

GDCh-Advisory Committee
on Existing Chemicals (BUA)

**N-Cetylpyridinium Chloride
Monohydrate**

BUA Report 247

(October 2003)



S. Hirzel

Wissenschaftliche Verlagsgesellschaft 2005

GDCh-Advisory Committee
on Existing Chemicals (BUA, Status 10/2003)

Chairman:

Prof. Dr. H. GREIM, Technische Universität München, Weihenstephan

Members:

Frau Dr. M. BETH-HÜBNER, Berufgenossenschaft der Chemischen Industrie, Heidelberg
Prof. Dr. N. CASPERS, Bayer AG, BIS-SUA-PUA I, Leverkusen
Prof. Dr. H. DREXLER, Institut für Arbeits- Sozial- und Umweltmedizin, Universität Erlangen
Frau Prof. Dr. H. FOTH, Institut für Umwelttoxikologie, Universität Halle an der Salle
Prof. Dr. Dr. H. GELBKE, BASF AG, Toxikologie, Ludwigshafen am Rhein
Dr. W. KÖRDEL, Fraunhofer-Gesellschaft, IME, Schmallenberg
Prof. Dr. R. NAGEL, Institut für Hydrobiologie, Technischen Universität Dresden
Prof. Dr. Dr. H. PARLAR, Institut für Lebensmitteltechnologie und Analytische Chemie, Technische Universität München
Dr. M. SCHÜMMANN, Arbeitsgruppe Epidemiologie der BAGS und des IMDM, Universitätsklinik Hamburg-Eppendorf
Dr. B. STOCK, Bayer AG, BIS-SUA-PUA I, Leverkusen
Prof. Dr. R. ZELLNER, Institut für Physikalische und Theoretische Chemie der Universität – Gesamthochschule – Essen (Vice Chairman)

Guests:

Dr. E. GOEDECKE, Anmeldestelle Chemikaliengesetz, Dortmund
Frau Prof. Dr. U. GUNDELT-REMY, Fachgebiet 8, Bundesinstitut für Risikobewertung, Berlin
MinR Dr. H. A. KLEIN, Bundesministerium für Wirtschaft und Arbeit, Bonn
Dr. M. LULEI, Verband der Chemischen Industrie, Frankfurt am Main
Dr. N. RUPPRICH, Bundesanstalt für Arbeitsschutz und Arbeitsmedizin, Dortmund
Dr. K. STEINHÄUSER, Umweltbundesamt, Berlin

With the collaboration of:

Dr. T. BROSCARD, Merck KGaA, Darmstadt/Main
Dr. S. ETTTEL, Institut für Physikalische und Theoretische Chemie, Universität Essen
Frau Dr. H. GREIM, Technische Universität München, Weihenstephan
Dr. G.-R. JÄNIG, Fachgebiet 8, Bundesinstitut für Risikobewertung, Berlin
Frau Dr. B. LOHMANN, Essen
Frau Dr. I. NEUMANN, Technische Universität München, Weihenstephan
Frau Dipl.-Biol. B. PRIESMANN, Institut für Hydrobiologie, Technischen Universität Dresden
Frau Dr. B. SCHWARZ-SCHULZ, Umweltbundesamt, Berlin
Frau Dr. K. WIDMANN, Technische Universität München, Weihenstephan

Responsible at BMU:

MinR Prof. Dr. A. BASLER, Bundesministerium für Umwelt, Naturschutz und Reaktorsicherheit, Bonn

GDCh Office:

Dr. H. BEHRET, GDCh, Frankfurt am Main

N-Cetylpyridinium Chloride Monohydrate

BUA Report 247

(October 2003)

edited by the GDCh-Advisory Committee
on Existing Chemicals

GDCh-Beratergremium
für Altstoffe (BUA)



S. Hirzel

Wissenschaftliche Verlagsgesellschaft 2005

Dr. K. Begitt
Gesellschaft Deutscher Chemiker
Postfach 90 04 40
D-60444 Frankfurt am Main
E-Mail: buag@gdch.de
Homepage: <http://www.gdch.de>

Responsible at the BMU:
MinR Prof. Dr. A. Basler
BMU
Postfach 12 06 29
D-53048 Bonn
E-Mail: armin.basler@bmu.bund.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)

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.

Bibliographic information published by Die Deutsche Bibliothek
Die Deutsche Bibliothek lists this publication in the
Deutsche Nationalbibliografie; detailed bibliographic
data are available in the internet at <http://dnb.ddb.de>.

ISBN 3-7776-1419-X

ISBN 978-3-7776-1419-9

Translated by P. Karbe.

© 2005 S. Hirzel Verlag, Stuttgart

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.

Printed on acid-free and low-chlorine paper.

Printing and binding: Druckpartner Rübelmann GmbH, Hemsbach
Printed in 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. Since the beginning of 2001 the BUA has been composed of scientists from the research areas of chemistry, analytics, monitoring, toxicology, primary and secondary exposition, aquatic and terrestrial toxicology as well as the fate and behaviour of compounds in water, soil, air. The BUA is supported by experts from federal government agencies and the German Chemical Industry Association (Verband der Chemischen Industrie [VCI]).

No other national or international body has dealt with the ecological and health-related effects of as many existing chemicals as the BUA. Upon the recommendation of the federal government, the BUA has participated as a Peer-Review Group in the evaluation of ICCA-compounds (ICCA: International Council of Chemical Associations) since 2000 and also acts as the Contact Point in the OECD-HPV-Chemicals Programme (High Production Volume). The goal of the initiative is on the one hand to complete the data on the HPV chemicals and on the other to undertake an internationally coordinated evaluation of their hazard potential.

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 datasets for such substances each year, for which the BUA sets the priority. Comprehensive reports are published on chemicals suspected of having a hazard potential. If the data available for substance assessment are insufficient, the gaps in knowledge are documented and, if necessary, investigations recommended. On the national level, the BUA has produced comprehensive reports on about 330 substances and carried out preliminary evaluation and classification (priority-setting) for approximately 200 more. The processes leading to priority-setting and the BUA reports are published to lend transparency to the Committee's work.

Moreover, BUA, as a group of expert advisors, is increasingly addressing scientific questions and problems, which apply simultaneously to many compounds, among others: "Marine Risk Assessment: Concept and Criteria" (BUA Report 220), "Biological Impact of Synthetic and Natural Endocrine Active Substances – Effects on Human Health" (BUA Report 228), Risk Assessment of Substances in Soils" (BUA Report 230), Persistent Organic Pollutants (POPs) (BUA Report 232) and "Safety Factors in Toxicological Risk Assessment". For each of these themes an analysis is made of the scientific state of the art, is documented and the results published in reports such as the current volume. 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
October, 2003

Helmut Greim
BUA Chairman

Contents

List of Abbreviations	IX
Summary	XI
Data Gaps.....	XIII

N-CETYLPIRIDINIUM CHLORIDE MONOHYDRATE (CPC) **(CAS No. 6004-24-6)**

1	Characterisation of CPC	1
1.1	Chemical Identity	1
1.2	Composition of the Technical Product.....	1
1.3	Chemical and Physical Properties.....	1
2	Analysis	4
2.1	Environmental Samples.....	4
2.2	Detergents, Cosmetics, Pharmaceuticals and Other Sample Types	5
3	Production, Processing, Application, Environmental Emissions	9
3.1	Production.....	9
3.2	Processing, Application, Consumption Quantities.....	10
3.3	Atmospheric Emissions	10
3.4	Hydrospheric Emissions	10
3.5	Introduction into the Geosphere and Biosphere.....	11
3.6	Overview of Environmental Emissions	11
4	Environmental Occurrence	12
4.1	Occurrence in Environmental Compartments	12
4.2	Occurrence in Products	12
5	Environmental Behaviour	13
5.1	Biodegradation.....	13
5.2	Abiotic Degradation	13
5.3	Accumulation	14
5.4	Distribution in the Environment.....	15
5.5	Environmental Fate.....	16

6.	Ecotoxicity	17
6.1	Aquatic Organisms	17
6.2	Terrestrial Organisms	19
6.3	Eco-Systems	20
7	Toxicity in Warm-Blooded Animals	21
7.1	General Effects	21
7.2	Mechanism of Action	22
7.3	Toxicokinetics	22
7.4	Acute Toxicity	22
7.5	Subacute, Subchronic and Chronic Toxicity	24
7.6	Skin and Mucous Membrane Tolerance	26
7.7	Sensitisation	28
7.8	Genotoxicity	29
7.9	Carcinogenicity	29
7.10	Reproductive Toxicity	29
7.10.1	Fertility	29
7.10.2	Developmental Toxicity	30
7.11	Other Effects	30
7.12	Experiences in Humans	31
8	Substance-Specific Regulations	32
9	References	33
Annex: Data Set of the Merck Company		1 – 30