DESCRIPTION

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:-
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 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
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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ABOUT THE AUTHOR

**Stephen Wilson** has published over 300 scientific papers and reviews, principally in theoretical and computational chemistry and molecular physics, but also in computing science and numerical analysis. He has authored two books - *Electron Correlation in Molecules*, Clarendon Press, Oxford, 1984, and *Chemistry by Computer: An Overview of the Applications of Computers in Chemistry*, Plenum Press, New York, 1986, and has edited some 21 volumes. He is an Editor-in-Chief of *Progress in Theoretical Chemistry and Physics* and Series Editor of *Methods in Computational Chemistry*. Dr. Wilson holds a D.Sc. from the University of Bristol.

**Peter F. Bernath** was born in Ottawa, Ontario, Canada and was educated at the University of Waterloo (B. Sc. in chemistry 1976) and Massachusetts Institute of Technology (Ph. D. in physical chemistry 1980). After a post-doctoral stint at the Herzberg Institute of Astrophysics of the National Research Council of Canada, he began his academic career at the University of Arizona in 1982. In 1991, he moved to the University of Waterloo as Professor of Chemistry and of Physics and now holds an Industrial Research Chair in Fourier Transform Spectroscopy. Prof. Bernath has interests in high resolution spectroscopy of molecules with applications in astronomy and atmospheric science. He is the author of the textbook *Spectra of Atoms and Molecules*. 
Roy McWeeny's academic career spans five decades. After a first degree in Physics (Leeds University) and a D.Phil. from Oxford University (where he worked with C.A. Coulson), he was appointed Lecturer in Physical Chemistry, University of Durham. In the mid-1950s he was an invited member of J.C. Slater's famous Solid-State and Molecular Theory Group at MIT; and in 1960 spent a year as Associate Director of P.-O. Lowdin's Quantum Theory Group at Uppsala University. His other University appointments include a Lectureship in Mathematics, Physics and Chemistry (University of Keele, UK); a Readership in Quantum Theory, a personal Chair of Theoretical Physics and Theoretical Chemistry, and a Chair of Chemistry (University of Sheffield, UK). In 1982 he became the first foreign scholar (following a Ministerial Decree) to be called to an Italian University Chair, taking up the position of Professore Ordinario di Chimica Teorica, Università di Pisa, where he became Professore Emerito in 1998. He is a Member of the International Academy of Quantum Molecular Science (elected 1973); and a Member of the European Academy of Arts, Sciences and the Humanities (elected 1986). In 1996 a Special Issue of the International Journal of Quantum Chemistry (Volume 60) was published in his honour: it contains sixty scientific papers, contributed by authors from many countries.

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