German Chemical Society
Gesellschaft Deutscher Chemiker

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

BUA Reports 71 - 73

Benzal chloride
BUA Report 71 (December 1991)

Benzotrichloride
BUA Report 72 (December 1991)

Benzoyl chloride
BUA Report 73 (December 1991)

S. Hirzel
Wissenschaftliche Verlagsgesellschaft 1997

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

Chairman:
Prof. Dr. E. Bayer, Institut für Organische Chemie der Universität Tübingen

Members:
Dr. G. Alfke, Mineralölwirtschaftsverband e. V., Hamburg
Prof. Dr. K. Ballschmiter, Abteilung Analytische Chemie und Umweltchemie der Universität Ulm
Dr. R. Bias, BASF AG, Emissionsüberwachung und Ökologie, Ludwigshafen a. Rh.
Dr. B. Broecker, HOECHST AG, Abteilung Umweltchemikalien/Verbrauchersicherheit, Frankfurt am Main
Prof. Dr. O. Fränzle, Geographisches Institut der Universität Kiel
Prof. Dr. F. H. Frimmel, DVGW-Forschungsstelle am Engler-Bunte-Institut der Universität Karlsruhe
Prof. Dr. H.-P. Gelbke, BASF AG, Toxikologie, Ludwigshafen a. Rh.
Prof. Dr. H. Greim, GSF - Institut für Toxikologie, Neuherberg (Vice Chairman)
Dr. H. Jungen, Deutsche Wissenschaftliche Gesellschaft für Erdöl, Erdgas und Kohle e. V., Hamburg
Dir. und Prof. Dr. D. Kayser, Bundesgesundheitsamt, Berlin
Prof. Dr. P. Müller, Institut für Biogeographie, Universität des Saarlandes, Saarbrücken
Prof. Dr. E. Offhaus, Umweltbundesamt, Berlin
Dr. R. Ott, Deutsche Shell Chemie GmbH, Eschborn/Ts.
Prof. Dr. U. Schlottmann, Bundesministerium für Umwelt, Naturschutz und Reaktorsicherheit, Bonn
Dr. N. Schön, BAYER AG, LE Umweltschutz/AWALU, Leverkusen
Dr. A. Troge, Umweltbundesamt, Berlin

Guests:
Dr. K. H. Adlfinger, Initiative umweltrelevante Altstoffe, Frankfurt am Main
Prof. Dr. R. Kümmel, Technische Hochschule Leuna-Merseburg
Prof. Dr. Dr. W. Mücke, Institut für Toxikologie und Umwelthygiene der TU München
Dr. J. Oberhansberg, BG Chemie, Heidelberg

In collaboration with:
Priv.-Doz. Dr. J. Ahlers, Umweltbundesamt, Berlin
Dr. S. Ettel, Institut für Organische Chemie der Universität Tübingen
Dr. R. Koch, Bayer AG, Umweltschutz, Leverkusen
Frau Dr. U. Koch, Bayer AG, Toxikologie, Wuppertal
Dr. W. Koch, Umweltbundesamt, Berlin
Frau Dr. I. Mangelsdorf, GSF - Institut für Toxikologie, Neuherberg
Frau Dr. H. Sterzl-Eckert, GSF - Institut für Toxikologie, Neuherberg
Dr. D. Vogel, Institut für Organische Chemie der Universität Tübingen
Frau Dipl.-Biol. L. Weis, Institut für Organische Chemie der Universität Tübingen
Frau Dr. K. Widmann, Institut für Organische Chemie der Universität Tübingen

GDCh Office:
Dr. H. Behret, GDCh, Frankfurt am Main

BUA Reports 71 - 73

Benzal chloride

BUA Report 71 (December 1991)

Benzotrichloride

BUA Report 72 (December 1991)

Benzoyl chloride

BUA Report 73 (December 1991)

edited by the GDCh-Advisory Committee on Existing Chemicals of Environmental Relevance

Beratergremium für Umweltrelevante Altstoffe (BUA)

S. Hirzel

Wissenschaftliche Verlagsgesellschaft 1997

Dr. H. Behret
Gesellschaft Deutscher Chemiker
Postfach 90 04 40
D-60444 Frankfurt am Main

Translated by P. Arend

Die Deutsche Bibliothek — CIP-Einheitsaufnahme

Benzal chloride : (December 1991). **Benzotrichloride** :
(December 1991) [u.a.] - Ed by the GDCh Advisory Committee
on Existing Chemicals of Environmental Relevance [Transl. by
P. Arend]. - Stuttgart: Hirzel ; Stuttgart : Wiss. Verl.-Ges.,
1997
(BUA report; 71/73)
Dt. Ausg. u.d.T.: Benzalchlorid
ISBN 3-7776-0751-7
NE: Arend, P. [Übers.]; Benzotrichloride; Gesellschaft Deutscher Chemiker / Beratergremium für
Chemiker / Beratergremium für Umweltrelevante Altstoffe: BUA
report

Printed in acid-free and low-chlorine paper.

Printing and binding: Druckhaus Beltz, Hemsbach
Printed in F.R. Germany

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

Benzal chloride

BUA Report 71
(December 1991)

edited by the GDCh-Advisory
Committee on Existing Chemicals
of Environmental Relevance

Beratergremium für
Umweltrelevante Altstoffe (BUA)

Contents

Benzal chloride

BUA Report on Benzal chloride

7 Summary

In the manufacture and processing of benzal chloride, roughly 150 kg/a are discharged with industrial sewage into a biological sewage treatment plant. Benzal chloride has not been detected in the sewage treatment plant effluent.

After disposal of exhaust gas by means of thermal exhaust air purification treatment with flue gas scrubbing, the benzal chloride discharge into the atmosphere is << 25 kg/a.

Substantial discharges of benzal chloride by Bayer AG into the environment are therefore not taking place at the present time.

Benzal chloride hydrolyses rapidly (t½ = 13 mm). The hydrolysis product benzaldehyde is readily biodegradable. Given the rapid hydrolysis of the low amounts discharged and the ready biodegradation of the hydrolysis product benzaldehyde, neither a major long-term exposure of outdoor organisms, nor a substantial bio- or geoaccumulation under humid climatic conditions, is to be expected.

For *Pseudomonas fluorescens*, the no-observed-effect concentration is given as EC_0 (2 hours) = 100 mg/l. Concentrations of 4.6 mg/l and 32 mg/l lead in photobacteria to a 50 % inhibition (EC_{50}) of luminescence over 30 minutes.

Random sampling over a period of 48 hours with the golden orfe (*Leuciscus idus*) indicated acute toxicity in the range of 50 - 100 mg/l.

Given the rapid hydrolysis of benzal chloride, the ecotoxic effect can be traced back to the hydrolysis product benzaldehyde.

Benzal chloride has only a low acute toxicity to mammals. It has a local irritant effect and is mutagenic. The formation of tumours has been observed in animal tests. In man tumours have occurred after mixed exposure with benzotrichloride and benzoyl chloride.

The Deutsche Forschungsgemeinschaft has classified benzal chloride as a substance with a reasoned suspicion of a carcinogenic risk (MAK III B).

Benzal chloride has been classified in Group IV. This present work has shown that exposure is only possible in the workplace, not in the environment or by the consumer. Further investigation of the substance does not therefore come under the terms of reference of BUA.

Benzotrichloride

BUA Report 72
(December 1991)

edited by the GDCh-Advisory
Committee on Existing Chemicals
of Environmental Relevance

Beratergremium für
Umweltrelevante Altstoffe (BUA)

Contents

Benzotrichloride

BUA Report on Benzotrichloride

7 Summary

Benzotrichloride discharged into industrial sewage during manufacture and processing hydrolysises rapidly into benzoic acid and hydrogene chloride ($t_{½}$ = 2.4 min in model study). The total amount of benzoic acid in the industrial sewage of chlorination plants, which does not stern only from the production of benzotrichloride, is ca. 35 t/a. It is disposed of in a biological sewage treatment plant.

The total release of benzoic acid from the Bayer AG sewage treatment plant into surface waters is < 1 t/a.

The discharges of benzotrichloride into the atmosphere during the production and manufacturing phases amount to << 25 kg/a. It is disposed of in a thermal exhaust air treatment plant with flue gas scrubbing.

Distillation residues are disposed of in hazardous waste incineration plant.

Substantial discharges of benzotrichloride into the environment from Bayer AG and Hoechst AG are not to be expected.

Given the rapid hydrolysis of the low amounts discharged and the ready biodegradability of the hydrolysis product, benzoic acid, neither a major long-term exposure of outdoor organisms nor a substantial bio- or geoaccumulation under humid climatic conditions is to be expected.

Studies on the ecotoxic effect were conducted with aquatic organisms only. In the case of *Photobacterium phosphoreum*, this led after 30 min to EC_{50} values of 17.8 or 19 mg/l (E = luminescence inhibition). The toxic limit concentration for proliferation inhibition of *Pseudomonas putida* (with an exposure time of 16 hours) is, as for *Scenedesmus quadricauda* (8 d), more than 100 mg/l. The lowest determined 24 h EC_{50} for Daphnia is 50 mg/l, for the golden orfe (*Leuciscus idus*) a 48h LC_{50} of 4,140 mg/l was determined.

In animal experiments benzotrichloride is only toxic after inhalation. Repeated applications lead to marked irritations and inflammation up to necrosis. Benzotrichloride is mutagenic, and

carcinogenic in animal experiments. In humans, tumours have occurred in mixed exposure with benzal chloride and benzoyl chloride.

The Deutsche Forschungsgemeinschaft has classified benzotrichloride as a substance with a reasoned suspicion of a carcinogenic risk (MAK III B).

Benzotrichloride has been classified in Group IV. This work has shown that exposure is only possible in the workplace, not in the environment or by the consumer. Further investigation of the substance does not, therefore, come under the terms of reference of BUA.

Benzoyl chloride

BUA Report 73
(December 1991)

edited by the GDCh-Advisory
Committee on Existing Chemicals
of Environmental Relevance

Beratergremium für
Umweltrelevante Altstoffe (BUA)

Contents

Benzoyl chloride

BUA Report on Benzoyl chloride

7 Summary

Given rapid hydrolysis to benzoic acid, the release of benzoyl chloride into the sewage of the production plant is not quantifiable. The total amount of benzoic acid (ca. 35 t/a) which passes into industrial sewage from a chlorination plant is disposed of in a biological sewage treatment plant.

In the processing of benzoyl chloride, the benzoic acid emissions into industrial sewage amount to around 26 t/a (Dormagen) or around 100 t/a (Leverkusen) with subsequent disposal in a biological sewage treatment plant. The overall discharge of benzoic acid from the sewage treatment plant into surface waters by Bayer AG is < 1 t/a.

The benzoyl chloride which reaches exhaust air from the production and processing stages is disposed of in a thermal exhaust air treatment plant with flue gas scrubbing. The discharge into the atmosphere is < 25 kg/a.

Around 900 t/a of distillation residues are disposed of in a hazardous waste incineration plant. Discharges by other downstream processors are not known.

Substantial discharges of benzoyl chloride into the environment are not to be expected.

Given the rapid hydrolysis of the 10w discharges and the ready biodegradation of the hydrolysis product, benzoic acid, no major long-term exposure of outdoor organisms is to be expected, nor is bio- or geoaccumulation likely under humid climatic conditions.

In the respiratory inhibition test with activated sludge, an EC_{50} of > 100 mg/l was determined.

For fish the highest non-lethal concentrations were given as 72 h LC_0 = 200 mg/l for the golden orfe (*Leuciscus idus*) and as 96 h LC_0 = 7.5 mg/l (96 h LC_{100} = 10 mg/l) for the zebra fish (*Brachydanio rerio*). For the fathead minnow (*Pimephales promelas*) the mean lethal concentration is 24 h LC_{50} = 42.6 mg/l.

Benzoyl chloride has only a low acute toxicity. When applied locally, it is highly irritant. Indications of mutagenic activity are not given. After repeated dermal application no tumours were observed in animal experiments. In man tumours have appeared after mixed exposure with benzotrichloride and benzal chloride.

Benzoyl chloride has been classified in Group IV. This work has shown that exposure is only possible in the workplace not in the environment or by the consumer. Further investigation of the substance does not, therefore, come under the terms of reference of BUA.