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A Textbook on Quantum Chemistry

Dr. Trilochan Swain

Kripa Drishti Publications, Pune.

A TEXTBOOK ON QUANTUM CHEMISTRY

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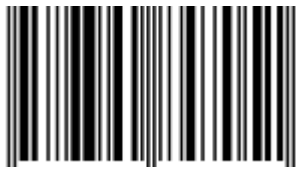
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PREFACE

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.

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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.

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