

# **The Handbook of Environmental Chemistry**

**Volume 3 Anthropogenic Compounds  
Part Q**

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# Phthalate Esters

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ISSN 1433-6847

ISBN 3-540-00992-2

DOI 10.1007/b11472

Springer-Verlag Berlin Heidelberg New York

## Library of Congress Cataloging-in-Publication Data

The Natural environment and the biogeochemical cycles / with contributions by P. Craig ... [et al.].

v. <A-F > : ill. ; 25 cm. – (The Handbook of environmental chemistry :

v. 1) Includes bibliographical references and indexes.

ISBN 0-387-09688-4 (U.S.) – ISBN 3-540-55255-3 (pt. F : Berlin). –

ISBN 0-387-55255-3 (pt. F : New York)

1. Biogeochemical cycles. 2. Environmental chemistry.

I. Craig, P. J., 1944- . II. Series.

QD31. H335 vol. 1 [QH344] 628.5 s

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Springer-Verlag Berlin Heidelberg New York

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Production Editor: Christiane Messerschmidt, Rheinau

Cover Design: E. Kirchner, Springer-Verlag

Typesetting: Fotosatz-Service Köhler GmbH, Würzburg

Printed on acid-free paper 52/3020 – 5 4 3 2 1 0

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## The Handbook of Environmental Chemistry Also Available Electronically

Environmental chemistry is a rather young and interdisciplinary field of science. Its aim is a complete description of the environment and of transformations occurring on a local or global scale. Environmental chemistry also gives an account of the impact of man's activities on the natural environment by describing observed changes.

"The Handbook of Environmental Chemistry" provides the compilation of today's knowledge. Contributions are written by leading experts with practical experience in their fields. The Handbook will grow with the increase in our scientific understanding and should provide a valuable source not only for scientists, but also for environmental managers and decision makers.

As a rule, contributions are specially commissioned. The editors and publishers will, however always be pleased to receive suggestions and supplements information. Papers for *The Handbook of Environmental Chemistry* are accepted in English.

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## Preface

Environmental Chemistry is a relatively young science. Interest in this subject, however, is growing very rapidly and, although no agreement has been reached as yet about the exact content and limits of this interdisciplinary discipline, there appears to be increasing interest in seeing environmental topics which are based on chemistry embodied in this subject. One of the first objectives of Environmental Chemistry must be the study of the environment and of natural chemical processes which occur in the environment. A major purpose of this series on Environmental Chemistry, therefore, is to present a reasonably uniform view of various aspects of the chemistry of the environment and chemical reactions occurring in the environment.

The industrial activities of man have given a new dimension to Environmental Chemistry. We have now synthesized and described over five million chemical compounds and chemical industry produces about hundred and fifty million tons of synthetic chemicals annually. We ship billions of tons of oil per year and through mining operations and other geophysical modifications, large quantities of inorganic and organic materials are released from their natural deposits. Cities and metropolitan areas of up to 15 million inhabitants produce large quantities of waste in relatively small and confined areas. Much of the chemical products and waste products of modern society are released into the environment either during production, storage, transport, use or ultimate disposal. These released materials participate in natural cycles and reactions and frequently lead to interference and disturbance of natural systems.

Environmental Chemistry is concerned with reactions in the environment. It is about distribution and equilibria between environmental compartments. It is about reactions, pathways, thermodynamics and kinetics. An important purpose of this Handbook, is to aid understanding of the basic distribution and chemical reaction processes which occur in the environment.

Laws regulating toxic substances in various countries are designed to assess and control risk of chemicals to man and his environment. Science can contribute in two areas to this assessment; firstly in the area of toxicology and secondly in the area of chemical exposure. The available concentration ("environmental exposure concentration") depends on the fate of chemical compounds in the environment and thus their distribution and reaction behaviour in the environment. One very important contribution of Environmental Chemistry to the above mentioned toxic substances laws is to develop laboratory test methods, or mathematical correlations and models that predict the environ-

mental fate of new chemical compounds. The third purpose of this Handbook is to help in the basic understanding and development of such test methods and models.

The last explicit purpose of the Handbook is to present, in concise form, the most important properties relating to environmental chemistry and hazard assessment for the most important series of chemical compounds.

At the moment three volumes of the Handbook are planned. Volume 1 deals with the natural environment and the biogeochemical cycles therein, including some background information such as energetics and ecology. Volume 2 is concerned with reactions and processes in the environment and deals with physical factors such as transport and adsorption, and chemical, photochemical and biochemical reactions in the environment, as well as some aspects of pharmacokinetics and metabolism within organisms. Volume 3 deals with anthropogenic compounds, their chemical backgrounds, production methods and information about their use, their environmental behaviour, analytical methodology and some important aspects of their toxic effects. The material for volume 1, 2 and 3 was each more than could easily be fitted into a single volume, and for this reason, as well as for the purpose of rapid publication of available manuscripts, all three volumes were divided in the parts A and B. Part A of all three volumes is now being published and the second part of each of these volumes should appear about six months thereafter. Publisher and editor hope to keep materials of the volumes one to three up to date and to extend coverage in the subject areas by publishing further parts in the future. Plans also exist for volumes dealing with different subject matter such as analysis, chemical technology and toxicology, and readers are encouraged to offer suggestions and advice as to future editions of "The Handbook of Environmental Chemistry".

Most chapters in the Handbook are written to a fairly advanced level and should be of interest to the graduate student and practising scientist. I also hope that the subject matter treated will be of interest to people outside chemistry and to scientists in industry as well as government and regulatory bodies. It would be very satisfying for me to see the books used as a basis for developing graduate courses in Environmental Chemistry.

Due to the breadth of the subject matter, it was not easy to edit this Handbook. Specialists had to be found in quite different areas of science who were willing to contribute a chapter within the prescribed schedule. It is with great satisfaction that I thank all 52 authors from 8 countries for their understanding and for devoting their time to this effort. Special thanks are due to Dr. F. Boschke of Springer for his advice and discussions throughout all stages of preparation of the Handbook. Mrs. A. Heinrich of Springer has significantly contributed to the technical development of the book through her conscientious and efficient work. Finally I like to thank my family, students and colleagues for being so patient with me during several critical phases of preparation for the Handbook, and to some colleagues and the secretaries for technical help.

I consider it a privilege to see my chosen subject grow. My interest in Environmental Chemistry dates back to my early college days in Vienna. I received significant impulses during my postdoctoral period at the University of California and my interest slowly developed during my time with the National Research



Council of Canada, before I could devote my full time of Environmental Chemistry, here in Amsterdam. I hope this Handbook may help deepen the interest of other scientists in this subject.

Amsterdam, May 1980

*O. Hutzinger*

Twentyone years have now passed since the appearance of the first volumes of the Handbook. Although the basic concept has remained the same changes and adjustments were necessary.

Some years ago publishers and editors agreed to expand the Handbook by two new open-end volume series: Air Pollution and Water Pollution. These broad topics could not be fitted easily into the headings of the first three volumes. All five volume series are integrated through the choice of topics and by a system of cross referencing.

The outline of the Handbook is thus as follows:

1. The Natural Environment and the Biochemical Cycles,
2. Reaction and Processes,
3. Anthropogenic Compounds,
4. Air Pollution,
5. Water Pollution.

Rapid developments in Environmental Chemistry and the increasing breadth of the subject matter covered made it necessary to establish volume-editors. Each subject is now supervised by specialists in their respective fields.

A recent development is the accessibility of all new volumes of the Handbook from 1990 onwards, available via the Springer Homepage <http://www.springer.de> or <http://Link.springer.de/series/hec/> or <http://Link.springer.com/series/hec/>.

During the last 5 to 10 years there was a growing tendency to include subject matters of societal relevance into a broad view of Environmental Chemistry. Topics include LCA (Life Cycle Analysis), Environmental Management, Sustainable Development and others. Whilst these topics are of great importance for the development and acceptance of Environmental Chemistry Publishers and Editors have decided to keep the Handbook essentially a source of information on "hard sciences".

With books in press and in preparation we have now well over 40 volumes available. Authors, volume-editors and editor-in-chief are rewarded by the broad acceptance of the "Handbook" in the scientific community.

Bayreuth, July 2001

*Otto Hutzinger*

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## Foreword

Phthalate ester plasticizers are widely used and commercially very important products that are primarily used in commercial applications to make vinyl products. These compounds have been in commercial use for several decades. Simultaneously with their long use has been the conduct of scientific research related to their physical properties, analytical chemistry, abiotic and biological degradation, effects on human and ecological health, exposure, and risk assessment. Literally thousands of studies and experiments with these compounds have been conducted by scientists employed by academia, industry and governments over the course of decades. Scientists from every continent have participated in such research. All of these data are available to support the close regulatory scrutiny to which these compounds are subject.

Adding to the complexity of this large database, the properties of phthalate ester plasticizers and hence their commercial applications vary widely across the class of compounds. Thus, a research result obtained for one compound cannot necessarily be directly extrapolated to the class of compounds and therefore, research has been needed to cover the full range of phthalate ester plasticizers. Given the large body of research available for phthalate esters, it becomes necessary and hopefully useful to compile relevant research results in such a way as to make the data accessible, to critically review all the data for quality and relevance issues, and to provide useful and appropriate context for the information. This book seeks to accomplish these tasks.

Thus, the aim of this book is to bring together the available data on phthalate esters to be used by scientists and their students who may be new to this field, by regulatory experts charged with managing these compounds, and by practicing scientists who need relevant information regarding phthalate esters to support their own studies. This book is divided into chapters that have been prepared by invited scientists who have worked with these compounds. The first chapter introduces the phthalate esters as a class of compounds and identifies the specific compounds that are the subject of this book. The second chapter deals with the analytical chemistry of phthalate esters. Besides a review of the various highly sensitive methods now available for these compounds in a wide variety of media, this chapter reviews the tremendous analytical challenges facing the chemist due to the well-documented interferences they cause. The next chapters deal with aspects of how phthalate esters behave in the environment. The physical properties are defined and used to support evaluative fate modeling. Environmental degradation processes are then reviewed and used to support more

extensive multi-media fate modeling. Modeling results are compared with measured observations from the environment. Moving to the biosphere, an extensive field study of the accumulation of phthalate esters in a marine food web is presented. The next chapters deal with the definition of critical pathways of exposure to phthalate esters, and review of the effects of these substances on humans and other biota. The last chapter deals with potential risks to sediment and soil dwelling organisms.

In support of full disclosure, the professional affiliation of each co-author is disclosed on the first page of each chapter. Many of the co-authors are scientists who work with industry, including the producers of these compounds, while other co-authors are academics. In all cases, there have been long and fruitful collaborations between industry and academic scientists to further the research agenda.

The preparation of this book has been both challenging and rewarding. The challenge has been that the immense amount of information that is available has been somewhat of a double-edged sword. On one side, a wealth of data on a chemical substance is vital to understanding its potential impact on human health and the environment and on the other side, it can be difficult to fully and appropriately utilize all the data that are available. The reward has been the close work with so many scientists truly well versed in the subject of their research.

Fairfax, June 2003

*Charles A. Staples*