



# Principles and Applications of Quantum Chemistry

*V.P. Gupta*

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## Principles and Applications of Quantum Chemistry V.P. Gupta

*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)
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