



**German Chemical Society
Gesellschaft Deutscher Chemiker**

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

**p-Toluene
sulphonic acid**
BUA Report 63
(June 1991)



S. Hirzel

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p-Toluene sulphonic acid

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of Environmental Relevance

Beratergremium für
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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

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BUA Report on p-Toluene sulphonic acid

Summary and conclusions

Ecological aspects

Occurrence and distribution in the compartments

p-Toluenesulfonic acid (PTSA) produced in the Federal Republic of Germany is a mixture of o-, m- and p-isomers containing about 85 % PTSA. The forms supplied are chiefly an aqueous solution containing approximately 65 % toluenesulfonic acid and flakes with approximately 90 % toluenesulfonic acid monohydrate. The volume produced in the Federal Republic of Germany in 1990 amounted to about 5000 tonnes (calculated as anhydrous PTSA), half of which was exported. About 440 tonnes PTSA (calculated as anhydrous product) was used in the Federal Republic of Germany in 1990 in the manufacture of about 500 tonnes sodium p-toluenesulfonate. About half of the amount produced was exported. Sodium p-toluenesulfonate serves as an additive to detergents and cleansing agents and as a hydrotrope. No information is available on the use of PTSA as an intermediate in the manufacture of antioxidants, pigments, plant protection products, pharmaceutical products and additives to mineral oil in the Federal Republic of Germany. PTSA as such is used in the Federal Republic of Germany as a hardening accelerator for foundry sand binder resins, acid curing varnishes, laminating resins and acid-proof cements and as a catalyst in esterification.

Discharge into the environment from industrial production takes place mostly via waste water (in the Federal Republic of Germany in 1990 < 68 kg), and to a lesser extent, via exhaust air (about 1 kg). The discharge from use and application takes place almost exclusively via waste water and is essentially caused by the application of sodium p-toluenesulfonate as an additive to detergents and cleansing agents and as a hydrotrope, and by the application of PTSA as a catalyst in esterification. This discharge is estimated to have been less than 37 tonnes in the Federal Republic of Germany in 1990.

An additional discharge into the environment can take place by biotic or abiotic degradation of the herbicide pyrazolate, which is used in Japan for the control of weeds in paddy fields.

No Information is available on the occurrence in the atmosphere (ambient air). The concentrations in the air at the workplace in foundries amounted to less than 0.1 ppm (corresponding 0.72 mg/m³). PTSA was detected (concentration not stated) in drinking water derived from groundwater and river water in the United Kingdom. No data are available on the occurrence in the geosphere. Although metabolic formation from the herbicide pyrazolate in soil and aquatic organisms is possible, no data on concentrations are available.

Degradability

As a readily biodegradable substance, PTSA in an aquatic environment under aerobic conditions undergoes biodegradation, which rapidly takes place following adaptation of the microorganisms. Marsh and water plants with the microflora in their rhizosphere are also able to mineralize PTSA. Biodegradation under anaerobic conditions does not occur, and degradation by hydrolysis under environmental conditions is unlikely.

Gaseous PTSA emitted into the atmosphere undergoes degradation by reaction with photochemically produced OH radicals. The half-life is calculated to be 14 days.

Accumulation

In view of the n-octanol/water partition coefficient ($\log P_{ow} = 0.784$ (calculated)), bioaccumulation is not to be expected. In fish a bioconcentration factor < 1 has been found experimentally.

Geoaccumulation is unlikely to occur due to low tendency to sorption on soils. Transport by leachates to the groundwater would seem to be possible.

Ecotoxic effects

The toxicity threshold at adjusted pH value (7 to 7.3) extends up to 1000 mg/l for aerobic bacteria and has been determined to be 2500 mg/l (at pH 6.5 to 7.5) for anaerobic bacteria. Fungistatic activity has been observed at concentrations (EC_{50}) \geq 48 mg/l (sodium salt).

In algae, slow population growth with symptoms of sulphur deficiency compared with sodium sulfate as a sulphur source has been observed at 51.7 mg/l. The growth of plants of limnic habitats is inhibited in most cases only at concentrations $>$ 81 mg/l. In a sensitive species, however, growth inhibition has been observed at as low as \geq 9 mg/l. This toxic effect can be ascribed partly to lowering of the pH in the nutrient solution, partly to a specific influence on the metabolic processes in the plant.

The results of studies on a toxic effect (of the sodium salt) on water fleas (*Daphnia magna*) are inconsistent. EC_0 values (immobilization; duration of exposure not stated) of 250 to 1000 mg/l and a 24-hr EC_0 value of 1625 mg/l contrast with an EC_{50} value (duration of exposure not stated) of 300 mg/l and a 24-hr EC_{100} value of 350 mg/l.

In two tests on acute toxicity to fish (golden orfe) no lethality has been observed following exposure to 200 mg/l (sodium salt) for 48 hours and to 325 mg/l (PTSA; pH 6.8 to 7.2) for 96 hours. As opposed to this a further test in the same species resulted in a 48-hr LC_{50} value of 66 mg/l (sodium salt).

The acute LD_{50} for birds is greater than 100 mg/kg body weight. A single dose of 158 mg/kg body weight had no significant toxic effect on reproduction in male quail.

Toxicological Aspects

PTSA is rapidly absorbed after oral administration. Elimination takes place in unchanged form; 90 % of the dose applied is excreted within one day chiefly via the urine. An accumulation of PTSA in the organism has not been observed even after repeated exposure.

Following acute oral exposure PTSA is regarded to have low toxicity. In such cases the principal effect consists of injury to the gastro-intestinal tract.

PTSA causes burns on the skin and mucous membranes and in the eyes. Dilute solutions (0.5 to 5 %) irritate the skin.

The maximization test yielded no indication of skin sensitization.

In a 28-day feeding study on rats dosed with 4 to 500 mg/kg body weight and day there were no signs of toxicological relevance.

No information is available on chronic toxicity, cancerogenicity and reproductive toxicity (apart from a corresponding study on birds).

PTSA has been proved to be non-mutagenic in the Ames test with and without metabolic activation. In vitro studies on the induction of chromosome aberrations in mammalian cells did not give evidence of a genotoxic effect.

Recommendations

Ecology

The available results of studies of ecotoxicology and environmental fate are regarded as sufficient for an evaluation of the environmental relevance.

Toxicology

Results of studies of reproductive toxicity and cancerogenic effect are not available. Tests on mutagenicity did not give evidence of a genotoxic potential of PTSA, therefore experimental clarification of the cancerogenic potential is not regarded as having priority. In view of the application of PTSA also in consumer products the reproductive toxicity potential of PTSA should be clarified. Hence it would be advisable to wait until the results of studies planned with the sodium salt of the homologous cumenesulfonic acid are available.