CHAPTER 4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

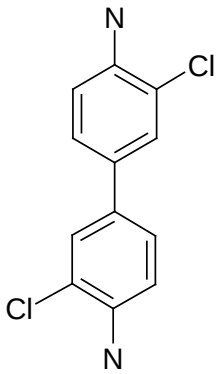
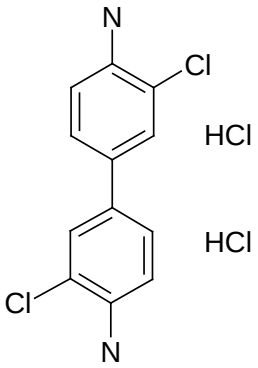
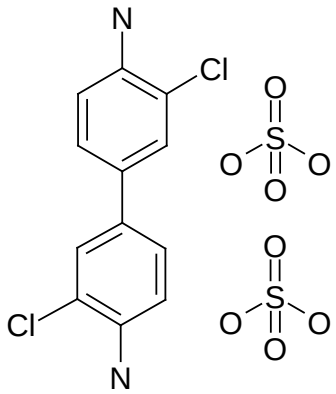
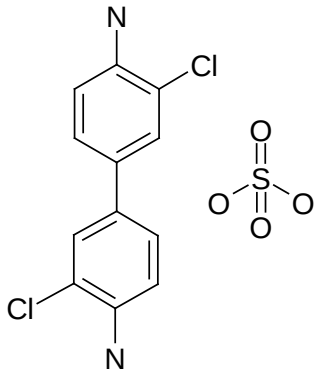
3,3'-Dichlorobenzidine is a solid crystalline powder composed of two conjoined benzene rings each with chlorine groups in the "3" positions and amino groups in the "4" positions. The primary Chemical Abstracts Service Registry Number (CASRN) for the compound includes the various salts that the base substance can form in the presence of certain compounds, especially inorganic acids. In addition to the general CASRN, 3,3'-dichlorobenzidine dihydrochloride and 3,3'-dichlorobenzidine sulfate are salts that have their own unique CASRNs, and may exhibit unique toxicological properties. 3,3'-Dichlorobenzidine is manufactured from o-nitrochlorobenzene by reduction with zinc dust and sodium hydroxide, followed by rearrangement with hydrochloric acid or sulfuric acid. Different salts are formed when 3,3'-dichlorobenzidine is exposed to certain compounds. 3,3'-Dichlorobenzidine (and its salts) was previously used in the manufacture of dyes in the United States. However, the 2016 Chemical Data Reporting (CDR) rule indicates that 3,3'-dichlorobenzidine dihydrochloride is currently used in pigment manufacturing. Information was not available on past or current uses of 3,3'-dichlorobenzidine sulfate (NLM 2019).

Table 4-1 lists common synonyms, trade names, and other pertinent identification information for 3,3'-dichlorobenzidine (and its salts), 3,3'-dichlorobenzidine dihydrochloride, and 3,3'-dichlorobenzidine sulphate, and 3,3'-dichlorobenzidine dihydrogen bis(sulphate).

4.2 PHYSICAL AND CHEMICAL PROPERTIES

3,3'-Dichlorobenzidine and its salts are solid crystalline substances. 3,3'-Dichlorobenzidine has a relatively high log K_{oc}, suggesting that it will have a low mobility in soil and will bind strongly to solid phases in soil, sediment, and sludges. The compound and its salts have relatively low (but not negligible) solubility in water. Table 4-2 lists important physical and chemical properties of 3,3'-dichlorobenzidine (and its salts), 3,3'-dichlorobenzidine dihydrochloride, 3,3'-dichlorobenzidine dihydrogen bis(sulphate), and 3,3'-dichlorobenzidine sulphate. This information includes synonyms, chemical formulas and structures, and identification numbers.

Table 4-1. Chemical Identity of 3,3'-Dichlorobenzidine (and its Salts), 3,3'-Dichlorobenzidine Dihydrochloride, 3,3'-Dichlorobenzidine Dihydrogen Bis(sulphate), and 3,3'-Dichlorobenzidine Sulphate

Characteristic	3,3’-Dichlorobenzidine (and its salts)	3,3’-Dichlorobenzidine dihydrochloride	3,3’-Dichlorobenzidine dihydrogen bis(sulphate)	3,3’-Dichlorobenzidine sulphate
Synonym(s) and Registered trade name(s)	Dichlorobenzidine; (1,1'-biphenyl)-4,4'-diamine, 3,3'-dichloro-; benzidine, 3,3'-dichloro-; DCB; 4,4'-diamino-3,3'-dichlorodiphenyl; Curithane[a]	Benzidine, 3,3'-dichloro-, dihydrochloride; (1,1'-biphenyl)-4,4'-diamine, 3,3'-dichloro-, dihydrochloride[a]	(1,1'-Biphenyl)-4,4'-diamine, 3,3'-dichloro-, sulfate (1:2)[a]	3,3'-Dichlorobenzidine sulphate; benzidine, 3,3'-dichloro-, sulfate; (1,1'-biphenyl)-4,4'-diamine, 3,3'-dichloro-, sulfate (1:1)[a]
Chemical formula	$C_{12}H_{10}Cl_2N_2$[a]	$C_{12}H_{12}Cl_4N_2$[a]	$C_{12}H_{14}Cl_2N_2O_8S_2$[a]	$C_{12}H_{12}Cl_2N_2O_4S$[a]
Chemical structure				
CAS registry number(s)	91-94-1[a]	612-83-9[a]	64969-34-2	64414-68-2 74332-73-3

[a]NLM 2019.

CAS = Chemical Abstracts Service

Table 4-2. Physical and Chemical Properties of 3,3'-Dichlorobenzidine (and its Salts), 3,3'-Dichlorobenzidine Dihydrochloride, 3,3'-Dichlorobenzidine Dihydrogen Bis(sulphate), and 3,3'-Dichlorobenzidine Dihydrogen Bis(sulphate)

Property	3,3'-Dichlorobenzidine (and its salts)	3,3'-Dichlorobenzidine dihydrochloride	3,3'-Dichlorobenzidine dihydrogen bis(sulphate)	3,3'-Dichlorobenzidine sulphate
Molecular weight	253.126 g/mol[b]	326.06 g/mol[b]	449.27 g/mol[b]	351.2 g/mol[b]
Color	White crystalline solid; gray to purple crystalline solid[b]	White crystals; white to light-gray powder; needles[b]	White crystalline powder[b]	White crystalline powder[b]
Physical state	Solid[b] (ionic species)	Solid[b] (ionic species)	Solid[b] (ionic species)	Solid[b] (ionic species)
Melting point(s)	132.5°C[b]	No data	No data	No data
Boiling point(s)	402°C[b]	No data	No data	No data
Density	Not applicable	Not applicable	Not applicable	Not applicable
Taste	No data	No data	No data	No data
Taste threshold:	No data	No data	No data	No data
Odor	No data	Mild odor[b]	No data	No data
Odor threshold:	No data	No data	No data	No data
Solubility:				
Water at 25°C	3.1 mg/L[b]	Slightly soluble in water	Slightly soluble in water	Slightly soluble in water
Organic solvent(s)	Soluble in alcohol, ether, acetic acid, and benzene; slightly soluble in hydrochloric acid[b]	Readily soluble in alcohol	No data	No data
Partition coefficients:				
Log K_{ow}	3.02–3.78[c]	No data	No data	No data
Log K_{oc}	2.86–4.67[d]	No data	No data	No data
Vapor pressure at 25°C	4.1×10^{-6} mmHg[b]	No data	No data	No data
Henry's law constant at 25°C	2.8×10^{-11} atm-m^3/mol[b]	No data	No data	No data
Dissociation constants:				
$pK_{a,1}$	1.6[a]	No data	No data	No data
$pK_{a,2}$	3.2[a]	No data	No data	No data

Table 4-2. Physical and Chemical Properties of 3,3'-Dichlorobenzidine (and its Salts), 3,3'-Dichlorobenzidine Dihydrochloride, 3,3'-Dichlorobenzidine Dihydrogen Bis(sulphate), and 3,3'-Dichlorobenzidine Dihydrogen Bis(sulphate)

Property	3,3’-Dichlorobenzidine (and its salts)	3,3’-Dichlorobenzidine dihydrochloride	3,3’-Dichlorobenzidine dihydrogen bis(sulphate)	3,3’-Dichlorobenzidine sulphate
Autoignition temperature	No data	No data	No data	No data
Flashpoint	No data	No data	No data	No data
Flammability limits in air	No data	No data	No data	No data
Conversion factors:	ppm = 0.0966 times mg/m^{3}[b]	No data	No data	No data
Explosive limits	No data	No data	No data	No data
Incompatibilities and reactivity	No data	No data	Reactivity to acidic salts and aryl halides	No data

[a]Nyman et al. 1997.
[b]NLM 2019.
[c]DCMA 1989; EPA 1982.
[d]Donaldson and Nyman 2005; EPA 1982, 2014.