A Textbook on
Quantum Chemistry

Dr. Trilochan Swain

Kripa Drishti Publications, Pune.

A TEXTBOOK ON

QUANTUM CHEMISTRY

Dr. Trilochan Swain

Associate Professor in Post Graduate
Department of Chemistry,
Fakir Mohan University,
Balasore.

Kripa-Drishti Publications, Pune.

Book Title: **A Textbook on Quantum Chemistry**

Author by: **Dr. Trilochan Swain**

1st Edition

ISBN: 978-93-90847-00-6

Published: **September 2021**

Publisher:

Kripa-Drishti Publications

A/ 503, Poorva Height, SNO 148/1A/1/1A,
Sus Road, Pashan- 411021, Pune, Maharashtra, India.
Mob: +91-8007068686
Email: editor@kdpublications.in
Web: https://www.kdpublications.in

© **Copyright KRIPA-DRISHTI PUBLICATIONS**
All Rights Reserved. No part of this publication can be stored in any retrieval system or reproduced in any form or by any means without the prior written permission of the publisher. Any person who does any unauthorized act in relation to this publication may be liable to criminal prosecution and civil claims for damages. [The responsibility for the facts stated, conclusions reached, etc., is entirely that of the author. The publisher is not responsible for them, whatsoever.]

PREFACE

I honestly gratitude to the Post Graduate students of Fakir Mohan University, Balasore as well as graduate students of AIMS College, Sambalpur for tempting me to complete this manuscript. Initially, I did not have any intention to complete this manuscript as a graduation and post-graduation level textbook but encouragement of students helps me to convert it into textbook.

The basic materials of this textbook are based on from my lecturers of postgraduates as well as undergraduates for several years. This textbook is primarily intended for the students of undergraduate and postgraduate students. This book covers complete mathematical explanation of all chapters which is not found any other textbook. A mathematically dull student of undergraduate and postgraduate can understand the quantum chemistry without any hesitation. All mathematical problems are derived completely which is the unique of this textbook.

Dr. Trilochan Swain

Acknowledgements

"There are times when silence speaks so much more loudly than Words of praise to only as good as belittle a person, whose words do not express, but only put a veneer over true feelings, which are of gratitude at this point of time."

Where would I be without my family? My parents deserve special mention for their inseparable support and prayers. My Father, Bikei Charana Swain, in the first place is the person who put the fundament my learning character, showing me the joy of intellectual pursuit ever since I was a child. My Mother, Indumati Swain, is the one who sincerely raised me with her caring and gently love. Brothers, Sisters, and sister in law thanks for being supportive and caring siblings.

I would also like to thank everybody who was important to the successful realization of this book, as well as expressing my apology that I could not mention personally one by one.

Finally, my greatest regards to the **Almighty** for bestowing upon me the courage to face the complexities of life and complete this thesis successfully.

Dedication

This book is completely dedicated to my beloved students and friends that I came across in my life.

About the Book

The beginning this book contains developmental story of the Quantum Chemistry. At the very beginning the historical concept of light is described. Towards the end of the history, a Speech by A.G. Ekstrand, President of the Royal Swedish Academy of Sciences, for Nobel Prize in Physics is written.

In the second part, the different types of operators are described followed by the theorem of Quantum mechanics with proof. The six postulates of Quantum mechanics are written with explanation. The various applications of Schrodinger equation such as Particle in 1D and 3D box, linear simple harmonic oscillator, rigid rotator, Hydrogen atom with full mathematical derivation is derived. The detail calculation of p (B and C atom) and d (Sc, V and Ni atom) configuration are also carried out.

In the middle part the Huckel Molecular Orbital theory and its application to ethylene, butadiene, cyclopropenyl radical, cyclobutadiene, bicyclobutadiene and benzene are completely derived with full explanation.

In the later part the application of Quantum mechanics to the free electron is explained. The complete mathematical derivation of two models such as Kronig-Penney model and Bloch theorem are completely derived.

In the last part of this book describes the approximation method of Quantum mechanics. Both perturbation and variation method are completely derived. The various application of variation method such as particle in 1D box, harmonic oscillator and ground state helium is also described.

INDEX

Chapter 1: Quantum Mechanics 1

1 Blackbody Radiation and Planck Hypothesis: 2
2 Expectation Values: 8
3 Operator: 9
    3.1 Properties of Operator: 12
    3.2 Unitary Operator: 19
4 Important Theorem of Quantum Mechanics: 21
5 Postulates of Quantum Mechanics: 24
6 Derivation of Schrodinger Wave Equation Based on the Postulates of Quantum Mechanics: 27
7 Particle in One Dimensional (1D) Box: 29
8 Particle in a three Dimensional Box: 36
9 Linear Simple Harmonic Oscillator (SHO): 41
10 Rigid Rotator (Rotor): 49
11 Ordinary Angular Momentum: 65
    11.1 Generalized Angular Momentum: 65
    11.2 Addition of Angular Momenta: Clebsch Gordan Coefficients 68
12 Pauli's Exclusion Principle: 69
13 Electronic Configuration and Term Symbols of B-Atom: 70
14 Electronic Configuration and Term Symbols of C-Atom: 74
15 Determination of Term Symbols for d^1 Configuration: 80
16 Determination of Term Symbols for d^2 Configuration: 84
17 Energy Calculation of J States of ^3F Term: 91
18 Determination of Term Symbols for d^8 Configuration: 94
19 Hückel Molecular Orbital (HMO) Theory: 107
20 Application of HMO Theory: 109
21 Quantum Free Electron Theory: 176
22 Time Independent Perturbation Theory: 191
23 Time Independent Non-Degenerate Perturbation: 192
24 Application of Time-Independent Perturbation Theory: 198
    24.1 Particle in One Dimensional Box with Slanted Bottom: 199
    24.2 Helium Atom: 201

Dr. Trilochan Swain

is a versatile researcher as well as loves to teach variety of students in different levels. In his school carrier he played many games including football, Kho kho, badminton, etc. He is a nature lover right from his school carrier and took part many planation drives in school. He likes very old classical music.

About the Author

Dr. Trilochan swain is Associate Professor in Post Graduate Department of Chemistry, Fakir Mohan University, Balasore. He completed his post-graduation from Berhampur University. He has 21 years of teaching experience. He taught various degree engineering colleges in Odisha as well as in National Institute of Technology, Calicut. During his teaching period he taught physical chemistry basically Quantum mechanics. He completed his Ph.D from Utkal University from physical chemistry. He acquired two national fellowships in Indian Institute of Science, Bangalore and INST Mohali. During his tenure he worked on superconductivity basically iron based superconductor. He published many research papers in various International Journals such as Solar Energy, International Journal of Energy Research, Journal of Thermal Analysis and Calorimetry, etc.. He presented more than 50 research papers in various National and International conferences. The current research topic is based on superconductivity and thermal energy. The Author is a nature lover and worked on climate change with Mrs. Eveweed Aka Sheseed from Canada. Many short articles based on climate change, global warming, arsenic removal etc. are posted in davidsuzuki organization. This is a non-profit organization host from Canada. The Author also posted many short articles on acid rain and global warming with Mrs. Annabelle Diestro and Miss Rose Balingit, teacher- cum- environmentalist from Philippines.

About the Book

The beginning this book contains developmental story of the Quantum Chemistry. At the very beginning the historical concept of light is described. Towards the end of the history, a Speech by A.G. Ekstrand, President of the Royal Swedish Academy of Sciences, for Nobel Prize in Physics is written.

In the second part, the different types of operator are described followed by the theorem of Quantum mechanics with proof. The six postulates of Quantum mechanics is written with explanation. The various applications of Schrodinger equation such as Particle in 1D and 3D box, linear simple harmonic oscillator, rigid rotator, Hydrogen atom with full mathematical derivation are derived. The detail calculation of p (B and C atom) and d (Sc, V and Ni atom) configuration are also carried out.

In the middle part the Huckel Molecular Orbital theory and its application to ethylene, butadiene, cyclopropenyl radical, cyclobutadiene, bicyclobutadiene and benzene are completely derived with full explanation.

In the later part the application of Quantum mechanics to the free electron is explained. The complete mathematical derivation of two models such as Kronig-Penney model and Bloch theorem are completely derived.

In the last part of this book describes the approximation method of Quantum mechanics. Both perturbation and variation method are completely derived. The various application of variation method such as particle in 1D box, harmonic oscillator and ground state helium is also described.

KRIPA DRISHTI PUBLICATIONS

Price: ₹450

Kripa-Drishti Publications
A-503 Poorva Heights, Pashan-Sus Road, Near Sai Chowk,
Pune – 411021, Maharashtra, India.
Mob: +91 8007068686
Email: editor@kdpublications.in
Web: https://www.kdpublications.in

ISBN: 978-93-90847-00-6

9 789390 847006