Pentachlorobenzene (CAS 608-93-5, molecular weight 250.3) is a colourless, crystalline solid with a pleasant aroma. It is not in wide commercial use, but is used in small quantities as an intermediate in the synthesis of some specialty chemicals, and has been used for producing the pesticide pentachloronitrobenzene and in producing transformer dielectric fluids. Pentachlorobenzene is not produced in Canada and imports have been negligible (Camford Information Services 1991). However, approximately 200 000 kg of pentachlorobenzene are present in transformer dielectric fluids either in use or stored before disposal. Small amounts (about 40 kg) were imported into Canada in 1992 for the maintenance of existing transformer dielectric fluid (E.D. Brien 1993, Environment Canada, Ottawa, pers. com.). The principle sources of environmental contamination are likely spillage of dielectric fluids and long-range transborder transport and deposition (Government of Canada 1993). Releases of pentachlorobenzene are also associated with the manufacture and use of various chlorinated substances (especially pentachloronitrobenzene). It is estimated that releases of pentachlorobenzene to the Canadian environment are likely in excess of 500 kg a\(^{-1}\) (Government of Canada 1993).

Concentrations of pentachlorobenzene in watercourses in Canada have been reported to range from 0.000 09 to 0.022 µg·L\(^{-1}\) at various locations in the Great Lakes basin. Levels near the upper part of the range are from sites on the Niagara River near known sites of contamination, and higher levels have been reported in various industrial effluents in Ontario. Canadian data for pentachlorobenzene in groundwater is rare, e.g., landfill leachates in Sarnia, Ontario, contained from 0.003 to 0.12 µg·L\(^{-1}\) (Government of Canada 1993).

Pentachlorobenzene has been found in aquatic invertebrates and fish in the Great Lakes basin in Canada at levels of <0.01 to 93.3 µg·kg\(^{-1}\) ww, and as high as 3500 µg·kg\(^{-1}\) (lipid-adjusted). The high levels were found in organisms collected near sites on the Niagara River and Lake Ontario known to be contaminated (Government of Canada 1993).

The major transformation product is the corresponding chlorophenol (Mackay et al., 1992). The elimination half-life determined under long-term (8 years), natural conditions (lake) in yellow eels (Anguilla anguilla) is reported as 340 d (de Boer et al. 1994).

Mackay et al. (1992) have modelled the environmental fate of each of the chlorobenzenes using several versions of a fugacity-based model and available information. These modelling results indicate that chlorobenzene behaviour varies as a function of the degree of chlorination. The simplest model, Fugacity Level I, demonstrates that pentachlorobenzene tends to partition mainly into soil, some into the sediment, and a small amount into air, because of its low vapour pressure (0.22 Pa) and very low water solubility (0.65 mg·L\(^{-1}\)). Level II modelling indicates that the primary removal processes for all chlorobenzenes are in air. For pentachlorobenzene, removal is mainly by advection (e.g., deposition, sedimentation) and, to a much lesser degree, by chemical reaction. Photodegradation is very slow, resulting in atmospheric half-lives of 4.2–14 months. Fugacity Level III modelling indicates that it accumulates and persists primarily in soils and sediments, with transfer between media being slow, and moves in the environment largely by long-range airborne transport and atmospheric deposition. As the primary removal process is advection, soils and sediments end up being long-term sinks/storage sites. In the aquatic environment, pentachlorobenzene is found mostly in organic phases (organisms, sediments) or associated with suspended/dissolved organic material rather than dissolved in the water phase (log octanol–water partition coefficient 5.0), with half-lives in the water and in the sediment of 1.1–3.4 years.

**Water Quality Guideline Derivation**

The interim Canadian water quality guideline for pentachlorobenzene for the protection of freshwater life was developed based on the CCME protocol (CCME 1991). For more information, see the Canadian

<table>
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<th>Aquatic life</th>
<th>Guideline value (µg·L(^{-1}))</th>
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<tr>
<td>Freshwater</td>
<td>6.0(^{1})</td>
</tr>
<tr>
<td>Marine</td>
<td>NRG(^{1})</td>
</tr>
</tbody>
</table>

\(^{1}\)Interim guideline.

\(^{1}\)No recommended guideline.
Environmental Protection Act (CEPA) assessment report and supporting document (Government of Canada 1993) and the supporting document (Environment Canada 1997).

Freshwater Life

The lowest acute study for fish is a 6-d LC$_{50}$ of 270 µg·L$^{-1}$ for fathead minnows (Pimephales promelas) (Ahmad et al. 1984). The lowest acute study for invertebrates is a 48-h LC$_{50}$ estimate of 230 µg·L$^{-1}$ and a 48-h NOEC of 97 µg·L$^{-1}$ for the midge (Chironomus riparius) (Roghair et al. 1994).

The lowest chronic studies are a 28-d NOEC (based on growth) of 34 µg·L$^{-1}$ and a 28-d LC$_{50}$ of 140 µg·L$^{-1}$ for zebra fish (Brachydanio rerio) (van Leeuwen et al. 1990). A 32-d MATC of 55 µg·L$^{-1}$ (Ahmad et al. 1984) and a 33-d NOEC of 55 µg·L$^{-1}$ (Carlson and Kosian 1987), for fathead minnows (P. promelas) were also found.

The water quality guideline for pentachlorobenzene for the protection of freshwater life is 6.0 µg·L$^{-1}$. It was derived by multiplying the 16-d LC$_{50}$ of 60 µg·L$^{-1}$ for Daphnia magna (de Wolf et al. 1988) by a safety factor of 0.1 (CCME 1991). Chronic data for D. magna consist of a 16-d LC$_{50}$ of 69 µg·L$^{-1}$ (Hermens et al. 1985) and a 16-d NOEC of 32 µg·L$^{-1}$ (De Wolf et al. 1988).

The alga Selenastrum capricornutum exhibited a 96-h EC$_{50}$ of 6630 µg·L$^{-1}$ based on changes in cell numbers (USEPA 1978).

<table>
<thead>
<tr>
<th>Toxicity information</th>
<th>Species</th>
<th>Toxicity endpoint</th>
<th>Concentration (µg·L$^{-1}$)</th>
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<tbody>
<tr>
<td>Acute</td>
<td>P. promelas</td>
<td>6-d LC$_{50}$</td>
<td>[ ]</td>
</tr>
<tr>
<td></td>
<td>C. riparius</td>
<td>48-h LC$_{50}$</td>
<td>[ ]</td>
</tr>
<tr>
<td>Chronic</td>
<td>P. promelas</td>
<td>30-d MATC</td>
<td>[ ]</td>
</tr>
<tr>
<td></td>
<td>B. rerio</td>
<td>28-d LC$_{50}$</td>
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<tr>
<td></td>
<td>D. magna</td>
<td>16-d LC$_{50}$</td>
<td>[ ]</td>
</tr>
<tr>
<td></td>
<td>D. magna</td>
<td>16-d LC$_{50}$</td>
<td>[ ]</td>
</tr>
<tr>
<td></td>
<td>S. capricornutum</td>
<td>96-h EC$_{50}$</td>
<td>[ ]</td>
</tr>
<tr>
<td>Canadian Water Quality Guideline</td>
<td>6.0 µg·L$^{-1}$</td>
<td>[ ]</td>
<td>[ ]</td>
</tr>
</tbody>
</table>

Toxicity endpoints:

- primary
- critical value
- secondary

Figure 1. Select freshwater toxicity data for pentachlorobenzene.

Marine Life

Insufficient information exists to derive an interim marine guideline for pentachlorobenzene.

Using sheepshead minnows (Cyprindon aggregata), Hansen and Cripe (1991) obtained a 96-h LC$_{50}$ of 82 µg·L$^{-1}$, while Heitmuller et al. (1981) reported a 96-h LC$_{50}$ of 800 µg·L$^{-1}$. Mortimer and Connell (1994) reported a 96-h LC$_{50}$ of 91 µg·L$^{-1}$ for the sand crab (Portunus pelagicus), and a 96-h LC$_{50}$ of 160 µg·L$^{-1}$ for opossum shrimp (Mysidopsis bahia) was published (USEPA 1980) Mortimer and Connell (1995) reported growth rate reductions of 10 and 50% after 40-d exposures of 14.0 µg·L$^{-1}$ (the lowest-effect-level) and 40.5 µg·L$^{-1}$, respectively, for the sand crab, P. pelagicus. A 96-h EC$_{50}$ for reduction in cell numbers of 1980 µg·L$^{-1}$ was reported for the marine diatom Skeletonema costatum (USEPA 1978).

References


USEPA (U.S. Environmental Protection Agency) 1978. In-depth studies on health and environmental impacts of selected water pollutants. (Table of data available from Charles E. Stephan.) USEPA, Duluth, MN.


Reference listing:


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