GDCh-Advisory Committee
on Existing Chemicals (BUA)

2,4,5-Trichloroaniline

BUA Report 227

(June 2001)

S. Hirzel

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on Existing Chemicals (BUA, June 2001)

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GDCh-Office:
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für Altstoffe (BUA)

S. Hirzel
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Dr. H. Behret
Gesellschaft Deutscher Chemiker
Postfach 90 04 40
D-60444 Frankfurt am Main
E-Mail: bua@gdch.de
Homepage: http://www.gdch.de

Responsible at the BMU:
MinR Prof. Dr. U. Schlottmann
BMU
Postfach 12 06 29
D-53048 Bonn
E-Mail: schlottmann.ulrich@bmu.de

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Preface

The Advisory Committee on Existing Chemicals of Environmental Relevance, BUA for short, was established in May 1982 to help the German federal government cope with the large task of dealing with existing chemicals. In an agreement between federal government, scientific community, and the chemical industry, it was associated with the German Chemical Society (GDCh, Gesellschaft Deutscher Chemiker) to ensure objective work, carried out in accordance with scientific principles.

At the end of 1997, the Committee was renamed 'GDCh Advisory Committee on Existing Chemicals' (abbreviation 'BUA' as before) and the statutes were revised to include EU level aspects of occupational safety for the handling of existing chemicals from then on. The collaboration with the Employment Accident Insurance Fund of the Chemical Industry (BG-Chemie), with its knowledge on workplace exposure and the toxicologic properties of chemicals, is a valuable addition to the BUA's know-how.

The cooperation between authorities, industry, and the scientific community, upon which the BUA is based, has proven worthwhile. No other national or international body has dealt with the ecological and health-related effects of so many existing chemicals as the BUA. On the national level, the BUA has produced comprehensive reports on about 300 substances and carried out preliminary evaluation and classification (priority-setting) for approximately 200 more, as of 1997. Publication of the process leading to priority-setting, in addition to the BUA Reports, lends transparency to the Committee's work.

Since the EU presently considers only those substances with a production volume of more than 1000 tonnes/year, the BUA began an additional national project in 1997, which also selects and assesses existing chemicals with a lower production volume in the range of 100 - 1000 tonnes/year. The chemical industry presents about 50 databases for substances each year, for which the BUA sets the priority. Comprehensive reports are published on chemicals suspected of having a hazardous potential. If the data available for substance assessment are insufficient, the gaps in knowledge are documented and, if necessary, investigations recommended.

Moreover, BUA is increasingly addressing scientific questions and problems such as "endocrine disruptors", selection criteria for "persistent organic pollutants" (POPs),"risk assessment of substances in soils", "evaluation criteria for the marine sector" and "safety factors within the framework of toxicological risk assessment". The aim of BUA is to develop assessment concepts, determine data gaps, point out the need for further research and, last but not least, also to reduce information deficits in the general population.

Weihenstephan, April 2001

Helmut Greim
BUA Chairman

Contents

Abbreviations

b.w.	body weight
3-CA	3-chloroaniline
d	day(s)
d.l.	detection limit
d.m.	dry matter
2,5-DCA	2,5-dichloroaniline
EPA	U.S. Environmental Protection Agency
GPC	gel permeation chromatography
h	hour(s)
max.	maximum
min.	minimum
n	number of measurements
n.f.d.	no further details
n.s.	not specified
o.c.	organic carbon
o.m.	organic material
2,4,5-TCA	2,4,5-trichloroaniline
2,3,4,5-TeCA	2,3,4,5-tetrachloroaniline
w.w.	wet weight

BUA Report on 2,4,5-Trichloroaniline

Summary

Ecotoxicological Aspect

Emissions

A total of 500 - 1 000 t of 2,4,5-trichloroaniline (2,4,5-TCA) is produced annually in Germany. Most of this is further processed within the company as a raw material and reaction component to pigments. No significant emission of 2,4,5-TCA into the environment is expected as a result of being handled in closed units and because of the measures taken to prevent emissions. There are no data available on other possible emission sources. The 2,4,5-TCA concentrations measured in surface waters and wastewater treatment plants cannot be explained by the known emission sources.

Occurrence

2,4,5-TCA in a concentration ranging from 0.17 to 0.42 µg/l (90^{th} percentile) was measured from 1991-1997 in the Rhine at the German-Dutch border with a peak value of 0,96 µg/l measured in 1995. 2,4,5-TCA was also detectable in the Maas River and in the Ijssel Lake (Ijsselmeer). In contrast to this, in the period from 1994 to 2000, the 2,4,5-TCA concentration or the 90^{th} percentile in the upper course of the Rhine down to 588.3 km, as well as in the Danube, Neckar and Main Rivers was below the detection limit of 0.05 µg/l. An occurrence of 2,4,5-TCA in the Elbe River cannot be evaluated with a single random sample measurement.

In the Erft, Lippe, Ruhr, Sieg and Wupper Rivers all the measurement values taken in 1997 were below the determination limit of 1 µg 2,4,5-TCA/l, and those taken in 1998 were below 0.5 µg 2,4,5-TCA/l.

The concentration of 2,4,5-TCA in discharges of municipal wastewater treatment plants in Lower Saxony was under 0.01 µg/l. In municipal sewage sludge from Karlsruhe 2,4,5-TCA was found in a mean concentration of 0.32 mg/kg dry matter (maximum 0.61 mg/kg dry matter).

Degradation and Distribution in the Environment

2,4,5-TCA was nondegradable in a closed bottle test according to OECD 301 D and thus is to be classified as not readily biodegradable. Under aerobic conditions a dehalogenation is possible through bacteria strains adapted to dichlorobenzene. Under methanogenic and sulfate-reducing conditions 2,4,5-TCA can be formed after an adaptation period of several months as a metabolite during the degradation of 2,3,4,5-tetrachloroaniline.

In the atmosphere a half-life of 2.5 days is expected for the photooxidative degradation of 2,4,5-TCA. Under open-field conditions the half-life for the photo-transformation was 6-8 hours during studies with surface water, and the half-life for photomineralization was 42 hours at 29 °C and 87 hours at 16 °C.

Regarding the bioaccumulation potential of 2,4,5-TCA, a BCF of 214 was determined for the guppy (*Poecilia reticulata*) and that of 67.6 for the large sludge snail (*Lymnea stagnalis)*.

The sorption of 2,4,5-TCA is correlated with the humus content of the soil. At calculated K_{OC}-values of 595 to 2003, there is an increased to high tendency for 2,4,5-TCA to adsorb to humus. In soils, 2,4,5-TCA can be bound to the humus matrix through enzymatically catalyzed or spontaneous chemical reactions.

Based on the Henry's Law constants, 2,4,5-TCA is classified as being moderately volatile in water. According to Mackay Level I, Version 2.11 (Mackay 1991) 2,4,5-TCA in an equilibrium state is distributed to 67.5 % in water, 14.4 % in soil, 14.5 % in

sediment, 0.1 % in suspended particles and 3.6 % in air. Consequently, the target compartments are the hydrosphere followed by sediment and soil.

Ecotoxicity

Regarding the toxicity to bacteria a 30 minute EC_{50} value (bioluminescence) of 1.49 mg 2,4,5-TCA/l was measured for *Photobacterium phosphoreum* .

In the aquatic area a 96h EC_{50} value of 2.2 mg 2,4,5-TCA/l (95% confidence interval 1.8 - 2.7 mg/l; biomass) was determined for the unicellular green alga *Chlorella pyrenoidosa*. The lowest measured 48h EC_{50} value for the water flea (*Daphnia magna*) was 1.91 mg 2,4,5-TCA/l (95% confidence interval 1.59 - 2.29 mg/l). The 14d LC_{50} value for the guppy (*Poecilia reticulata*) was 1.96 mg 2,4,5-TCA/l. The embryonal stage of the zebra fish (*Danio rerio)* proved to be particularly sensitive. Based on the measurement parameters molt rate, growth in length and survival, the 28d NOEC was 0.056 mg 2,4,5-TCA/l and the 28d LC_{50} value 0,12 mg 2,4,5-TCA/l (95% confidence interval 0.06 – 0.18 mg/l).

The toxicity to the large sludge snail (*Lymnea stagnalis)* was established according to OECD 203 (modified) with a 96h LC_{50} value of 5.19 mg 2,4,5-TCA/l (95% confidence interval 4.01 – 6.72 mg/l).

In the terrestrial area the toxicity to the earthworm (*Eisenia foetida*) was shown by the lowest 14d LC_{50} value of 134 mg 2,4,5-TCA/kg soil dry matter and 3.54 mg 2,4,5-TCA/l based on the water concentration in the soil pores. For lettuce (*Lactuca sativa*), the lowest measured 14d EC_{50} value was 17 mg 2,4,5-TCA/kg soil dry matter (natural loam soil), and the 16d EC_{50} value was 1.3 mg 2,4,5-TCA/l nutrient solution.

Toxicological Aspect

2,4,5-Trichloroaniline can be absorbed orally, dermally and possibly also by inhalation. In acute toxicity studies with rats, symptoms such as narcosis, matted fur, prone position, weight loss, paralysis of the hind extremities, bloody eyes and a diminished state of well-being were described at high dosages. Depending on the dosage, cats showed a weakly pronounced methemoglobin formation, an increased number of Heinz bodies as well as leukocytosis, neutrophilia and lymphocytopenia.

2,4,5-Trichloraniline does not irritate the eyes or skin.

In 2- and 4-week studies, rats showed retarded growth and alterations in the liver (weight increase and hemosiderosis) and spleen (hemosiderosis, extramedullary hematopoiesis and vascular congestion) as well as a decreased hematocrit, hemoglobin concentration and erythrocyte count. They also showed an increased number of Heinz bodies, reticulocytes and thrombocytes. Because of the increased liver weights and the decreased hematocrit and hemoglobin concentration at the lowest dosage in the 4-week study, no NOEL can be derived for 2,4,5-TCA. Thus, the results reveal only a LOEL of 40 mg/kg b.w..

2,4,5-Trichloraniline does not induce any gene mutations in bacterial systems (Salmonella microsome test) but does slightly induce SOS-DNA repair (umu-test). No DNA repair (UDS) is caused in primary rat hepatocytes. At toxic dosages, no micronuclei are induced in the bone marrow erythrocytes of NMRI-mice.

Data Gaps

Ecological Aspects

The emissions of 2,4,5-TCA from production and use are uncritical. They lie considerably below the loads that were estimated for the Dutch section of the Rhine. There are gaps in knowledge about the possible emission sources for the detected 2,4,5-TCA near Lobith and in sewage sludge. The local measurement near Lobith would indicate a hazard. The 90th percentiles of the 2,4,5-TCA concentrations over 6 years were below 0.42 µg/l with a peak concentration of 0.96 µg 2,4,5-TCA/l measured in 1995. In other surface waters, all the measurement values were below the determination limit of 1 µg 2,4,5-TCA/l. The measurement values for most of the samples, however, were always below the analytical detection limit of 0,05 µg/l, so that a risk to the environment is expected neither here nor at the known locations of the manufacturer and processor in Germany. With respect to the aquatic area various studies are available on the toxicity of 2,4,5-TCA (alga: 96h EC_{50} 2.2 mg /l; daphnia: 48h EC_{50} 1.91 mg/l; guppy: 14d LC_{50} 1.96 mg/l; zebra fish: 28d NOEC 0.056 mg/l). The lowest NOEC amounts to 0.056 mg 2,4,5-TCA/l. Thus, a risk from 2,4,5-TCA for aquatic organisms cannot be excluded.

Because the water body represents an exposure route for sediment and 2,4,5-TCA has a sorption potential, an exposure to benthic organisms is also possible. Studies on the toxicity of 2,4,5-TCA-contaminated sediment to endobenthic organisms would be desirable from a scientific standpoint.

Toxicological Aspects

There are no studies available on metabolism, toxicokinetics, chronic toxicity, sensitization, carcinogenicity or reproduction toxicity.

The product databank of BgVV does not indicate any products which the consumer could come in contact with. Because of the known gaps in this databank (not all products that the consumer comes into contact with are found here), an exposure for the consumer cannot be ruled out. Experience gained from other cases has shown that there was, indeed, a considerable amount of consumer contact despite a missing entry in the BgVV-product databank.

According to the sole German producer and also by the company's clients, 2,4,5-trichloroaniline is produced at the company in a closed system and is processed exclusively to pigments (Clariant 2000). In the filling area contact with 2,4,5-TCA must be avoided by taking precautionary measures (wearing gas masks, safety glasses/face masks, protective gloves and clothing).