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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

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.

Intended for upper-level undergraduate and graduate courses in chemistry, physics, mathematics and engineering, this text is also suitable as a reference for advanced students in the physical sciences. Detailed problems and worked examples are included.

The canonical ensemble - Other ensembles and

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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.

This textbook facilitates students' ability to apply fundamental principles and concepts in classical thermodynamics to solve challenging problems relevant to industry and everyday life. It also introduces the reader to the fundamentals of statistical mechanics, including understanding how the microscopic properties of atoms and molecules, and their associated intermolecular interactions, can be accounted for to calculate various average properties of macroscopic systems. The author emphasizes application of the fundamental principles outlined above to the calculation of a variety of thermodynamic properties, to the estimation of conversion efficiencies for work production by heat interactions, and to the solution of practical thermodynamic problems related to the behavior of non-ideal pure fluids and fluid mixtures, including phase equilibria and chemical reaction equilibria. The book contains detailed solutions to many challenging sample problems in classical thermodynamics and statistical mechanics that will help the reader

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Crystallize the material taught. Class-tested and perfected over 30 years of use by nine-time Best Teaching Award recipient Professor Daniel Blankschtein of the Department of Chemical Engineering at MIT, the book is ideal for students of Chemical and Mechanical Engineering, Chemistry, and Materials Science, who will benefit greatly from in-depth discussions and pedagogical explanations of key concepts. Distills critical concepts, methods, and applications from leading full-length textbooks, along with the author's own deep understanding of the material taught, into a concise yet rigorous graduate and advanced undergraduate text; Enriches the standard curriculum with succinct, problem-based learning strategies derived from the content of 50 lectures given over the years in the Department of Chemical Engineering at MIT; Reinforces concepts covered with detailed solutions to illuminating and challenging homework problems.

This book will revolutionize the way physical chemistry is taught by bridging the gap between the traditional "solve a bunch of equations for a very simple model" approach and the computational methods that are used to solve research problems. While some recent textbooks include exercises using pre-packaged Hartree-Fock/DFT calculations, this is largely limited to giving students a proverbial black box. The DIY (do-it-yourself) approach taken in this book helps student gain understanding by building their own simulations from scratch. The reader of this book should come away with the ability to apply and adapt these techniques in computational chemistry to his or her own research problems, and have an

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enhanced ability to critically evaluate other computational results. This book is mainly intended to be used in conjunction with an existing physical chemistry text, but it is also well suited as a stand-alone text for upper level undergraduate or intro graduate computational chemistry courses.

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