

Arieh Ben-Naim

Solvation Thermodynamics

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Arieh Y. Ben-Naim



Solvation Thermodynamics:

Solvation Thermodynamics Arie Y. Ben-Naim, 2013-03-09 This book deals with a subject that has been studied since the beginning of physical chemistry. Despite the thousands of articles and scores of books devoted to solvation thermodynamics, I feel that some fundamental and well-established concepts underlying the traditional approach to this subject are not satisfactory and need revision. The main reason for this need is that solvation thermodynamics has traditionally been treated in the context of classical macroscopic thermodynamics alone. However, solvation is inherently a molecular process dependent upon local rather than macroscopic properties of the system. Therefore, the starting point should be based on statistical mechanical methods. For many years, it has been believed that certain thermodynamic quantities such as the standard free energy or enthalpy or entropy of solution may be used as measures of the corresponding functions of solvation of a given solute in a given solvent. I first challenged this notion in a paper published in 1978 based on analysis at the molecular level. During the past ten years, I have introduced several new quantities which, in my opinion, should replace the conventional measures of solvation thermodynamics. To avoid confusing the new quantities with those referred to conventionally in the literature as standard quantities of solvation, I called these nonconventional generalized and local standard quantities and attempted to point out the advantages of these new quantities over the conventional ones.

Solvation Thermodynamics Professor of Physical Chemistry Arie Ben-Naim, 2014-01-15 *Thermodynamics of Solvation* Gennadiĭ Alekseevich Krestov, 1991 Aimed at scientists interested in the structure and dynamics of aqueous electrolyte solutions, this work examines the concept of the chemical nature of solutions. It shows quantitatively in tabulations of thermodynamic data for metal ions and anions the role of solvents as chemical reagents. **Statistical Thermodynamics**

for Chemists and Biochemists Arie Y. Ben-Naim, 2013-11-11 This book was planned and written with one central goal in mind: to demonstrate that statistical thermodynamics can be used successfully by a broad group of scientists ranging from chemists through biochemists to biologists who are not and do not intend to become specialists in statistical thermodynamics. The book is addressed mainly to graduate students and research scientists interested in designing experiments the results of which may be interpreted at the molecular level or in interpreting such experimental results. It is not addressed to those who intend to practice statistical thermodynamics per se. With this goal in mind, I have expended a great deal of effort to make the book clear, readable, and I hope enjoyable. This does not necessarily mean that the book as a whole is easy to read. The first four chapters are very detailed. The last four become progressively more difficult to read for several reasons. First, presuming that the reader has already acquired familiarity with the methods and arguments presented in the first part, I felt that similar arguments could be skipped later on, leaving the details to be filled in by the reader. Second, the systems themselves become progressively more complicated as we proceed toward the last chapter. Single-Ion Solvation Philippe Hunenberger, Maria Reif, 2015-10-20 Ions are ubiquitous in chemical, technological, ecological, and biological processes. Characterizing their role in

these processes in the first place requires the evaluation of the thermodynamic parameters associated with the solvation of a given ion. However, due to the constraint of electroneutrality, the involvement of surface effects and the ambiguous connection between microscopic and macroscopic descriptions, the determination of single ion solvation properties via both experimental and theoretical approaches has turned out to be a very difficult and highly controversial problem. This unique book provides an up-to-date compact and consistent account of the research field of single ion solvation thermodynamics that has over one hundred years of history and still remains largely unsolved. By reviewing the various approaches employed to date, establishing the relevant connections between single ion thermodynamics and electrochemistry, resolving conceptual ambiguities, and giving an exhaustive data compilation in the context of alkali and halide hydration, this book provides a consistent synthesis in depth understanding and clarification of a large and sometimes very confusing research field. The book is primarily aimed at researchers, professors, postgraduates, graduates, and industrial researchers concerned with processes involving ionic solvation properties; these are ubiquitous, e.g., in physical organic, analytical chemistry, electrochemistry, biochemistry, pharmacology, geology, and ecology. Because of the concept definitions and data compilations it contains, it is also a useful reference book to have in a university library. Finally, it may be of general interest to anyone wanting to learn more about ions and solvation. Key features: discusses both experimental and theoretical approaches and establishes the connection between them; provides both an account of the past research covering over one hundred years and a discussion of current directions in particular on the theoretical side; involves a comprehensive reference list of over 2000 citations; employs a very consistent notation including table of symbols and unambiguous definitions of all introduced quantities; provides a discussion and clarification of ambiguous concepts, i.e., concepts that have not been defined clearly or have been defined differently by different authors, leading to confusion in past literature; encompasses an exhaustive data compilation in the restricted context of alkali and halide hydration along with recommended values after critical analysis of this literature; data is illustrated by a number of synoptic colour figures that will help the reader to grasp the connections between different concepts in one single picture.

Fundamentals and Practice in Statistical Thermodynamics

Jianzhong Wu, John M. Prausnitz, 2024-08-20. Bridge the gap between thermodynamic theory and engineering practice with this essential textbook. Thermodynamics is a discipline which straddles the fields of chemistry, physics, and engineering and has long been a mainstay of undergraduate and graduate curricula. Conventional thermodynamics courses, however, often ignore modern developments in statistical mechanics such as molecular simulation methods, cooperative phenomena, phase transitions, universality, as well as liquid state and polymer theories despite their close relevance to both fundamental research and engineering practice. *Fundamentals and Practice in Statistical Thermodynamics* fills this gap with an essential book that applies up-to-date statistical mechanical techniques to address the most crucial thermodynamics problems found in chemical and materials systems. It is ideally suited to introduce a new generation of researchers and molecular engineers to

modern thermodynamic topics with numerous cutting edge applications From Fundamentals and Practice in Statistical Thermodynamics readers will also find An introduction to statistical mechanical methods including molecular dynamics simulation Monte Carlo simulation as well as the molecular theories of phase transitions classical fluids electrolyte solutions polymeric materials and more Illustrative examples and exercise problems with solutions to facilitate student understanding Supplementary online materials covering the basics of quantum mechanics density functional theory variational principles of classical mechanics intermolecular interactions and many more subjects Fundamentals and Practice in Statistical Thermodynamics is ideal for graduate and advanced undergraduate students in chemical engineering biomolecular engineering environmental engineering materials science and engineering and all related scientific subfields of physics and chemistry

Molecular Theory of Solutions Arieh Ben-Naim, 2006-07-27 This book presents new and updated developments in the molecular theory of mixtures and solutions It is based on the theory of Kirkwood and Buff which was published more than fifty years ago This theory has been dormant for almost two decades It has recently become a very powerful and general tool to analyze study and understand any type of mixtures from the molecular or the microscopic point of view The traditional approach to mixture has been for many years based on the study of excess thermodynamic quantities This provides a kind of global information on the system The new approach provides information on the local properties of the same system Thus the new approach supplements and enriches our information on mixtures and solutions

Thermodynamics of Geothermal Fluids Andri Stefánsson, Thomas Driesner, Pascale Bénézech, 2018-12-17 Volume 76 of Reviews in Mineralogy and Geochemistry presents an extended review of the topics conveyed in a short course on Geothermal Fluid Thermodynamics held prior to the 23rd Annual V M Goldschmidt Conference in Florence Italy August 24 25 2013 It covers Thermodynamics of Geothermal Fluids The Molecular Scale Fundament of Geothermal Fluid Thermodynamics Thermodynamics of Aqueous Species at High Temperatures and Pressures Equations of State and Transport Theory Mineral Solubility and Aqueous Speciation Under Hydrothermal Conditions to 300 C The Carbonate System as an Example Thermodynamic Modeling of Fluid Rock Interaction at Mid Crustal to Upper Mantle Conditions Speciation and Transport of Metals and Metalloids in Geological Vapors Solution Calorimetry Under Hydrothermal Conditions Structure and Thermodynamics of Subduction Zone Fluids from Spectroscopic Studies and Thermodynamics of Organic Transformations in Hydrothermal Fluids

Classical and Molecular Thermodynamics of Fluid Systems Juan H. Vera, Grazyna Wilczek-Vera, Claudio Olivera-Fuentes, Costas Panayiotou, 2024-11-14 This text explores the connections between different thermodynamic subjects related to fluid systems In an innovative way it covers the subject from first principles to the state of the art in fundamental and applied topics Using simple nomenclature and algebra it clarifies concepts by returning to the conceptual foundation of thermodynamics The structural elements of classical and molecular thermodynamics of fluid systems presented cover via examples and references both the usefulness and the limitations of thermodynamics for the

treatment of practical problems This new edition explores recent advances in statistical associated fluid theories and contains creative end of chapter problems connecting the theory with real life situations It includes new chapters on thermodynamics of polymer solutions and molecular thermodynamics and also presents advances in the study of the activity of individual ions Provides a concise structure of concepts using simple nomenclature and algebra Clarifies problems usually overlooked by standard texts Features end of chapter problems to enhance the reader's understanding of the concepts Includes diverse topics of interest to researchers and advanced students including elements of statistical thermodynamics models of solutions statistical associated fluid theory and the activity of individual ions Offers four appendices giving step by step procedures and parameters for direct use of the PRSV equation of state and the ASOG KT group method for fugacity and activity coefficient calculations Features a complete set of solutions to problems throughout the book available for download on the book's webpage under Support Material This textbook is written for advanced undergraduate and graduate students studying chemical engineering and chemistry as well as for practicing engineers and researchers

Water and Biological Macromolecules Westhof, 1993-08-16 *Water and Biological Macromolecules* presents an excellent description of the structural aspects of water molecules around biological macromolecules Topics discussed include the properties of water in solid and liquid states proteins nucleic acids polysaccharides and lipids and theoretical approaches for understanding the macroscopic observations and integrating microscopic descriptions The nature and roles of hydration forces in macromolecular complexation and cell cell interactions are explained in addition to phenomena such as entropy enthalpy compensation and the thermodynamic treatment of water bridging *Water and Biological Macromolecules* will be a valuable reference for biophysicists biochemists and macromolecular biologists

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