3. CHEMICAL AND PHYSICAL INFORMATION

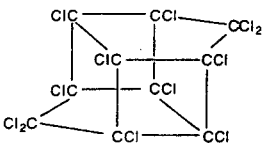
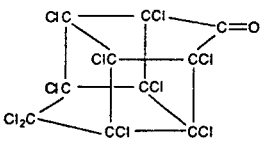
3.1 CHEMICAL IDENTITY

Information regarding the chemical identity of mirex and chlordecone is located in Table 3-l.

3.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of mirex and chlordecone is located in Table 3-2.

TABLE 3-1. Chemical Identity of Mirex and Chlordecone[a]

Characteristic	Mirex	Chlordecone
Chemical name	1,1a,2,2,3,3a,4,5,5,5a,5b,6-Dodecachlorooctahydro-1,3,4-metheno-1H-cyclobuta[cd]-pentalene	1,1a,3,3a,4,5,5,5a,5b,6-Decachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd] pentalen-2-one
Synonym(s)	1,2,3,4,5,5-Hexachloro-1,3-cyclopentadiene dimer[b]; dodecachlorooctahydro-1,3,4-metheno-1H-cyclobuta[cd] pentalene[b]	Decachloroketone[c]; decachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalen-2-one[c]
Registered trade name(s)	CG-1283; Dechlorane; HRS1276b[e]; ENT 25719[d]	GC 1189; ENT16391[e]; Kepone; Merex[c]
Chemical formula	$C_{10}Cl_{12}$	$C_{10}Cl_{10}O$
Chemical structure	b 	c 
Identification numbers:		
CAS registry	2385-85-5	143-50-0
NIOSH RTECS	PC8225000[e]	PC8575000[c]
EPA hazardous waste	No data	U142
OHM/TADS	No data	No data
DOT/UN/NA/IMCO shipping	No data	NA 2761; UN 2588[e]
HSDB	1659[d]	1558[f]
NCI	CO6428[d]	CO0191[f]

[a]All information for mirex and chlordecone is from Merck 1989 unless otherwise indicated.
[b] IARC 1979c
[c] IARC 1979a
[d] HSDB 1994b
[e] Sittig 1985
[f] HSDB 1994a

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 and Hazardous Materials/Technical Assistance Data System; RTECS = Registry of Toxic Effects of Chemical Substances

TABLE 3-2. Physical and Chemical Properties of Mirex and Chlordecone[a]

Property	Mirex	Chlordecone
Molecular weight	545.59	490.68
Color	Snow-white	Tan-white[b]
Physical state	Crystalline solid	Crystalline solid
Melting point	485 °C (decomposes)	350 °C (decomposes)[b]
Boiling point	No data	No data
Density:		
at 25 °C	No data	No data
Odor	Odorless[c] 5.0667 mg/m^3 [d]	Odorless[e]
Solubility:		
Water	Practically insoluble 0.60 mg/L[f] insoluble[g] 0.2 mg/L at 24 °C (practical grade)[g]	Slightly soluble 3.0 mg/L[f] practically insoluble[b]
Organic solvent(s)	Dioxane (15.3%); xylene (14.3%); benzene (12.2%); CCl_4 (7.2%) methyl ethyl ketone (5.6%)	Soluble in hydrocarbon solvents, alcohols, ketones
Partition coefficients:		
Log K_{ow}	5.28[h]	4.50[i]
Log K_{oc}	3.763[f]	3.38–3.415[i]
Vapor pressure at 25 °C	3×10^{-7} mm Hg[g]	$<3\times10^{-7}$ mm Hg[b]
Henry's law constant:		
at 20 °C	839.37 Pa m^3/mole[j]	2.50×10^{-8} atm m^3/mole[i]
at 22 °C	5.16×10^{-4} atm m^3/mole (22 °C)[k]	
Autoignition temperature	Nonflammable[b]	Nonflammable
Flashpoint	No data	No data
Flammability limits	Nonflammable[d] Supports combustion	Nonflammable
Conversion factors	1 ppm = 0.041 mg/m^3	1 ppm = 0.046 mg/m^3
Explosive limits	No data	No data

[a]All information for mirex and chlordecone is from Merck 1989, unless otherwise indicated.
[b]IARC 1979a
[c]Sittig 1985
[d]HSDB 1994b
[e]Verschueren 1983
[f]Kenaga 1980
[g]IARC 1979c
[h]Niimi 1991
[i]Howard 1991
[j]Domine et al. 1992
[k]Yin and Hassett 1986

CCl_4 = carbon tetrachloride