



Thermodynamics of Solutions: From Gases to Pharmaceutics to Proteins

Eli Ruckenstein, Ivan L. Shulgin



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This book consists of a number of papers regarding the thermodynamics and structure of multicomponent systems that we have published during the last decade. Even though they involve different topics and different systems, they have something in common which can be considered as the “signature” of the present book. First, these papers are concerned with “difficult” or very nonideal systems, i. e. systems with very strong interactions (e. g. , hyd- gen bonding) between components or systems with large differences in the partial molar v- umes of the components (e. g. , the aqueous solutions of proteins), or systems that are far from “normal” conditions (e. g. , critical or near-critical mixtures). Second, the conventional th- modynamic methods are not sufficient for the accurate treatment of these mixtures. Last but not least, these systems are of interest for the pharmaceutical, biomedical, and related ind- tries. In order to meet the thermodynamic challenges involved in these complex mixtures, we employed a variety of traditional methods but also new methods, such as the fluctuation t- ory of Kirkwood and Buff and ab initio quantum mechanical techniques. The Kirkwood-Buff (KB) theory is a rigorous formalism which is free of any of the - proximations usually used in the thermodynamic treatment of multicomponent systems. This theory appears to be very fruitful when applied to the above mentioned “difficult” systems.



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