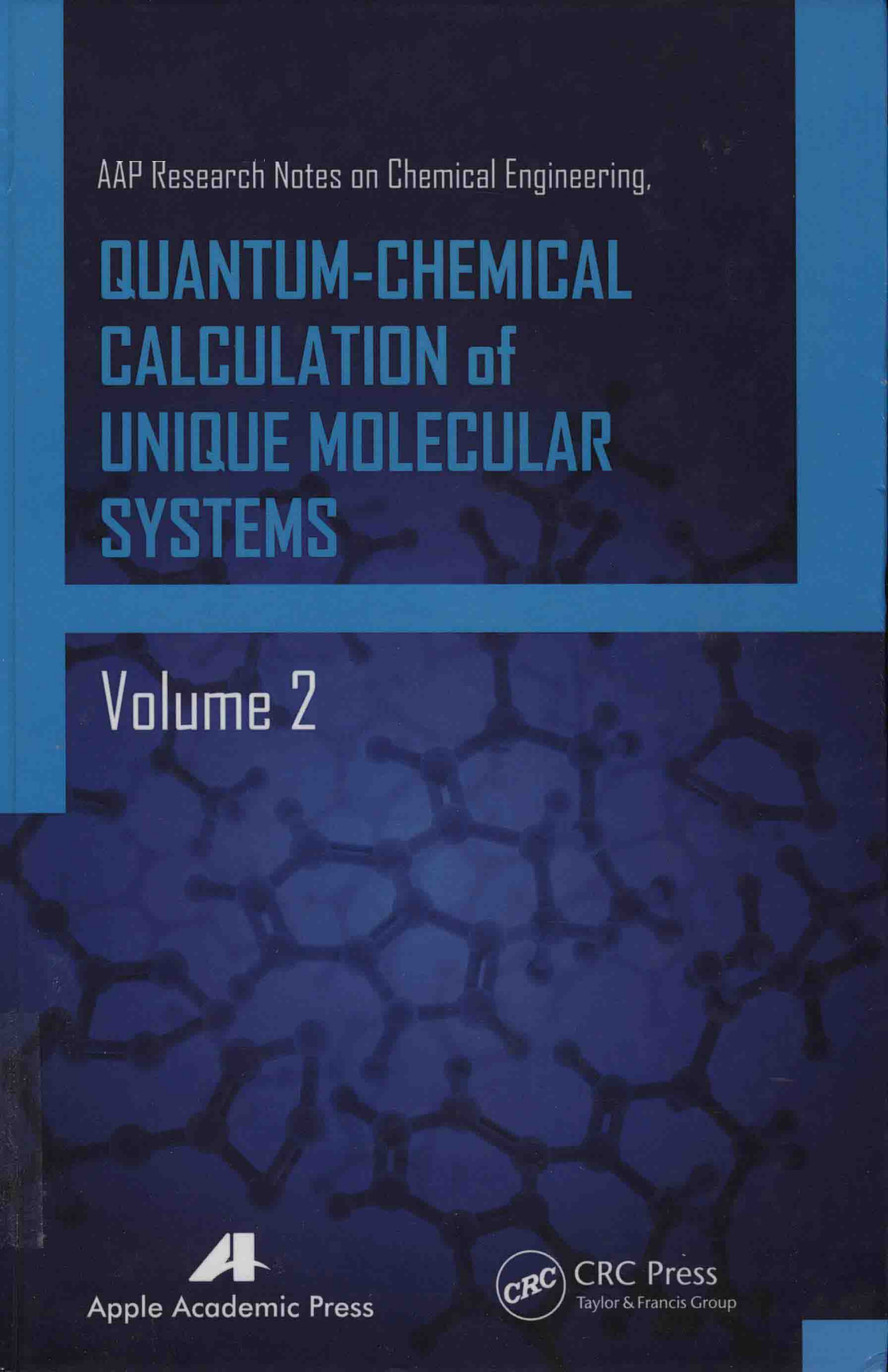
AAP Research Notes on Chemical Engineering,

QUANTUM-CHEMICAL CALCULATION of UNIQUE MOLECULAR SYSTEMS

Volume 2



Apple Academic Press

CRC Press
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QUANTUM-CHEMICAL CALCULATION OF UNIQUE MOLECULAR SYSTEMS

VOLUME 2

Edited by

Vladimir A. Babkin, DSc, Gennady E. Zaikov, DSc, and
A.K. Haghi, PhD

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Apple Academic Press

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

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

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

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

International Standard Book Number-13: 978-1-926895-75-8 (Hardcover)

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Library of Congress Control Number: 2013955808

Library and Archives Canada Cataloguing in Publication

Quantum-chemical calculation of unique molecular systems/edited by Vladimir A. Babkin, DSc, Gennady E. Zaikov, DSc, and A. K. Haghi, PhD.

Includes bibliographical references and index.
ISBN 978-1-926895-75-8 (bound).--ISBN 978-1-926895-75-8 (set)
1. Quantum chemistry--Data processing. 2. Quantum chemistry--Mathematics--Data processing. 3. Molecular structure--Data processing. I. Haghi, A. K., editor of compilation II. Zaikov, G. E. (Gennadiĭ Efremovich), 1935-, author, editor of compilation III. Babkin, V. A. (Vladimir Aleksandrovich), 1952-, author, editor of compilation

QD462.6.D38Q82 2014 541'.28 C2013-907916-5

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VOLUME 2

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PREFACE

Quantum chemistry, a special field of the quantum-mechanical theory, has always been a very tricky course for chemistry students around the world, because of the demanding mathematical background they have to possess in order to comprehend the extremely difficult concepts and applications and to understand phenomena at the atomic and molecular level. Quantum chemistry is a branch of theoretical chemistry that applies quantum mechanics and quantum field theory to address issues and problems in chemistry. The description of the electronic behavior of atoms and molecules as pertaining to their reactivity is one of the applications of quantum chemistry. Quantum chemistry lies on the border between chemistry and physics, and significant contributions have been made by scientists from both fields. It has a strong and active overlap with the field of atomic physics and molecular physics, as well as physical chemistry. This new book presents leading research in the field.

Practical for readers in all branches of chemistry, the new edition (in two volumes) reflects the latest quantum chemistry research and methods of computational chemistry and clearly demonstrates the usefulness and limitations of current quantum-mechanical methods for the calculation of molecular properties.

Integrating many new computer-oriented examples and problems throughout, this book demonstrates the usefulness and limitations of current quantum-chemical methods for the calculation of molecular properties. It offers full, step-by-step examinations of derivations that are easy to follow and understand and offers comprehensive coverage of recent, revolutionary advances in modern quantum-chemistry methods for molecular calculations. Many are integrated problems, throughout, with a substantial amount of computer applications utilized.

This book presents the structure and unity of the theoretical framework of modern chemistry in a progression from the single atom to the bulk limit. Employing an engaging and somewhat informal tone, this new

book delivers a superior presentation of rigorous mathematical derivations and quantum theory in a manner that is accessible and applicable to diverse readers.

— Prof. A. K. Haghi

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Section 2: Quantum-Chemical Calculations of Compounds with Low Cycles

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