

CHAPTER 4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

Data pertaining to the chemical identity of chlordane are listed in Table 4-1. Technical chlordane is a mixture of >140 related compounds, 120 of which have been 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 (1 α ,2 α ,3 $\alpha\alpha$,4 β ,7 β ,7 $\alpha\alpha$) is also known as α -chlordane. *trans*-Chlordane (1 α ,2 β ,3 $\alpha\alpha$,4 β ,7 β ,7 $\alpha\alpha$) is commonly known as γ -chlordane, although it is occasionally referred to as β -chlordane (CAS 1992; EPA 1984; 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. This toxicological profile for chlordane uses the names *cis*- and *trans*-chlordane to avoid confusion.

Table 4-1. 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(s) and registered trade name(s)	1,2,4,5,6,7,8,9-Octachloro-3a,4,7,7a-tetrahydro-4,7-methanoinden; Chlordan; Velsicol 1068®; Octachlor®	Anonymous 1988; CAS 1987
Chemical formula	C ₁₀ H ₆ Cl ₈	CAS 1988
Chemical structure	<div style="display: flex; justify-content: space-around; align-items: center;"> <div style="text-align: center;"> <p><i>trans</i></p> </div> <div style="text-align: center;"> <p><i>cis</i></p> </div> </div>	CAS 1988
CAS Registry Number	12789-03-6 (technical) 57-74-9 (nonstereospecific) 5103-71-9 (<i>cis</i> -chlordane or α -chlordane) 5103-74-2 (<i>trans</i> -chlordane or γ -chlordane)	CAS 1988; Worthing and Walker 1987

CAS = Chemical Abstracts Service

Other major constituents of technical chlordane are chlordene; heptachlor; *cis*-, and *trans*-nonachlor; α -, β -, and γ -chlordene; 3a,4,5,5a,6-exo-hexachloro-1a,2,3,3a,5a,5b-hexahydro-1,4-methano-

4. CHEMICAL AND PHYSICAL INFORMATION

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).

4.2 PHYSICAL AND CHEMICAL PROPERTIES

The physical and chemical properties of chlordane are presented in Table 4-2. 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 determine the specific properties of the product. For example, the vapor pressure of individual components of chlordane will be lower than that of the technical product because individual components 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 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.

4. CHEMICAL AND PHYSICAL INFORMATION

Table 4-2. Physical and Chemical Properties of Chlordane

Property	Information	Reference
Molecular weight	409.76 (pure chlordane)	Windholz 1983
Color	Amber Colorless	Windholz 1983 Hawley 1981
Physical state	Viscous liquid (technical product)	Windholz 1983
Melting point		
<i>cis</i> -chlordane	106–107°C	Worthing and Walker 1987
<i>trans</i> -chlordane	104–1-5°C	Worthing and Walker 1987
Boiling point	175°C at 2 mmHg	Hawley 1981
Density at 25°C	1.59–1.63 g/cm ³	Windholz 1983
Odor	Odorless Mild pungent	Hawley 1981 NRCC 1974
Odor threshold:	0.0084–0.0419 mg/m ³	Ruth 1986
Solubility: ^a		
Water at 25°C	0.056 mg/L for <i>cis:trans</i> (75:25) 1.850 mg/L ^b	Sanborn et al. 1976 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 6.3 (<i>trans</i> -) suspended solids	Lyman 1982 Lau et al. 1989
Vapor pressure: ^d		Foreman and Bidleman 1987
<i>cis</i> -chlordane (supercooled liquid) (crystal) ^e	2.2x10 ⁻⁵ mmHg 3.0x10 ⁻⁶ mmHg	
<i>trans</i> -chlordane (supercooled liquid) (crystal) ^e	2.9x10 ⁻⁵ mmHg 3.9x10 ⁻⁶ mmHg	
Henry's law constant at 25°C	4.85x10 ⁻⁵ atm-m ³ /mol ^b 8.31x10 ⁻⁵ atm-m ³ /mol (<i>trans</i> -) 4.8x10 ⁻⁵ atm-m ³ /mol	Suntio et al. 1988 Fendinger et al. 1989 Cotham and Bidleman 1991
Autoignition temperature	No data	
Flashpoint	56°C (open cup)	OHM/TADS 1988
Flammability limits	No data	
Conversion factors	1 ppm (v/v) = 16.75 mg/m ³ in air 1 mg/m ³ = 0.0597 ppm (v/v) in air	HSDB 1988
Explosive limits	No data	

^aThe solubility of the components of technical chlordane may differ from the solubility of the technical product.

^bStudy did not specify whether test substance was technical grade or a mixture.

^cEstimated for pure chlordane using Equations 4-5 and 4-8 in Lyman (1982).

^dVapor pressure for technical chlordane may differ from that of individual components of technical chlordane.

^eCalculated from the supercooled value.