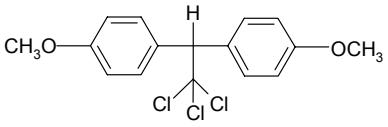
4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

Information regarding the chemical identity of methoxychlor is located in Table 4-1.

Methoxychlor is produced commercially in the United States as a technical grade containing 88–90% of the pure chemical and 10–12% of impurities consisting of isomers and other reaction products (IARC 1979; Lamoureux and Feil 1980). Twenty-five of these impurities were characterized in studies conducted on technical methoxychlor; evidence for >50 impurities was obtained through gas chromatography/mass spectrometry (GC/MS) (Lamoureux and Feil 1980). Purification of technical grade (nominally 90%) 1,1,1-trichloro-2,2-bis(4-methoxyphenyl)ethane (*p,p'*-methoxychlor; *p,p'*-DMDT) by recrystalization gave 76% *p,p'*-methoxychlor (99.8% pure by normal phase high performance liquid chromatography [HPLC]) and 24% impurities (West et al. 1982). The impurities were found to contain approximately 40 components. The major components were identified (HPLC and GC/MS) using reference standards. Component identities and percent (w/w) in technical grade methoxychlor were found to be as follows: 1,1,1,2-tetrachloro-2-(4-methoxyphenyl)ethane (1.73%), 1,1,1-trichloro-2-(2-methoxyphenyl)-2-(4-methoxyphenyl)ethane (*o,p'*-methoxychlor; *o,p'*-DMDT; 4.03%), 1,1-dichloro-2,2-di(4-methoxyphenyl)ethene (DMDE; 0.39%), a condensation product of *p,p'*-methoxychlor (*p,p'*-DMDT; 0.48%), a condensation product of *o,p'*-methoxychlor (*o,p'*-DMDT; 0.4%), and 1,2,2,2-tetrakis(4-methoxybenzyl)ethene (0.5%). The percentages were calculated relative to the quantity of methoxychlor contained in technical grade material and were found to vary depending upon manufacturing conditions. Another impurity is 1-chloro-1,2,2-tris(4-methoxyphenyl)ethene (chlorotrianisene; TACE), a triphenylethylene derivative, that exhibits estrogenic/anti-estrogenic characteristics. Other impurities include polycylic hydrocarbons (e.g., 3,6-dimethoxy-9,10-bis (p-methoxyphenyl)phenanthrene, tetrakis(p-methoxyphenyl)ethylene, and 3,6,11,14-tetramethoxydibenzo(g,p)chrysene), which have been studied for mutagenicity and putative carcinogenicity (Grant et al. 1976). The substance, 3,6,11,14-tetramethoxydibenzo(g,p)chrysene, was found to be mutagenic.

Table 4-1. Chemical Identity of Methoxychlor

Characteristic	Information	Reference
Chemical name	Methoxychlor	Howard 1991
Synonym(s)	2,2-bis(p-methoxyphenyl)-1,1,1-trichoroethane; 1,1,1-trichloro-2,2-bis(4-methoxyphenyl) ethane; methoxy-DDT; 1,1r-(2,2,2-trichloroethylidene)-bis(4-methoxybenzene)	HSDB 2000
Registered trade name(s)	Marlate® Metox® Prentox®; Methoxcide®	EPA 1988b; HSDB 2000; Sittig 1980
Chemical formula	$C_{16}H_{15}Cl_3O_2$	Howard 1991
Chemical structure	 1,1,1-Trichloro-2,2-bis(4-methoxyphenyl)ethane (*p,p'*-methoxychlor; DMDT)	EPA 1988c
Identification numbers:		
CAS registry	72-43-5	Howard 1991
NIOSH RTECS	KJ 3675000	Sax and Lewis 1989
EPA hazardous waste	U247; D014	HSDB 2000
OHM/TADS	OHM 7216536	HSDB 2000
DOT/UN/NA/IMCO shipping	DOT 2761 UN 2761 NA 2761 IMCO 6.1	Sax and Lewis 1989 HSDB 2000
HSDB	1173	HSDB 2000
NCI	C00497	HSDB 2000

CAS = Chemical Abstracts Services; DOT/UN/NA/IMCO = 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; OHM/TADS = Oil Hazardous Materials/Technical Assistance Data System; RTECS = Registry of Toxic Effects of Chemical Substance

4.2 PHYSICAL AND CHEMICAL PROPERTIES

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

Table 4-2. Physical and Chemical Properties of Methoxychlor

Property	Information	Reference
Molecular weight	345.65	Howard 1991
Color	Pale yellow	EPA 1988c
Physical state	Crystalline solid	EPA 1988c
Melting point	89 EC 77 EC (technical grade) No data (decomposes)	HSDB 2000 Montgomery and Welkom 1990
Density: at 25 EC	1.41 g/cm^3	Montgomery and Welkom 1990
Odor	Slightly fruity; musty; chlorine-like	HSDB 2000; Sigworth 1965
Odor threshold: Water 60 EC Air	 4.7 ppm No data	 Sigworth 1965
Solubility: Water at 25 EC at 15 EC at 24 EC at 35 EC at 45 EC	 0.045 mg/L 0.02 mg/L 0.04 mg/L 0.095 mg/L 0.185 mg/L	
Organic solvent(s)	Soluble in chlorinated aromatic solvents, ketonic solvents, ethanol, methylene chloride, methylated naphthalene, carbon tetrachloride, chloroform, xylene, methanol, petroleum ether, benzene	Budavari et al. 1989; EPA 1988a; HSDB 2000; Montgomery and Welkom 1990
Partition coefficients: Log K_{ow} Log K_{oc}	 4.68–5.08 4.9	 Howard 1991 Montgomery and Welkom 1990
Vapor pressure at 25 EC	1.4x10^{-6} mmHg (estimated)	Howard 1991
Henry's law constant: at 25 EC	 1.6x10^{-5} atm-m^3/mol (estimated)	 Howard 1991
Autoignition temperature	No data	
Flashpoint	No data	
Flammability limits	No data	
Conversion factors[a]	No data	
Explosive limits	No data	

[a]Exists partially in particulate form in air. Conversion factors are only applicable for compounds that are entirely in the vapor phase.