GDCh-Advisory Committee
on Existing Chemicals (BUA)

Monochloroacetone

BUA Report 226

(November 2000)

S. Hirzel

Wissenschaftliche Verlagsgesellschaft 2002

GDCh-Advisory Committee
on Existing Chemicals (BUA, November 2000)

Chairman:
Prof. Dr. H. GREIM, TU München, Weihenstephan

Members:
Prof. Dr. H. DREXLER, Institut für Arbeits-, Sozial- und Umweltmedizin, Universität Erlangen
Prof. Dr. Dr. H.-P. GELBKE, BASF AG, Toxikologie, Ludwigshafen am Rhein
Frau Prof. Dr. U. GUNDERT-REMY, Bundesinstitut für gesundheitlichen Verbraucherschutz und Veterinärmedizin, Berlin
Dr. H. von HOLLEBEN, Verband der Chemischen Industrie, Frankfurt am Main
Prof. Dr. H. HULPKE, Bayer AG, Konzernstab KS-QUS, Leverkusen
Priv.-Doz. Dr. Dr. A. KAPPOS, Behörde für Arbeit, Gesundheit und Soziales der Freien Hansestadt Hamburg
Dr. J. KUTSCHER, Berufsgenossenschaft der Chemischen Industrie, Heidelberg
Dr. C. MEICHSNER, Infraserv GmbH & Co. Höchst KG, Umwelt/Sicherheit, Frankfurt/Main
Prof. Dr. R. NAGEL, Institut für Hydrobiologie der Technischen Universität Dresden
Dr. N. RUPPRICH, Bundesanstalt für Arbeitsschutz und Arbeitsmedizin, Dortmund
Prof. Dr. R. ZELLNER, Institut für Physikalische und Theoretische Chemie der Universität Essen (stellvertretender Vorsitzender)

Collaborators and Guests:
Priv.-Doz. Dr. J. AHLERS, Fachgebiet IV 1.2 des Umweltbundesamtes, Berlin
Dr. T. BROCK, Berufsgenossenschaft der Chemischen Industrie, Heidelberg
Dr. F. ENGEL, Wacker Chemie GmbH, Abt. A-CG, Burghausen
Dr. D. FINK, Verband der Chemischen Industrie, Frankfurt am Main
Dr. E. GOEDECKE, Anmeldestelle Chemikaliengesetz, Dortmund
Frau Dr. H. GREIM, Technische Universität München, Weihenstephan
Dr. G.-R. JÄNIG, Fachgebiet 821 des Bundesinstituts für gesundheitlichen Verbraucherschutz und Veterinärmedizin, Berlin
MinR Dr. H. A. KLEIN, Bundesministerium für Arbeit und Sozialordnung, Bonn
Dr. W. KÖRDEL, Institut für Umweltchemie und Ökotoxikologie der Fraunhofer-Gesellschaft, Schmallenberg
Frau Dr. P. KREIS, Technische Universität München, Weihenstephan
Frau Dr. M. LANGE, Institut für Hydrobiologie der Technischen Universität Dresden
Dipl.-Ökol. T. SCHMIEGELT, Universität Essen
Dr. R. SCHWABE, Technische Universität München, Weihenstephan
Frau Dr. K. WIDMANN, Technische Universität München, Weihenstephan

Responsible at the BMU:
MinR Prof. Dr. U. SCHLOTTMANN, Bundesministerium für Umwelt, Naturschutz und Reaktorsicherheit, Bonn

GDCh-Office:
Dr. H. BEHRET, GDCh, Frankfurt am Main

Monochloroacetone

BUA Report 226
(November 2000)

edited by the GDCh-Advisory Committee
on Existing Chemicals

GDCh-Beratergremium
für Altstoffe (BUA)

S. Hirzel
Wissenschaftliche Verlagsgesellschaft 2002

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

The work for this publication was sponsored by the Federal Ministry for the Environment, Nature Conservation and Nuclear Safety (Bundesministerium für Umwelt, Naturschutz und Reaktorsicherheit (BMU) / Federal Environmental Agency (Umweltbundesamt)) and the German Chemical Industry Association (Verband der Chemischen Industrie, VCI)

Die Deutsche Bibliothek – CIP-Einheitsaufnahme

Monochloroacetone / ed. by the GDCh Advisory Committee on Existing Chemicals. [Transl. by P. Karbe] – (November 2000). – Stuttgart Hirzel ; Stuttgart : Wiss. Verl.-Ges., 2002
(BUA Report ; 226)
Dt. Ausg. u. d. T.: Monochloraceton
ISBN 3-7776-1173-5

Printed on acid-free and low-chlorine paper.

Printing and binding: Druckpartner Rübelmann GmbH, Hemsbach
Printed in F.R. Germany

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 and evaluation models for soils and sediments", "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.

Munich, November 2000

Helmut Greim
BUA Chairman

Contents

BUA report on Monochloroacetone

Summary

Ecological Aspect

The only manufacturer of monochloroacetone in Europe is Wacker-Chemie GmbH in Burghausen (Germany); one other manufacturer is located in India.

The sole European manufacturer produces about 500 – 1 000 tonnes/year; no figures are available from the Indian manufacturer.

Due to the various possibilities for synthesizing heterocyclic compounds, monochloroacetone is used mainly as a building block in the synthesis of pharmaceuticals and plant-protection agents. Other applications concern the formulation of emulsifiers, tanning agents, fragrances, antioxidants, enzyme activators, and photosensitizers. Figures are not available on the quantities used in these areas.

According to the manufacturer, no emissions, wastewater, or wastes occur through production in a closed system. No data are available on emissions into the atmosphere, hydrosphere, geosphere, or biosphere through processing or application. Due to the lack of data on emissions into the various environmental media, no overview statement can be made.

Little information is available on the occurrence in the environment. A 1979 publication reported air concentrations of 0.004 – 0.01 mg/m^3 (= 1.0 – 2.6 ppb) in the area of Jones State Forest (Texas). No data are available on the occurrence in the hydrosphere or geosphere. Monochloroacetone was qualitatively identified as a natural component of mazzard cherries (*Prunus avium*).

Test results (closed bottle test according to OECD 301 D) have shown monochloroacetone to be non-biodegradable (0 % after 28 days). However, various other investigations indicate a degradation of monochloroacetone by bacteria, yeasts, and enzymes.

With respect to the abiotic degradation in the atmosphere, monochloroacetone should be classified as barely degradable. It has no chromophoric components. However, as the absorption maximum in the UV spectrum is λ = 292 nm, some weak photolysis cannot be excluded completely. For photochemical-oxidative degradation, a reaction rate constant of $0.3682 \bullet 10^{-12}$ $cm^3 \bullet molecules^{-1} \bullet s^{-1}$ was calculated by the AOPWIN program at room temperature. At an assumed OH-radical concentration of $5 \bullet 10^5$ molecules/cm^3, this gives a half-life of 43.6 days.
The experimentally determined hydrolytic rate of $k = 8 \bullet 10^{-6}$ (1/h) at 25 °C indicates the substance to be stable in water. The half-life of an added concentration of 0.01 M was calculated to be 989 years.

For the bioconcentration of monochloroacetone in aquatic organisms, a log BCF of approximately 2.6 – 3.2 can be calculated. Due to the hydrophilic nature of the compound, there thus appears to be little likelihood of bioconcentration in aquatic organisms.
Sorption values of 1.2 – 1.3 for soils and sediments can be calculated from the octanol-water partition coefficients, so that very little sorption to organic matter in soils and sediments may be assumed.
The data on vapor pressure at room temperature vary between 14.6 and 42 hPa and are seen to be considerable.
The solubility in water at room temperature is between 100 – 124 g/l; data for Henry's law constants at room temperature are 1.7 – 3.13 Pa $\bullet$ m^3/mol. Thus, the volatilization of monochloroacetone from an aqueous solution is classified as moderate.
The calculation of the equilibrium distribution into target compartments according to Mackay level 1 gives 57.7 % for air and 42.3 % for water; soil, sediment, and biota make up <<1 %.

Valid data for an ecotoxicological assessment are sparse: Investigations on golden orfe (*Leuciscus idus*) to determine the acute fish toxicity according to DIN 38412, Part 15, gave the following 48-hour mortality values (nominal) in a semistatic test:

48-h LC_0 = 0.2 mg/l
48-h LC_{50} = 0.6 mg/l
48-h LC_{100} = 1.6 mg/l.

In toxicity studies on guppies (*Poecilia reticulata*), an LC_{50} of 0.7 mg/l was determined in a 14-day test.

In a cell growth inhibition test according to DIN 38412, Part 8, with *Pseudomonas putida* the following values were determined for the 16-hour incubation time:

16-h EC_{10} = 0.14 mg/l
16-h EC_{50} = 2.00 mg/l.

Tests are not available on the ecotoxicity to algae or daphniae. Thus, the ecotoxicity results at hand do not yet allow an assessment of the environmental relevance.

Toxicological Aspect

Data on the metabolism are missing. Investigations on rat hepatocytes have shown that monochloroacetone reacts directly with a biologically relevant macromolecule containing sulfhydryl groups and with glutathione. After splitting off the chloride ion, the compound may act as an alkylating agent. Monochloroacetone is a potent tear gas. In humans, monochloroacetone causes irritation of the eyes and upper respiratory tract. Skin contact causes painful blistering. In animal experiments, lung edema and hydrothorax were observed after inhalation exposure. Male rats are more sensitive to acute toxicity through inhalation than females. After oral and i.p. administration

to the mouse and rat and dermal application to the rabbit, the compound shows comparable, very high acute toxicity. Repeated oral administration to rats causes necrosis of the liver, spleen, adrenal gland, and testis, as well as ulceration and perforation in the gastric area. Repeated inhalation exposure to the rat causes congestion of blood in the liver and lung. Higher exposure rates causing blood congestion in the heart, kidney, and spleen, as well. Repeated spreading onto the skin causes inflammations in guinea pigs, and additionally causes necroses in rabbits. In an inadequately documented experiment in guinea pigs, no sensitizing effect was demonstrated.

The available genotoxicity studies on bacteria, drosophila, and newts, none of which meet present methodical requirements, gave contradictory results and do not permit unequivocal conclusions. In the studies at hand, no tumor-initiating effect was shown. Carcinogenicity studies are not available.

Data Gaps

Ecological Aspects

No tests are available on the ecotoxicity to algae and daphniae. Thus, the available results on ecotoxicity do not yet allow an assessment of the environmental relevance.

Toxicological Aspects

There is a lack of meaningful data from animal experiments on the target organs of systemic toxicity and the NOEL after repeated administration. Information is also lacking on the toxic effect on reproduction and on the assessment of genotoxic and carcinogenic properties. No statement can be made on a sensitizing effect of the compound, due to a lack of valid data.

The BgVV Product Data Sheet gives no indication of products which reach the consumer. It is therefore assumed that no consumer exposure occurs. According to the sole German manufacturer, monochloroacetone is produced in a closed system and 75 % of it is exported. From its former use as tear gas, a strong irritant effect is known. However, a more extensive assessment of this compound's active properties is not possible, due to insufficient data.

Monochloroacetone is also being considered by the US Challenge/HPV Program, which fills out data sets on selected bulk compounds at the OECD-SIDS level. It is recommended that the data gaps be closed within this framework.