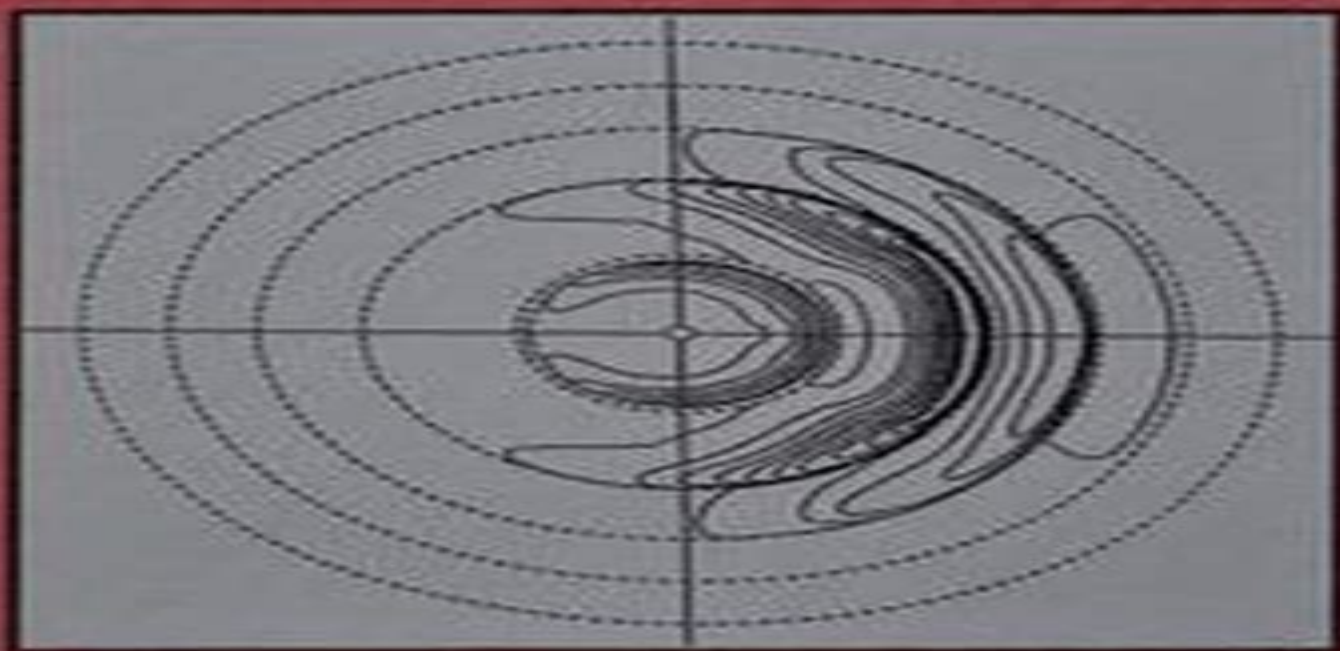


PHYSICAL CHEMISTRY

A MOLECULAR APPROACH

Donald A. McQuarrie • John D. Simon



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McQuarrie Simon's Physical Chemistry: A Molecular Approach but it is also well suited as a stand alone text for upper level undergraduate or intro graduate computational chemistry courses Assumes no computational background Enables students to build simulations from scratch to reproduce famous literature calculations Teaches a variety of computational numerical simulation methods applicable to solving chemical problems Designed to play well with McQuarrie Simon's landmark P CHEM text but can be used with others as well *Physical Chemistry* Donald A. McQuarrie, John D. Simon, 2013

Basiswissen Physikalische Chemie Claus Czeslik, Heiko Seemann, Roland Winter, 2010-05-12 Das Basiswissen der Physikalischen Chemie wird in klarer und kompakter Weise dargestellt Angesichts des Umfangs traditioneller Lehrbücher der Physikalischen Chemie soll der hier dargebotene Stoff das Lernen für Prüfungen und Klausuren erleichtern Ziel des Buches ist es für die fortgeschrittene und spezielle Ausbildung in diesem Fach ein tragfähiges mathematisch fundiertes Fundament zu legen Neben der makroskopischen phänomenologischen Beschreibungsweise kommt der molekularen theoretischen Deutung der Begriffe und Gesetzmäßigkeiten eine zentrale Rolle zu Wichtige Aspekte der quantenmechanischen Darstellung molekularer Eigenschaften werden ebenfalls besprochen *Mathematical Methods for Scientists and Engineers* Donald

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Shillady, 2011-07-27 At a time when U S high school students are producing low scores in mathematics and science on international examinations a thorough grounding in physical chemistry should not be considered optional for science undergraduates Based on the author's thirty years of teaching Essentials of Physical Chemistry merges coverage of calculus with chemistry and molecular physics in a friendly yet thorough manner Reflecting the latest ACS guidelines the book can be used as a one or two semester course and includes special topics suitable for senior projects The book begins with a math and physics review to ensure all students start on the same level and then discusses the basics of thermodynamics and kinetics with mathematics tuned to a level that stretches students abilities It then provides material for an optional second semester course that shows students how to apply their enhanced mathematical skills in a brief historical development of the quantum mechanics of molecules Emphasizing spectroscopy the text is built on a foundation of quantum chemistry and more mathematical detail and examples It contains sample classroom tested exams to gauge how well students know how to use relevant formulas and to display successful understanding of key concepts Coupling the development of mathematical skills

with chemistry concepts encourages students to learn mathematical derivations Mini biographies of famous scientists make the presentation more interesting from a people point of view Stating the basic concepts of quantum chemistry in terms of analogies provides a pedagogically useful technique Covering key topics such as the critical point of a van der Waals gas the Michaelis Menten equation and the entropy of mixing this classroom tested text highlights applications across the range of chemistry forensic science pre medical science and chemical engineering In a presentation of fundamental topics held together by clearly established mathematical models the book supplies a quantitative discussion of the merged science of physical chemistry

Physical Chemistry Henry Eyring, Douglas Henderson, Wilhelm Jost, 1971

Statistical Mechanics Donald A. McQuarrie, 2000-06-16 The canonical ensemble Other ensembles and fluctuations Boltzmann statistics fermi dirac statistics and bose einstein statistics Ideal monatomic gas Ideal diatomic Classical statistical mechanics Ideal polyatomic Chemical equilibrium Quantum statistics Crystals Imperfect gases Distribution functions in classical monatomic liquids Perturbation theories of liquids Solutions of strong electrolytes Kinetic theory of gases and molecular collisions Continuum mechanics Kinetic theory of gases and the boltzmann equation Transport processes in dilute gases Theory of brownian motion The time correlation function formalism

Physical Chemistry for the Chemical Sciences Raymond Chang, 2014-06-15 Following in the wake of Chang's two other best selling physical chemistry textbooks Physical Chemistry for the Chemical and Biological Sciences and Physical Chemistry for the Biosciences this new title introduces laser spectroscopist Jay Thoman Williams College as co author Following in the wake of Chang's two other best selling physical chemistry textbooks Physical Chemistry for the Chemical and Biological Sciences and Physical Chemistry for the Biosciences this new title introduces laser spectroscopist Jay Thoman Williams College as co author This comprehensive new text has been extensively revised both in level and scope Targeted to a mainstream physical chemistry course this text features extensively revised chapters on quantum mechanics and spectroscopy many new chapter ending problems and updated references while biological topics have been largely relegated to the previous two textbooks Other topics added include the law of corresponding states the Joule Thomson effect the meaning of entropy multiple equilibria and coupled reactions and chemiluminescence and bioluminescence One way to gauge the level of this new text is that students who have used it will be well prepared for their GRE exams in the subject Careful pedagogy and clear writing throughout combine to make this an excellent choice for your physical chemistry course

Concise Physical Chemistry Donald W. Rogers, 2011-03-31 This book is a physical chemistry textbook that presents the essentials of physical chemistry as a logical sequence from its most modest beginning to contemporary research topics Many books currently on the market focus on the problem sets with a cursory treatment of the conceptual background and theoretical material whereas this book is concerned only with the conceptual development of the subject Comprised of 19 chapters the book will address ideal gas laws real gases the thermodynamics of simple systems thermochemistry entropy and the second law the Gibbs free energy equilibrium statistical approaches to

thermodynamics the phase rule chemical kinetics liquids and solids solution chemistry conductivity electrochemical cells atomic theory wave mechanics of simple systems molecular orbital theory experimental determination of molecular structure and photochemistry and the theory of chemical kinetics

Molecular Physical Chemistry for Engineering Applications

Florin Emilian Daneş, Silvia Daneş, Valeria Petrescu, Eleonora-Mihaela Ungureanu, 2021-07-06 This textbook introduces the molecular side of physical chemistry It offers students and practitioners a new approach to the subject by presenting numerous applications and solved problems that illustrate the concepts introduced for varied and complex technical situations The book offers a balance between theory tools and practical applications The text aims to be a practical manual for solving engineering problems in industries where processes depend on the chemical composition and physical properties of matter The book is organized into three main topics I the molecular structure of matter II molecular models in thermodynamics and III transport phenomena and mechanisms Part I presents methods of analysis of the molecular behavior in a given system while the following parts use these methods to study the equilibrium states of a material system and to analyze the processes that can take place when the system is in a state of non equilibrium in particular the transport phenomena Molecular Physical Chemistry for Engineering Applications is designed for upper level undergraduate and graduate courses in physical chemistry for engineers applied physical chemistry transport phenomena colloidal chemistry and transport transfer processes The book will also be a valuable reference guide for engineers technicians and scientists working in industry Offers modeling techniques and tools for solving exercises and practical cases Provides solutions and conclusions so students can follow results more closely Step by step problem solving enables students to understand how to approach complex issues

Physical Chemistry

Robert G. Mortimer, 2000-04-28 This new edition of Robert G Mortimer s Physical Chemistry has been thoroughly revised for use in a full year course in modern physical chemistry In this edition Mortimer has included recent developments in the theories of chemical reaction kinetics and molecular quantum mechanics as well as in the experimental study of extremely rapid chemical reactions While Mortimer has made substantial improvements in the selection and updating of topics he has retained the clarity of presentation the integration of description and theory and the level of rigor that made the first edition so successful Emphasizes clarity every aspect of the first edition has been examined and revised as needed to make the principles and applications of physical chemistry as clear as possible Proceeds from fundamental principles or postulates and shows how the consequences of these principles and postulates apply to the chemical and physical phenomena being studied Encourages the student not only to know the applications in physical chemistry but to understand where they come from Treats all topics relevant to undergraduate physical chemistry

Molecular Thermodynamics Donald A. McQuarrie, John D. Simon, 1999-02-24 This text covers the principles of quantum mechanics before engaging those ideas in the subsequent development of thermodynamics It includes worked examples and chapter ending problems with solutions

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