96 mg/m^3	
mg/m^3 to ppm (v/v) in air at 25 °C	1 mg/m^3 = 0.25 ppm (v/v)	1 mg/m^3 = 0.25 ppm (v/v)	
Explosive limits	9.7–12.8% in air	9.7–12.8% in air	HSDB 1995; Stevens 1979

HSDB = Hazardous Substances Data Bank; v/v = volume per volume