



**German Chemical Society
Gesellschaft Deutscher Chemiker**

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

Triisopropanolamine

BUA Report 148

(December 1993)



S. Hirzel

Wissenschaftliche Verlagsgesellschaft 1996

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)
Dir. und Prof. Dr. J. Hahn, Institut für Wasser-, Boden- und Lufthygiene des Umweltbundesamtes, Berlin
Dr. H. Jungen, Deutsche Wissenschaftliche Gesellschaft für Erdöl, Erdgas und Kohle e. V., Hamburg
Dir. und Prof. Dr. D. Kayser, Bundesinstitut für gesundheitlichen Verbraucherschutz und Veterinärmedizin, Berlin
Dr. W. Mühlhölzl, Bayerische Landesanstalt für Wasserforschung, München
Prof. Dr. P. Müller, Institut für Biogeographie, Universität des Saarlandes, Saarbrücken
Dir. und Prof. Dr. E. Offhaus, Umweltbundesamt, Berlin
Dr. R. Ott, Deutsche Shell Chemie GmbH, Eschborn/Ts.
MinRat Prof. Dr. U. Schlottmann, Bundesministerium für Umwelt, Naturschutz und Reaktorsicherheit, Bonn
Dr. N. Schön, BAYER AG, Umweltschutz/Produktsicherheit, Leverkusen
Vizepräsident Dr. A. Troge, Umweltbundesamt, Berlin

Collaborators and Guests:

Dr. K. H. Adlfinger, Initiative Umweltrelevante Altstoffe, Frankfurt am Main
Priv.-Doz. Dr. J. Ahlers, Fachgebiet IV 1.2 des Umweltbundesamtes, Berlin
Dr. S. Ettel, Institut für Organische Chemie der Universität Tübingen
Dr. J. Feltes, Fraunhofer-Institut für Toxikologie und Aerosolforschung, Hannover
Dr. R. F. Hertel, Fachgruppe 821 des Bundesinstituts für gesundheitlichen Verbraucherschutz und Veterinärmedizin, Berlin
Dr. H.-J. Klimisch, BASF AG, Toxikologie, Ludwigshafen a. Rh.
Dr. G. Könnecker, Fraunhofer-Institut für Toxikologie und Aerosolforschung, Hannover
Dr. J. Koppenhöfer, Institut für Organische Chemie der Universität Tübingen
Prof. Dr. R. Kümmel, Institut für Umwelt- und Sicherheitstechnik der Fraunhofer Management-Gesellschaft, Oberhausen
Frau Dr. I. Mangelsdorf, GSF - Institut für Toxikologie, Neuherberg
Frau Dr. I. Neumann, GSF - Institut für Toxikologie, Neuherberg
Dr. J. Oberhansberg, BG Chemie, Heidelberg
Frau Dr. U. Reuter, GSF - Institut für Toxikologie, Neuherberg
Dr. G. Rosner, Fraunhofer-Institut für Toxikologie und Aerosolforschung, Hannover
Dr. P. Stahnecker, BASF AG, Ludwigshafen a. Rh.
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

Triisopropanolamine

BUA Report 148

(December 1993)

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

Beratergremium für
Umweltrelevante Altstoffe (BUA)



S. Hirzel

Wissenschaftliche Verlagsgesellschaft 1996

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

Translated by R. Brown

This book was carefully produced. Nevertheless, authors, editors and publisher do not warrant the information contained therein to be free of errors. Readers are advised to keep in mind that statements, data, illustrations, procedural details or other items may inadvertently be inaccurate.

The use of general descriptive names, trade names, trademarks, etc. in a publication, even if not specifically identified, does not imply that these names are not protected by the relevant law and regulations.

Die Deutsche Bibliothek — CIP-Einheitsaufnahme

Triisopropanolamine / GDCh Advisory Committee on Existing Chemicals of Environmental Relevance. – (BUA). [Transl. by R. Brown]. - (December 1993). - Stuttgart: Hirzel ; Stuttgart : Wiss. Verl.-Ges., 1996
(BUA report; 148)
Dt. Ausg. u.d.T.: Triisopropanolamin
ISBN 3-7776-0702-9
NE: Brown, R. [Übers.]; Gesellschaft Deutscher Chemiker / Beratergremium für Umweltrelevante Altstoffe: BUA report

All rights reserved. No part of this publication may be translated, stored in a retrieval system, or transmitted, in any form or by any means, electronic, mechanical, photocopying, microfilming, recording or otherwise, without permission in writing from the publisher.

© 1996 S. Hirzel Verlag, Birkenwaldstraße 44, 70191 Stuttgart

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

Contents

Summary and conclusions	XI	
Recommendations	XVI	
1	Chemistry of triisopropanolamine	1
1.1	Chemical identity	1
1.2	Composition of the industrial product	2
1.3	Chemical properties	4
2	Physical properties	6
3	Analytical methods	9
3.1	Determination in air	9
3.2	Determination in water	10
3.3	Determination in soil, sediment and biological material	10
3.4	Determination in consumer products	10
4	Discharge into the environment during manufacture, processing, use and waste disposal	11
4.1	Manufacture	11
4.2	Manufacturers and processors production levels exports, imports, total consumption	12
4.3	Processing, use, consumption	14
4.3.1	Processing	14
4.3.2	Use	16
4.4	Discharge into the atmosphere	18
4.4.1	Discharge during manufacture and processing	18
4.4.2	Discharge during application	18
4.5	Discharge into the hydrosphere	19
4.5.1	Discharge during manufacture and processing	19
4.5.2	Discharge during use	19
4.6	Discharge into the geosphere and biosphere	20
4.7	Discharge via waste and waste disposal	20
4.8	Summary of discharge into the environment	20

5	Occurrence in the environment	22
5.1	Atmosphere.....	22
5.2	Hydrosphere	22
5.3	Geosphere	22
5.4	Biosphere.....	22
5.5	Natural sources.....	22
6	Behaviour in the environment	23
6.1	Transformation, degradation and degradation products	23
6.1.1	Biodegradation.....	23
6.1.2	Hydrolytic degradation	23
6.1.3	Photochemical degradation	24
6.1.3.1	Photooxidative degradation in air.....	24
6.1.3.2	Photochemical degradation in water	24
6.2	Accumulation	25
6.2.1	Bioaccumulation.....	25
6.2.2	Geoaccumulation	25
6.3	Distribution behaviour and transport processes in and between environmental compartments	25
6.3.1	Henry's constant	25
6.3.2	n-Octanol/water partition coefficient.....	26
6.3.3	Soil-sorption coefficients.....	26
6.4	Fate in the environment	27
7	Ecotoxicology	28
7.1	Effects on aquatic organisms.....	28
7.1.1	Micro-organisms	28
7.1.2	Plants.....	29
7.1.3	Invertebrates.....	29
7.1.4	Vertebrates	29
7.2	Effects on terrestrial organisms.....	30
7.2.1	Micro-organisms	30
7.2.2	Plants.....	30
7.2.3	Invertebrates.....	31
7.2.4	Vertebrates	31
7.3	Effects on ecosystems	31

8	Toxicity to mammals	32
8.1	General nature of effects	32
8.2	Mode of action	32
8.3	Metabolism, toxicokinetics	32
8.4	Acute toxicity	33
8.5	Skin and mucous membrane tolerance	35
8.6	Sensitizing effect	37
8.7	Subacute, subchronic and chronic toxicity	37
8.7.1	Subacute toxicity	37
8.7.2	Chronic toxicity	38
8.8	Genotoxicity	39
8.9	Carcinogenicity	39
8.9.1	Triisopropanolamine	39
8.9.2	N-Nitrosobis(2-hydroxypropyl)amine (ND2HPA)	39
8.10	Reproduction toxicity	40
8.11	Miscellaneous effects	41
8.12	Experience in humans	41
9	Substance-specific legal regulations	43
9.1	Gefahrstoffverordnung (Hazardous Substances Regulation)	43
9.2	Bundes-Immissionsschutzgesetz (Federal Emissions Act)	43
9.3	Wasserhaushaltsgesetz (Water Conservation Act)	43
9.4	Abfallgesetz (Waste-Disposal Act)	44
9.5	Kosmetikverordnung (Cosmetics Ordinance)	45
9.6	Gefahrgutverordnung (Dangerous Goods Regulation)	45
10	Literature	46

BUA Report on Triisopropanolamine

Summary and conclusions

Ecological aspects

Discharge during manufacture and usage

In the Federal Republic of Germany, triisopropanolamine is manufactured jointly with the other two isopropanolamines by three companies. Production totals 350 to 750 t/a.

Domestic sales approximate 80 t/a; 30 t/a are blended with triethanolamine. In addition, 95 t triisopropanolamine produced exclusively in the USA were sold in the Federal Republic of Germany in 1991. This yields overall consumption of about 200 t/a. The remaining production volume (250 - 650 t/a) is exported.

By far the most triisopropanolamine sold by a German manufacturer (50 t/a) is processed into textile auxiliaries and polyurethanes (approx. 17 and 13 t/a respectively). The remainder (approx. 20 t/a) finds use in various products, including cosmetics, surfactants and emulsifiers. Some of the product is sold via traders to recipients of small amounts.

Blended with triethanolamine, 30 t/a triisopropanolamine sold by another German manufacturer in the home market are also processed to detergents raw materials.

In the literature, a series of other possible uses is mentioned whose importance in the Federal Republic of Germany, however, is unknown. Thus, possible applications for triisopropanolamine are in the manufacture of polyurethane foams as neutralizing agent, in the form of triisopropanolamine salts with alkylsulphonic acid for degreasing; as a component of cleaners; as triisopropanolamine lauryl sulphate in detergents; as an ingredient of special soaps and cosmetics in the USA; as a corrosion inhibitor in lubricating oils

and cutting oils; as mould-release agent; as textile finishing agent; as coating agent for paper and wood; as well as blending component of developers for photocopy systems.

Discharge of triisopropanolamine into the atmosphere via manufacture and processing is negligible since production is performed in closed plants and the compound has a low vapour pressure.

At one manufacturer's, discharge into the wastewater treatment plant via manufacture and processing is estimated at 2.9 t/a. No information is available at the two other manufacturers'.

Estimation of discharge during usage and processing is difficult on account of the data situation. Discharge into the atmosphere, hydrosphere and geosphere is possible. It is, however, not quantifiable owing to the numerous applications possible in some cases.

Production residues containing triisopropanolamine that accumulate at two German manufacturers' (one not quantifiable, the other 3 t/a) are disposed of by incineration in suitable residue incinerators. At the third manufacturer's, no waste containing the compound is generated.

Occurrence in the environment

Owing to the low vapour pressure and the pronounced polar nature of the compound, occurrence in the atmosphere of quantities of relevance to the environment is not expected. Measurements are not available.

Triisopropanolamine could not be detected in 1981 in Japanese surface waters or in soil sediment (limit of detection: 10 µg/l and 80 ng/kg).

Distribution behaviour and degradability

Whereas direct photolytic degradation of triisopropanolamine does not occur due to the lack of UV absorption above 290 nm, atmospheric photooxidative degradation of the compound by OH free radicals with a calculated half-life of 3.3 hours is expected. Judging from the value of Henry's constant, the compound has extremely low volatility from aqueous solution. According to estimates, sorption of triisopropanolamine on soil is very slight to weak. Its mobilization potential is correspondingly high. Transportation of the compound with leachate to the ground water is possible. Bioaccumulation is not expected owing to the measured bioconcentration factors (< 0.57) and the measured $\log P_{OW}$ value of -0.015 .

Triisopropanolamine proved to be heavily eliminable in the modified Zahn-Wellens Test and non-degradable in the BOD Test.

In the investigations published, triisopropanolamine proved stable to hydrolysis.

Ecotoxic effects

In the short term respiration inhibition test with activated sludge from an industrial wastewater-treatment plant, no inhibition of the respiration activity was recorded for tested concentrations of up to 2,000 mg/l. In another respiration-inhibition test, triisopropanolamine concentrations of 10 and 50 mg/l led to short-term, reversible inhibition of up to 20 %.

The toxicity threshold concentration in the cell multiplication inhibition test involving *Pseudomonas putida* in neutralized medium was 20,000 mg/l.

In a standardized algae test on the green alga *Scenedesmus subspicatus* CHODAT, the 72-h EC_{50} value was 35 mg/l; the EC_{20} value was 11 mg/l and the EC_{90} value was > 100 mg/l.

A standardized *Daphnia* test on *Daphnia magna* returned a 48-h EC₀ value of 250 mg/l; the EG value was > 500 mg/l. The medium was not neutralized.

In a standardized golden orfe test on *Leuciscus idus*, the following values were obtained: NOEC 2,150 mg/l (48/96 h), 2,150 < LC₅₀ (48/96 h) < 4,640 mg/l, LC₁₀₀ 10,000 mg/l (48 h) and 4,640 mg/l (96 h). Neutralization of the medium reduced the harmful effect of 24 hours' exposure.

Toxicological aspects

Alkanolamines are generally resorbed well from the intestine and respiratory tract. Structure-related compounds like triethanolamine (see Toxicological Evaluation No. 57, BG Chemie) and diisopropanolamine (see Toxicological Evaluation No. 178, BG Chemie) are eliminated mainly unchanged and predominantly via the urine. Studies on the kinetics and metabolism of triisopropanolamine are not available.

Triisopropanolamine exhibits very minor toxicity after single oral, dermal, or inhalation exposure. In animals, the compound caused either only slight skin irritation or none at all. In clinical studies, cosmetic products that contained up to 1.1% triisopropanolamine irritated the skin either only slightly or not at all. Various investigations showed that, in the eye, triisopropanolamine causes slight to moderate irritation of the mucous membrane.

In man, triisopropanolamine proved to be non-sensitizing. Inadequately documented animal experiment findings also produced no evidence of a sensitizing effect.

Two weeks' administration of triisopropanolamine via the drinking water showed that effects in rats occurred only at relatively high dosages: at 0.6 and 2 g/kg b.w. per day (males) and 2 g/kg b.w. per day (females) the kidney weight was significantly higher. In a 30- day drinking water study, 0.14 g/kg b.w. per day was tolerated

without symptoms by rats. 0.26 g/kg b.w. per day led to changes in the liver, kidney, spleen and testicles that were not explained in more detail. A chronic study that satisfies current standards is not available.

The Ames test, both with and without metabolic activation, disclosed no evidence of a mutagenic effect exerted by triisopropanolamine.

In an inadequately documented study on rats, no evidence of teratogenic or other reproduction-toxic effects was found.

A two-year study on male Wistar rats (n=19) returned no evidence of a carcinogenic effect in the form of either tumours or preneoplastic liver foci, after oral application of triisopropanolamine (2 % in the feed). In the same study, application of 2 % triisopropanolamine in the feed, together with 0.15 or 0.3% sodium nitrite in the drinking water, led to a significantly higher tumour incidence only in the adrenal glands (in the 0.3% sodium nitrite group).

Recommendations

Ecological Aspects

Exposure cannot be estimated owing to data gaps on processing and usage. However, because of low toxic effects clarification of the open issues is not of priority.

Toxicological Aspects

Except for genotoxicity and reproduction toxicity, the relevant end points are generally so well clarified experimentally that a conclusive toxicological evaluation is possible. The Point Mutation (Ames) Test produced no evidence of a potential for genotoxicity. For further clarification, an in vivo Micro-Nucleus Test (mouse) is being performed on triisopropanolamine, acting as a representative of the trialkanolamines. To clarify the reproduction toxicity, a teratogenicity study (oral, rat) is being performed on triisopropanolamine, again acting as a representative of the trialkanolamines.