3. CHEMICAL AND PHYSICAL INFORMATION

3.1 CHEMICAL IDENTITY

Dibenzofuran is an organic compound that contains two benzene rings fused to a central furan ring. CDFs are a class of organic compounds in which one to eight chlorine atoms are attached to the benzene ring positions of a dibenzofuran structure. The general chemical structure for CDFs with the numbering system is as follows:

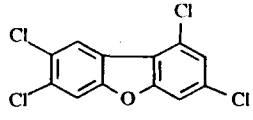
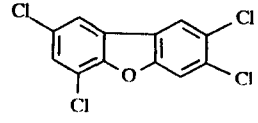
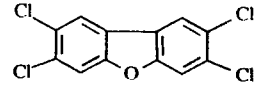
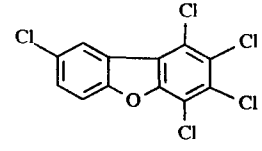
Based on the number of chlorine substituents (one to eight) on the benzene rings, there are eight homologues of CDFs (monochlorinated through octachlorinated). Each homologous group contains one or more isomers. There are 135 possible CDF isomers, including 4 monoCDFs, 16 diCDFs, 28 triCDFs, 38 tetraCDFs, 28 pentaCDFs, 16 hexaCDFs, 4 heptaCDFs, and one octaCDF. Each one of these compounds is called a congener. Because of molecular asymmetry, CDFs have 135 congeners, compared to 75 for CDDs.

The synonyms, chemical formulas, chemical structure, and identification numbers of selected CDFs are reported in Table 3-l. CDFs that are known or suspected to be most toxic (2,3,7,%substituted congeners) and other CDFs, for which health effects data are discussed in Section 2, have been selected for inclusion in Table 3-l.

3.2 PHYSICAL AND CHEMICAL PROPERTIES

CDFs have been synthesized in quantities <1 g. The methods needed to separate the isomeric compounds in a congener series make the isolation of an individual congener difficult. Therefore, data pertaining to the simplest physical and chemical properties of the individual congener are not generally available. The extremely low water solubilities and vapor pressures contribute to the difficulty in determining these and related physico-chemical properties (e.g., K_{OW} and Henry's law constant) of these compounds. In general, the melting point increases and the vapor pressures and water

TABLE 3-1. Chemical Identities of CDFs

Characteristic	1,3,7,8-TetraCDF	2,3,6,8-TetraCDF	2,3,7,8-TetraCDF	1,2,3,4,8-PentaCDF
Synonyms[a]	1,3,7,8-Tetrachlorodiphenylene oxide	2,3,6,8-Tetrachlorodiphenylene oxide	2,3,7,8-Tetrachlorodiphenylene oxide	1,2,3,4,8-Pentachlodiphenylene oxide
Registered trade names	No data	No data	No data	No data
Chemical formula	$C_{12}H_4Cl_4O$	$C_{12}H_4Cl_4O$	$C_{12}H_4Cl_4O$	$C_{12}H_3Cl_5O$
Chemical structure				
Identification numbers:				
CAS registry[b]	57117-35-8	57117-37-0	51207-31-9	67517-48-0
NIOSH RTECS	No data	No data	HP5295200[c]	No data
EPA hazardous waste	No data	No data	No data	No data
OHM/TADS	No data	No data	No data	No data
DOT/UN/NA/IMCO shipping	No data	No data	No data	No data
HSDB	No data	No data	4306	No data
NCI	No data	No data	C56611	No data

[a]Weast 1985
[b]EPA 1986
[c]NIOSH 1987

CAS = Chemical Abstracts Services; CDF = Chlorodibenzofuran; 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 3-1. Chemical Identities of CDFs *(continued)*

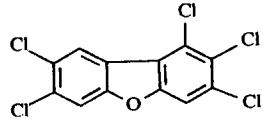
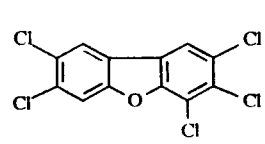
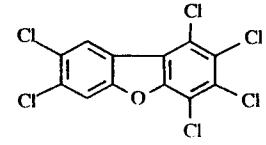
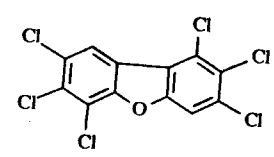
Characteristic	1,2,3,7,8-PentaCDF	2,3,4,7,8-PentaCDF	1,2,3,4,7,8-HexaCDF	1,2,3,6,7,8-HexaCDF
Synonyms[a]	1,2,3,7,8-Pentachlorodiphenylene oxide	2,3,4,7,8-Pentachlorodiphenylene oxide	1,2,3,4,7,8-Hexachlorodiphenylene oxide	1,2,3,6,7,8-Hexachlorodiphenylene oxide
Registered trade names	No data	No data	No data	No data
Chemical formula	$C_{12}H_3Cl_5O$	$C_{12}H_3Cl_5O$	$C_{12}H_2Cl_6O$	$C_{12}H_2Cl_6O$
Chemical structure				
Identification numbers:				
CAS registry[b]	57117-41-6	57117-31-4	70648-26-9	57117-44-9
NIOSH RTECS	No data	HP52955150[c]	No data	No data
EPA hazardous waste	No data	No data	No data	No data
OHM/TADS	No data	No data	No data	No data
DOT/UN/NA/IMCO shipping	No data	No data	No data	No data
HSDB	No data	No data	No data	No data
NCI	No data	No data	No data	No data

TABLE 3-1. Chemical Identities of CDFs *(continued)*

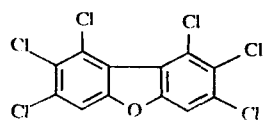
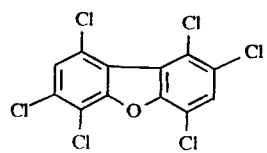
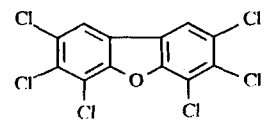
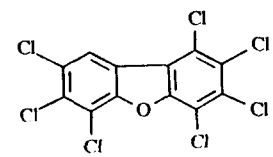
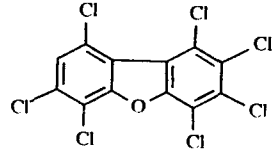
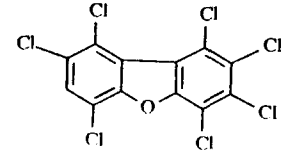
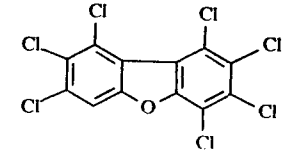
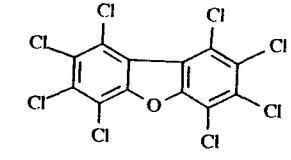
Characteristic	1,2,3,7,8,9-HexaCDF	1,2,4,6,7,9-HexaCDF	2,3,4,6,7,8-HexaCDF	1,2,3,4,6,7,8-HeptaCDF
Synonyms[a]	1,2,3,7,8,9-Hexachlorodiphenylene oxide	1,2,4,6,7,9-Hexachlorodiphenylene oxide	2,3,4,6,7,8-Hexachlorodiphenylene oxide	1,2,3,4,6,7,8-Heptachlorodiphenylene oxide
Registered trade names	No data	No data	No data	No data
Chemical formula	$C_{12}H_2Cl_6O$	$C_{12}H_2Cl_6O$	$C_{12}H_2Cl_6O$	$C_{12}HCl_7O$
Chemical structure				
Identification numbers:				
CAS registry[b]	72918-21-9	75627-02-0	60851-34-5	67562-39-4
NIOSH RTECS	No data	No data	No data	No data
EPA hazardous waste	No data	No data	No data	No data
OHM/TADS	No data	No data	No data	No data
DOT/UN/NA/IMCO shipping	No data	No data	No data	No data
HSDB	No data	No data	No data	No data
NCI	No data	No data	No data	No data

TABLE 3-1. Chemical Identities of CDFs *(continued)*

Characteristic	1,2,3,4,6,7,9-HeptaCDF	1,2,3,4,6,8,9-HeptaCDF	1,2,3,4,7,8,9-HeptaCDF	1,2,3,4,6,7,8,9-OctaCDF
Synonyms[a]	1,2,3,4,6,7,9-Heptachlorodiphenylene oxide	1,2,3,4,6,8,9-Heptachlorodiphenylene oxide	1,2,3,4,7,8,9-Heptachlorodiphenylene oxide	1,2,3,4,6,7,8,9-Octachlorodiphenylene oxide
Registered trade names	No data	No data	No data	No data
Chemical formula	$C_{12}HCl_7O$	$C_{12}HCl_7O$	$C_{12}HCl_7O$	$C_{12}Cl_8O$
Chemical structure				
Identification numbers:				
CAS registry[b]	70648-25-8	69698-58-4	55673-89-7	39001-02-0
NIOSH RTECS	No data	No data	No data	No data
EPA hazardous waste	No data	No data	No data	No data
OHM/TADS	No data	No data	No data	No data
DOT/UN/NA/IMCO shipping	No data	No data	No data	No data
HSDB	No data	No data	No data	No data
NCI	No data	No data	No data	No data

solubilities of the CDFs decrease as the number of chlorine substituents increases (see Table 3-2). These hydrophobic compounds are generally colorless solids and are soluble in nonpolar organic solvents (Gray et al. 1976). The CDFs are relatively stable towards acid and alkali attack, but they start to decompose at 700°C (see Section 4.4) (Van den Berg et al. 1985). The physical and chemical properties of CDFs are given in Table 3-2.

TABLE 3-2. Physical and Chemical Properties of CDFs

Property	1,3,7,8-TetraCDF	2,3,6,8-TetraCDF	2,3,7,8-TetraCDF	1,2,3,4,8-PentaCDF
Molecular weight	305.96	305.96	305.96	340.42
Color[a]	No data	Colorless[b]	Colorless	No data
Physical state[a]	No data	Solid[c]	Solid	No data
Melting point, °C[a]	No data	197-198	219-221	177-178
Boiling point	No data	No data	No data	No data
Density	No data	No data	No data	No data
Odor	No data	No data	No data	No data
Odor threshold:				
Water	No data	No data	No data	No data
Air	No data	No data	No data	No data
Solubility:				
Water[d]	No data	No data	1.37×10^{-9} mol/L (0.42 µg/L)	No data
Organic solvent(s)[e]	Soluble in toluene	Soluble in toluene and chloroform	Soluble in toluene	Soluble in toluene
Partition coefficients:				
Log K_{ow}[f]	No data	No data	5.82[g]	6.79
Log K_{oc}[h]	No data	No data	5.61 (estimated)	No data
Vapor pressure, mm Hg[i] (25°C)	No data	No data	9.21×10^{-7}	No data
Henry's law constant[j] (atm-m^3/mol)[k]	1.48×10^{-5}	1.48×10^{-5}	1.48×10^{-5}	2.63×10^{-5}
Autoignition temperature	No data	No data	No data	No data
Flashpoint	No data	No data	No data	No data
Flammability limits	No data	No data	No data	No data
Conversion factors				
Air[b] (at 20°C)	1 ppb = 12.719 µg/m^3	1 ppb = 12.719 µg/m^3	1 ppb = 12.719 µg/m^3	1 ppb = 14.151 µg/m^3
Water	1 ppb = 1 µg/L	1 ppb = 1 µg/L	1 ppb = 1 µg/L	1 ppb = 1 µg/L
Soil	1 ppb = 1 µg/kg	1 ppb = 1 µg/kg	1 ppb = 1 µg/kg	1 ppd = 1 µg/kg
Explosive limits	No data	No data	No data	No data

[a]Kuroki et al. 1984 unless otherwise stated
[b]The PCDFs are present predominantly in the particulate phase in ambient air (Hunt and Maisel 1990)
[c]Gray et al. 1976
[d]Friesen et al. 1990 unless otherwise stated
[e]Ryan et al. 1991 unless otherwise stated
[f]Sijm et al. 1989 unless otherwise stated; some of the values are for two isomers that could not be separated.
[g]Burkhard and Kuehl 1986
[h]EPA 1986
[i]Eitzer and Hites 1988
[j]Eitzer and Hites 1989; the values are for unseparated isomers of each homologous series
[k]Frank and Schrap 1990

CDF = chlorodibenzofuran

TABLE 3-2. Physical and Chemical Properties of CDFs *(continued)*

Property	1,2,3,7,8-PentaCDF	2,3,4,7,8-PentaCDF	1,2,3,4,7,8-HexaCDF	1,2,3,6,7,8-HexaCDF
Molecular weight	340.42	340.42	374.87	374.87
Color[a]	Colorless	No data	No data	No data
Physical state[a]	Solid	No data	No data	No data
Melting point, °C[a]	225-227	196-196.5	225.5-226.5	232-234
Boiling point	No data	No data	No data	No data
Density	No data	No data	No data	No data
Odor	No data	No data	No data	No data
Odor threshold:				
Water	No data	No data	No data	No data
Air	No data	No data	No data	No data
Solubility:				
Water[d]	No data	6.92×10^{-10} mol/L (0.24 µg/L)	2.20×10^{-11} mol/L (0.008 µg/L)	4.72×10^{-11} mol/L (0.018 µg/L)
Organic solvent(s)[e]	Soluble in hexane[a] and toluene	Soluble in toluene	Soluble in toluene	Soluble in toluene
Partition coefficients:				
Log K_{ow}[f]	6.79	6.92	No data	No data
Log K_{oc}[h]	No data	No data	No data	No data
Vapor pressure, mm Hg[i] (25°C)	2.73×10^{-7}	1.63×10^{-7}	6.07×10^{-8}	6.07×10^{-8}
Henry's law constant (atm-m^3/mol)[j]	2.63×10^{-5}	2.63×10^{-5}	2.78×10^{-5}	2.78×10^{-5}
Autoignition temperature	No data	No data	No data	No data
Flashpoint	No data	No data	No data	No data
Flammability limits	No data	No data	No data	No data
Conversion factors				
Air[b] (at 20°C)	1 ppb = 14.151 µg/m^3	1 ppb = 14.151 µg/m^3	1 ppb = 15.583 µg/m^3	1 ppb = 15.583 µg/m^3
Water	1 ppb = 1 µg/L	1 ppb = 1 µg/L	1 ppb = 1 µg/L	1 ppb = 1 µg/L
Soil	1 ppb = 1 µg/kg	1 ppb = 1 µg/kg	1 ppb = 1 µg/kg	1 ppb = 1 µg/kg
Explosive limits	No data	No data	No data	No data

TABLE 3-2. Physical and Chemical Properties of CDFs *(continued)*

Property	1,2,3,7,8,9-HexaCDF	1,2,4,6,7,9-HexaCDF	2,3,4,6,7,8-HexaCDF	1,2,3,4,6,7,8-HeptaCDF
Molecular weight	374.87	374.87	374.87	409.31
Color[a]	No data	No data	No data	No data
Physical state[a]	No data	No data	No data	No data
Melting point, °C[a]	No data	180-181	239-240	236-237
Boiling point	No data	No data	No data	No data
Density	No data	No data	No data	No data
Odor	No data	No data	No data	No data
Odor threshold:				
Water	No data	No data	No data	No data
Air	No data	No data	No data	No data
Solubility:				
Water[d]	No data	No data	No data	3.31×10^{-12} mol/L (0.014 µg/L)
Organic solvent(s)[e]	Soluble in toluene	Soluble in toluene	Soluble in toluene	Soluble in toluene
Partition coefficients:				
Log K_{ow}[f]	No data	No data	No data	7.92
Log K_{oc}[h]	No data	No data	No data	No data
Vapor pressure, mm Hg[i] (25°C)	3.74×10^{-8}	No data	3.74×10^{-8}	1.68×10^{-8}
Henry's law constant (atm-m^3/mol)[j]	2.78×10^{-5}	2.78×10^{-5}	2.78×10^{-5}	4.1×10^{-6}
Autoignition temperature	No data	No data	No data	No data
Flashpoint	No data	No data	No data	No data
Flammability limits	No data	No data	No data	No data
Conversion factors				
Air[b] (at 20°C)	1 ppb = 15.583 µg/m^3	1 ppb = 15.583 µg/m^3	1 ppb = 15.583 µg/m^3	1 ppb = 17.015 µg/m^3
Water	1 ppb = 1 µg/L	1 ppb = 1 µg/L	1 ppb = 1 µg/L	1 ppb = 1 µg/L
Soil	1 ppb = 1 µg/kg	1 ppb = 1 µg/kg	1 ppb = 1 µg/kg	1 ppb = 1 µg/kg
Explosive limits	No data	No data	No data	No data

TABLE 3-2. Physical and Chemical Properties of CDFs *(continued)*

Property	1,2,3,4,6,7,9-HeptaCDF	1,2,3,4,6,8,9-HeptaCDF	1,2,3,4,7,8,9-HeptaCDF	1,2,3,4,6,7,8,9-OctaCDF
Molecular weight	409.31	409.31	409.31	443.76
Color[a]	No data	No data	No data	No data
Physical state[a]	No data	No data	No data	No data
Melting point, °C[a]	No data	211-212	212-223	259[c]
Boiling point	No data	No data	No data	537[c]
Density	No data	No data	No data	No data
Odor	No data	No data	No data	No data
Odor threshold:				
Water	No data	No data	No data	No data
Air	No data	No data	No data	No data
Solubility:				
Water[d]	No data	No data	No data	2.61×10^{-12} mol/L (0.0012 µg/L) (3.0 µg/L)[k]
Organic solvent(s)[e]	Soluble in toluene	Soluble in toluene	Soluble in toluene	Soluble in toluene
Partition coefficients:				
Log K_{ow}[f]	No data	No data	No data	8.20 (7.97)[i]
Log K_{oc}[h]	No data	No data	No data	8.57 (estimated)
Vapor pressure, mm Hg[i] (25°C)	No data	No data	9.79×10^{-9}	No data
Henry's law constant (atm-m^3/mol)[j]	4.1×10^{-6}	4.1×10^{-6}	4.1×10^{-6}	1.7×10^{-6}
Autoignition temperature	No data	No data	No data	No data
Flashpoint	No data	No data	No data	No data
Flammability limits	No data	No data	No data	No data
Conversion factors				
Air[b] (at 20°C)	1 ppb = 17.015 µg/m^3	1 ppb = 17.015 µg/m^3	1 ppb = 17.015 µg/m^3	1 ppb = 18.447 µg/m^3
Water	1 ppb = 1 µg/L	1 ppb = 1 µg/L	1 ppb = 1 µg/L	1 ppb = 1 µg/L
Soil	1 ppb = 1 µg/kg	1 ppb = 1 µg/kg	1 ppb = 1 µg/kg	1 ppb = 1 µg/kg
Explosive limits	No data	No data	No data	No data