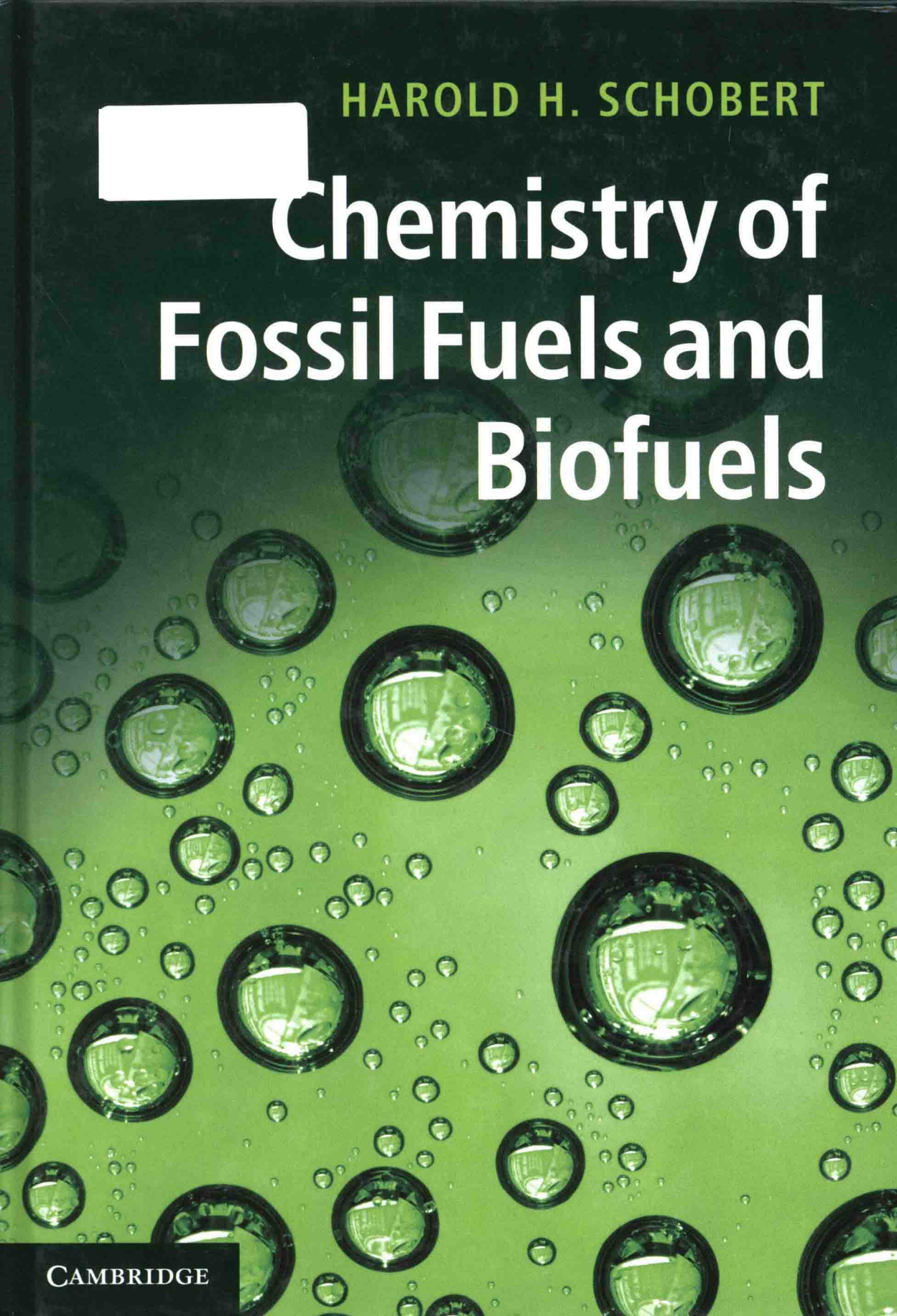
HAROLD H. SCHOBERT

Chemistry of Fossil Fuels and Biofuels



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Chemistry of Fossil Fuels and Biofuels

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The Pennsylvania State University
and
North-West University

CAMBRIDGE
UNIVERSITY PRESS

CAMBRIDGE UNIVERSITY PRESS
Cambridge, New York, Melbourne, Madrid, Cape Town,
Singapore, São Paulo, Delhi, Mexico City

Cambridge University Press
The Edinburgh Building, Cambridge CB2 8RU, UK

Published in the United States of America by
Cambridge University Press, New York

www.cambridge.org
Information on this title: www.cambridge.org/9780521114004

First published 2013

Printed and bound in the United Kingdom by the MPG Books Group

A catalog record for this publication is available from the British Library

Library of Congress Cataloging-in-Publication Data

Schobert, Harold H., 1943–
Chemistry of fossil fuels and biofuels / Harold Schobert.
p. cm. – (Cambridge series in chemical engineering)
ISBN 978-0-521-11400-4 (Hardback)
1. Fossil fuels–Analysis. 2. Biomass energy. 3. Energy crops–Composition.
4. Fuelwood crops–Composition. I. Title.
TP318.S368 2012
553.2–dc23

2012020435

ISBN 978-0-521-11400-4 Hardback

Chemistry of Fossil Fuels and Biofuels

Focusing on today's major fuel resources – ethanol, biodiesel, wood, natural gas, petroleum products, and coal – this book discusses the formation, composition and properties of the fuels, and the ways in which they are processed for commercial use. The book examines the origin of fuels through natural processes such as photosynthesis and the geological transformation of ancient plant material; the relationships between their composition, molecular structures, and physical properties; and the various processes by which they are converted or refined into the fuel products appearing on today's market. Fundamental chemical aspects such as catalysis and the behaviour of reactive intermediates are presented, and global warming and anthropogenic carbon dioxide emissions are also discussed. The book is suitable for graduate students in energy engineering, chemical engineering, mechanical engineering, and chemistry, as well as for professional scientists and engineers.

Harold H. Schobert is Professor Emeritus of Fuel Science, The Pennsylvania State University, and Extra-ordinary Professor, Coal Research Group, North-West University. A recognized leading authority on energy technology, he has over 30 years' experience in teaching and research on fuel chemistry.

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"The book is a welcome modern update to the available literature regarding the genesis, characteristics, processing and conversion of fossil and bio-derived fuels. Its comprehensive coverage of the chemistry involved with each of these aspects makes it an important source for upper-level undergraduates, graduate students, and professionals who need a strong understanding of the field. It is an interesting read for anyone who really wants to understand the nature of fuels."

Robert G. Jenkins, University of Vermont

"There is no other book like this in field of energy science. It is the perfect introduction to the topic; but Professor Schobert has packed so much in, that it is just as much a valuable reference for more experienced professionals. It touches on all aspects of fuel formation, transformation and use as well as strategies for managing the end product, carbon dioxide. I will be using it as a text in my own teaching to both senior undergraduate and graduate students."

Alan L. Chaffee, Monash University, Australia

"This is an excellent reference for the student of modern fuel science or the practitioner wishing to sharpen their 'big-picture' understanding of the field. The book offers a seasoned balance between technical rigor and readability, providing many helpful references for the reader interested in further study. I found the text engaging and enlightening, with the end-of-chapter notes a particularly thought-provoking and entertaining bonus."

Charles J. Mueller, Sandia National Laboratories

Preface

About twenty years ago I wrote a short book, *The Chemistry of Hydrocarbon Fuels**, that was based on lectures I had been giving at Penn State University for a course on Chemistry of Fuels. In the years since, that book has long been out of print, and the energy community has seen a significant increase in interest in biofuels, and concern for carbon dioxide emissions from fuel utilization. It seemed time, therefore, for a new book in the area. While this present book owes much to the earlier one, the changes are so extensive that it is not simply a second edition of its predecessor, but merits a new title and new organization of chapters.

The life cycle of any fuel begins with its formation in nature, followed by its harvesting or extraction. Many fuels then undergo one or more processes of refining, upgrading, or conversion to improve their properties or to remove undesirable impurities. Finally, the fuel is put to use, usually in a combustion process, but sometimes by further conversion to useful materials such as carbon products or polymers. *Chemistry of Fossil Fuels and Biofuels* focuses primarily on the origins of fuels, their chemical constitution and physical properties, and the chemical reactions involved in their refining or conversion. Most fuels are complex mixtures of compounds or have macromolecular structures that are, in some cases, ill-defined. But that does not mean that we throw away the laws of chemistry and physics in studying these materials. The composition, molecular structures, and properties of fuels are not some curious, random outcome of nature, but result from straightforward chemical processes. Any use of the fuels necessarily involves breaking and forming chemical bonds.

This book has been written for several potential audiences: those who are new to the field of fuel and energy science, especially students, who seek an introduction to fuel chemistry; practicing scientists or engineers in any field who feel that some knowledge of fuel chemistry would be of use in their activities; and fuel scientists who have been specializing in one type of fuel but who would like to learn about other fuels. I have presumed that the reader of this book will have had an introductory course in organic chemistry, so is familiar with the basic principles of structure, nomenclature, and reactivity of functional groups. I have also presumed that the reader is familiar with aspects of the descriptive inorganic chemistry of the major elements of importance in fuels, and with some of the basic principles of physical chemistry. As a textbook, this book would therefore be suitable for third- or fourth-year undergraduates or first-year graduate students in the physical sciences or engineering. However, anyone with some elementary knowledge of chemistry and who is willing to refer to other appropriate texts as needed could certainly derive much from this book.

Our civilization once relied almost entirely on biomass fuel (wood) for its energy needs. Then, for about two centuries, the fossil fuels – coal, oil, and natural gas – have dominated the energy scene. In recent decades biomass has experienced increasing interest – a revival of interest in wood, as well as ethanol and biodiesel. Anything that we do in daily life requires use of energy, and, in most parts of the world, much of that energy derives from using fossil or biofuels. Despite the critical importance of fuels, few, if any, texts in introductory chemistry or organic chemistry give more than passing mention to these resources. So, I hope that this book might also be of use to chemists or chemical engineers curious to learn about new areas.

This book does not intend, nor pretend, to provide encyclopedic coverage of fuel formation or of refining and conversion processes. At the end of each chapter I have provided a number of suggested sources for those wishing to probe further. The material in the book is the distillation of having taught Chemistry of Fuels at least twenty times to students in fuel science, energy engineering, and chemical engineering. The course has changed somewhat each year, incorporating student feedback as appropriate. The person using this book, either as a textbook or for self-study, should become equipped with enough knowledge then to follow his or her interests with confidence in the professional journals or monographs in the field.

**The Chemistry of Hydrocarbon Fuels*, London, Butterworths, 1990.

Acknowledgments

I could not have done this without the help and support of my dear wife Nita, who assisted in many, many ways. This book has been developed from more than twenty years' worth of notes for a course, Chemistry of Fuels, that I taught at Penn State University. Every year I started over again making entirely new notes for the lectures. My good friend and colleague, Omer Gül, provided invaluable assistance in converting many of my hand-drawn sketches, used off and on for years, into diagrams for this book. Two staff assistants, Carol Brantner and Nicole Arias, typed some of the versions of hand-written notes and created some of the diagrams. Their work was of great help in pulling the manuscript together. Lee Ann Nolan and Linda Musser, of the Fletcher Byrom Earth and Mineral Sciences Library at Penn State, helped in tracking down information, particularly biographical sketches of fuel scientists. I am also indebted to the staff of the Shakopee branch of the Scott County (Minnesota) Library, who made me welcome and provided a quiet room to work on visits to Minnesota. Many friends and colleagues at Penn State, especially Gary Mitchell and Caroline Clifford, helped in many different ways to provide information or ideas. Professor Christien Strydom, Director of the School of Physical and Chemical Sciences, North-West University, Potchefstroom, South Africa, helped by providing office space and computer access, as well as many splendid discussions. Many other friends at North-West and at Sasol provided assistance in various ways as well. Mohammad Fatemi, President of Middle East PetroChem Engineering and Technology, generously provided the software used to create the chemical structures and reactions. The two people at Cambridge University Press with whom I have worked, Michelle Carey and Sarah Marsh, deserve thanks for their long-suffering perseverance that would make Job seem a pretty impatient fellow. Finally, special thanks are due to the generations of students in Chemistry of Fuels, whose comments and suggestions were actually listened to, and often useful. Despite all this help, which I am very pleased to acknowledge and thank, any mistakes are my own.

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