3. CHEMICAL AND PHYSICAL INFORMATION

3.1 CHEMICAL IDENTITY

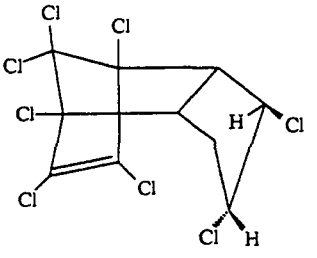
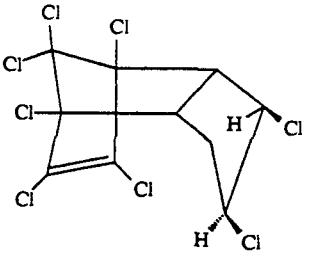
Data pertaining to the chemical identity of chlordane are listed in Table 3-l. Technical chlordane is a mixture of >140 related compounds, 120 of which have been recently identified by high resolution gas spectroscopy with electron capture, negative ionization mass spectroscopy (Dearth and Hites 1991c). Most of these compounds are minor or trace components. Sixty to 85% of technical chlordane consists of the stereoisomers *cis*- and *trans*-chlordane (Buchert et al. 1989; Worthing and Walker 1987). The ratio of the *cis* and *trans* isomers depends on the manufacturing process (Buchert et al. 1989). *Cis*-chlordane (lα,2α,3aα,4ß,7ß,7aα) is also known as α-chlordane. *trans*-chlordane (1α,2ß,3aα,4ß,7ß,7aα) is commonly known as γ-chlordane, although it is occasionally referred to as ß-chlordane (EPA 1984; CAS 1992; Worthing and Walker 1987). This is particularly confusing because γ-chlordane is also the common name of the 2,2,4,5,6,7,8,8 octachloro isomer. We will use the names *cis*- and *trans*-chlordane in this document to avoid confusion.

Other major constituents of technical chlordane are chlordene; heptachlor; *cis*-, and *trans*-nonachlor; α-, ß-, and γ-chlordene; 3a,4,5,5a,6-exo-hexachloro-la,2,3,3a5a,5b-hexahydro-1,4-methano-1H-cyclobuta[cd]pentalene; and 2,4,4,5,6,6,7,8-octachloro-2,3,3a,4,5,7a-hexahydro-1,4-methano-1H-indene (Miyazaki et al. 1985; Parlar et al. 1979).

3.2 PHYSICAL AND CHEMICAL PROPERTIES

The physical and chemical properties of chlordane are presented in Table 3-2. The physical and chemical properties of technical chlordane are difficult to specify since there are many components in the technical mixture. For example, technical chlordane is a viscous liquid made of a mixture of many compounds that are solids when pure (a eutectic mixture). The state of the technical product alone will effect the properties of the product. For example, the vapor pressure of the pure components of chlordane will be lower than the technical product because they are solids and have crystal lattice energies that reduce their vapor pressures relative to a liquid (Bidleman and Foreman 1987). The vapor pressure of the mixture will also change over time since the more volatile components will be removed faster, changing the composition of the mixture. Compositional changes with time may also

TABLE 3-1. Chemical Identity of Chlordane

Characteristic	Information	Reference
Chemical name	1,2,4,5,6,7,8,8-Octachloro-2,3,3a,4,7,7a-hexahydro-4,7-methano-1H-indene	CAS 1987
Synonym	1,2,4,5,6,7,8,8-Octachloro-3a,4,7,7a-tetrahydro-4,7-methanoindan	CAS 1987
Trade name(s)	Chlordan; Velsicol 1068®; Octachlor®	Anonymous 1988
Chemical formula	$C_{10}H_6Cl_8$	CAS 1988
Chemical structure	*trans*  *cis* 	CAS 1988
Identification Numbers:		
CAS Registry	12789-03-6 (technical) 57-74-9 (nonstereospecific) 5103-71-9 (*cis*-chlordane or α-chlordane) 5103-74-2 (*trans*-chlordane or γ-chlordane)	CAS 1988 Worthing and Walker 1987
NIOSH RTECS	PB9800000	NIOSH 1988
EPA Hazardous Waste[a]	U036	EPA 1982a
OHM-TADS	7215092	OHM-TADS 1988
DOT/UN/NA/IMCO	NA 2762	OHM-TADS 1988
HSDB	802	HSDB 1988
NCI	C00099	NIOSH 1988

[a]Related EPA hazardous waste numbers are as follows (EPA 1982a):
KO32: wastewater treatment sludge from the production of chlordane
KO33: wastewater and scrub water from the chlorination of cyclopentadiene in the production of chlordane
KO34: filter solids from the filtration of hexachlorocylclopentadiene in the production of chlordane
KO97: vacuum stripper discharge from the chlordane chlorinator in the production of chlordane

CAS = Chemical Abstract Service; DOT/UN/NA/IMCO = Department of Transportation/United Nations/North America/International Maritime Consultive Organization; 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 Base; RTECS = Registry of Toxic Effects of Chemical Substances

TABLE 3-2. Physical and Chemical Properties of Chlordane

Property	Information	Reference
Molecular weight	409.76 (pure chlordane)	
Color	Amber	Windholz 1983
	Colorless	Hawley 1981
Physical state	Viscous liquid (technical product)	Windholz 1983
Melting point		
cis-chlordane	106-107°C	Worthing and Walker 1987
trans-chlordane	104-105°C	Worthing and Walker 1987
Boiling point	175°C at 2 mmHg	Hawley 1981
Density (25°C)	1.59-1.63 g/cm^3	Windholz 1983
Odor	Odorless	Hawley 1981
	Mild pungent	NRCC 1974
Odor threshold	Not available	
Solubility[a]:		
Water	0.056 mg/L at 25°C for *cis*:*trans* (75:25)	Sanborn et al. 1976
	1.850 mg/L at 25°C[b]	Weil et al. 1974
Organic solvents	Miscible with hydrocarbon solvents	Whetstone 1964; Worthing and Walker 1987
Partition coefficients:		
Log K_{ow}	5.54 (estimated for pure chlordane)	EPA 1986b
Log K_{oc}	3.49-4.64[c]	Lyman 1982
	6.3 (*trans*-) suspended solids	Lau et al. 1989
Vapor pressure[d]:		
cis-chlordane		
(supercooled liquid)	2.2x10^{-5} mmHg	Foreman and Bidleman 1987
(crystal)[e]	3.0x10^{-6} mmHg	
trans-chlordane		
(supercooled liquid)	2.9x10^{-5} mmHg	Foreman and Bidleman 1987
(crystal)[e]	3.9x10^{-6} mmHg	
Henry's Law constant (25°C)	4.85x10^{-5} atm-m^3/mol[b]	Suntio et al. 1988
	8.31x10^{-5} atm-m^3/mol (*trans*-)	Fendinger et al. 1989
	4.8x10^{-5} atm-m^3/mol	Cotham and Bidleman 1991
Autoignition temperature	Not available	
Flashpoint	56°C (open cup)	OHM-TADS 1988
Flammability limits	Not available	
Conversion factors (25°C)		
ppm (v/v) to mg/m^3 in air	ppm (v/v) x 16.75 = mg/m^3	HSDB 1988
mg/m^3 to ppm (v/v) in air	mg/m^3 x 0.0597 = ppm (v/v)	
Explosive limits	Not available	Not available

[a]The solubility of the components of technical chlordane may differ from the solubility of the technical product.
[b]There was no indication whether the chlordane used in this study was technical grade chlordane or a mixture of chlordane isomers.
[c]Estimated for pure chlordane, using Equations 4-5 and 4-8 in Lyman 1982
[d]The vapor pressure of the components of technical chlordane may differ from the vapor pressure of the technical product.
[e]Calculated from the supercooled value

result from different rates of degradation and transport among the constituents of the mixture. Additionally, physical properties are not always available for the technical product, which makes comparing properties difficult and increases the uncertainty of any calculated properties. Finally, the overall effect of these differences cannot be evaluated since a complete set of physical properties for the components and technical product is not available.