

RABAH ALI KHALIL

A Simple Approach to

Quantum Chemistry

CHEMISTRY RESEARCH AND APPLICATIONS

NOVA

CHEMISTRY RESEARCH AND APPLICATIONS

A SIMPLE APPROACH TO QUANTUM CHEMISTRY

No part of this digital document may be reproduced, stored in a retrieval system or transmitted in any form or by any means. The publisher has taken reasonable care in the preparation of this digital document, but makes no expressed or implied warranty of any kind and assumes no responsibility for any errors or omissions. No liability is assumed for incidental or consequential damages in connection with or arising out of information contained herein. This digital document is sold with the clear understanding that the publisher is not engaged in rendering legal, medical or any other professional services.

CHEMISTRY RESEARCH AND APPLICATIONS

Additional books and e-books in this series can be found
on Nova's website under the Series tab.

CHEMISTRY RESEARCH AND APPLICATIONS

A SIMPLE APPROACH TO QUANTUM CHEMISTRY

RABAH ALI KHALIL



Copyright © 2020 by Nova Science Publishers, Inc.

All rights reserved. No part of this book may be reproduced, stored in a retrieval system or transmitted in any form or by any means: electronic, electrostatic, magnetic, tape, mechanical photocopying, recording or otherwise without the written permission of the Publisher.

We have partnered with Copyright Clearance Center to make it easy for you to obtain permissions to reuse content from this publication. Simply navigate to this publication's page on Nova's website and locate the "Get Permission" button below the title description. This button is linked directly to the title's permission page on copyright.com. Alternatively, you can visit copyright.com and search by title, ISBN, or ISSN.

For further questions about using the service on copyright.com, please contact:

Copyright Clearance Center

Phone: +1-(978) 750-8400

Fax: +1-(978) 750-4470

E-mail: info@copyright.com.

NOTICE TO THE READER

The Publisher has taken reasonable care in the preparation of this book, but makes no expressed or implied warranty of any kind and assumes no responsibility for any errors or omissions. No liability is assumed for incidental or consequential damages in connection with or arising out of information contained in this book. The Publisher shall not be liable for any special, consequential, or exemplary damages resulting, in whole or in part, from the readers' use of, or reliance upon, this material. Any parts of this book based on government reports are so indicated and copyright is claimed for those parts to the extent applicable to compilations of such works.

Independent verification should be sought for any data, advice or recommendations contained in this book. In addition, no responsibility is assumed by the Publisher for any injury and/or damage to persons or property arising from any methods, products, instructions, ideas or otherwise contained in this publication.

This publication is designed to provide accurate and authoritative information with regard to the subject matter covered herein. It is sold with the clear understanding that the Publisher is not engaged in rendering legal or any other professional services. If legal or any other expert assistance is required, the services of a competent person should be sought. FROM A DECLARATION OF PARTICIPANTS JOINTLY ADOPTED BY A COMMITTEE OF THE AMERICAN BAR ASSOCIATION AND A COMMITTEE OF PUBLISHERS.

Additional color graphics may be available in the e-book version of this book.

Library of Congress Cataloging-in-Publication Data

ISBN: 978-1-53618-138-8

Published by Nova Science Publishers, Inc. † New York

In Memory of my Father and Mother

CONTENTS

Preface		ix
Chapter 1	General Introduction	1
Chapter 2	Quantum Theory	15
Chapter 3	Quantum Mechanics	29
Chapter 4	Applications of Quantum Mechanics for Some Simple Systems	49
Chapter 5	Approximate Methods for Treating Multi-Electron Atoms	71
Chapter 6	Approximate Solutions of the Schrödinger Equation in Molecular Systems	93
Chapter 7	Introduction to Computational Chemistry	119
References		129
About the Author		131
Index		133

PREFACE

Rabah Ali Khalil*

Professor and Chair of Physical Chemistry,
Department of Chemistry, College of Science,
University of Mosul, Mosul, Iraq

Remarkable improvements in the applications of quantum mechanical calculations for developing and understanding essential issues in different aspects are necessary. These are including medicinal, pharmaceutical, renewable energies, and some others. Moreover, this will be the probable success in developing what the so-called “quantum computer” encourages people in order to know about the subject of quantum mechanics. Therefore, an adopted book for simply introducing the principle of quantum mechanics seems to be interesting. The presented book may be considered as a textbook for undergraduate students of the chemistry department as a basic course, and also can be considered as a background for beginners who desire to understand this subject. Indeed, this book may reflect the two decades of experience of

* Corresponding Author's E-mail: rakhalil64@yahoo.com

the author in teaching quantum chemistry to undergraduate students. The presented textbook includes seven chapters, starting from the requested classical mechanics, quantum theory, quantum mechanics, applications of quantum mechanics for some simple systems, approximate methods, atoms, and molecules to the introductory chapter of computational chemistry. As an advanced book in quantum chemistry, many published books have been covered this subject by many respected authors.