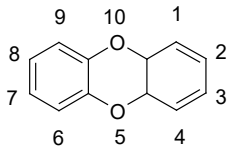
CHAPTER 4. CHEMICAL AND PHYSICAL INFORMATION

CDDs are a class of related chlorinated hydrocarbons that are structurally similar. The basic structure is a dibenzo-*p*-dioxin (DD) molecule, which is comprised of two benzene rings joined at their *para* carbons by two oxygen atoms. There are eight homologues of CDDs, monochlorinated through octachlorinated. The class of CDDs contains 75 congeners, consisting of 2 monochlorodibenzo-*p*-dioxins (MCDDs), 10 dichlorodibenzo-*p*-dioxins (DCDDs), 14 trichlorodibenzo-*p*-dioxins (TrCDDs), 22 tetrachlorodibenzo-*p*-dioxins (TCDDs), 14 pentachlorodibenzo-*p*-dioxins (PeCDD), 10 hexachlorodibenzo-*p*-dioxins (HxCDDs), 2 heptachlorodibenzo-*p*-dioxins (HpCDDs), and a single octachlorodibenzo-*p*-dioxin (OCDD) (Ryan et al. 1991). The general structure of the dibenzo-*p*-dioxins is shown below. The numbers indicate the positions for chlorine substitutions, excluding, of course, positions 5 and 10.



Not all congeners have been studied for their chemical and physical properties, but basic properties are known for the CDDs as a chemical family and for the homologous groups. Chlorinated dioxins exist as colorless solids or crystals in the pure state. They have low solubility in water and low volatility. Chlorinated dioxins have an affinity for particulates and readily partition to particles in air, water, and soil. The more toxic compounds appear to be the 2,3,7,8-substituted tetra-, penta-, and hexachloro-compounds (i.e., 2,3,7,8-TCDD, 1,2,3,7,8-PeCDD, 1,2,3,4,7,8-HxCDD, 1,2,3,6,7,8-HxCDD, and 1,2,3,7,8,9-HxCDD). These are also the congeners, along with OCDD, that have the greatest tendency to bioaccumulate. One of the most toxic congeners in mammals is believed to be 2,3,7,8-TCDD; this compound has also been the most studied of the TCDD congeners.

4.1 CHEMICAL IDENTITY

Information regarding the chemical identities of CDDs is presented in Table 4-1.

Table 4-1. Chemical Identity of CDDs[a]

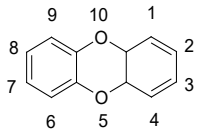
Characteristic	Monochlorodibenzo-*p*-dioxins	Dichlorodibenzo-*p*-dioxins
Chemical name	1-Chlorodibenzo-*p*-dioxin (CAS Registry Number 39227-53-7); 2-Chlorodibenzo-*p*-dioxin (CAS Registry Number 39227-54-8)[b]	2,7-Dichlorobenzo-*p*-dioxin (CAS Registry Number 33857-26-0)[c]
Synonym(s) and registered trade name(s)[d]	1-Chlorodibenzo-*p*-dioxin; 1-Chlorodibenzo-*p*-dioxin; 1-Chlorodibenzo[*b,e*](1,4)dioxin[b]; 2-Chlorodibenzo[*b,e*](1,4)dioxin[b]	1,3- or 1,6- or 2,3- or 2,7- or 2,8-Dichlorodibenzo-*p*-dioxin; 1,3- or 1,6- or 2,3- or 2,7- or 2,8-Dichlorodibenzo[b,e](1,4)dioxin; 1,3- or 1,6- or 2,3- or 2,7- or 2,8-Dichlorodibenzodioxin[b]
Total number of possible isomers	2	10
Chemical formula	$C_{12}H_7ClO_2$[e]	$C_{12}H_6Cl_2O_2$[b]
SMILES	c1(Cl)c2c(ccc1)Oc1c(cccc1)O2	c1(Cl)c(Cl)cc2c(c1)Oc1c(cccc1)O2
Chemical structure[b,f]		See footnote "f"
CAS Registry Number(s)[g]	39227-53-7 (1-)[e] 39227-54-8 (2-)[b]	50585-39-2 (1,3-); 38178-38-0 (1,6-); 29446-15-9 (2,3-)[e]; 33857-26-0 (2,7-)[c]; 38964-22-6 (2,8-)[e]

Table 4-1. Chemical Identity of CDDs[a]

Characteristic	Trichlorodibenzo-*p*-dioxins	Tetrachlorodibenzo-*p*-dioxins
Chemical name	1,2,4-Trichlorodibenzo-*p*-dioxin (CAS Registry Number 39227-58-2); 2,3,7-Trichlorodibenzo-*p*-dioxin (CAS Registry Number 33857-28-2)[b]	2,3,7,8-Tetrachlorodibenzo-*p*-dioxin (CAS Registry Number 1746-01-6)[c]
Synonym(s) and registered trade name(s)[d]	1,2,4- or 2,3,7-Trichlorodibenzo-*para*-dioxin; 1,2,4- or 2,3,7-Trichloro-dibenzo[b,e](1,4)dioxin; 1,2,4- or 2,3,7-Trichlorodibenzodioxin[b]	1,2,3,4- or 1,2,3,8- or 1,3,6,8- or 1,3,7,8- or 1,2,7,8- or 2,3,7,8-Tetrachlorodibenzo-*p*-dioxin[h]; 1,2,3,4- or 1,2,3,8- or 1,2,7,8- or 1,3,6,8- or 1,3,7,8- or 2,3,7,8-Tetrachlorodibenzodioxin; 1,2,3,4- or 1,2,3,8- or 1,3,6,8- or 1,3,7,8- or 1,2,7,8- or 2,3,7,8-Tetrachloro-dibenzo[b,e](1,4)dioxin; 1,2,7,8- or 2,3,7,8-Tetrachlorodibenzo-1,4-dioxin; 2,3,6,7-Tetrachloro-dibenzodioxin; 1,2,7,8-Tetrachlorodibenzo-*p*-dioxin; Dioxin; TCDBD; TCDD[b]
Total number of possible isomers	14	22
Chemical formula	$C_{12}H_5Cl_3O_2$[e]	$C_{12}H_4Cl_4O_2$[b]
SMILES	c1(Cl)c(Cl)c(Cl)c2c(c1)Oc1c(cccc1)O2	c1(Cl)c(Cl)c(Cl)c(Cl)c2c1Oc1c(cccc1)O2
Chemical structure[b,f]	See footnote "f"	See footnote "f"
CAS Registry Numbers[g]	39227-58-2 (1,2,4-); 33857-28-2 (2,3,7-)[e]	30746-58-8 (1,2,3,4-); 53555-02-5 (1,2,3,8-); 34816-53-0 (1,2,7,8-); 33423-92-6 (1,3,6,8-); 50585-46-1 (1,3,7,8-)[e] 1746-01-6 (2,3,7,8-)[c]

Table 4-1. Chemical Identity of CDDs[a]

Characteristics	Pentachlorodibenzo-*p*-dioxins	Hexachlorodibenzo-*p*-dioxins
Chemical name	1,2,3,7,8-Pentachlorodibenzo-*p*-dioxin (CAS Registry Number 40321-76-4)[e]	1,2,3,6,7,8-Hexachlorodibenzo-*p*-dioxin (CAS Registry Number 57653-85-7); 1,2,3,7,8,9- Hexachlorodibenzo-*p*-dioxin (CAS Registry Number 19408-74-3); Hexachlorodibenzo-*p*-dioxin (CAS Registry Number 34465-46-8)[c]
Synonym(s) and registered trade name(s)[d]	1,2,3,4,7- or 1,2,3,7,8- or 1,2,4,7,8-Pentachlorodibenzo-para-dioxin; 1,2,3,4,7- or 1,2,3,7,8- or 1,2,4,7,8-Pentachlorodibenzodioxin; 1,2,3,4,7- or 1,2,3,7,8- or 1,2,4,7,8-Pentachlorodibenzo[b,e] (1,4)dioxin[b]	1,2,3,4,7,8- or 1,2,3,6,7,8- or 1,2,3,6,7,9- or 1,2,3,7,8,9- or 1,2,4,6,7,9-Hexachlorodi-benzo-para-dioxin; 1,2,3,4,7,8- or 1,2,3,6,7,8- or 1,2,3,6,7,9- or 1,2,3,7,8,9- or 1,2,4,6,7,9-Hexachlorodibenzodioxin[b]; Hexachlorodibenzo-4-dioxin[c]
Total number of possible isomers	14	10
Chemical formula	$C_{12}H_3Cl_5O_2$[e]	$C_{12}H_2Cl_6O_2$[b]
SMILES	c1(Cl)c(Cl)c(Cl)c(Cl)c2c1Oc1c(c(Cl)ccc 1)O2	c1(Cl)c(Cl)c(Cl)c(Cl)c2c1Oc1c(c(Cl)c(Cl) cc1)O2
Chemical structure[b,f]	See footnote "f"	See footnote "f"
CAS Registry Numbers[g]	39227-61-7 (1,2,3,4,7-); 40321-76-4 (1,2,3,7,8-); 58802-08-7 (1,2,4,7,8-)[e]	57653-85-7 (1,2,3,6,7,8-)[c]; 64461-98-9 (1,2,3,6,7,9-)[e]; 19408-74-3 (1,2,3,7,8,9-)[c]; 39227-62-8 (1,2,4,6,7,9-)[c]; 34465-46-8[e]

Table 4-1. Chemical Identity of CDDs[a]

Characteristic	Heptachlorodibenzo-*p*-dioxins	Octachlorodibenzo-*p*-dioxin
Chemical name	Heptachlorodibenzo-*p*-dioxin (CAS Registry Number 35822-46-9)[c]	Octachlorodibenzo-*p*-dioxin[c]
Synonym(s) and registered trade name(s)[d]	1,2,3,4,6,7,8- or 1,2,3,4,6,7,9-Heptachlorodibenzo-*p*-dioxin; 1,2,3,4,6,7,8- or 1,2,3,4,6,7,9-Heptachlorodibenzo[b,e](1,4) dioxin; 1,2,3,4,6,7,8- or 1,2,3,4,6,7,9-Heptachlorodibenzodioxin; 1,2,3,4,6,7,8- or 1,2,3,4,6,7,9-Heptachlorodibenzo-*para*-dioxin[e]; Heptachlorodibenzo[b,e](1,4)dioxin[c]	1,2,3,4,6,7,8,9-Octachlorodibenzo-*p*-dioxin; OCDD; Octachlorodibenzodioxin; Octachlorodibenzo[b,e](1,4)dioxin; Octachlorodibenzo-*p*-dioxin; 1,2,3,4,6,7,8,9-Octachlorodibenzodioxin; 1,2,3,4,6,7,8,9-Octachlorodibenzo[b,e](1,4)dioxin; Octachloro-*para*-dibenzodioxin[b]
Total number of possible isomers	2	1
Chemical formula	$C_{12}HCl_7O_2$[e]	$C_{12}Cl_8O_2$[c]
SMILES	c1(Cl)c(Cl)c(Cl)c(Cl)c2c1Oc1c(c(Cl)c(Cl)c(Cl)c1)O2	Clc3c(Cl)c(Cl)c2Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Oc2c3Cl
Chemical structure[b,f]	See footnote "f"	See footnote "f"
CAS Registry Numbers[g]	35822-46-9 (1,2,3,4,6,7,8-)[i]; 58200-70-7 (1,2,3,4,6,7,9-)[e]; 37871-00-4 (b,e)(1,4)[c]	3268-87-9[c]

[a]In some cases, information regarding chemical identity was not available for all isomers of a homologous class.
[b]IARC 1977.
[c]IARC 1997.
[d]Example, alternative nomenclature shown; not all possible isomers are listed but can be extrapolated from the general structure or from the literature (Ryan et al. 1991).
[e]RTECS 1996.
[f]The structural formula of unsubstituted dibenzo-*p*-dioxin and the numbering of the carbon atoms in the ring are given under monochlorodibenzo-*p*-dioxins. The chlorinated dibenzo-*p*-dioxins contain chlorine atoms at the positions indicated in their names (IARC 1977).
[g]Specific chlorine substitutions are given in parentheses following the identification numbers when multiple identification numbers are given.
[h]1,2,7,8- is the same isomer as 2,3,6,7- in tetrachlorodibenzo-*p*-dioxins.
[i]NLM 2024.

CAS = Chemical Abstracts Services; CDD = chlorinated dibenzo-*p*-dioxin; SMILES = simplified molecular-input line-entry system

4.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of CDDs is presented in Table 4-2.

Table 4-2. Physical and Chemical Properties of CDDs[a]

Characteristic	Monochlorodibenzo-*p*-dioxins	Dichlorodibenzo-*p*-dioxins	Trichlorodibenzo-*p*-dioxins
Molecular weight	218.6	253.1	287.5
Color	Colorless[b]	Colorless[b]	Colorless (1,2,4-)[b]
Physical state	Crystals (1-); solid (2-)[b]	Needles (1,6-); solid (2,3-, 2,8-); crystals (2,7-)[b]	Solid (1,2,4-)[b]
Melting point	105.5°C (1-); 89.0°C (2-)[c]	114–115°C (1,3-); 184–185°C (1,6-)[b]; 164°C (2,3-); 210°C (2,7-); 151°C (2,8-)[c]	129°C (1,2,4-)[c]; 128–129°C (1,2,4-)[b]; 153–163°C (2,3,7-)[b]
Boiling point	No data	No data	No data
Density at 25°C	No data	No data	No data
Odor	No data	No data	No data
Odor threshold: Water Air	 No data No data	 No data No data	 No data No data
Solubility: Water at 25°C[d]	0.417 mg/L (1-); 0.278–0.318 mg/L (2-)[c]	0.0149 mg/L (2,3-); 0.00375 mg/L (2,7-); 0.0167 mg/L (2,8-)[c]	0.00841 mg/L (1,2,4-)[c]
Organic solvent(s)[e]	No data	No data	No data
Partition coefficients: Log K_{ow} Log K_{oc}	 4.52–5.45 (1-, 2-)[f] No data	 5.86–6.39 (2,7-)[f] No data	 6.86–7.45 (1,2,4-)[f] No data
Vapor pressure at 25°C	9.0×10^{-5} mm Hg (1-); 1.3×10^{-4} mm Hg (2-)[g]	2.9×10^{-6} mm Hg (2,3-); 9.0×10^{-7} mm Hg (2,7-); 1.1×10^{-6} mm Hg (2,8-)[g]	2.7×10^{-7} mm Hg (1,3,7-); 7.5×10^{-7} mm Hg (1,2,4-)[g]
Henry's law constant at 25°C	82.7×10^{-6} to 146.26×10^{-6} atm·m^3/mol[c]	21.02×10^{-6} to 80.04×10^{-6} atm·m^3/mol (2,3-, 2,7-, 2,8-)[c]	37.9×10^{-6} atm·m^3/mol (1,2,4-)[c]
Degradation	Atmospheric lifetime using gas-phase reaction with OH radical=0.5 days[h]	Atmospheric lifetime using gas-phase reaction with OH radical=0.5–0.7 days[h]	Atmospheric lifetime using gas-phase reaction with OH radical=0.7–0.9 days[h]
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 in air at 25°C, 760 mm Hg	1 mg/m^3 = 0.112 ppm; 1 ppm = 8.94 mg/m^3	1 mg/m^3 = 0.0966 ppm; 1 ppm = 10.35 mg/m^3	1 mg/m^3 = 0.0850 ppm; 1 ppm = 11.76 mg/m^3
Explosive limits	No data	No data	No data

Table 4-2. Physical and Chemical Properties of CDDs[a]

Characteristic	Tetrachlorodibenzo-*p*-dioxins[i]	Pentachlorodibenzo-*p*-dioxins	Hexachlorodibenzo-*p*-dioxins
Molecular weight	322	356.4	390.9
Color	White or colorless[b,j] (2,3,7,8-); colorless (1,2,3,4-, 1,3,6,8-)[b]	Colorless (1,2,3,4,7-)[b]	Colorless (1,2,3,4,7,8-, 1,2,4,6,7,9-)[b]
Physical state	Crystalline solid[j] (2,3,7,8-)	Solid (1,2,3,4,7-)[b]	Solid (1,2,3,4,7,8-, 1,2,4,6,7,9-)[b]
Melting point	190°C (1,2,3,4-); 175°C (1,2,3,7-)[c]; 219–219.5°C (1,3,6,8-); 193.5–195°C (1,3,7,8-); 305–306°C (2,3,7,8-)[b]	195–196°C (1,2,3,4,7-); 240–241°C (1,2,3,7,8-); 205–206°C (1,2,4,7,8-)[b]	273°C (1,2,3,4,7,8-)[c]; 275°C (1,2,3,4,7,8-)[b]; 285–286°C (1,2,3,6,7,8-); 243–244°C (1,2,3,7,8,9-); 238–240°C (1,2,4,6,7,9-)[b]
Boiling point	446.5°C[f] (2,3,7,8-)	No data	No data
Density at 25°C	1.827 g/mL[k] (2,3,7,8-)	No data	No data
Odor	No data	No data	No data
Odor threshold:			
Water	No data	No data	No data
Air	No data	No data	No data
Solubility:			
Water at 25°C[d]	4.7×10^{-4}–6.3×10^{-4} mg/L (1,2,3,4-)[c,l] 4.2×10^{-4} mg/L (20°C) (1,2,3,7-); 3.2×10^{-4} mg/L (20°C) (1,3,6,8-); 1.9×10^{-5} mg/L (2,3,7,8-)[m] 7.9×10^{-6}–3.2×10^{-4} mg/L (2,3,7,8-)[c]	1.18×10^{-4} mg/L (20°C) (1,2,3,4,7-)[c]	4.42×10^{-6} mg/L (20°C) (1,2,3,4,7,8-)[c]
Organic solvent(s)[e]	*o*-Dichlorobenzene, chloro-benzene, benzene, chloroform, n-octanol[b]	No data	No data
Partition coefficients:			
Log K_{ow}	7.02–8.7 (1,2,3,7-)[f,g]; 7.02–8.93 (2,3,7,8-)[c]; 7.39–7.58 (2,3,7,8-)[n]; 6.8 (2,3,7,8-TCDD)[o;] 6.6 (1,2,3,4-TCDD)[o]	5.80–9.65 (1,2,3,4,7-)[c]	9.19–10.4 (1,2,3,4,7,8-)[f]
Log K_{oc}	No data	No data	No data

Table 4-2. Physical and Chemical Properties of CDDs[a]

Vapor pressure at 25°C	$7.5x10^{-9}$ mm Hg (1,2,3,7-)[c]; $4.8x10^{-8}$ mm Hg (1,2,3,4-)[g]; $1.5x10^{-9}$–$3.4x10^{-5}$ mm Hg (2,3,7,8-)[g]; $5.3x10^{-9}$–$4.0x10^{-3}$ mm Hg (1,3,6,8-)[c]; $7.4x10^{-10}$ mm Hg (2,3,7,8-)[p]	$6.6x10^{-10}$ mm Hg (1,2,3,4,7-)[c]	$3.8x10^{-11}$ mm Hg (1,2,3,4,7,8-)[c]
Henry's law constant at 25°C	$16.1x10^{-6}$–$101.7x10^{-6}$ atm·m^3/mol (2,3,7,8-); $7.01x10^{-6}$–$101.7x10^{-6}$ atm·m^3/mol[c]	$2.6x10^{-6}$ atm·m^3/mol (1,2,3,4,7-)[c]	$44.6x10^{-6}$ atm·m^3/mol (1,2,3,4,7,8-)[c]
Degradation	Photodegradation half-life on grass (2,3,7,8-)=44 hours (k_2=0.0156 h^{-1})[o,q]; atmospheric lifetime using gas-phase reaction with OH radical=0.8–2 days[h]	Atmospheric lifetime using gas-phase reaction with OH radical=1.1–2.4 days[h]	Atmospheric lifetime using gas-phase reaction with OH radical=1.5–3.4 days[h]
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 in air at 25°C, 760 mm Hg	1 mg/m^3=0.0759 ppm 1 ppm=13.17 mg/m^3	1 mg/m^3=0.0686 ppm 1 ppm=14.58 mg/m^3	1 mg/m^3=0.0625 ppm 1 ppm=15.99 mg/m^3
Explosive limits	No data	No data	No data

Characteristic	Heptachlorodibenzo-*p*-dioxins	Octachlorodibenzo-*p*-dioxin
Molecular weight	425.3	459.8
Color	No data	No data
Physical state	No data	No data
Melting point	265°C (1,2,3,4,6,7,8-)[c]	332°C[c]; 325–326°C[p]
Boiling point	507.2°C[g]	510°C[g]; 485°C[o]
Density at 25°C	No data	No data
Odor	No data	No data
Odor threshold:		
Water	No data	No data
Air	No data	No data
Solubility:		
Water at 25°C[d]	$2.4x10^{-6}$ mg/L at 20°C (1,2,3,4,6,7,8-)[c]	$7.4x10^{-8}$ mg/L[c]
Organic solvent(s)[e]	No data	Acetic acid, anisole, chloroform, *o*-dichlorobenzene, dioxane, diphenyl oxide, pyridine, xylene[b]

Table 4-2. Physical and Chemical Properties of CDDs[a]

Partition coefficients:		
Log K_{ow}	9.69–11.38 (1,2,3,4,6,7,8-)[f]	10.07–12.26[f]; 8.20[p]
Log K_{oc}	No data	No data
Vapor pressure at 25°C	$5.6x10^{-12}$ mm Hg (1,2,3,4,6,7,8-)[g]	$8.25x10^{-13}$ mm Hg[g]; $1.68x10^{-12}$ [o]
Henry's law constant at 25°C	$1.31x10^{-6}$ atm–m^3/mol (1,2,3,4,6,7,8-)[c]	$6.74x10^{-6}$ atm·m^3/mol[c]
Degradation	Atmospheric lifetime using gas-phase reaction with OH radical=4.4 days[h]	Atmospheric lifetime using gas-phase reaction with OH radical=9.6 days[h]
Autoignition temperature	No data	No data
Flashpoint	No data	No data
Flammability limits	No data	No data
Conversion factors in air at 25°C, 760 mm Hg	1 mg/m^3=0.0575 ppm 1 ppm=17.39 mg/m^3	1 mg/m^3=0.0532 ppm 1 ppm=18.81 mg/m^3
Explosive limits	No data	No data

[a]In some cases, information regarding chemical and physical properties was not available for all isomers of a homologous class.
[b]IARC 1977.
[c]Shiu et al. 1988.
[d]Solubility is given for 25°C unless noted otherwise in text.
[e]In most cases, no specific solubilities were found. However, solvation in organic solvents such as toluene, hexane, and methylene chloride is possible given that these solvents are used in extraction and analysis methods.
[f]Webster et al. 1985.
[g]Rordorf 1989.
[h]Atkinson 1991.
[i]Physical and chemical properties of 2,3,7,8-TCDD are shown in bold.
[j]Sax and Lewis 1987.
[k]Schroy et al. 1985.
[l]Doucette and Andren 1988.
[m]Marple et al. 1986.
[n]Des Rosiers 1986.
[o]McCrady and Maggard 1993.
[p]IARC 1997.
[q]k_2 = elimination rate constants.

CDD = chlorinated dibenzo-*p*-dioxin