

Protein - Water Interactions: A Differential Approach, 2014, pages 1-132

Protein - water interactions: A differential approach

Sirotkin V.

Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

© 2014 by Nova Science Publishers, Inc. All rights reserved. This book is aimed at understanding which molecular parameters control the thermodynamics, structure, and functions of the protein-water systems. Proteins are one of the most important classes of biological molecules. Water binding (hydration or biological water) plays a crucial role in determining the structure, stability, and functions of proteins. Knowledge of processes occurring upon hydration or dehydration of protein macromolecules is very important in biotechnological and pharmaceutical applications of proteins such as their use as biocatalysts, biosensors, and selective adsorbents. There are essential differences between hydration and bulk water surrounding a protein. This means that a characterization of the hydration of protein macromolecules requires elucidating the effects of both the protein on water and vice versa. Therefore, a quantitative estimation of the protein and water contributions to the thermodynamic functions of binary protein-water systems is of considerable fundamental importance and practical interest. This book describes the basic principles of a novel methodology to investigate the protein-water interactions. This methodology is based on the analysis of the excess thermodynamic functions of mixing. The thermodynamic properties (volume V , enthalpy H , entropy S , heat capacity C_p , and Gibbs free energy G) of a real binary water-protein system can be expressed in terms of the excess functions. They are the difference between the thermodynamic function of mixing in a real system and the value corresponding to an ideal system at the same temperature, pressure and composition. For an ideal system, all excess functions are zero. Deviations of the excess functions from zero indicate the extent to which the studied binary system is non-ideal due to strong specific interactions between components (i.e., hydrogen bonding and charge-charge interactions).
