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Map: Physical Chemistry (McQuarrie and Simon) - Chemistry ...  
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Physical Chemistry, A Molecular Approach, by Donald McQuarrie and John Simon, published by University Science Books, 0-935702-99-7, the definitive new textbook for physical chemistry. Physical Chemistry, A Molecular Approach, Donald A. McQuarrie and John D.

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Physical Chemistry: A Molecular Approach - Donald A ...

The field of bioscience methodologies in physical chemistry stands at the intersection of the power and generality of classical and quantum physics with the minute molecular complexity of chemistry and biology. This book provides an application of physical principles in explaining and rationalizing chemical and biological phenomena.

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Unlike most physical chemistry texts, modern physical chemistry research is based on quantum mechanics, and this state-of-the-art approach is the one adopted by McQuarrie and Simon. Quantum theory is introduced at the outset, and the molecular viewpoint of quantum chemistry informs the authors' investigation of physical chemistry's other main topic areas - thermodynamics and chemical kinetics.

Emphasizes a molecular approach to physical chemistry, discussing principles of quantum mechanics first and then using those ideas in development of thermodynamics and kinetics. Chapters on quantum subjects are interspersed with ten math chapters reviewing mathematical topics used in subsequent chapters. Includes material on current physical chemical research, with chapters on computational quantum chemistry, group theory, NMR spectroscopy, and lasers. Units and symbols used in the text follow IUPAC recommendations. Includes exercises. Annotation copyrighted by Book News, Inc., Portland, OR

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This text provides students with concise reviews of mathematical topics that are used throughout physical chemistry. By reading these reviews before the mathematics is applied to physical chemical problems, a student will be able to spend less time worrying about the math and more time learning the physical chemistry.

This is the physical chemistry textbook for students with an affinity for computers! It offers basic and advanced knowledge for students in the second year of chemistry masters studies and beyond. In seven chapters, the book presents thermodynamics, chemical kinetics, quantum mechanics and molecular structure (including an introduction to quantum chemical calculations), molecular symmetry and crystals. The application of physical-chemical knowledge and problem solving is demonstrated in a chapter on water, treating both the water molecule as well as water in condensed phases. Instead of a traditional textbook top-down approach, this book presents the subjects on the basis of examples, exploring and running computer programs (Mathematica®), discussing the results of molecular orbital

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calculations (performed using Gaussian) on small molecules and turning to suitable reference works to obtain thermodynamic data. Selected Mathematica® codes are explained at the end of each chapter and cross-referenced with the text, enabling students to plot functions, solve equations, fit data, normalize probability functions, manipulate matrices and test physical models. In addition, the book presents clear and step-by-step explanations and provides detailed and complete answers to all exercises. In this way, it creates an active learning environment that can prepare students for pursuing their own research projects further down the road. Students who are not yet familiar with Mathematica® or Gaussian will find a valuable introduction to computer-based problem solving in the molecular sciences. Other computer applications can alternatively be used. For every chapter learning goals are clearly listed in the beginning, so that readers can easily spot the highlights, and a glossary in the end of the chapter offers a quick look-up of important terms.

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In this new textbook on physical chemistry, fundamentals are introduced simply yet in more depth than is common. Topics are arranged in a progressive pattern, with simpler theory early and more complicated theory later. General principles are induced from key experimental results. Some mathematical background is supplied where it would be helpful. Each chapter includes worked-out examples and numerous references. Extensive problems, review, and discussion questions are included for each chapter. More detail than is common is devoted to the nature of work and heat and how they differ. Introductory Caratheodory theory and the standard integrating factor for  $dG_{rev}$  are carefully developed. The fundamental role played by uncertainty and symmetry in quantum mechanics is emphasized. In chemical kinetics, various methods for determined rate laws are presented. The key mechanisms are detailed. Considerable statistical mechanics and reaction rate theory are then surveyed. Professor Duffey has given us a most readable, easily followed text in physical chemistry.

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

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