

## 4. CHEMICAL AND PHYSICAL INFORMATION

### 4.1 CHEMICAL IDENTITY

When we refer to DDT, we are generally referring to *p,p'*-DDT, which was produced and used for its insecticidal properties. However, technical grade DDT, the grade that was generally used as an insecticide, was composed of up to fourteen chemical compounds, of which only 65–80% was the active ingredient, *p,p'*-DDT. The other components included 15–21% of the nearly inactive *o,p'*-DDT, up to 4% of *p,p'*-DDD, and up to 1.5% of 1-(*p*-chlorophenyl)-2,2,2-trichloroethanol (Metcalf 1995).

The chemical formulas, structures, and identification numbers for *p,p'*-DDT, *p,p'*-DDE, *p,p'*-DDD, *o,p'*-DDT, *o,p'*-DDE, and *o,p'*-DDD are listed in Table 4-1. The latter five compounds are either impurities or metabolites of technical DDT.

### 4.2 PHYSICAL AND CHEMICAL PROPERTIES

Technical DDT is a white amorphous powder that melts over the range of 80–94 EC (Metcalf 1995). Physical and chemical properties of *p,p'*-DDT, *p,p'*-DDE, *p,p'*-DDD, *o,p'*-DDT, *o,p'*-DDE, and *o,p'*-DDD are listed in Table 4-2.

Table 4-1. Chemical Identity of *p,p'*- and *o,p'*-DDT, DDE, and DDD<sup>a</sup>

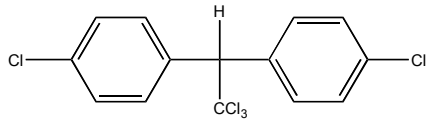
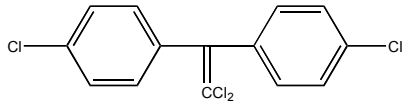
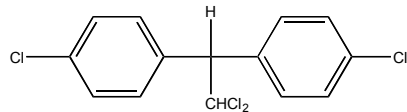
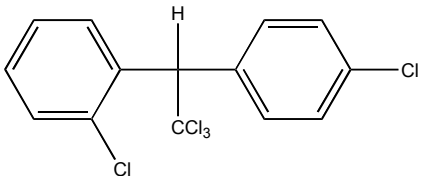
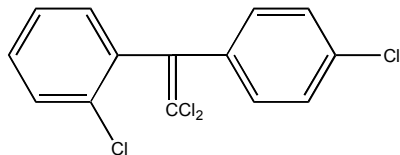
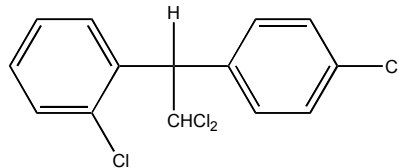
Characteristic	<i>p,p'</i> -DDT	<i>p,p'</i> -DDE	<i>p,p'</i> -DDD
Synonym(s)	4,4'-DDT; 1,1,1-trichloro-2,2-bis( <i>p</i> -chlorophenyl)ethane; dichloro-diphenyl trichloroethane; DDT; 1,1'-(2,2,2-trichloroethylidene)bis(4-chlorobenzene); $\alpha$ - $\alpha$ -bis( <i>p</i> -chlorophenyl)- $\beta$ , $\beta$ , $\beta$ -trichloroethane	4,4'-DDE; dichlorodiphenyl-dichloroethane; 1,1-dichloro-2,2-bis( <i>p</i> -chlorophenyl) ethylene; 1,1'-(2,2-dichloroethylidene)bis(4-chlorobenzene); DDE	4,4'-DDD; DDD; 1,1-dichloro-2,2-bis( <i>p</i> -chlorophenyl)ethane; 1,1-bis(4-chlorophenyl)-2,2-dichloroethane; TDE; tetrachlorodiphenylethane
Registered trade name(s)	Genitox, Anofex, Detoxan, Neocid, Gesarol, Pentachlorin, Dicophane, Chlorophenothane <sup>b</sup>	No data	DDD; Rothane; Dilene, TDE
Chemical formula	C <sub>14</sub> H <sub>9</sub> Cl <sub>5</sub>	C <sub>14</sub> H <sub>8</sub> Cl <sub>4</sub>	C <sub>14</sub> H <sub>10</sub> Cl <sub>4</sub>
Chemical structure			
Identification numbers:			
CAS registry	50-29-3	72-55-9	72-54-8
NIOSH RTECS	KJ3325000	KV9450000	KI0700000
EPA hazardous waste	U061	No data	U060
OHM/TADS	7216510	No data	7215098
DOT/UN/NA/IMCO shipping	IMCO 6.1; UN2761	No data	NA2761; TDE
HSDB	200	1625	285
NCI	C00465	C00555	C00475

Table 4-1. Chemical Identity of *p,p'*- and *o,p'*-DDT, DDE, and DDD<sup>a</sup> (continued)

Characteristic	<i>o,p'</i> -DDT	<i>o,p'</i> -DDE	<i>o,p'</i> -DDD
Synonym(s)	4,4'-DDT; 1,1,1-trichloro-2-( <i>o</i> -chlorophenyl)-2-( <i>p</i> -chlorophenyl)ethane; <i>o,p'</i> -dichlorodiphenyltrichloroethane	2,4'-DDE; 1,1-dichloro-2-( <i>o</i> -chlorophenyl)-2-( <i>p</i> -chlorophenyl)ethylene; 1-chloro-2-(2,2-dichloro-1-(4-chlorophenyl)ethenyl)benzene	2,4'-DDD; Mitotane; <i>o,p'</i> -DDD; 1,1-dichloro-2-( <i>o</i> -chlorophenyl)-2-( <i>p</i> -chlorophenyl)ethane; <i>o,p'</i> -TDE; Choditane; 2-( <i>o</i> -chlorophenyl)-2-( <i>p</i> -chlorophenyl)-1,1-dichloroethane
Registered trade name(s)	No data	No data	Lysodren
Chemical formula	C <sub>14</sub> H <sub>9</sub> Cl <sub>5</sub>	C <sub>14</sub> H <sub>8</sub> Cl <sub>4</sub>	C <sub>14</sub> H <sub>10</sub> Cl <sub>4</sub>
Chemical structure			
Identification numbers:			
CAS registry	789-02-6	3424-82-6	53-19-0
NIOSH RTECS	No data	No data	KH7880000
EPA hazardous waste	No data	No data	No data
OHM/TADS	No data	No data	No data
DOT/UN/NA/IMCO shipping	No data	No data	No data
HSDB	No data	No data	3240
NCI	No data	No data	C04933

<sup>a</sup>All information obtained from HSDB 1999a, 1999b, 1999c, 1999d, or Howard and Neal 1992 except where noted.

<sup>b</sup>Klassen et al. 1991

CAS = Chemical Abstracts Service; 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

## 4. CHEMICAL AND PHYSICAL INFORMATION

**Table 4-2. Physical and Chemical Properties of *p,p'*- and *o,p'*-DDT, DDE, and DDD<sup>a</sup>**

Property	<i>p,p'</i> -DDT	<i>p,p'</i> -DDE	<i>p,p'</i> -DDD
Molecular weight	354.49 <sup>b</sup>	318.03 <sup>b</sup>	320.05 <sup>b</sup>
Color	Colorless crystals, white powder <sup>c</sup>	White	Colorless crystals, white powder
Physical state	Solid <sup>d</sup>	Crystalline solid	Solid
Melting point	109 EC <sup>b</sup>	89 EC <sup>b</sup>	109–110 EC <sup>b</sup>
Boiling point	Decomposes	336 EC <sup>b</sup>	350 EC <sup>b</sup>
Density	0.98–0.99 g/cm <sup>3</sup>	No data	1.385 g/cm <sup>3</sup>
Odor	Odorless or weak aromatic odor <sup>e</sup>	No data	Odorless
Odor threshold:			
Water	0.35 mg/kg <sup>c</sup>	No data	No data
Air	No data	No data	No data
Solubility:			
Water	0.025 mg/L at 25 EC <sup>b</sup>	0.12 mg/L at 25 EC <sup>b</sup>	0.090 mg/L at 25 EC <sup>b</sup>
Organic solvents	Slightly soluble in ethanol, very soluble in ethyl ether and acetone <sup>f</sup>	Lipids and most organic solvents	No data <sup>g</sup>
Partition coefficients:			
Log K <sub>ow</sub>	6.91 <sup>b</sup>	6.51 <sup>b</sup>	6.02 <sup>b</sup>
Log K <sub>oc</sub>	5.18 <sup>h</sup>	4.70 <sup>i</sup>	5.18 <sup>i</sup>
Vapor pressure	1.60x10 <sup>-7</sup> at 20 EC, torr <sup>b</sup>	6.0x10 <sup>-6</sup> at 25 EC, torr <sup>b</sup>	1.35x10 <sup>-6</sup> at 25 EC, torr <sup>b</sup>
Henry's law constant	8.3x10 <sup>-6</sup> atm-m <sup>3</sup> /mol <sup>b</sup>	2.1x10 <sup>-5</sup> atm-m <sup>3</sup> /mol <sup>b</sup>	4.0x10 <sup>-6</sup> atm-m <sup>3</sup> /mol <sup>b</sup>
Autoignition temperature	No data	No data	No data
Flashpoint	72.2–77.2 EC	No data	No data
Flammability limits	No data	No data	No data
Conversion factors			
ppm(v/v) to mg/m <sup>3</sup> in air at 20 EC	Not applicable <sup>k</sup>	Not applicable <sup>k</sup>	Not applicable <sup>k</sup>
mg/m <sup>3</sup> to ppm(v/v) in air at 20 EC	Not applicable	Not applicable	Not applicable
Explosive limits	No data	No data	No data

## 4. CHEMICAL AND PHYSICAL INFORMATION

**Table 4-2. Physical and Chemical Properties of *p,p'*- and *o,p'*-DDT, DDE, and DDD<sup>a</sup> (continued)**

Property	<i>o,p'</i> -DDT	<i>o,p'</i> -DDE	<i>o,p'</i> -DDD
Molecular weight	354.49 <sup>b</sup>	318.03 <sup>b</sup>	320.05 <sup>b</sup>
Color	White crystalline powder <sup>c</sup>	No data	No data
Physical state	Solid <sup>d</sup>	No data	Solid
Melting point	74.2 EC <sup>e</sup>	No data	76–78 EC
Boiling point	No data	No data	No data
Density	0.98–0.99 g/cm <sup>3</sup>	No data	No data
Odor	Odorless or weak aromatic odor <sup>e</sup>	No data	No data
Odor threshold:			
Water	No data	No data	No data
Air	No data	No data	No data
Solubility:			
Water	0.085 mg/L at 25 EC <sup>b</sup>	0.14 mg/L at 25 EC <sup>b</sup>	0.1 mg/L at 25 EC <sup>b</sup>
Organic solvents	No data <sup>g</sup>	No data <sup>g</sup>	Soluble in ethanol, isooctane, carbon tetrachloride <sup>j</sup>
Partition coefficients:			
Log K <sub>ow</sub>	6.79 <sup>h</sup>	6.00 <sup>b</sup>	5.87 <sup>b</sup>
Log K <sub>oc</sub>	5.35 <sup>j</sup>	5.19 <sup>j</sup>	5.19 <sup>j</sup>
Vapor pressure	1.1x10 <sup>-7</sup> at 20 EC, torr <sup>b</sup>	6.2x10 <sup>-6</sup> at 25 EC, torr <sup>b</sup>	1.94x10 <sup>-6</sup> at 30 EC, torr <sup>b</sup>
Henry's law constant	5.9x10 <sup>-7</sup> atm-m <sup>3</sup> /mol <sup>b</sup>	1.8x10 <sup>-5</sup> atm-m <sup>3</sup> /mol <sup>b</sup>	8.17x10 <sup>-6</sup> atm-m <sup>3</sup> /mol <sup>b</sup>
Autoignition temperature	No data	No data	No data
Flashpoint	No data	No data	No data
Flammability limits	No data	No data	No data
Conversion factors			
ppm(v/v) to mg/m <sup>3</sup> in air at 20 EC	Not applicable <sup>k</sup>	Not applicable <sup>k</sup>	Not applicable <sup>k</sup>
mg/m <sup>3</sup> to ppm(v/v) in air at 20 EC	Not applicable	Not applicable	Not applicable
Explosive limits	No data	No data	No data

<sup>a</sup>All information obtained from HSDB 1999a, 1999b, 1999c, 1999d unless otherwise noted

<sup>b</sup>Howard and Meylan 1997

<sup>c</sup>Verschueren 1988

<sup>d</sup>NIOSH 1985

<sup>e</sup>Sax 1979

<sup>f</sup>Lide 1998

<sup>g</sup>Chemical is expected to be soluble in most organic compounds.

<sup>h</sup>Swann et al. 1981

<sup>i</sup>Sablejic 1984

<sup>j</sup>Meylan et al. 1992 (values estimated from a fragment constant method)

<sup>k</sup>Exists partially in particulate form in air. Conversion factors are only applicable for compounds that are entirely in the vapor phase.

