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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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Genre/Form: Electronic books: Additional Physical Format: Print version: Atkins, P.W. (Peter William), 1940-Molecular quantum mechanics. New York : Oxford University ...

This text unravels those fundamental physical principles which explain how all matter behaves. It takes us from the foundations of quantum mechanics, through quantum models of atomic, molecular, and electronic structure, and on to discussions of spectroscopy, and the electronic and magnetic properties of molecules.

This manual contains the authors' detailed solutions to the 353 problems at the ends of the chapters in the third edition of Molecular Quantum Mechanics. Most problem solutions are accompanied by a further related exercise. The manual will be invaluable both to the instructors and lecturers who adopt the parent text and to the students themselves.

aspects of the learning process are fully supported, including the understanding of terminology, notation, mathematical concepts, and the application of physical chemistry to other branches of science." "Building on the heritage of the world-renowned Atkins' Physical Chemistry , Quanta, Matter, and Change gives a refreshing new insight into the familiar by illuminating physical chemistry from a new direction." --Book Jacket.

This textbook offers an introduction to the foundations of spectroscopic methods and provides a bridge between basic concepts and experimental applications in fields as diverse as materials science, biology, solar energy conversion, and environmental science. The author emphasizes the use of time-dependent theory to link the spectral response in the frequency domain to the behavior of molecules in the time domain, strengthened by two brand new chapters on nonlinear optical spectroscopy and time-resolved spectroscopy. Theoretical underpinnings are presented to the extent necessary for readers to understand how to apply spectroscopic tools to their own interests.

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 Hückel 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.

A 'travel guide' to the periodic table, explaining the history, geography and the rules of behaviour in this imagined land. The Periodic Kingdom is a journey of imagination in which Peter Atkins treats the periodic table of elements - the 109 chemical elements in the world, from which everything is made - as a country, a periodic kingdom, each region of which corresponds to an element. Arranged much like a travel guide, the book introduces the reader to the general features of the table, the history of the elements, and the underlying arrangement of the table in terms of the structure and properties of atoms. Atkins sees elements as finely balanced living personalities, with quirks of character and certain, not always outward, dispositions, and the kingdom is thus a land of intellectual satisfaction and infinite delight.

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.

Atkins' Physical Chemistry: Molecular Thermodynamics and Kinetics is designed for use on the second semester of a quantum-first physical chemistry course. Based on the hugely popular Atkins' Physical Chemistry, this volume approaches molecular thermodynamics with the assumption that students will have studied quantum mechanics in their first semester. The exceptional quality of previous editions has been built upon to make this new edition of Atkins' Physical Chemistry even more closely suited to the needs of both lecturers and students. Re-organised into discrete 'topics', the text is more flexible to teach from and more readable for students. Now in its eleventh edition, the text has been enhanced with additional learning features and maths support to demonstrate the absolute centrality of mathematics to physical chemistry. Increasing the digestibility of the text in this new approach, the reader is brought to a question, then the math is used to show how it can be answered and progress made. The expanded and redistributed maths support also includes new 'Chemist's toolkits' which provide students with succinct reminders of mathematical concepts and techniques right where they need them. Checklists of key concepts at the end of each topic add to the extensive learning support provided throughout the book, to reinforce the main take-home messages in each section. The coupling of the broad coverage of the subject with a structure and use of pedagogy that is even more innovative will ensure Atkins' Physical Chemistry remains the textbook of choice for studying physical chemistry.

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