CHAPTER 4. CHEMICAL AND PHYSICAL INFORMATION

4.1 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.

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 1 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 4-1. CDFs that are known or suspected to be most toxic (2,3,7,8-substituted congeners) and other CDFs, for which health effects data are discussed in Chapter 2, have been selected for inclusion in Table 4-1.

4.2 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 solubilities of the CDFs decrease as the number of chlorine substituents increases (see Table 4-2). 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 (van den Berg et al. 1985). The physical and chemical properties of CDFs are given in Table 4-2.

Table 4-1. Chemical Identity of Chlorodibenzofurans (CDFs)

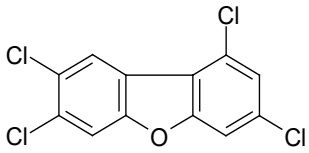
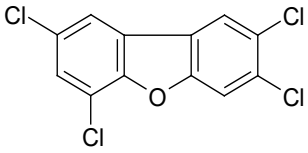
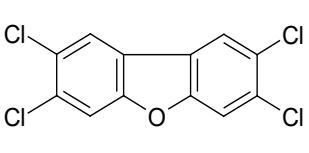
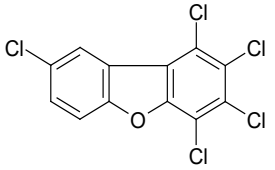
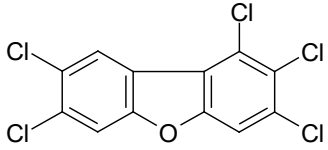
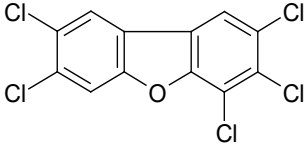
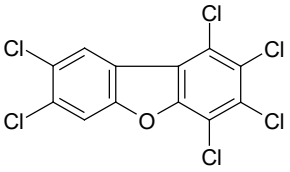
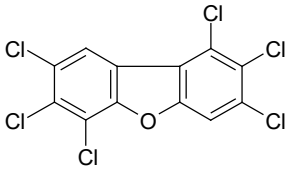
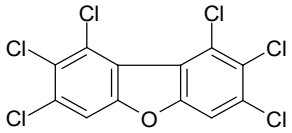
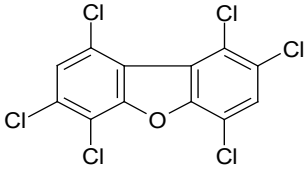
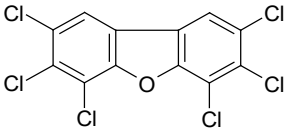
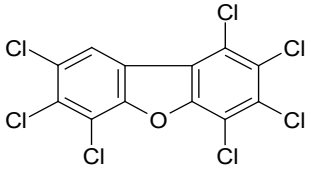
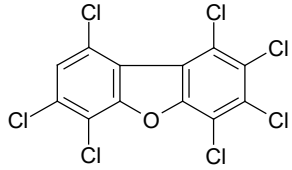
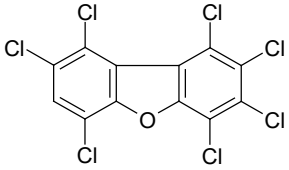
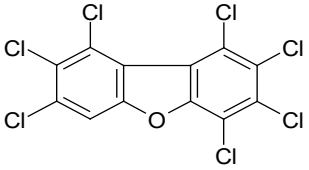
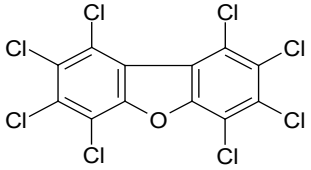
Characteristic	Information			
Chemical name	1,3,7,8-TetraCDF	2,3,6,8-TetraCDF	2,3,7,8-TetraCDF	1,2,3,4,8-PentaCDF
Registered trade name(s)	No data	No data	No data	No data
Chemical formula	$C_{12}H_4Cl_4O$	$C_{12}H_4Cl_4O$	$C_{12}H_4Cl_4O$	$C_{12}H_3Cl_5O$
Chemical structure				
CAS Registry Number[a]	57117-35-8	57117-37-0	51207-31-9	67517-48-0
Chemical name	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
Registered trade name(s)	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				
CAS Registry Number[a]	57117-41-6	57117-31-4	70648-26-9	57117-44-9
Chemical name	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
Registered trade name(s)	No data	No data	No data	No data
Chemical formula				
Chemical structure	$C_{12}H_2Cl_6O$	$C_{12}H_2Cl_6O$	$C_{12}H_2Cl_6O$	$C_{12}HCl_7O$
CAS Registry Number[a]	72918-21-9	75627-02-0	60851-34-5	67562-39-4

Table 4-1. Chemical Identity of Chlorodibenzofurans (CDFs)

Characteristic	Information			
Chemical name	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
Registered trade name(s)	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				
CAS Registry Number[a]	70648-25-8	69698-58-4	55673-89-7	39001-02-0

[a]EPA 1985

CAS = Chemical Abstracts Services

Table 4-2. Physical and Chemical Properties of Chlorodibenzofurans (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	305.9	305.9	305.9	340.42
Color[a]	No data	Colorless[b]	Colorless	No data
Physical state[c]	Solid	Solid	Solid	Solid
Melting point, °C[a]	No data	197–198	219–221	177–178
Boiling point °C	No data	No data	No data	No data
Density at 20°C	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 (0.43 µg/L)	No data
Organic solvents[e]	Soluble in toluene	Soluble in toluene and chloroform	Soluble in toluene	Soluble in toluene
Partition coefficients:				
Log K_{ow}[f]	6.73	6.73	6.53	6.79
Log K_{oc}[h]	No data	No data	5.61 (estimated)	No data
pKa	Not applicable	Not applicable	Not applicable	Not applicable
Vapor pressure at 25°C[i]	1.95×10^{-8}[j]	1.95×10^{-8}[j]	9.21×10^{-7}	No data
Henry's law constant[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[a] Water Soil	1 ppb = 12.72 µg/m^3 1 ppb = 1 µg/L 1 ppb = 1 µg/kg	1 ppb = 12.72 µg/m^3 1 ppb = 1 µg/L 1 ppb = 1 µg/kg	1 ppb = 12.72 µg/m^3 1 ppb = 1 µg/L 1 ppb = 1 µg/kg	1 ppb = 14.15 µg/m^3 1 ppb = 1 µg/L 1 ppb = 1 µg/kg
Explosive limits	No data	No data	No data	No data

Table 4-2. Physical and Chemical Properties of Chlorodibenzofurans (CDFs)

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[c]	Solid	Solid	Solid	Solid
Melting point °C[a]	225–227	196–16.5	225.5-226.5	232–234
Boiling point °C	No data	No data	No data	No data
Density at 20°C	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 solvents[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
pKa	Not applicable	Not applicable	Not applicable	Not applicable
Vapor pressure at 25°C[i]	2.73×10^{-7}	1.63×10^{-7}	6.07×10^{-8}	6.07×10^{-8}
Henry's law constant[k]	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[a] Water Soil	1 ppb = 14.15 µg/m^3 1 ppb = 1 µg/L 1 ppb = 1 µg/kg	1 ppb = 14.15 µg/m^3 1 ppb = 1 µg/L 1 ppb = 1 µg/kg	1 ppb = 15.58 µg/m^3 1 ppb = 1 µg/L 1 ppb = 1 µg/kg	1 ppb = 15.58 µg/m^3 1 ppb = 1 µg/L 1 ppb = 1 µg/kg
Explosive limits	No data	No data	No data	No data

Table 4-2. Physical and Chemical Properties of Chlorodibenzofurans (CDFs)

Property	1,2,3,7,8,9-HexaCDF	1,2,3,7,8,9-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[c]	Solid	Solid	Solid	Solid
Melting point, °C[a]	No data	180–181	239–240	236–237
Boiling point, °C	No data	No data	No data	No data
Density at 20°C	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 solvents[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	No data
Log K_{oc}[h]	No data	No data	No data	No data
pKa	Not applicable	Not applicable	Not applicable	Not applicable
Vapor pressure at 25°C[i]	3.74×10^{-8}	No data	3.74×10^{-8}	1.68×10^{-8}
Henry's law constant[k]	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[a] Water Soil	1 ppb = 15.58 µg/m^3 1 ppb = 1 µg/L 1 ppb = 1 µg/kg	1 ppb = 15.58 µg/m^3 1 ppb = 1 µg/L 1 ppb = 1 µg/kg	1 ppb = 15.58 µg/m^3 1 ppb = 1 µg/L 1 ppb = 1 µg/kg	1 ppb = 17.02 µg/m^3 1 ppb = 1 µg/L 1 ppb = 1 µg/kg
Explosive limits	No data	No data	No data	No data

Table 4-2. Physical and Chemical Properties of Chlorodibenzofurans (CDFs)

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[c]	Solid	Solid	Solid	Solid
Melting point, °C[a]	No data	211–212	212–223	25[c]
Boiling point, °C	No data	No data	No data	537[c]
Density at 20°C	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)[l]
Organic solvents[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)
pKa	Not applicable	Not applicable	Not applicable	Not applicable
Vapor pressure at 25°C[i]	No data	No data	9.79×10^{-9}	No data
Henry's law constant[k]	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[a]	1 ppb = 17.02 µg/m^3	1 ppb = 17.02 µg/m^3	1 ppb = 17.02 µg/m^3	1 ppb = 18.45 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

Table 4-2. Physical and Chemical Properties of Chlorodibenzofurans (CDFs)

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
Explosive limits	No data	No data	No data	No data

[a]Kuroki et al. 1984 unless otherwise stated.
[b]The polychlorinated dibenzofurans are present predominantly in the particulate phase in ambient air (Hunt and Maisel 1990).
[c]WHO 2000.
[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 1985.
[i]Eitzer and Hites 1988.
[j]Rordorf 1989.
[k]Eitzer and Hites 1989a; the values are for unseparated isomers of each homologous series.
[l]Frank and Schrap 1990.