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A Molecular Approach

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Donald A. McQuarrie
John D. Simon

Physical Chemistry A Molecular Approach

Praveen Kaushik



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Physical Chemistry Donald A. McQuarrie, 2023-08-07 As the first modern physical chemistry textbook to cover quantum mechanics before thermodynamics and kinetics this book provides a contemporary approach to the study of physical chemistry As the first modern physical chemistry textbook to cover quantum mechanics before thermodynamics and kinetics this book provides a contemporary approach to the study of physical chemistry By beginning with quantum chemistry students will learn the fundamental principles upon which all modern physical chemistry is built The text includes a special set of Math Chapters to review and summarize the mathematical tools required to master the material Thermodynamics is simultaneously taught from a bulk and microscopic viewpoint that enables the student to understand how bulk properties of materials are related to the properties of individual constituent molecules This new text includes a variety of modern research topics in physical chemistry as well as hundreds of worked problems and examples Translated into French Italian Japanese Spanish and Polish *Physical Chemistry* Donald A. McQuarrie, John D. Simon, 2013 **Physical Chemistry: a Molecular Approach** McQuarrie Donald A, Simon John D, 1988 Modern Physical Chemistry George H. Duffey,

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understanding With its emphasis on modern perspectives interdisciplinary approaches and practical applications Innovative Physical Chemistry Perspectives is set to become an essential reference for anyone seeking to explore physical chemistry from new and exciting angles

Problems and Solutions to Accompany McQuarrie and Simon, Physical Chemistry: a Molecular Approach Heather Cox, 1997 *Molecular Physical Chemistry* José J. C. Teixeira-Dias, 2017-01-16 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 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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