



Handbook of Molecular Physics and Quantum Chemistry, 3 Volume Set

Stephen Wilson, Roy McWeeny, Peter F. Bernath

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Published in three volumes, this comprehensive reference work brings together in a single source for the first time, a detailed presentation of the most important theoretical concepts and methods for the study of molecules and molecular systems.

The logical format of the Handbook allows the reader to progress from the foundations of the field to the most important and exciting areas of current research. Edited and written by an outstanding international team, and containing over 100 articles written by more than 50 contributors, it will be invaluable for both the expert researcher and the graduate student or postdoctoral worker active in any of the broad range of fields where these concepts and methods are important.

Comprises three themed volumes:

- Fundamentals
- Molecular Electronic Structure
- Molecules in the Physico-Chemical Environment: Spectroscopy, Dynamics and Bulk Properties
- Presents detailed articles covering the key topics, presented in a didactic manner
- Focuses both on theory and the relation of experiment to theory

Volume 1, *Fundamentals* presents the foundations of molecular physics and quantum chemistry. It consists of 7 parts arranged as follows:-

Part 1 Introduction

Part 2 Elements of Quantum Mechanics

Part 3 Orbital Models for Atomic, Molecular and Crystal Structure

Part 4 Symmetry Groups and Molecular Structure

Part 5 Second Quantization and Many-Body Methods

Part 6 Approximate Separation of Electronic and Nuclear Motion

Part 7 Quantum Electrodynamics of Atoms and Molecules

The central problem of molecular physics and quantum chemistry is the description of atomic and molecular electronic structure. The development of appropriate models for the description of the effects of electron

correlation and of relativity are key components of the analysis. Volume 2, *Molecular Electronic Structure*, addresses these topics, and consists of 7 parts arranged as follows:

Part 1 Approximation methods

Part 2 Orbital Models and Generalized Product Functions

Part 3 Electron correlation

Part 4 Relativistic molecular electronic structure

Part 5 Electronic structure of large molecules

Part 6 Computational quantum chemistry

Part 7 Visualization and interpretation of molecular electronic structure

In reality no molecular system exists in isolation. Molecules interact with other atoms and molecules, and with their environment. Volume 3, *Molecules in the Physico-Chemical Environment - Spectroscopy, Dynamics and Bulk Properties*, consists of 7 parts arranged as follows:-

Part 1 Response theory and propagator methods

Part 2 Interactions between molecules

Part 3 Molecules in different environments

Part 4 Molecular Electronic spectra

Part 5 Atomic Spectroscopy and Molecular Vibration-Rotation Spectroscopy

Part 6 Molecular dynamics and dynamical processes

Part 7 Bulk properties

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