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GDCh-Advisory Committee
on Existing Chemicals of
Environmental Relevance (BUA)

1,3-Dichloro-4-nitrobenzene

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S. Hirzel
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on Existing Chemicals of Environmental Relevance (BUA)

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Beratergremium für Umweltrelevante Altstoffe (BUA)

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Foreword

The German Chemicals Act (Chemikaliengesetz - ChemG) of 1980 stipulates that certain existing chemicals must be reported to the competent authority, if they exhibit properties which indicate that they may be hazardous, either alone or in combination with other substances.

In the summer of 1982, an Advisory Committee on Existing Chemicals of Environmental Relevance (BUA) was set up by the German Chemical Society (Gesellschaft Deutscher Chemiker - GDCh). It brings together representatives from the scientific community, the chemical industry and the governmental authorities. This Advisory Committee is responsible for elaborating appropriate solutions for substances of relevance for health and the environment on the basis of voluntary measures. It selects and examines existing chemicals from the aforementioned angles. The testing and evaluation are based on scientific criteria alone.

It was, therefore, necessary to develop priority setting procedures. In a first phase reports were only prepared for priority chemicals. Within the framework of a first priority setting procedure, chemicals were compiled from several priority lists and 135 chemicals were selected for detailed substance reports.

In a second priority setting procedure the survey of the German Chemical Industry Association (VCI) on all substances with a production volume of more than 10 tons per year was used as a starting list. Since this survey covered 4,600 chemicals, BUA decided to process the corresponding list in several stages. The first stage included approx. 1,050 substances with a production volume of more than 1,000 tons per year.

Detailed reports are drawn up on chemicals suspected of having a hazard potential and abridged reports on those presenting only a minor hazard potential, according to the current state of knowledge.

The detailed BUA reports take in both the published literature and data from industry. If data for the evaluation of the chemicals are not available, additional studies are recommended and the results are published as updates to the reports. The reports serve as a basis for the instigation of administrative measures, when there are indications of risks to health or the environment.

Tübingen, May 1993

Ernst Bayer
Chairman of the Advisory Committee
on Existing Chemicals
of Environmental Relevance

Contents

BUA Report on 1,3-Dichloro-4-nitrobenzene

Summary and conclusions

Ecological aspects

Occurrence and distribution in the compartments

1,3-Dichloro-4-nitrobenzene is an intermediate in the manufacture of herbicides, pharmaceutical products and dyes (pigments). The volume produced in the Federal Republic of Germany in 1990 amounted to about 1500 tonnes/yr; about 500 tonnes/yr were exported. There is no information available on importation.

Discharge into the environment from industrial production and use of 1,3-dichloro-4-nitrobenzene takes place both via waste water (> 75 %) and exhaust air (< 25 %). As a result a maximum of 200 kg entered the hydrosphere and less than 50 kg were released into the atmosphere in 1990.

Due to its physico-chemical properties, slow transfer of 1,3-dichloro-4-nitrobenzene from water to the atmosphere is possible.

No information is available on the occurrence in the atmosphere or in the soil. Maximum concentration of dichloronitrobenzene (non-specific isomeric mixture) of 3 µg/l was found in the Rhine River in the Netherlands in 1978 and of 0.2 µg/l in 1983.

In routine measurements in North Rhine-Westphalia, 1,3-dichloro-4-nitrobenzene could not be detected in the Rhine River or near the mouths of its affluents from 1984 to 1989 at a detection limit of 0.1 µg/l (except the Lippe River where a concentration of 0.1 µg/l was found in 1985) and in Rhine sediments in 1987/88 at a detection limit of 1 µg/kg. In the Main River, 1,3-dichloro-4-nitrobenzene was found repeatedly at a maximum concentration of 1.0 µg/l from 1984 to 1987; the 90-percentile value amounted to 0.24 µg/l. From 1988 to 1991 the maximum concentration was 0.2 µg/l.

1,3-Dichloro-4-nitrobenzene has been found in Main River fish (1982) and in Mississippi River fish (concentrations not stated).

Degradability

Tests for ready biodegradability using various inocula at a wide range of concentrations of the compound gave no evidence of such degradation in the aquatic environment. Degradation by hydrolysis under environmental conditions is unlikely to occur. Non-adapted terrestrial mould fungi are able to metabolize 1,3-dichloro-4-nitrobenzene, via its reduction to 2,4-dichloroaniline or the formation of a conjugate with glutathione, which undergoes further biotransformation.

In the atmosphere, slow photodegradation takes place by reaction with photochemically produced OH radicals. The half-life is calculated to be 130 days.

Accumulation

In view of the n-octanol/water partition coefficient (log P_{OW} = 2.78 - 3.09) bioaccumulation is likely to occur. In fish (on a wet-weight basis) bioconcentration factors of 118 ± 21 (log BCF = 2.07 ± 0.07) and, in another study, of 88 ± 22 (log BCF = 1.94 ± 0.1) have been found experimentally. Following oral intake the biological half-life in fish is less than 3 days.

There are indications that 1,3-dichloro-4-nitrobenzene is moderately adsorbed on soils.

Ecotoxic effects

Inhibition of the oxygen consumption of aerobic bacteria and of gas production of anaerobic bacteria by 1,3-dichloro-4-nitrobenzene does not take place at concentrations of 62.5 mg/l and 5 mg/l respectively. For soil fungi, the EC_{50} value (fungistatic activity) of 1,3-dichloro-4-nitrobenzene amounts to ≥ 9.6 mg/l.

Following the exposure of algae for 96 hours to 2.4 mg/l 1,3-dichloro-4-nitrobenzene, 50 percent inhibition of growth has been observed. Oxygen production of algae is diminished by 50 percent when they are exposed for 4 hours to 4 mg/l 1,3-dichloro-4-nitrobenzene.

For water fleas (*Daphnia magna*), the EC_{50} values (immobilization)

range from 2 to 4.4 mg/l following the exposure for 24 hours to 21 days. In a semistatic 21-day reproduction test the lowest concentration of 1,3-dichloro-4-nitrobenzene at which the population growth rate and mean length of the animals significantly ($p < 0.01$) decreased were 1.0 mg/l and 3.2 mg/l respectively.

In a study of the acute toxicity to fish, 1,3-dichloro-4-nitrobenzene yields a steep dose-response curve, extending from a 96-hr LC_0 value of 9 mg/l to a 96-hr LC_{100} value of 10 mg/l. In the prolonged fish toxicity test under semistatic conditions a 14-d LC_{50} value of 6.6 mg/l has been found.

A solution of 30 mg/l 1,3-dichloro-4-nitrobenzene, when fed to male fruit flies for 72 hours, was not lethal but proved to be sterilizing for 30 % of the insects.

Toxicological Aspects

1,3-Dichloro-4-nitrobenzene is readily absorbed after oral or dermal application and is rapidly excreted from the organism, predominantly via the urine. Excretion takes place primarily in the form of the mercapturic acid derivative N-acetyl-S-(5-chloro-2-nitrophenol)-L-cysteine and to a lesser extent as glucuronide and sulphuric esters of dichloronitro- and dichloroamino-substituted phenols and as free 2,4-dichloroaniline.

Studies of acute toxicity in rats yielded a median lethal dose (LD_{50}) of about 380 mg/kg body weight following oral administration and of 921 mg/kg body weight following dermal application. Symptoms of acute intoxication were non-specific and no pathological changes were observed macroscopically.

1,3-Dichloro-4-nitrobenzene is slightly irritating to skin and eyes. 1,3-Dichloro-4-nitro-benzene has been proved to be a sensitizer in experimental animals; corresponding data published for man are possibly based an confusion with 2,4-dinitro-1-chlorobenzene.

No data are available on subacute, subchronic and chronic toxicity or on cancerogenicity and reproductive toxicity.

Studies on genotoxicity indicate that 1,3-dichloro-4-nitrobenzene induces point mutations in bacteria, whereas the compound does not induce gene mutations in mammalian cells (HGPRT-test).

An increased incidence of chromosomal aberrations was observed in mammalian cell cultures. In *Drosophila melanogaster* 1,3-dichloro-4-nitrobenzene failed to induce sex-linked recessive lethal mutations.

Recommendations

Ecology

A test for inherent biodegradability is recommended to enable final evaluation of the environmental relevance. As to biodegradation under anaerobic conditions, it is advisable to wait for the results of the corresponding study with the isomer 1,4-dichloro-2-nitrobenzene.

Toxicology

Due to a lack of data on toxicity following repeated administration it is necessary to carry out a 28-day study on rats with oral administration to obtain information an the symptoms of intoxication, possible target organs and the no-observable-effect level.

On the basis of the findings an genotoxicity and of chemical structure a cancerogenic potential of 1,3-dichloro-4-nitrobenzene cannot be ruled out. However, the product is used only as an intermediate in industrial manufacture. If measurements reveal that no relevant exposure occurs at the workplace, the experimental clarification of the cancerogenic potential will not be regarded as having priority. The same applies to the performance of studies on reproductive toxicity.