Horst Surburg and Johannes Panten

Common Fragrance and Flavor Materials

Preparation, Properties and Uses 5th completely revised and enlarged edition



WILEY-VCH Verlag GmbH & Co. KGaA

Horst Surburg and Johannes Panten

Common Fragrance and Flavor Materials

Related Titles

Ziegler, H. (ed.) Flavourings Production, Composition, Applications, Regulations 2nd edition, 2006, ISBN 3-527-31406-7

Kraft, Philip; Swift, Karl A. D. (eds.) Perspectives in Flavor and Fragrance Chemistry 2005, ISBN: 3-906-390-36-5

Oetjen, G.-W., Haseley, P. Freeze-Drying 2004, ISBN 3-527-30620-X

Mollet, H., Grubenmann, A. Formulation Technology Emulsions, Suspensions, Solid Forms 2001, ISBN 3-527-30201-8 Horst Surburg and Johannes Panten

Common Fragrance and Flavor Materials

Preparation, Properties and Uses 5th completely revised and enlarged edition



WILEY-VCH Verlag GmbH & Co. KGaA

The Authors

Dr. Horst Surburg Symrise GmbH & C. KG RD Synthesis Mühlenfeldstr. 1 37603 Holzminden

Dr. Johannes Panten Symrise GmbH & C. KG RD Synthesis Mühlenfeldstr. 1 37603 Holzminden

1st edition 1985 2nd, revised edition 1990 3rd, completely revised edition 1997 4th, completely revised edition 2001 5th, completely revised and enlarged edition 2006

All books published by Wiley-VCH are carefully produced. Nevertheless, authors, editors, and publisher do not warrant the information contained in these books, including this book, 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.

Library of Congress Card No.: applied for.

British Library Cataloguing-in-Publication Data:

A catalogue record for this book is available from the British Library.

Bibliographic information published by Die Deutsche Bibliothek

Die Deutsche Bibliothek lists this publication in the Deutsche Nationalbibliografie; detailed bibliographic data is available in the Internet at http://dnb.ddb.de

© 2006 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim

All rights reserved (including those of translation into other languages). No part of this book may be reproduced in any form – by photoprinting, microfilm, or any other means – nor transmitted or translated into a machine language without written permission from the publishers. Registered names, trademarks etc. used in this book, even when not specifically marked as such, are not to be considered unprotected by law.

Printed in the Federal Republic of Germany Printed on acid-free paper

Cover Design4t Matthes + Traut, DarmstadtCompositionMitterweger & Partner, Kommunikationsgesellschaft mbH, PlankstadtPrintingbetz-druck GmbH, DarmstadtBookbindingLitges & Dopf Buchbinderei GmbH, Heppenheim

ISBN-13: 978-3-527-31315-0 **ISBN-10:** 3-527-31315-X

Contents

1	Introduction 1
1.1 1.2 1.3 1.4	History1Definition2Physiological Importance2Natural, Nature-identical, and Artificial Products3
1.5	Sensory Properties and Structure
1.6	Volatility
1.7	Odor Description 4
2	Individual Fragrance and Flavor Materials 7
2.1	Aliphatic Compounds
2.1.1	Hydrocarbons
2.1.2	Alcohols
2.1.3	Aldehydes and Acetals 12
2.1.4	Ketones
2.1.5	Acids and Esters 18
2.1.6	Miscellaneous Compounds
2.2	Acyclic Terpenes
2.2.1	Hydrocarbons
2.2.2	Alcohols
2.2.3	Aldenydes and Acetals
2.2.4	Acids and Esters 45
2.2.5	Miscellaneous Compounds 49
2.2.0	Cyclic Tornonos
2.3	Hydrocarbons 51
2.3.1	Alcohols and Ethers 54
2.3.3	Aldehydes and Ketones
2.3.4	Esters
2.3.5	Miscellaneous Compounds
2.4	Other Cycloaliphatic Compounds
2.4.1	Alcohols and Ethers
2.4.2	Aldehydes
2.4.3	Ketones
2.4.4	Esters
2.4.5	Miscellaneous Compounds

VI Contents

Aromatic Compounds	
Hydrocarbons	105
Alcohols and Ethers	105
Aldehydes and Acetals	111
Ketones	119
Esters of Araliphatic Alconois and Aliphatic Acids	124
Aromatic Acids	127
Miscellaneous Compounds	130
Phenols and Phenol Derivatives	132
Phenols, Phenyl Esters, and Phenyl Ethers	132
Phenol Alcohols and their Esters	139
Phenol Aldehydes	140
Phenol Ketones	145
	140
O-, O,S- and S,S-Heterocycles	149
Cyclic Ethers	149
Lactones	162
Glycidates	1/1
N- and N S-Heterocycles	172
	172
Natural Raw Materials in the Flavor and Fragrance Industry	177
Introduction	177
	1//
Isolation of Natural Fragrance and Flavor Concentrates	178
Isolation of Natural Fragrance and Flavor Concentrates Essential Oils Essential Oils Essential Oils Essential Oils	177 178 179
Isolation of Natural Fragrance and Flavor Concentrates Essential Oils Extracts	177 178 179 180
Isolation of Natural Fragrance and Flavor Concentrates Essential Oils Extracts Survey of Natural Raw Materials	177 178 179 180 181
Isolation of Natural Fragrance and Flavor Concentrates Essential Oils Extracts Survey of Natural Raw Materials Analytical Methods/Quality Control	177 178 179 180 181 239
Isolation of Natural Fragrance and Flavor Concentrates Essential Oils Extracts Survey of Natural Raw Materials Analytical Methods/Quality Control Safety Evaluation and Legal Aspects	177 178 179 180 181 239 241
Isolation of Natural Fragrance and Flavor Concentrates Essential Oils Extracts Survey of Natural Raw Materials Analytical Methods/Quality Control Safety Evaluation and Legal Aspects Flavoring Substances	177 178 179 180 181 239 241 241
Isolation of Natural Fragrance and Flavor Concentrates Essential Oils Extracts Survey of Natural Raw Materials Analytical Methods/Quality Control Safety Evaluation and Legal Aspects Flavoring Substances Fragrance Materials	177 178 179 180 181 239 241 241 242
Isolation of Natural Fragrance and Flavor Concentrates Essential Oils Extracts Survey of Natural Raw Materials Analytical Methods/Quality Control Safety Evaluation and Legal Aspects Flavoring Substances Fragrance Materials References	177 178 179 180 181 239 241 241 242 245
Isolation of Natural Fragrance and Flavor Concentrates Essential Oils Extracts Survey of Natural Raw Materials Analytical Methods/Quality Control Safety Evaluation and Legal Aspects Flavoring Substances Fragrance Materials References Formula Index: CAS Registry Number Index	177 178 179 180 181 239 241 241 242 245 289
	Hydrocarbons Alcohols and Ethers Aldehydes and Acetals Aldehydes and Acetals Ketones Esters of Araliphatic Alcohols and Aliphatic Acids Aromatic Acids Esters Derived from Aromatic and Araliphatic Acids Miscellaneous Compounds Phenols and Phenol Derivatives Phenols, Phenyl Esters, and Phenyl Ethers Phenol Alcohols and their Esters Phenol Aldehydes Phenol Ketones Phenol carboxylates O-, O,S- and S,S-Heterocycles Cyclic Ethers Lactones Glycidates Miscellaneous Compounds

Preface to the Fifth Edition

In the last two decades, "Common Fragrance and Flavor Materials" has developed to become probably the most cited standard work in the field of fragrance and flavor chemistry, and continual demand has now made it necessary to publish a new edition.

With regard to the contents, an update was required for several reasons, as some remarkable changes in the compositions of perfume oils – increasing use of macrocyclic musk materials has been observed, for example – have occurred since the publication of the 4^{th} edition. Consequently, chapter 2 has had to be extended with some new monographs.

Some other trend-setting materials have also had to be included, whilst other materials that had lost their importance have had to be eliminated.

The changes in the landscape of fragrance and flavor materials producers also required corresponding adjustments.

The class of cooling agents – materials that create a cold sensation on skin or mucosa – has been admitted for the first time. Although known in principle for a long time, cooling agents have recently acquired increasing importance.

Chapter 3 has been partly revised and updated with regard to recent literature. Since it is impossible to cite the whole literature comprehensively, it was decided to refer to current review literature where possible. Otherwise, some of the very recent original references have been cited.

In general, the successful conception of this book, established about 20 years ago by Kurt Bauer and Dorothea Garbe, has been maintained. For a long time both of these authors worked in the research department of the flavor and fragrance company Haarmann & Reimer in Holzminden, Germany, Kurt Bauer as director of research and Dorothea Garbe as head of the department for scientific literature and documentation. Both retired some years ago and are therefore no longer engaged in the preparation of the 5th edition.

The responsible authors are now Horst Surburg and Johannes Panten, both of whom work in the synthesis department of the corporate research division of "Symrise", the company formed by the merger of the flavor and fragrance houses "Dragoco" and "Haarmann & Reimer" in Holzminden.

Both authors are indebted to many colleagues for their support and to the management of Symrise for the opportunity to prepare the 5th edition of this book.

December, 2005

Horst Surburg Johannes Panten

Preface to the Fourth Edition

The constant interest in "Common Fragrance and Flavor Materials" has encouraged us to proceed with the publication of a new edition within a relatively short period of time. The proven concept of the book has remained unchanged because of positive feedback from readers.

After a critical examination of the text, some material that has lost significance has been removed. A certain amount of new material, mainly components that have influenced modern fragrance trends over the past few years, have been added. The literature references in the chapter on "Natural Raw Materials" have been updated and the newest international standards for the characterization of materials have been included.

The authors would like to point out particularly that the present book can only provide a selection of the many commercially available fragrance and flavor materials. Also not included are compounds with exclusive uses that are not commonly/generally available ("captives") as well as substances that are too new to be judged as to whether they will find a successful place in the market. Analytical data on natural raw materials that can be obtained by means of new analytical techniques are not explicitly mentioned if the analytical techniques have not yet reached international standardization. However, reference is made to this in the corresponding literature and in the chapter on "Quality Control."

We thank our critics for numerous suggestions and we especially thank our colleagues, who prompted our work on the new edition through their kind support.

Holzminden, June 2001

K. BauerD. GarbeH. Surburg

Preface to the Third Edition

Twelve years after its first publication comes the third edition of "Common Fragrance and Flavor Materials". The content has been updated in many respects while retaining the proven concept.

In the case of the single-component fragrance and flavor materials, those compounds have been included which have become established on the market, as well as those which have attracted considerable interest on account of their outstanding organoleptic properties and have contributed to the composition of new fragrance types. The production processes for all fragrance and flavor materials described in the book have been critically reviewed. New processes have been taken into account, and those that are clearly outdated have been eliminated. A few compounds that have declined in importance or whose use is now restricted for toxicological reasons have been removed from the text, as have several essential oils. The latest publications and standards concerning essential oils and natural raw materials have been included in the new edition, making it an up-to-date reference work. For the first time references are cited for all essential oils, giving newcomers to the field a quick overview of the original literature. The chapters on quality control and product safety have been expanded and brought up to date.

The authors wish to thank all the colleagues whose specialist advice assisted us in revising the book.

Holzminden, February 1997

K. BauerD. GarbeH. Surburg

Preface to the Second Edition

Within three years of publication the first edition of "Common Fragrance and Flavor Materials" was out of print and is now followed by this second edition. As in the case of the first edition this book is based mainly on a chapter on "Flavors and Fragrances" which has since been published in English in Ullmann's Encyclopedia of Industrial Chemistry.

We would like to thank our readers for their suggestions for improvement and further development of the contents which were contained in several book reviews. We have not followed up all the suggestions for the simple reason that we did not wish to change the character of the book, which is expressly aimed at a general audience interested in commonly used fragrance and flavor materials, and not at experts in the field.

The chapter on "Single Fragrance and Flavor Compounds" has been updated to include new developments, production methods have been brought up-to-date and CAS registry numbers have been added to all single compounds described. The former chapters "Essential Oils" and "Animal Secretions" have been grouped together under the heading "Natural Raw Materials in the Flavor and Fragrance Industry" and thoroughly revised to include new literature references.

Holzminden, February 1990

K. BauerD. GarbeH. Surburg

Preface to the First Edition

Fragrance and flavor materials are used in a wide variety of products, such as soaps, cosmetics, toiletries, detergents, alcoholic and non-alcoholic beverages, ice cream, confectioneries, baked goods, convenience foods, tobacco products, and pharmaceutical preparations. This book presents a survey of those natural and synthetic fragrance and flavor materials which are produced commercially on a relatively large scale, or which are important because of their specific organoleptic properties. It provides information concerning their properties, methods employed in their manufacture, and areas of application. Therefore, the book should be of interest to anyone involved or interested in fragrance and flavor, e.g., perfumers, flavorists, individuals active in perfume and flavor application, food technologists, chemists, and even laymen.

The book is, essentially, a translation of the chapter on fragrance and flavor materials in Ullmanns Encyklopädie der technischen Chemie, Volume 20, 4th Edition, Verlag Chemie GmbH, Weinheim (Federal Republic of Germany), 1981. The original (German) text has been supplemented by inclusion of recent developments and of relevant information from other sections of the Encyclopedia. The present English version will make the information available to a wider circle of interested readers.

The condensed style of presentation of "Ullmann's" has been maintained. A more detailed treatment of various items and aspects was considered but was believed to be outside the scope of this book. Additional information, however, can be obtained from the literature cited.

To improve its usefulness, the book contains

- a formula index, including CAS registry numbers;
- an alphabetical index of single fragrance and flavor compounds, essential oils, and animal secretions.

Starting materials and intermediates are not covered by these indexes. The authors wish to express their gratitude to:

- Haarmann & Reimer Company, in particular to its General Manager, Dr. C. Skopalik, who suggested the publication of this book in English and who, at an earlier stage, provided time and facilities for writing the chapter on fragrance and flavor materials in Ullmanns Encyklopädie der technischen Chemie (1981), and to Dr. Hopp, Vice President Research, for valuable additions to his book;
- all others who provided information and suggestions for the chapter in Ullmann's Encyclopedia and thereby for this book.

XII Preface to the First Edition

The authors are most grateful to Dr. J. J. Kettenes-van den Bosch and Dr. D. K. Kettenes for translating the original German text into English and for their suggestions and help in shaping the present book. Drs. Kettenes thank Mr. W. S. Alexander, Hockessin, Delaware (USA), for critically reviewing the English.

Holzminden, June 1984

K. Bauer D. Garbe

1 Introduction

1.1 History

Since early antiquity, spices and resins from animal and plant sources have been used extensively for perfumery and flavor purposes, and to a lesser extent for their observed or presumed preservative properties. Fragrance and flavor materials vary from highly complex mixtures to single chemicals. Their history began when people discovered that components characteristic of the aroma of natural products could be enriched by simple methods. Recipes for extraction with olive oil and for distillation have survived from pre-Christian times to this day.

Although distillation techniques were improved, particularly in the 9th century A.D. by the Arabs, the production and application of these concoctions remained essentially unchanged for centuries. Systematic development began in the 13th century, when pharmacies started to prepare so-called remedy oils and later recorded the properties and physiological effects of these oils in pharmacopoeias. Many essential oils currently used by perfumers and flavorists were originally prepared by distillation in pharmacies in the 16th and 17th centuries.

Another important step in the history of natural fragrance materials occurred in the first half of the 19th century, when the production of essential oils was industrialized due to the increased demand for these oils as perfume and flavor ingredients. Around 1850, single organic compounds were also used for the same purposes. This development resulted from the isolation of cinnamaldehyde from cinnamon oil by DUMAS and PÈLIGOT in 1834, and the isolation of benzaldehyde from bitter almond oil by LIEBIG and WöHLER in 1837. The first synthetic "aroma oils" were introduced between 1845 and 1850. These consisted of lower molecular mass fatty acid esters of several alcohols and were synthesized by the chemical industry for their fruity odor. Methyl salicylate followed in 1859 as "artificial wintergreen oil" and benzaldehyde in 1870 as "artificial bitter almond oil." With the industrial synthesis of vanillin (1874) and coumarin (1878) by Haarmann & Reimer (Holzminden, Federal Republic of Germany), a new branch of the chemical industry was founded.

The number of synthetically produced fragrance and flavor chemicals has since expanded continually as a result of the systematic investigation of essential oils and fragrance complexes for odoriferous compounds. Initially, only major components were isolated from natural products; their structure was then elucidated and processes were developed for their isolation or synthesis. With the development of modern analytical techniques, however, it became possible to isolate and identify characteristic fragrance and flavor substances that occur in the natural products in only trace amounts. The isolation and structure elucidation of these components re-