
STATISTICAL MECHANICS

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John Dirk Walecka



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Computational Approaches for the Prediction of pKa Values George C. Shields, Paul G. Seybold, 2013-12-07 The pKa of a compound describes its acidity or basicity and therefore is one of its most important properties Its value determines what form of the compound positive ion negative ion or neutral species will be present under different circumstances This is crucial to the action and detection of the compound as a drug pollutant or other active chemical agent In many cases it is desirable to predict pKa values prior to synthesizing a compound and enough is now known about the salient features that influence a molecule's acidity to make these predictions Computational Approaches for the Prediction of pKa Values describes the insights that have been gained on the intrinsic and extrinsic features that influence a molecule's acidity and discusses the computational methods developed to estimate acidity from a compound's molecular structure The authors examine the strengths and weaknesses of the theoretical techniques and show how they have been used to obtain information about the acidities of different classes of chemical compounds The book presents theoretical methods for both general and more specific applications covering methods for various acids in aqueous solutions including oxyacids and related compounds nitrogen acids inorganic acids and excited state acids as well as acids in nonaqueous solvents It also considers temperature effects isotope effects and other important factors that influence pKa This book provides a resource for predicting pKa values and understanding the bases for these determinations which can be helpful in designing better chemicals for future uses

Gibbs Energy and Helmholtz Energy Trevor M. Letcher, Emmerich Wilhelm, 2021-09-15 This book contains the latest information on all aspects of the most important chemical thermodynamic properties of Gibbs energy and Helmholtz energy as related to fluids Both the Gibbs energy and Helmholtz energy are very important in the fields of thermodynamics and material properties as many other properties are obtained from the temperature or pressure dependence Bringing all the information into one authoritative survey the book is written by acknowledged world experts in their respective fields Each of the chapters will cover theory experimental methods and techniques and results for all types of liquids and vapours This book is the fourth in the series of Thermodynamic Properties related to liquids solutions and vapours edited by Emmerich Wilhelm and Trevor Letcher The previous books were Heat Capacities 2010 Volume Properties 2015 and Enthalpy 2017 This book fills the gap in fundamental thermodynamic properties and is the last in the series

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Continuum mechanics Kinetic theory of gases and the boltzmann equation Transport processes in dilute gases Theory of brownian motion The time correlation function formalism **Viscoelasticity of Polymers** Kwang Soo Cho, 2016-05-30 This book offers a comprehensive introduction to polymer rheology with a focus on the viscoelastic characterization of polymeric materials It contains various numerical algorithms for the processing of viscoelastic data from basic principles to advanced examples which are hard to find in the existing literature The book takes a multidisciplinary approach to the study of the viscoelasticity of polymers and is self contained including the essential mathematics continuum mechanics polymer science and statistical mechanics needed to understand the theories of polymer viscoelasticity It covers recent achievements in polymer rheology such as theoretical and experimental aspects of large amplitude oscillatory shear LAOS and numerical methods for linear viscoelasticity as well as new insights into the interpretation of experimental data Although the book is balanced between the theoretical and experimental aspects of polymer rheology the author s particular interest in the theoretical side will not remain hidden Aimed at readers familiar with the mathematics and physics of engineering at an undergraduate level the multidisciplinary approach employed enables researchers with various scientific backgrounds to expand their knowledge of polymer rheology in a systematic way Statistical Mechanics Donald Allan McQuarrie, 1975

Encyclopedia of Materials Science and Engineering , 1989 **Federal Executive Directory** , 1985 Covers only the management sector of the executive branch **Problems on Statistical Mechanics** D.A.R Dalvit, J Frastai, Ian Lawrie, 1999-01-01 A thorough understanding of statistical mechanics depends strongly on the insights and manipulative skills that are acquired through the solving of problems Problems on Statistical Mechanics provides over 120 problems with model solutions illustrating both basic principles and applications that range from solid state physics to cosmology An introductory chapter provides a summary of the basic concepts and results that are needed to tackle the problems and also serves to establish the notation that is used throughout the book The problems themselves occupy five chapters progressing from the simpler aspects of thermodynamics and equilibrium statistical ensembles to the more challenging ideas associated with strongly interacting systems and nonequilibrium processes Comprehensive solutions to all of the problems are designed to illustrate efficient and elegant problem solving techniques Where appropriate the authors incorporate extended discussions of the points of principle that arise in the course of the solutions The appendix provides useful mathematical formulae *Introduction To Statistical Mechanics: Solutions To Problems* John Dirk Walecka, 2016-08-25 Statistical mechanics is concerned with defining the thermodynamic properties of a macroscopic sample in terms of the properties of the microscopic systems of which it is composed The previous book Introduction to Statistical Mechanics provided a clear logical and self contained treatment of equilibrium statistical mechanics starting from Boltzmann s two statistical assumptions and presented a wide variety of applications to diverse physical assemblies An appendix provided an introduction to non equilibrium statistical mechanics through the Boltzmann equation and its extensions The coverage in that

book was enhanced and extended through the inclusion of many accessible problems The current book provides solutions to those problems These texts assume only introductory courses in classical and quantum mechanics as well as familiarity with multi variable calculus and the essentials of complex analysis Some knowledge of thermodynamics is also assumed although the analysis starts with an appropriate review of that topic The targeted audience is first year graduate students and advanced undergraduates in physics chemistry and the related physical sciences The goal of these texts is to help the reader obtain a clear working knowledge of the very useful and powerful methods of equilibrium statistical mechanics and to enhance the understanding and appreciation of the more advanced texts **Solutions to Accompany McQuarrie's**

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include result discussions that enhance the lecture material For reader s convenience the problem assignments are reproduced in this volume Prov de l editor **Elementary Lectures in Statistical Mechanics** George D.J. Phillies,2012-12-06 This volume is based on courses on Statistical Mechanics which I have taught for many years at the Worcester Polytechnic Institute My objective is to treat classical statistical mechanics and its modern applications especially interacting particles correlation functions and time dependent phenomena My development is based primarily on Gibbs s ensemble formulation Elementary Lectures in Statistical Mechanics is meant as a relatively sophisticated undergraduate or relatively straightforward graduate text for physics students It should also be suitable as a graduate text for physical chemistry students Physicists may find my treatment of algebraic manipulation to be more explicit than some other volumes In my experience some of our colleagues are perhaps a bit over enthusiastic about the ability or tendency of our students to complete gaps in the derivations I emphasize a cyclic development of major themes I could have begun with a fully detailed formal treatment of ensemble mechanics as found in Gibbs s volume and then given material realizations I instead interleave formal discussions with simple concrete models The models illustrate the formal definitions The approach here gives students a chance to identify fundamental principles and methods before getting buried in ancillary details

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