

# HEXACHLOROCYCLO- PENTADIENE HEALTH AND SAFETY GUIDE



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**IPCS**

Health and Safety Guide No. 63

**HEXACHLOROCYCLO-  
PENTADIENE  
HEALTH AND  
SAFETY GUIDE**

This is a companion volume to  
Environmental Health Criteria 120: Hexachlorocyclopentadiene

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## INTRODUCTION

The Environmental Health Criteria (EHC) documents produced by the International Programme on Chemical Safety include an assessment of the effects on the environment and on human health of exposure to a chemical or combination of chemicals, or physical or biological agents. They also provide guidelines for setting exposure limits.

The purpose of a Health and Safety Guide is to facilitate the application of these guidelines in national chemical safety programmes. The first three sections of a Health and Safety Guide highlight the relevant technical information in the corresponding EHC. Section 4 includes advice on preventive and protective measures and emergency action; health workers should be thoroughly familiar with the medical information to ensure that they can act efficiently in an emergency. Within the Guide is a Summary of Chemical Safety Information which should be readily available, and should be clearly explained, to all who could come into contact with the chemical. The section on regulatory information has been extracted from the legal file of the International Register of Potentially Toxic Chemicals (IRPTC) and from other United Nations sources.

The target readership includes occupational health services, those in ministries, governmental agencies, industry, and trade unions who are involved in the safe use of chemicals and the avoidance of environmental health hazards, and those wanting more information on this topic. An attempt has been made to use only terms that will be familiar to the intended user. However, sections 1 and 2 inevitably contain some technical terms. A bibliography has been included for readers who require further background information.

Revision of the information in this Guide will take place in due course, and the eventual aim is to use standardized terminology. Comments on any difficulties encountered in using the Guide would be very helpful and should be addressed to:

The Manager  
International Programme on Chemical Safety  
Division of Environmental Health  
World Health Organization  
1211 Geneva 27  
Switzerland

**THE INFORMATION IN THIS GUIDE  
SHOULD BE CONSIDERED AS A  
STARTING POINT TO A COMPREHENSIVE  
HEALTH AND SAFETY PROGRAMME**



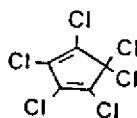
# 1. PRODUCT IDENTITY AND USES

## 1.1 Identity

Common name: hexachlorocyclopentadiene (HEX)

Molecular formula:  $C_5Cl_6$

Chemical structure:



Common synonyms: perchlorocyclopentadiene (HCCPD)

Common trade names: C-56, HRS 1655, Graphlox

CAS chemical name: 1,2,3,4,5,5'-hexachloro-1,3-cyclopentadiene

CAS registry number: 77-47-4

EINEC number: 2010293

Relative molecular mass: 272.77

Conversion factor  
(20 °C):  $1 \text{ ppm} = 11.3 \text{ mg/m}^3$   
 $1 \text{ mg/m}^3 = 0.088 \text{ ppm}$

## 1.2 Physical and Chemical Properties

Pure hexachlorocyclopentadiene (HEX) is a light, lemon-yellow liquid that has a pungent, musty odour. The odour threshold is reported to be 0.0014–0.0016  $\text{mg/m}^3$ . HEX is highly reactive and volatile at low temperatures. Other physical and chemical properties of HEX are given in the Summary of Chemical Safety Information (section 6).

## PRODUCT IDENTITY AND USES

### 1.3 Composition

Commercially available HEX contains several impurities, depending on the method of synthesis. HEX with a purity exceeding 90% is produced by thermal dechlorination of octachlorocyclopentene. HEX with a purity of 75% contains many lower chlorinated cyclopentadienes as well as hexachlorobenzene and octachlorocyclopentene.

### 1.4 Uses

HEX is an intermediate in the manufacture of chlorinated cyclodiene pesticides, such as heptachlor, chlordane, aldrin, dieldrin, endrin, and mirex, and in the manufacture of resins, dyes, and pharmaceutical products. Another major use is in the manufacture of flame retardants, including Dechlorane Plus® and chlorendic anhydride.

## 2. SUMMARY AND EVALUATION

### 2.1 Exposure

Few data are available on the relative contribution of different sources of HEX to the environment. Human exposure via air, soil, or water is expected to be minimal, except for that of persons living in the vicinity of manufacturing, shipping, or disposal sites. Occupational exposure is probably the major source of human exposure.

Short-term laboratory tests have shown that HEX is highly toxic for aquatic microorganisms, invertebrates, and fish, and less toxic for soil microorganisms. Information obtained under environmentally realistic conditions is limited, but the potential hazard for the general environment is expected to be low.

### 2.2 Uptake, Metabolism, and Excretion

Absorption from the gastrointestinal tract is relatively low compared with that from the lungs or skin. HEX appears to be almost completely metabolized in the body. The primary metabolites are described as polar compounds, but they have not been identified. Most of the retained HEX and its metabolites are found in the liver and kidneys, though after inhalation exposure, the highest tissue concentrations are found in the lung and trachea. The major routes of elimination are the urine and faeces. Excretion in the bile has been shown to occur with all routes of exposure.

### 2.3 Effects on Animals

HEX is moderately toxic for animals via the oral and dermal routes of exposure, and extremely toxic via inhalation. The main cause of death following acute exposure via any route is respiratory failure, suggesting that the respiratory tract is the major target organ of toxicity. HEX is also a primary skin irritant and causes severe eye irritation in rabbits.

Short-term oral exposure (91 days) to HEX resulted in kidney damage. No data have been found on effects associated with long-term oral exposure to HEX.

## SUMMARY AND EVALUATION

The inhalation of HEX vapour at concentrations of  $4.52 \text{ mg/m}^3$  (0.4 ppm) or more, for 90 days, resulted in respiratory-tract effects, including inflammation and respiratory distress, in mice and rats. The inhalation of  $5.65 \text{ mg/m}^3$  (0.5 ppm) for 6 h/day, 5 days/week, over 30 weeks, resulted in lung damage in mice and rats. No data on the effects of long-term inhalation exposure to HEX were available.

HEX has not been shown to affect reproduction and development in animals. There is good evidence that HEX is not mutagenic in bacterial or mammalian cells, or in the fruit fly. Data on the carcinogenic potential of HEX in experimental animals are not currently available.

### 2.4 Effects on Human Beings

There is limited information on human health effects. Acute exposure can result in severe irritation of the eyes, nose, throat, and gastrointestinal tract. In a well-documented incident at a waste-water treatment plant, exposed workers exhibited eye irritation, headaches, nausea, and eye and throat irritation. These effects persisted for several weeks. Exposure levels could not be estimated accurately, but airborne concentrations in primary treatment areas, measured 4 days after closing the facility, ranged from  $3.05$  to  $10.96 \text{ mg/m}^3$  (270 to 970 ppb).

No excess cancer mortality was reported in an epidemiological study of workers employed at a chemical plant producing and processing HEX. Using the criteria of the International Agency for Research on Cancer (IARC), the available data on carcinogenicity are classified in Group 3, i.e., because of major qualitative or quantitative limitations, the available studies cannot be interpreted as showing either the presence or absence of a carcinogenic effect.

### 2.5 Effects on Organisms in the Environment

HEX is highly toxic for aquatic organisms. There is a lack of information on the effects of HEX on animals and vegetation.

### 3. CONCLUSIONS AND RECOMMENDATIONS

- (i) Environmental monitoring is needed to examine the persistence and fate of HEX in all media near production, processing, and disposal sites, and also hazardous waste incinerators. Monitoring data are needed for HEX in drinking-water, and surface, shower, and ground waters.
- (ii) Biomarker techniques should be developed to indicate the possible past or current actions of HEX. Such biomarkers could be stable metabolites derived from HEX, or the contaminants present in the original preparation.
- (iii) Research is needed on the metabolic, degradation, and reactive products, to understand the fate of HEX in humans and the environment.
- (iv) Further study of the apparent disparity between degradation under laboratory conditions and that observed in the environment is needed.
- (v) The efficacy and safety of current disposal methods should be evaluated, and their present and future health impacts assessed.
- (vi) Developmental and reproductive studies on HEX need to be conducted, with emphasis on the inhalation route of exposure.
- (vii) Methods for the early warning of the presence of HEX should be developed.

## CONCLUSIONS AND RECOMMENDATIONS

(viii) Occupational exposure to HEX should be minimized by the use of closed systems. Guidelines should be followed on the disposal of HEX and HEX wastes.

## 4. HUMAN HEALTH HAZARDS, PREVENTION AND PROTECTION, EMERGENCY ACTION

### 4.1 Main Human Health Hazards, Prevention and Protection, First Aid

HEX is toxic via all routes of exposure, but is particularly dangerous via inhalation. This chemical is extremely irritating to the mucous membranes, eyes, and skin, causing lacrimation, sneezing, and salivation. Contact with the skin can result in discoloration, blisters, and burns. Inhalation or ingestion can result in nausea, vomiting, diarrhoea, headaches, lethargy, breathing difficulties, and liver and kidney damage. Inhalation exposure may cause severe irritation to the throat, respiratory tract, and the lungs. The human health hazards associated with certain types of exposure, as well as preventive and protective measures and first-aid recommendations, are presented in the Summary of Chemical Safety Information (section 6).

#### 4.1.1 *Advice to physicians*

Following the ingestion of HEX, oxygen should be administered, if respiration is depressed. Toxic symptoms resulting from inhalation exposure should be treated symptomatically and supportively. Oxygen should be administered as needed. In the case of eye contact, the eyes should be washed immediately with large amounts of water for at least 15 minutes, to remove any remaining chemical. The eyes should then be irrigated with physiological saline solution for 30–60 minutes, or until the pH returns to normal. Following dermal contact, the affected area should be washed immediately with soap and large amounts of water. If blistering develops, the skin should be covered with loosely wrapped sterile bandages.

#### 4.1.2 *Health surveillance advice*

Persons employed in the manufacture, transportation, or disposal of HEX should undergo periodic medical examinations.

## HUMAN HEALTH HAZARDS, PREVENTION AND PROTECTION, EMERGENCY ACTION

### 4.2 Explosion and Fire Hazards

#### 4.2.1 *Explosion hazards*

HEX is not explosive. However, containers may explode in the heat of fires. Furthermore, HEX may form explosive mixtures with sodium.

#### 4.2.2 *Fire hazards*

HEX is not flammable. However, toxic fumes, such as hydrogen chloride, chlorine, and phosgene, are formed in fires.

#### 4.2.3 *Prevention*

Enclosed processing equipment, local exhaust, or ventilation that is adequate to meet published exposure limits, should be provided.

#### 4.2.4 *Extinguishing agents*

For fires, dry chemical powder, carbon dioxide, water spray, or standard foam is recommended. If possible, containers should be moved away from the fire. Water used to control fires should be contained, or diked, for later disposal.

### 4.3 Storage

HEX should be stored in tightly closed containers, labelled as corrosive, and stored in a cool, dry place, away from moisture, heat, and strong oxidizing agents.

### 4.4 Transport

HEX can be transported at ambient temperatures and does not require an inert atmosphere; it is stable under normal conditions. For shipping, 55-gallon (250-litre) drums or tank cars are recommended. Label as corrosive.



## HUMAN HEALTH HAZARDS, PREVENTION AND PROTECTION, EMERGENCY ACTION

### 4.5 Spillage

In the case of a spill or leak, earth, sand, or some other noncombustible absorbent material (cement powder or soda ash) can be used to absorb the chemical. This material is then placed in a clean, dry, covered container for later disposal. Dry spills can be removed using a clean shovel. For large spills, the liquid should be contained, or diked, at a distance from the spill for later disposal. In the case of an air release, vapours should be knocked down with a water spray. Persons should remain upwind of the vapour cloud. Water spills can be trapped at the bottom of deep water pockets (since HEX is heavier than water), in excavated holding areas, or within sandbag barriers, to avoid contamination of sewers and surface waters. Damaged containers should be destroyed to prevent further use. Suction hoses can then be used to remove the spilled material.

### 4.6 Disposal

HEX can be incinerated after mixing with a combustible fuel. This mixture should be completely combusted to prevent the formation of phosgene. An acid scrubber should be used to remove the halo acids produced. HEX can be buried in specially designated chemical landfills. However, HEX and organic solvents should not be disposed of in the same landfill area, to prevent possible migration of HEX from the disposal site. Dumping into sewer systems is not an acceptable method of disposal. Deep well injection can be used.

## 5. HAZARDS FOR THE ENVIRONMENT AND THEIR PREVENTION

Since environmental pollution is expected to occur as a result of releases during the production, processing, and disposal of HEX, contamination can be avoided by the use of proper methods of storage, transport, handling, and waste disposal (sections 4.3, 4.4, and 4.6). In the case of spillage, the clean-up methods described in section 4.5 should be used.

When the fate and transport of HEX in the atmosphere was modelled on the basis of available laboratory data, a tropospheric residence time of approximately 5 h was calculated. The atmospheric transport of HEX has been reported from an area where waste was stored, and from wet wells during the treatment of industrial wastes.

In water, HEX may undergo photolysis, hydrolysis, and biodegradation. In shallow water, it has a photolytic half-life of <1 h. In deeper water, where photolysis was precluded, the hydrolytic half-life of HEX ranged from several days to approximately 3 months; biodegradation is predicted to occur more slowly. HEX is known to volatilize from surface water, and its volatilization is affected by turbulence and by sorption on to sediments.

Because of its low solubility in water, HEX should be relatively immobile in soil; however, HEX has been found in ground water. Volatilization, which is likely to occur primarily at the soil surface, is inversely related to the levels of organic matter in the soil. From laboratory studies, chemical hydrolysis and microbial metabolism, both aerobic and anaerobic, would be expected to reduce HEX levels in soils.

Low concentrations of HEX have been shown to be toxic for aquatic life. Lethality in acute exposures (48–96 h) was observed in both freshwater and saltwater crustaceans and fish at nominal concentrations of 32–180 µg/litre in static exposure systems where the water was not renewed during the test. As the photolytic half-life is <1 h, the concentration of the HEX would have decreased substantially during the 48–96 h of exposure.

In aqueous media, HEX is toxic for many other microorganisms at nominal concentrations of 0.2–10 mg/litre, or levels substantially higher than those needed to kill most aquatic animals or plants. HEX appears to be less

## HAZARDS FOR THE ENVIRONMENT AND THEIR PROTECTION

toxic for microorganisms in the soil than in aquatic media, probably because of the sorption of HEX on to the soil matrix.

Although exposure is expected to be low, data currently available are insufficient to determine the effects of HEX exposure on terrestrial vegetation or wildlife.



## 6. SUMMARY OF CHEMICAL SAFETY INFORMATION

*This summary should be easily available to all health workers concerned with, and users of, hexachlorocyclopentadiene. It should be displayed at, or near, entrances to areas where there is potential exposure to hexachlorocyclopentadiene, and on processing equipment and containers. The summary should be translated into the appropriate language(s). All persons potentially exposed to the chemical should also have the instructions in the summary clearly explained.*

*Space is available for insertion of the National Occupational Exposure Limit, the address and telephone number of the National Poison Control Centre, and local trade names.*

## SUMMARY OF CHEMICAL SAFETY INFORMATION

### HEXACHLOROCYCLOPENTADIENE (C<sub>5</sub>Cl<sub>6</sub>)

#### PHYSICAL PROPERTIES

Relative molecular mass  
 Appearance  
 Odour threshold  
 Odour  
 Melting point (°C)  
 Boiling point (°C)  
 Solubility in water (25 °C)  
 Relative vapour density (air = 1)  
 Density (25 °C)  
 Vapour pressure (25 °C)  
 Electronegativity  
 Flame colouration test  
 Octanol/water partition coefficient (K<sub>ow</sub>)

272.77  
 lemon-yellow liquid  
 0.00019 mg/m<sup>3</sup>  
 pungent, musty  
 -9.6  
 239  
 1.03-1.25 mg/litre  
 9.42  
 1.702  
 0.08 mmHg  
 ND  
 ND  
 1.1 × 10<sup>5</sup>

#### OTHER CHARACTERISTICS

Reacts slowly with water to form hydrochloric acid; may form explosive mixture with sodium; corrosive to iron and other metals, in the presence of moisture

#### HAZARDS/SYMPTOMS

**SKIN:** Severe irritation; burns, blisters; readily absorbed through intact skin

#### PREVENTION AND PROTECTION

Avoid exposure; wear protective clothing and rubber gloves and shoes

#### FIRST AID

Remove contaminated clothing and shoes; flush skin with plenty of water; cover burns with sterile bandages, loosely wrapped

**EYES:** Severe irritation; redness; pain

Wear a face-shield if there is a possibility of eye contact

Flush the eyes with plenty of water for 15 minutes, making sure to remove any remaining chemical; seek medical attention

**INHALATION:** Severe irritation to mucous membranes and upper respiratory tract; sore throat, coughing, shortness of breath, headache, vomiting, lacrimation, pulmonary oedema, degenerative changes in lung, liver, and kidney; death may occur from respiratory failure

Avoid exposure by using ventilation, local exhaust, or respiratory protection, such as a self-contained breathing apparatus and a face-shield

Fresh air, rest; if breathing has stopped, apply artificial respiration; administer oxygen, if required; seek medical attention immediately

**INGESTION:** Salivation, diarrhoea, lethargy, shortness of breath or difficulty in breathing, degenerative changes in the lung, liver, kidney, adrenal glands, heart, and brain

Do not eat, drink, or smoke when handling the compound

Rinse mouth; seek medical attention

**HEX** is highly toxic to aquatic environments

Do not contaminate surface waters or sewers

## SUMMARY OF CHEMICAL SAFETY INFORMATION

<b>SPILLAGE</b>	<b>STORAGE</b>	<b>FIRE AND EXPLOSION</b>	
Do not touch spilled material; for dry spills, using clean shovel place material into a clean, dry container; for small liquid spills, take up with sand or other absorbent material and place into containers for disposal; for large liquid spills, dike far ahead of spill for later disposal	Store in a cool, dry place in tightly closed containers	Negligible fire hazard; hydrogen chloride, chlorine, and phosgene may be formed in the heat of fires; closed containers may explode in the heat of fires	
<b>WASTE DISPOSAL</b>	<b>NATIONAL INFORMATION</b>		
Incinerate after mixing with combustible fuel; take care to ensure complete combustion; apply acid scrubbers; can also be disposed of in specially designated chemical landfill; care should be taken to avoid disposal together with organic solvents	National Occupational Exposure Limit:  National Poison Control Centre:  Local trade names:	Code of Federal Regulations: Poison, Class B	



## **7. CURRENT REGULATIONS, GUIDELINES AND STANDARDS**

The information given in this section has been extracted from the International Register of Potentially Toxic Chemicals (IRPTC) legal file. A full reference to the original national document from which the information was extracted can be obtained from IRPTC. When no effective date appears in the IRPTC legal file, the year of the reference from which the data are taken is indicated by (r).

The reader should be aware that regulatory decisions about chemicals taken in a certain country can only be fully understood in the framework of the legislation of that country. Furthermore, the regulations and guidelines of all countries are subject to change and should always be verified with appropriate regulatory authorities before application.

### **7.1 Previous Evaluations by International Bodies**

Data are insufficient to assess the carcinogenic potential of HEX in humans. No previous evaluations have been carried out by international bodies.

### **7.2 Exposure Limit Values**

See table on pages 24–25.

### **7.3 Specific Restrictions**

No specific restrictions were found.

### **7.4 Labelling, Packaging, and Transport**

The United Nations Committee of Experts on the Transport of Dangerous Goods classifies HEX as a poisonous substance (Hazard Class 6.1), and as a very dangerous substance (Packing Group I) with regard to packing.

## CURRENT REGULATIONS, GUIDELINES, AND STANDARDS

Country	Type	Media	Level/remark <sup>a</sup>	Date
Australia	recommendation	air/occupational	TLV/TWA = 0.1 mg/m <sup>3</sup> (0.01 ppm) STEL = 0.3 mg/m <sup>3</sup> (0.03 ppm)	1983
Belgium	recommendation	air/occupational	TLV/TWA = 0.1 mg/m <sup>3</sup> (0.01 ppm)	1988
Canada	regulation	air/occupational	TLV/TWA = 0.01 ppm (0.1 mg/m <sup>3</sup> )	1980
Canada	regulation	transport	specific transportation regulations	1987
Finland	recommendation	air/occupational skin	TWA = 1.0 mg/m <sup>3</sup> (0.1 ppm) STEL = 3.0 mg/m <sup>3</sup> (0.3 ppm)	1989 1989
Germany, Federal Republic of	regulation	waste	"toxic waste" subject to specific handling, transport, treatment, storage, and disposal regulation/permits	1981
Netherlands	recommendation	air/occupational	TWA/OCC = 0.11 mg/m <sup>3</sup> (0.01 ppm)	1986
Switzerland	regulation	air/occupational	TWA = 0.1 mg/m <sup>3</sup> (0.01 ppm)	1987
USA	regulation	water	1 µg/litre ambient water quality criteria (organoleptic)	1980

USA (ACGIH)	recommendation	air/occupational	TWA = 0.1 mg/m <sup>3</sup> (0.01 ppm)	1980
USA	regulation	air/occupational	TWA = 0.1 mg/m <sup>3</sup> (0.01 ppm)	1989
USA	regulation	water/land	notification of spill of 1 lb (0.454 kg) in 24-h period	1983
USA	regulation	waste/transport	"toxic waste" subject to specific handling, transport, treatment, storage, and disposal regulation/permits	1980
USA	draft recommendation	drinking-water	7 µg/kg per day (lifetime)	1990
USSR	regulation	air/occupational	TLV = 0.01 mg/m <sup>3</sup> (0.01 ppm vapour)	1989
USSR	regulation	water	MAC = 0.001 mg/ml (organoleptic)	1985
USSR	regulation	air/ambient	STEL = 0.001 mg/m <sup>3</sup>	1987
Yugoslavia	regulation	air/occupational	TWA = 0.1 mg/m <sup>3</sup> (skin)	1985

<sup>1</sup> TLV = threshold limit value; TWA = time-weighted average; STEL = short-term exposure level; OCC = occupational; MAC = maximum allowable concentration.

## CURRENT REGULATIONS, GUIDELINES AND STANDARDS

The US Code of Federal Regulations lists HEX as a Class B poison and recommends that the label presented below be placed on packaging. Label as a corrosive.



### 7.5 Other Measures

None found.

### 7.6 Waste Disposal

The US EPA classifies HEX as a toxic pollutant and is required to set effluent limitations and pretreatment standards for 21 major industries. Permits are required for the discharge of any pollutant from any point source into US waters. Applicants who have reason to believe that HEX is contained in any of the outfalls produced, or applicants using specific industrial processes listed in the Code of Federal Regulations (40 CFR 122.53; 1981), must report quantitative data for HEX. Inspecting, monitoring, and reporting requirements are specified after the permit is issued. Discharge of the substance must be reported, regardless of permit requirements, if levels exceed 10  $\mu\text{g/litre}$ , five times the maximum concentration reported in the application, or the level established by the US EPA administrator. The US EPA further classifies certain specified industrial solid wastes containing HEX as hazardous substances.

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