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Volume 17

Water and Biological Macromolecules

Edited by

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Preface

The Makonde people of Mozambica, well-known for their wood sculptures, tell the following legendary story of their origins. A long time ago came to the Rovuma valley a living being, not yet quite human. He did not eat, drank little, never went into the river and did not cut his hair. Once out of boredom, he took a piece of wood and carved something looking like him. In the evening, he left the wooden sculpture standing on the earth. The next morning, the statue was alive and it was a woman. They both swam in the river and settled next to the river. Later, the woman gave birth, but the child was still-born. They moved to another spot close to the water and, again, they had a still-born baby. They moved several times to different sites along the river without any more luck. Finally, they decided to run away from water, took refuge on a dry table-land, and the woman gave birth to a large descendance. From then on, Makonde built their villages one-hour's walking distance from a water spot.

This legend renders the constant love-hate story of life and water. Indeed, although life, as we know it, is inconceivable without water, life could only emerge and develop together with systems for controlling and confining water. Whatever the nature of the prebiotic soup (warm little ponds or clays), alternation of wet and dry periods is required. From lipid bilayers to the amniotic egg, life evolved around the containment of water. This subtle and parsimonious use of water constitutes a recurrent theme in the present book.

The book is organized in five sections. The first describes the peculiar and narcissistic properties of water in the solid and liquid states. Analysis of the hydrogen bonded water networks in the ice polymorphs indicate that they are characterized by a maximization of the number of hydrogen bonds and a minimization of the short-range repulsive restrictions. Although the formation and breaking of the hydrogen bonds occur on the picosecond time scale, the three-dimensional hydrogen bond network has a retarding influence on the rotational and translational molecular mobility, as measured by nuclear magnetic resonance techniques. A vision of water in constant conflict between order and chaos illustrates the links between

structure and movement and stresses how molecular dynamics is constrained by molecular geometry.

The three central sections treat the main types of biological macromolecules: proteins, nucleic acids, polysaccharides, and lipids. They all exploit rather extensively the data obtained by X-ray diffraction analysis of crystals. The fundamental driving force for the folding of a macromolecule into a three-dimensional architecture with potential biological functions is the hydrophobic effect, arising much less from the macromolecule's phobia of water than from the self-loving properties of water molecules. Depending on the chemical entities constituting the macromolecule, there is a constant interplay between the hydrophobic effect and the specific interactions of hydrophilic sites on the macromolecule with water molecules. The wealth of structural information gathered by crystallographers on protein crystals allows extensive comparative studies on the arrangement of water molecules around amino acids and elements of secondary structures. Furthermore, careful analysis of those static tertiary structures led to understanding of the role of water molecules in the formation and denaturation of the main repetitive secondary structures of proteins. In contrast to the case of proteins, the folding and stability of nucleic acids are not principally governed by the hydrophobic effect, as indicated by the thermodynamic characteristics of their denaturation. Since the discovery of the A to B transition in DNA made by Franklin and Gosling and which was so instrumental for the establishment of the double-stranded DNA helix by Watson and Crick, the role of water in stabilizing or inducing DNA conformations has been repeatedly stressed. The chapters describe the beautiful and striking arrangements of water molecules around nucleic acids both from the point of view of their observation, stressing the geometry and periodicity of nucleic acid helices, and of their theoretical interpretation, emphasizing movements and water exchanges. Polysaccharides and lipids delineate extreme cases. Stereochemistry imposes the precise spacings and arrangements of hydroxyl groups in polysaccharides so that hydrophilic interactions with water molecules are facilitated. Bilayers formed by polar lipids, although susceptible to specific interactions, display striking electrostatic properties partly governed by geometry. In the last section, theoretical approaches for understanding the macroscopic observations and integrating the microscopic descriptions of the previous sections are developed. Thus, the nature and roles of hydration forces in macromolecular complexation and cell-cell interactions are explained, as well as phenomena such as entropy-enthalpy compensation and the thermodynamic treatment of water bridging.

Most of the chapters accentuate the structural aspects of water molecules around biological macromolecules. Water is so pervasive that attempting to cover all of its features becomes an impossible task. Each contributor has taken special care to refer to other review articles or books, either more

general or specialized, so that the interested reader can complement his knowledge. Finally, with respectful awe, mention should be made to the books and reviews edited by F. Franks, *Water: A Comprehensive Treatise*, published by Plenum Press, and *Water Science Reviews*, published by Cambridge University Press.

The power of iconography is well appreciated outside the realm of science. Indeed, scientists consider pictures just as mirrors of nature, more or less accurate, and besides, there is always the danger of equating ideas with descriptions. Nevertheless, the insertion of a large number of figures was actively pursued in each contribution because descriptions of molecular patterns, of the way water molecules repeatedly arrange themselves around macromolecules, while certainly not helping to organize our thought, constitute a rich soil on which our insight and intuition feed and grow. At the onset of each section, an artistic drawing tries to convey the tension between geometry and dynamics so strongly inherent to the nature of water. I thank Marc Westhof (Hoboken, N. J.) for letting me publish these drawings in black-and-white and not with their original colours.

I thank all the authors for their contributions and I hope they learnt as much from writing as I did from editing.

Strasbourg, 1992

E. W.

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