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Peter Atkins Peter William Atkins (born 10 August 1940) is an English chemist and a Fellow of Lincoln College at the University of Oxford.He retired in 2007. He is a prolific writer of popular chemistry textbooks, including "Physical Chemistry", "Inorganic Chemistry", and "Molecular Quantum Mechanics". Atkins is also the author of a number of popular science books, including "Atkins ...

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Computational chemistry has become extremely important in the last decade, being widely used in academic and industrial research. Yet there have been few books designed to teach the subject to nonspecialists. Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics is an invaluable tool for teaching and researchers alike. The book provides an overview of the field, explains the basic underlying theory at a meaningful level that is not beyond beginners, and it gives numerous comparisons of different methods with one another and with experiment. The following concepts are illustrated and their possibilities and limitations are given: - potential energy surfaces; - simple and extended H ü ckel methods; - ab initio, AM1 and related semiempirical methods; - density functional theory (DFT). Topics are placed in a historical context, adding interest to them and removing much of their apparently arbitrary aspect. The large number of references, to all significant topics mentioned, should make this book useful not only to undergraduates but also to graduate students and academic and industrial researchers.

Thoroughly rewritten from start to finish, the second edition of this text provides a complete, highly accessible introduction to quantum chemistry.

Ab initio quantum chemistry has emerged as an important tool in chemical research and is applied to a wide variety of problems in chemistry and molecular physics. Recent developments of computational methods have enabled previously intractable chemical problems to be solved using rigorous quantum-mechanical methods. This is the first comprehensive, up-to-date and technical work to cover all the important aspects of modern molecular electronic-structure theory. Topics covered in the book include: \* Second quantization with spin adaptation \* Gaussian basis sets and molecular-integral evaluation \* Hartree-Fock theory \* Configuration-interaction and multi-configurational self-consistent theory \* Coupled-cluster theory for ground and excited states \* Perturbation theory for single- and multi-configurational states \* Linear-scaling techniques and the fast multipole method \* Explicitly correlated wave functions \* Basis-set convergence and extrapolation \* Calibration and benchmarking of computational methods, with applications to molecular equilibrium structure, atomization energies and reaction enthalpies. Molecular Electronic-Structure Theory makes extensive use of numerical examples, designed to illustrate the strengths and weaknesses of each method treated. In addition, statements about the usefulness and deficiencies of the various methods are supported by actual examples, not just model calculations. Problems and exercises are provided at the end of each chapter, complete with hints and solutions. This book is a must for researchers in the field of quantum chemistry as well as for nonspecialists who wish to acquire a thorough understanding of ab initio molecular electronic-structure theory and its applications to problems in chemistry and physics. It is also highly recommended for the teaching of graduates and advanced undergraduates.

Supplementing "Quantum Mechanics. An Introduction" and "Quantum Mechanics. Symmetries", this book covers an important additional course on quantum mechanics, including an introduction to quantum statistics, the structure of atoms and molecules, and the Schr ö dinger wave equation. 72 fully worked examples and problems consolidate the material.

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Introduction to problems of molecular structure and motion covers calculus of orthogonal functions, algebra of vector spaces, and Lagrangian and Hamiltonian formulation of classical mechanics. Answers to problems. 1966 edition.

The Instructor's solutions manual to accompany Atkins' Physical Chemistry provides detailed solutions to the 'b' exercises and the even-numbered discussion questions and problems that feature in the ninth edition of Atkins' Physical Chemistry . The manual is intended for instructors and consists of material that is not available to undergraduates. The manual is free to all adopters of the main text.