



Structure and Dynamics of Solutions (Studies in Physical and Theoretical Chemistry)

Hitohsi Ohtaki

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Recent advances in the study of structural and dynamic properties of solutions have provided a molecular picture of solute-solvent interactions. Although the study of thermodynamic as well as electronic properties of solutions have played a role in the development of research on the rate and mechanism of chemical reactions, such macroscopic and microscopic properties are insufficient for a deeper understanding of fast chemical and biological reactions. In order to fill the gap between the two extremes, it is necessary to know how molecules are arranged in solution and how they change their positions in both the short and long range. This book has been designed to meet these criteria.

It is possible to develop a sound microscopic picture for reaction dynamics in solution without molecular-level knowledge of how reacting ionic or neutral species are solvated and how rapidly the molecular environment is changing with time. A variety of actual examples is given as to how and when modern molecular approaches can be used to solve specific solution problems. The following tools are discussed: x-ray and neutron diffraction, EXAFS, and XANES, molecular dynamics and Monte Carlo computer simulations, Raman, infrared, NMR, fluorescence, and photoelectron emission spectroscopic methods, conductance and viscosity measurements, high pressure techniques, and statistical mechanics methods. Static and dynamic properties of ionic solvation, molecular solvation, ion-pair formation, ligand exchange reactions, and typical organic solvents are useful for bridging the gap between classical thermodynamic studies and modern single-molecule studies in the gas phase.

The book will be of interest to solution, physical, inorganic, analytical and structural chemists as well as to chemical kineticists.

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