



CHEMISTRY and PHYSICS of COMPLEX MATERIALS

Concepts and Applications

Editors

Maria Rajkiewicz, DSc

Wiktor Tyszkiewicz, PhD

Zbigniew Wertejuk, PhD



Apple Academic Press



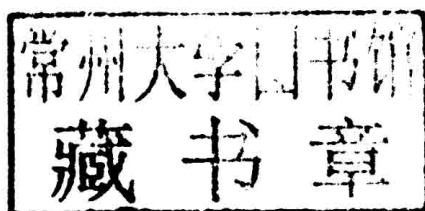
CRC Press
Taylor & Francis Group

CHEMISTRY AND PHYSICS OF COMPLEX MATERIALS

Concepts and Applications

Edited by

**Maria Rajkiewicz, DSc, Wiktor Tyszkiewicz, PhD,
and Zbigniew Wertejuk, PhD**



Apple Academic Press

TORONTO NEW JERSEY

Apple Academic Press Inc.
3333 Mistwell Crescent
Oakville, ON L6L 0A2
Canada

Apple Academic Press Inc.
9 Spinnaker Way
Waretown, NJ 08758
USA

©2014 by Apple Academic Press, Inc.

Exclusive worldwide distribution by CRC Press, a member of Taylor & Francis Group

No claim to original U.S. Government works

Printed in the United States of America on acid-free paper

International Standard Book Number-13: 978-1-926895-60-4 (Hardcover)

This book contains information obtained from authentic and highly regarded sources. Reprinted material is quoted with permission and sources are indicated. Copyright for individual articles remains with the authors as indicated. A wide variety of references are listed. Reasonable efforts have been made to publish reliable data and information, but the authors, editors, and the publisher cannot assume responsibility for the validity of all materials or the consequences of their use. The authors, editors, and the publisher have attempted to trace the copyright holders of all material reproduced in this publication and apologize to copyright holders if permission to publish in this form has not been obtained. If any copyright material has not been acknowledged, please write and let us know so we may rectify in any future reprint.

Trademark Notice: Registered trademark of products or corporate names are used only for explanation and identification without intent to infringe.

Library of Congress Control Number: 2013951881

Library and Archives Canada Cataloguing in Publication

Chemistry and physics of complex materials: concepts and applications/edited by
Maria Rajkiewicz, DSc, Wiktor Tyszkiewicz, PhD, and Zbigniew Wertekuk, PhD.

Includes bibliographical references and index.

ISBN 978-1-926895-60-4

1. Materials. 2. Materials--Analysis. 3. Chemistry, Technical. 4. Materials science.

I. Rajkiewicz, Maria, editor of compilation II. Tyszkiewicz, Wiktor, editor of compilation

III. Wertekuk, Zbigniew, editor of compilation

TA403.6.C54 2013

620.1'1

C2013-906848-1

Apple Academic Press also publishes its books in a variety of electronic formats. Some content that appears in print may not be available in electronic format. For information about Apple Academic Press products, visit our website at www.appleacademicpress.com and the CRC Press website at www.crcpress.com

CHEMISTRY AND PHYSICS OF COMPLEX MATERIALS

Concepts and Applications

ABOUT THE EDITORS

Maria Rajkiewicz, DSc

Professor Maria Rajkiewicz is Head of the Division of the Institute for Engineering of Polymer Materials and Dyes, in Warsaw, Poland. She is a well-known specialist in the field of synthesis, investigation of properties and applications of low molecular compounds, oligomers, polymers, composites, and nanocomposites. She is a contributor or co-contributor to several monographs and the author of about 100 original papers.

Wiktor Tyszkiewicz, PhD

Wiktor Tyszkiewicz, PhD, is Professor at the Military Institute of Chemistry and Radiometry in Warsaw, Poland. He has a long and varied career, including being a member of the Polish Delegation to ICCS in Vietnam; he has participated in many NATO workshops on environmental problems emanating from military installations and activities. He has headed the Biological Laboratory at the Military Institute of Chemistry and Radiometry, among many other roles.

Zbigniew Wertejuk, PhD

Zbigniew Wertejuk, PhD, is Professor at the Military Institute of Chemistry and Radiometry in Warsaw, Poland. He has worked as a researcher and was also Research and Development Deputy Director and Director of the Institute. He has served as the Head of the Organization for the Prohibition of Chemical Weapons Expert Team as well as a NATO Long-Term Scientific Study national representative.

LIST OF CONTRIBUTORS

M. Anachkov

Institute of Catalysis, Bulgarian Academy of Sciences, "11 Acad. G. Bonchev" str., 1113 Sofia Bulgaria

J. Aneli

Iv. Javakhishvili Tbilisi State University, Institute of Macromolecular Chemistry and Polymeric Materials, I. Chavchavadze Ave., 13, Tbilisi 0179, Georgia, E-mail: JimAneli@yahoo.com

V. A. Babkin

403343 SF VolgSABU, c. Mikhailovka, Region Volgograd, Michurina 21, Russia. E-mail: sfi@reg.avtlg.ru

M. Belitski

Institute of Catalysis, Bulgarian Academy of Sciences, 11 Bonchev Str., 1113 Sofia, Bulgaria

Ana Beltrán

Analytical Chemistry, Nutrition and Food Sciences Department, University of Alicante, P.O. Box 99, 03080. Alicante, Spain

A. Berlin

N. N. Semenov Institute of Chemical Physics, Russian Academy of Sciences, 4 Kosygin str., Moscow 119991 Russia, email: Berlin@chph.ras.ru

V. I. Binyukov

N M Emanuel Institute of Biochemical Physics, Russian Academy of Sciences, ul. Kosygina 4, 119334 Moscow, Russian Federation. Tel. (7-495) 939 71 40, Fax (7-495) 137 41 01

C. Bueno-Ferrer

Analytical Chemistry, Nutrition and Food Sciences Department, University of Alicante, P.O. Box 99, E-03080, Alicante, Spain

N. Burgos

Analytical Chemistry, Nutrition and Food Sciences Department, University of Alicante, P.O. Box 99, E-03080, Alicante, Spain

E. B. Burlakova

Emanuel Institute of Biochemical Physics of the Russian Academy of Sciences, Moscow, Russia

L. B. Dudnik

Emanuel Institute of Biochemical Physics of Russian Academy of Sciences, Moscow, Russia

N. M. Evteeva

Establishment of the Russian Academy of Sciences Institute of biochemical physics of N.M. Emanuelja, Kosygina, 4, 119991 Moscow, Russia, Fax: (095 1374101)

C. Garrigós, María

Analytical Chemistry, Nutrition and Food Sciences Department, University of Alicante, P.O. Box 99, 03080. Alicante, Spain

V. Georgiev

Institute of Catalysis, Bulgarian Academy of Sciences, 11 Bonchev Str., 1113 Sofia, Bulgaria

A. K. Haghi

University of Guilan, Rsaht, Iran, E-mail: Haghi@Guilan.ac.ir

Alfonso Jiménez

Analytical Chemistry, Nutrition and Food Sciences Department, University of Alicante, P.O. Box 99, E-03080, Alicante, Spain; Telephone: +34-965909660; E-mail: alfjimenez@ua.es

N. Koiava

Iv. Javakhishvili Tbilisi State University, Institute of Macromolecular Chemistry and Polymeric Materials, I. Chavchavadze Ave., 13, Tbilisi 0179, Georgia

S. M. Lomakin

Establishment of the Russian Academy of Sciences Institute of biochemical physics of N.M. Emanuelja, Kosygina, 4, 119991 Moscow, Russia, Fax: (095 1374101)

E. Markarashvili

Iv. Javakhishvili Tbilisi State University, Institute of Chemistry, I. Chavchavadze 3, Tbilisi 0128, Georgia

L. I. Matienko

N M Emanuel Institute of Biochemical Physics, Russian Academy of Sciences, ul. Kosygina 4, 119334 Moscow, Russian Federation. Tel. (7-495) 939 71 40, Fax (7-495) 137 41 01, E-mail: matienko@sky.chph.ras.ru

L. I. Mazaletskaya

Emanuel Institute of Biochemical Physics of Russian Academy of Sciences, Moscow, Russia, E-mail: lim@sky.chph.ras.ru

L. A. Mosolova

N M Emanuel Institute of Biochemical Physics, Russian Academy of Sciences, ul. Kosygina 4, 119334 Moscow, Russian Federation. Tel. (7-495) 939 71 40, Fax (7-495) 137 41 01

O. Mukbaniani

Iv. Javakhishvili Tbilisi State University, Institute of Chemistry, I. Chavchavadze 3, Tbilisi 0128, Georgia, E-mail: Omarimui@yahoo.com

Elena Pekhtasheva

G. V. Plekhanov Russian Economic University, 36, Stremyannyi way, 117997 Moscow, Russia, E-mail: pekhtasheva@mail.ru

Mercedes A. Peltzer

Analytical Chemistry, Nutrition and Food Sciences Department, University of Alicante, P.O. Box 99, 03080. Alicante, Spain

S. Rakovsky

Institute of Catalysis, Bulgarian Academy of Sciences, "11 Acad. G. Bonchev" str., 1113 Sofia Bulgaria, E-mail: rakovsky@ic.bas.bg

Marina Ramos

Analytical Chemistry, Nutrition and Food Sciences Department, University of Alicante, P.O. Box 99, 03080. Alicante, Spain; E-mail: marina.ramos@ua.es, Tel: +34965903400 Ext. 1187, Fax: +34965903527

N. I. Sheludchenko

Emanuel Institute of Biochemical Physics of Russian Academy of Sciences, Moscow, Russia

L. N. Shishkina

Emanuel Institute of Biochemical Physics of Russian Academy of Sciences, Moscow, Russia

Anamika Singh

Division of Reproductive and Child Health, Indian Council of Medical Research, New Delhi

Rajeev Singh

Division of Reproductive and Child Health, Indian Council of Medical Research, New Delhi, E-mail: 10rsingh@gmail.com

T. Tatrishvili

Iv. Javakhishvili Tbilisi State University, Institute of Chemistry, I. Chavchavadze 3, Tbilisi 0128, Georgia

Arancha Valdés

Analytical Chemistry, Nutrition and Food Sciences Department, University of Alicante, P.O. Box 99, 03080. Alicante, Spain

A. A. Volodkin

Establishment of the Russian Academy of Sciences Institute of biochemical physics of N.M. Emanuelja, Kosygina, 4, 119991 Moscow, Russia, Fax: (095 1374101)

G. E. Zaikov

Institute of Biochemical Physics, Russian Academy of Sciences, 4 Kosygin Street, 117334 Moscow, Russia. E-mail: GEZaikov@Yahoo.com

Gennady Zaikov

N.M. Emanuel Institute of Biochemical Physics, Russian Academy of Sciences, 4, Kosygin str., 119334 Moscow, Russia, E-mail: chembio@sky.chph.ras.ru

V. Zhigacheva

Emanuel Institute of Biochemical Physics of the Russian Academy of Sciences, Moscow, Russia, E-mail: zhigacheva@mail.ru

LIST OF ABBREVIATIONS

AcP	acetophenone
AHH	acute hypobaric hypoxia
AO	antioxidants
BBIC	bioluminescent bioreporter integrated circuit
CEF	compensation effect
CHP	cumylhydroperoxide
CNF	carbon nanofiber
DADPM	diaminodiphenylmethane
DADPS	diaminodiphenylsulphone
DATPO	diaminotriphenyloxide
DCHP	dicumylhydroperoxide
DMA	dynamic mechanical analysis
DMPC	dimethylphenylcarbinol
DSC	differential scanning calorimetry
DTA	differential thermal analysis
DTBP	2,6-di- <i>tert</i> -butylphenol
ECH	epichlorohydrin
EMAP	equilibrium modified atmosphere packaging
ERM	estimation of reaction mechanism
FCCP	carbonylcyanide- <i>p</i> -trifluoromethoxyphenylhydrazone
GFP	green fluorescent protein
HAART	highly active retroviral therapy
HMTA	Hexamethylenetetramine
HPLC	high performance liquid chromatography
IW	insufficient watering
LPO	lipidperoxidation
MF	melaphen
MMD	molecular mass distribution
MPDA	methylphenyldiamine
MTHPA	methyltetrahydrophthalic anhydride

NSP	nanoscale particles
OIT	oxidation induction time
ONRL	Oak Ridge National Laboratory
P	pyraphen
PEPA	polyethylene polyamine
PGR	plant growth regulators
PPSSO	polyphenylsilsesquioxanes
PVC	polyvinylcyclohexane
ROS	reactive oxygen species
SPME	solid phase microextraction
TGA	thermogravimetric analysis
TP	terpenephenols

LIST OF SYMBOLS

ΔH_m (J g ⁻¹)	latent heat of fusion of the sample
ΔH_m^o	theoretical latent heat of fusion for 100% crystalline PP
C_v	the axis of symmetry
$d_{H...O}$	the bond length in the complex
D_{O_3}	diffusion coefficient of ozone in the solution
e	the base of natural logarithm
g	the earth acceleration
h	Planck's constant
I	the current intensity
I_o	the intensity of the chemiluminiscent signal
j	the number of axes of symmetry
k_B	Boltzmann's constant
K_d	the dissociation constant of the complex
k_L	coefficient of mass transfer in the liquid phase
m	the mass of the molecule
n	the number of carbon atoms in the cycle
N_a	Avogadro's number
r	the bond order
r_A and r_B	van der Waals radii of the reagents
s	time interval of renovation
SE	steric energy
T	absolute temperature
U	the height of tunneling occurrence
v	rate of the gas flow
V	volume of the liquid phase
W	PP weight fraction in the sample
W'_{DMPC}	the rate of DMPC formation at square termination
W_{O_3}	the rate of ozone absorption
Z_o	collision factor

Greek Symbols

α	Henry's coefficient
δ	thickness of the bound layer in hydrodynamic model
η	viscosity of the solvent
ν	kinematics viscosity of the solvent
ξ	empiric coefficient
ρ	solvent density
ω	relative rate

PREFACE

This book provides innovative chapters on the growth of educational, scientific, and industrial research activities among chemists, biologists and polymer and chemical engineers and provides a medium for mutual communication between international academia and the industry. This book publishes significant research and reviews reporting new methodologies and important applications in the fields of complex materials. This book also provides a comprehensive presentation of the concepts, properties, and applications of complex materials. It also provides the first unified treatment for the broad subject of materials. The authors of each chapter use a fundamental approach to define the structure and properties of a wide range of solids on the basis of the local chemical bonding and atomic order present in the material. Emphasizing the physical and chemical origins of different material properties, this important volume focuses on the most technologically important materials being utilized and developed by scientists and engineers.

In Chapter 1, active packaging based on the release of Carvacrol and Thymol for fresh food is presented. In Chapter 2, the importance of vegetable oils as platform chemicals for synthesis of thermoplastic bio-based polyurethanes is reviewed in detail. In Chapter 3, a new concept on genetically engineered microbial biosensors is reported. In Chapter 4, degradation and stabilization of fur and leather are well described. In Chapter 5, new developments in materials chemistry and physics are presented. In Chapter 6, the quantum-chemical calculation in chemical reaction is well described. In Chapter 7, energy of a homolytic cleavage of communication OH in 4-Replaced 2,6-di-*tert*.butyl phenols is investigated. Results of quantum-chemical calculations of phenols and phenoxyls radicals a method of Hartree-Fock with parameters UHF, RHF are used for calculations of energy of homolytic decomposition of communication OH bonds. Results of the analysis of dependences of calculations $D_{(OH)}$ from k_7 allow to recommend approach PM6 with parameter RHF for calculation $D_{(OH)}$ of sterically hindered phenols.

In Chapter 8, a study on reaction of ozone with some oxygen containing organic compounds is presented. This chapter, based on 92 references, is focused on degradation of organics by ozonation and it comprises various classes of oxygen-containing organic compounds – alcohols, ketones, ethers and hydroxybenzenes. The mechanisms of a multitude of ozone reactions with these compounds in organic solvents are discussed in detail, presenting the respective reaction schemes, and the corresponding kinetic parameters are given and some thermodynamic parameters are also listed. The dependences of the kinetics and the mechanism of the ozonation reactions on the structure of the compounds on the medium and on the reaction conditions are revealed. The various possible applications of ozonolysis are specified and discussed. All these reactions have practical importance for the protection of the environment. In Chapter 9, the kinetics and mechanism of the selective ethylbenzene oxidation is studied. In this chapter, AFM method in the analytical purposes to research the possibility of the formation of supramolecular structures on basis of heterobinuclear heteroligand triple complexes $\text{Ni(II)(acac)}_2 \cdot \text{NaSt(or LiSt)PhOH}$ were applied.

It is also shown what the self-assembly-driven growth seems to be due to H-bonding of triple complexes $\text{Ni(II)(acac)}_2 \cdot \text{NaSt(or LiSt)PhOH}$ with a surface of modified silicone, and further formation supramolecular nanostructures $\{\text{Ni(II)(acac)}_2 \cdot \text{NaSt(or LiSt)PhOH}\}_n$ due to directional intermolecular (phenol–carboxylate) H-bonds, and, possibly, other non-covalent interactions (van Der Waals-attractive and π -bonding).

In Chapter 10, a detailed study of composite materials on the basis of epoxy containing organosilicon compounds is presented. The synthesis of organosiloxane monomers and polymers of linear and cyclic structure with epoxy groups via catalytic oxidation reactions of compounds with vinyl group and condensation reactions of compounds with hydroxyl or ethoxyl groups with epichlorohydrin have been summarized in this chapter. The hydrosilylation reaction of linear polyhydromethylsiloxane with allyl glycidyl ether is also considered. Some ring opening reactions of epoxy groups have been studied.

The composite materials on the basis of epoxy containing organosiloxane compounds and their physical-chemical properties have been considered as well.