



LEARNING TOXICOLOGY  
THROUGH OPEN EDUCATIONAL

# PENTACHLOROPHENOL

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## INTRODUCTION

Pentachlorophenol (PCP) is a chlorinated aromatic organic compound used as insecticide, fungicide, herbicide, disinfectant, and additive in antifouling paint. The principal use of PCP was as wood preservative, applied to protect timber from fungal rot and wood-boring insects. PCP has also been used as a pre-harvest defoliant in cotton, and as biocide in industrial water systems. PCP was released to the environment as a result of its manufacture, storage, transport or use. Its sodium salt is used for similar purposes and readily degrades to PCP. Prior 1984 (when becomes a restricted-use pesticide), PCP was one of the most widely used biocides in the U.S. (EPA, 2010). Production of PCP and sodium pentachlorophenate (NaPCP) ceased in the EU in 1992. Although PCP is no longer produced in the U.S., it is still a high-volume chemical, imported into the U.S. in quantities of 1 million pounds or more per year. In 2012, PCP was reported to be manufactured by at least six companies worldwide, and the production and imports in U.S. were > 1 million to 10 million pounds (EPA, 2013). According to the Toxics Release Inventory (TRI), 54% of the total environmental release, was discharged to the atmosphere from manufacturing and processing facilities in the U.S. PCP can also be formed during the incineration of chlorine-containing waste materials. PCP constituted 8% of polychlorinated phenols formed in the flue gas and 10% of those formed in the stack gas during the incineration of waste materials containing chlorine. PCP may also be released in stack emissions as a result of pyrolysis of PVC. (UNEP.POPS.POPRC, 2013). In the period 1980–1996, about 37 tonnes of PCP per year are released from a municipal waste incinerator in Hungary (Kovács, G., 2002). Pentachlorophenol is extremely toxic to humans from acute (short-term) ingestion and inhalation exposure. (RoC Monograf, 2014).

## STRUCTURE AND PROPERTIES OF PCP AND NAPCP

During production of PCP, the elevated temperatures and pressures used in the processes result in the formation of several additional chlorinated molecules. The concentrations of these by-products can be altered somewhat by changes in the conditions of the manufacturing process, but all commercial forms of PCP contain by-products of its synthesis in detectable amounts (WHO, 2010). Technical grade PCP (86% pure) also contains polychlorinated phenols (tri- and tetra-), hexachlorobenzene dioxins (tetra-, hexa- and octachlorodibenzo-*p*-dioxins) and hexa-, hepta-, and octachlorodibenzo furans (Collins, 2013), as manufacturing by-products. PCP also is a major product of the metabolism of hexachlorobenzene in mammals.

**Formula of the pentachlorophenol** ( $C_6HCl_5O$ ).

**CAS registry:** 87-86-5.

**Formula of sodium pentachlorophenate** ( $C_6Cl_5ONa$ ).

**CAS registry:** 131-52-2

In the Figure 1 are presented the chemical structure of pentachlorophenol and Sodium pentachlorophenate

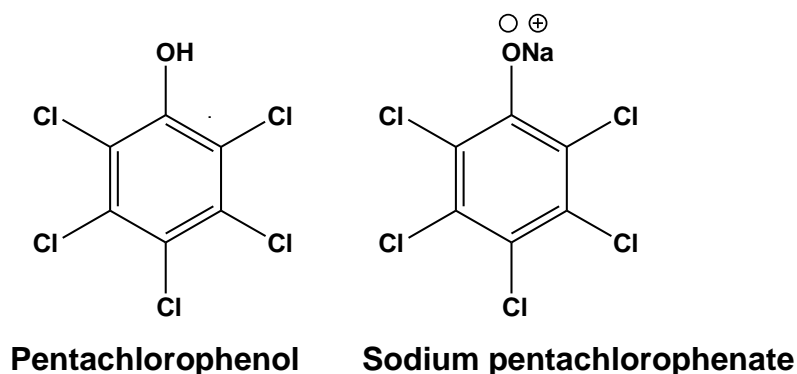


Figure 1. Chemical structure of pentachlorophenol and sodium pentachlorophenate

In Table 1. Are presented some physical properties of PCP

Table 1. Physical properties of PCP

Property	PCP
Molecular weight	266.35
Melting point	188°C
Boiling point	310°C
Vapor pressure (mm Hg)	0.0003 at 25°C
Vapor density (air = 1)	1.98
Density	1.978 g/cm <sup>3</sup> at 22°C
Solubility in water	14 mg/l at 20°C
Octanol/water partition coefficient (pK <sub>ow</sub> )	5.12
Henry's law constant at 25 °C	2.45 10 <sup>-8</sup> atm/m <sup>3</sup> /mole at 22°C

Source: ChemIDplus 2013

Pure PCP exists as light tan to white needle-like crystals at room temperature. Also known as chlorophen, penchlorol, and penta, the compound is relatively volatile, practically insoluble in water at the pH generated by its dissociation (pK<sub>a</sub> = 4.7), and soluble in most organic solvents (WHO, 2010). Salts of PCP, such as sodium pentachlorophenate, are readily soluble in water. Technical grade PCP consists of brown flakes; technical grade sodium PCP consists of cream-colored beads. The physical and chemical properties of the PCP suggest limited evaporation to the atmosphere, limited miscibility in water and association with soil particles. Movement of PCP in soils depends on soil acidity.

## PERSISTENCE IN WATER, SOIL AND SEDIMENT

PCP was ubiquitously distributed in the environment in the past, as evidenced by measured levels reported for surface water, groundwater, drinking water, ambient and indoor air, dust, soil, sediment, and food from several countries and time periods (EPA, 2013). PCP is rapidly degraded in the environment with environmental half-life estimates of less than 4 weeks in

water; less than 20 weeks in sediment and less than 10 weeks in soil. PCP is hydrolytically stable in water at pH 4 to pH 9. Chemical degradation of PCP in water occurs mainly through photo-degradation. In surface water, PCP will rapidly photo-degrade when exposed to direct sunlight. The photolysis of PCP in water is a process dependent on the pH (EPA, Office of Water 2010). The rapid degradation occurs with increased pH, when the compound is dissociated.. The ionized form is more sensitive to photodegradation than the protonated form. A degradation of 90% after 10 hours in surface water at pH =7.3, respectively a degradation of 40% at pH= 3 after 90 hours was reported (Zheng, 2011). Photolysis in water determines the formation of toxic organic compounds such as 2,3-dichloromaleic acid, 2,3,5,6- and 2,3,4,6-tetrachlorophenol, tetrachlororesorcinol, tetrachlorocatechol, benzoquinones and dioxins (UNEP. POPS.POPRC, 2013). In soil, wood treated with PCP (used as a solution in petroleum-based products or as its sodium salt in a water-based solution) may release toxic compounds through volatilization or leaching. PCP may be photo-degraded on the wood surface, making degraded compounds available for leaching. In wet soil, photolysis may produce 55% photodegradation of PCP during 14-day. Maximum degradation of 0.3–0.5 mg/kg per day in soils containing 30 mg/kg PCP and a degradation rate of 82% after 7 months have been reported. PCP released into the atmosphere from treated wood can be transported back to surface waters and soils via wet and dry deposition. Atmospheric PCP is transformed via photolysis, by free radical oxidation, with a half-life of 2 months, in the absence of water. Photolysis of sorbed or film-state PCP in the presence of oxygen has also been observed. The reaction products were similar to those found in aqueous photolysis. Adsorption of PCP to particulate matter will attenuate the rate of this process in the atmosphere. PCP released to air can be transported over substantial distances (1,500 to 3,000 km, with a half-life in the environment of approx. 1.5 months (Borysiewicz, 2008).

## BIOACCUMULATION OF PCP

The bioaccumulation of PCP in the aquatic organisms is high. Bioconcentration factors of 100–1000 have been reported and depends on the pH, increasing with falling pH. The toxicity is also dependent on the pH of the substrate tested. The investigation of the acute toxicity of PCP at pH =4, 6 and 9 in living organisms showed that toxicity was maximum at pH= 4 and minimum at pH =9. The difference in toxicity was attributed to variations in the degree to which PCP penetrated the organism tested, since at pH =4 the PCP is in protonated form and therefore lipophilic. At pH =9, PCP is fully ionized, which reduces both, the potential for penetration into the organisms, and the potential for toxic effects (UNEP.POPS.POPRC, 2013). Regarding the bioaccumulation of PCP in plants, no reliable data have been found. The physical and chemical properties of the PCP suggest limited evaporation to the atmosphere, the moving of PCP to water and association with soil organic particles. The mobility and volatilization of PCP from treated wood in the environment depends on the acidity of the medium and increases with temperature. In air, soil and surface water PCP is subjected to photolysis degradation, with atmospheric half-lives ranging from hours to weeks. PCP bioconcentrate in aquatic organisms and the BCF value increases with falling pH.

## SOURCES OF EXPOSURE

Present or past exposure to PCP can be correlated with its release during production and particularly during processing and use, which result in both occupational exposure to workers and to the general public. Sources of exposure to workers in the past have included (1) production plants, (2) wood treatment facilities and (3) contact during the use or disposal of the treated wood, through dermal contact with the substance or with treated wood /products and via inhalation of affected workplace air. Occupational exposure to PCP still occurs for workers who treat lumber or come in contact with treated lumber in their work activities and contact during the use or disposal of the

treated wood or waste. Elimination /reduction of half-lives of PCP between 4 and 72 days have been observed (UNEP, 2016.). By-products of PCP synthesis, have elimination half-lives of up to 10 years (Collins, 2013). Exposure to PCP is widespread for people due to its presence and persistence in the environment. This exposure has been determined by measurements of levels of PCP in blood, liver, brain, kidneys, spleen, and body fat and reflect more long-term exposure (RoC Monograf, 2014). The decrease in exposure from the period 30 to 40 years or more ago to the present, is consistent with actions taken by EPA to restrict PCP use as wood preservative, cancelling and restricting non-wood uses in the 1987. The main routes of exposure to the general public are through inhalation of air, ingestion of food and other potential sources. Releases of PCP can result from the presence of treated wood in the environment, as well as from the releases that occur during production, processing, and use in treating wood products. In food PCP was found at levels ranging from 0.01 to 0.02 ppm in ham, (cured or baked), chicken breast oven-roasted (skin removed), meats, fish, dairy products, grains and vegetables. High levels of exposure to people living in log homes or other houses treated with PCP and exposure for the general public to PCP from dust and hazardous waste sites also been identified (FDA, 2006). PCP has been detected in drinking water supplies as well as in groundwater and surface water (Zheng, 2011). In air, soil and surface water PCP lasts for hours to days. Chlorination of phenolic compounds during water treatment produced detectable levels of PCP and, in addition, common pesticides such as Lindane, HCHs, , PCB, etc., are known to be metabolized to PCP by plants, animals and microorganisms. PCP is an important environmental contaminant even in the countries where the use has been abandoned because it is imported via materials treated with PCP. The population can also be exposed to PCP from treated textiles, leather and paper products and, above all, through inhalation of contaminated indoor air. PCP is metabolized into other molecules and therefore its absence in animal tissues is not conclusive; on the other hand, it is a major product of the metabolism of HCHs and other common pesticides in mammals. Studies in humans and



experimental animals show that PCP is absorbed following oral, inhalation, or dermal exposure. Although PCP is widely distributed, accumulation in tissues appears to be limited by extensive binding to plasma proteins in rats and humans (RoC Monograf, 2014). Tissue distribution studies in experimental animals show that the highest concentrations are found in organs associated with metabolism and excretion and include the liver, gall bladder, kidneys, and gastrointestinal tract. PCP is mostly excreted in the urine, either unchanged or as metabolites. In the U.S. the levels are generally lower than three or four decades ago (before the use of PCP was restricted in the 1980s). PCP in the range of 10s to 100s of micrograms per liter in blood and generally around 10 mg/L in urine were reported for people living in the U.S. in studies published during 1960s and 1980s (Zheng, 2011).

## HEALTH HAZARD

**Toxicokinetics.** PCP is rapidly and completely absorbed by the digestive tract. After entering the blood, where it combines at least in part with plasma proteins, the highest concentrations of PCP are in the liver, kidneys and brain, but the tendency for bioaccumulation remains very low. Results from human and animal studies indicate that PCP is not extensively metabolized. For different species (including humans) and exposure route, the principal elimination route of PCP is the urine and via plasma proteins. In humans, NaPCP has a half-life of 30 hours in the plasma (RoC Monograph, 2014).

Regarding human health effects, the experimental data related to PCP are well documented for the oral low-dose chronic exposures and indicate impact on the liver characterized by biochemical, functional and histopathological changes; impact on the immune system; significant alteration of thyroid hormone levels at exposures of 1 or 2 mg/kg bw per day (RoC Monograf, 2014). Data on occupationally exposed workers confirm effects on the immune system and liver. The health characterization of PCP indicates a potential for a number of human health effects associated with low-level chronic exposure via the oral



route, as a result of occupational exposure. PCP introduced into the environment have the potential for LRTAP and may reach human foodstuffs and drinking-water (UNEP, 2016.) PCP is extremely toxic to humans from acute (short-term) ingestion and inhalation exposure. Acute inhalation exposures in humans have resulted in neurological, blood and liver effects, and eye irritation. Chronic (long-term) exposure to PCP by inhalation in humans has resulted in effects on the respiratory tract, blood, kidney, liver, immune system, eyes, nose, and skin. Human studies are inconclusive regarding PCP exposure and reproductive effects. Human studies suggest an association between exposure to PCP and cancer. EPA classified PCP and NaPCP as a Group B2, probable human carcinogen (EPA, 2010). Overall, monitoring data for PCP in abiotic matrices (air, soil and water) show a decreasing trend probably due to global regulatory actions (bans, restrictions and regulations) that have been put in place (UNEP, 2016.).

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