Properties and uses

Properties

The physical properties of the ortho, meta, and para isomers of nitrochlorobenzene are summarized in Table.

O-Nitrochlorobenzene

O-Nitrochlorobenzene crystallizes in light yellow, monoclinic needles. It is insoluble in water and is very soluble in benzene, diethyl ether, and hot ethanol.

O-Nitrochlorobenzene reactions involve the nitro groups, chlorine atom, and aromatic ring. The nitro group can be partially reduced to the corresponding intermediate or fully to the amino group. The aromatic ring can be nitrated, leading to the formation of 2,4-dinitro-1chlorobenzene and 2,6-dintro-1-chlorobenzene or it can be sulfonated, yielding 3-nitro-4-chlorobenzenesulfonic acid. The chlorine atom can be displaced easily by o-nitrophenol attack by-OH, $-OCH_3$, $-OC_6H_6$, $-NH_2$, etc. treatment of o-nitrochlorobenzene with aqueous sodium hydroxide at 130^0C results in the formation of o-nitrophenol, and with aqueous methanolic potassium hydroxide at high temperature and pressure, o-nitroanisole is formed. When o-nitrochlorobenzene is treated with aqueous ammonia under high temperature and pressure, o-nitroaniline is formed. O-Nitrochlorobenzene condenses with aniline to form 2-nitrodiphenylamine.

m-Nitrochlorobenzene

m-Nitrochlorobenzene is a pale yellow crystalline solid, which can exist as a stable or labile form in the solid state. It is insoluble in water, very soluble in benzene and diethyl ether, and soluble in acetone, chloroform, and hot ethanol. Unlike the ortho and para isomers, the chlorine atom of m-nitrochlorobenzene is not activated for nucleophilic substitution.

p-Nitrochlorobenzene

p-Nitrochlorobenzene crystallizes in light yellow monoclinic prisms. It is insoluble in water and very soluble in benzene, diethyl ether, and hot ethanol p- Nitrochlorobenzene undergoes the same reactions described for the ortho isomer to yield the analogous para derivatives. Tin (II) chloride and hydrochloric acid convert p-nitrochlorobenzene to p-chloroaniline. The aromatic ring of the para isomer can undergo additional substitution by nitration to yield 2,4-dinitro-1-chlorobenzene, by chlorination to yield 1,2-dichloro-4nitrobenzene, or by sulfonation to yield 2-chloro-5-nitrobenzene sulfonic acid. The chlorine atom is activated and, as with the ortho isomer, can be easily displaced by nucleophilic attack. Treatment with aqueous ammonia at elevated temperature and pressure results in the formation of p-nitrochlorobenzene, and with aqueous sodium hydroxide under pressure, p-nitrophenol is formed. p- nitrochlorobenzene reacts with sodium disulfide to form 4,4'-dinitrodiphenyl disulfide which is an intermediate in the preparation of sulfanilamide derivatives.

Physical Properties of Mononitrochlorobenzene

Property	o-Nitrochlorobenzene	m-Nitrochlorobenzene	p-Nitrochlorobenzene
melting point, ^0C	32.5	46 (stable) 24 (labile)	83
boiling point, $^0C_{kPa}{}^c$	245.5_{100} $119_{1.1}$	235.6_{101}	242_{101} $113_{1.1}$
density, g/cm^3			

	1.368	1.534	1.520
flash point, ^{0}C	127	127	---

Uses

o-Nitrochlorobenzene is used in the synthesis of azo dye intermediates, eg. o-chloroniline (Fast Yellow G Base), o-nitroaniline (fast Orange GR Base), o-anisidine (fast Red BB Base), o-phenetidine, and o-aminophenol. It also is used in corrosion inhibitors, pigments, and agricultural chemicals. p- Nitrochlorobenzene is used principally in the production of intermediates for azo and sulfur dyes. Other uses include pharmaceuticals, photo chemicals, rubber chemicals, and insecticides. Typical intermediates manufactured from the para isomer are p-phenylenediamine (Fast Red GC Base), p-anisidine, p-aminophenol, p-nitrophenol, p-phenylenedi- amine, 2-chloro-p-anisidine (Fast Red R Base), 2,4-dinitro-1-chlorobenzene, and 1,2-dichloro-4-nitrobenzene.