

Principles and Applications of Quantum Chemistry

By V. P. Gupta

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Principles and Applications of Quantum Chemistry offers clear and simple coverage based on the author's extensive teaching at advanced universities around the globe. Where needed, derivations are detailed in an easy-to-follow manner so that you will understand the physical and mathematical aspects of quantum chemistry and molecular electronic structure. Building on this foundation, this book then explores applications, using illustrative examples to demonstrate the use of quantum chemical tools in research problems. Each chapter also uses innovative problems and bibliographic references to guide you, and throughout the book chapters cover important advances in the field including: Density functional theory (DFT) and time-dependent DFT (TD-DFT), characterization of chemical reactions, prediction of molecular geometry, molecular electrostatic potential, and quantum theory of atoms in molecules.

- Simplified mathematical content and derivations for reader understanding
- Useful overview of advances in the field such as Density Functional Theory (DFT) and Time-Dependent DFT (TD-DFT)
- Accessible level for students and researchers interested in the use of quantum chemistry tools

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Editorial Review

Review
"A large number of examples to support different applications have been given. Bibliography at the end of each chapter aims at opening the door for those who intend to pursue quantum chemistry more deeply. Overall, a very useful book for researchers and graduate students." --**Zentralblatt MATH,** ***Principles and Applications of Quantum Chemistry***

From the Back Cover

Principles and Applications of Quantum Chemistry offers clear and simple coverage based on the author's extensive teaching at advanced universities around the globe. This book is ideal for graduate and postgraduate students in chemistry, physics, materials science, biochemistry, and chemical engineering as well as researchers in chemical-, biochemical-, and drug-related laboratories.

Where needed, derivations are detailed in an easy-to-follow manner so that you will understand the physical and mathematical aspects of quantum chemistry and molecular electronic structure. Building on this foundation, this book then explores applications, using illustrative examples to demonstrate the use of quantum chemical tools in research problems. Each chapter also uses innovative problems and bibliographic references to guide you, and chapters throughout the book cover important advances in the field including density functional theory (DFT) and time-dependent DFT (TD-DFT), characterization of chemical reactions, prediction of molecular geometry, molecular electrostatic potential, and quantum theory of atoms in molecules.

Key features

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About the Author
V.P. Gupta, Philosophy Doctor in Physics and Mathematics (1967) from Moscow (USSR), is an academician and researcher of long standing, with 45 years of teaching and research experience. He has held important positions of Professor and Chairman, Department of Physics, University of Jammu, Jammu-Tawi, India; Visiting Professor of Chemistry, Université de Provence, Marseille, France; Professor and Chairman, Department of Physics, University of Calabar, Calabar, Nigeria; Professor Emeritus (Emeritus Fellow), University Grants Commission (UGC), India; Emeritus Scientist, Council of Scientific & Industrial Research (CSIR), India; Emeritus Scientist, All India Council of Technical Education (AICTE), India; Visiting Scientist/Fellow, University of Helsinki, Helsinki, Finland; and International Centre for Theoretical Physics, Trieste, Italy. The major areas of his research interest are quantum chemistry, molecular spectroscopy and molecular structure, matrix isolation infrared studies, astrochemistry and laser spectroscopy in which he has approximately one hundred research publications in refereed journals. He has written two books, including a translation from Russian into English. V.P. Gupta has successfully executed 16 scientific research projects and a book-writing project supported by various funding agencies of the Government of India such as the Department of Science and Technology (DST), UGC, CSIR, AICTE, and Indian Space Research Organization (ISRO), Bangalore. His areas of current interest in theoretical chemistry are related to the accurate prediction of chemical structures, molecular properties and electronic and vibrational spectra,

formation of molecules under extraterrestrial conditions and their spectroscopic characterization, and characterization of drugs.

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