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George Némethy - *The Structure of Water and the
Thermodynamic Properties of Aqueous Solutions*

ANNALI DELL' ISTITUTO SUPERIORE DI SANITÀ



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THE STRUCTURE OF WATER AND
THE THERMODYNAMIC PROPERTIES OF
AQUEOUS SOLUTIONS

GEORGE NÉMETHY

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In recent years a great deal of progress has been made concerning the structure of water, aqueous solutions, and associations of organic molecules in solution.

One of the important results of such studies, using both experiments and theoretical models, has been to increase our knowledge of the conformation of proteins in solution. In this way, fundamental data for a better understanding of the biological properties of proteins have been obtained and this is basic to cell biology and physiology.

Prof. George Némethy, of the Rockefeller University, N. Y., is recognized as one of the most important scientists who have contributed to the development of new concepts and ideas on the structure of water, and thermodynamic properties of aqueous solutions. Prof. Némethy delivered a series of lectures on this topic at the Istituto Superiore di Sanità in the autumn 1970. The present monograph originated from these lectures, and it is a great privilege to present it as a special issue of the Annali dell'Istituto Superiore di Sanità.

The Istituto Superiore di Sanità is pleased to have been able, in collaboration with the Italian Research National Council (CNR); the Theoretical Chemistry Group, the Institute of Chemical-Physics, and the Institute of Physics of the University of Palermo; the Institute of Physics, Faculty of Engineering of the University of Rome, to offer to young Italian scientists the opportunity of personal contact and discussion with Prof. Némethy.

G. B. MARINI-BETTÒLO

George Némethy was born in 1934 in Budapest, Hungary, where he lived until 1951. Since 1954, he lives in the United States. He received the B. A. degree in chemistry in 1956 at Lincoln University, and the Ph. D. degree in physical chemistry in 1962 at Cornell University, with a thesis on «The Structure of Water and Hydrophobic Bonding in Proteins». In 1962-63, he worked as physical chemist at the General Electric Research Laboratory in New York. Since 1963, he is assistant professor of biophysical chemistry at the Rockefeller University in New York.

He has carried out research work in the following areas: structure of water and aqueous solutions, theoretical treatments of noncovalent interactions and of conformational stability of proteins, theoretical models for allosteric interactions, experimental and theoretical work on the association of organic molecules in aqueous solution.

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This survey of the structure of water and of aqueous solutions is based on the material presented in a series of lectures held at the Istituto Superiore di Sanità in Rome, under the auspices of the Laboratori di Fisica, from September 18 to October 26, 1970. It is not intended to present here an exhaustive review of the subjects covered, inasmuch as there exist several recent, detailed, and authoritative reviews on water (KAVANAU, 1964, BERENDSEN, 1967; HORNE, 1968; FLETCHER, 1970; HORNE, 1971; and others), first and foremost the excellent monograph *The Structure and Properties of Water* by EISENBERG & KAUZMANN (1969). I am particularly indebted to the latter for many useful insights obtained from the perusal of their book. A critical and lucid evaluation of the current standing of structural studies in water was presented recently by FRANK (1970).

Some topics are discussed here which seemed to me of greatest actuality and interest at the time of writing. Often only selected examples are used, instead of the detailed survey of a particular field. This may have led to incompleteness and some subjectivity. On the other hand, it is hoped that the emphasis on topics of current interest can offer some helpful guidelines in studies of the vast literature (*) on water structure.

Throughout this survey, those thermodynamic and related physico-chemical aspects of the properties of water are emphasized which lead to the generally accepted concept of liquid water being a more ordered substance than most other liquids. Obviously, other points of view are possible as well, as indicated very poignantly by the following inscription, discovered in Rome while preparing these lectures:

« Il disordine è nell'acqua,
l'equilibrio nel vino ».

(Anonimo romano)

(*) A thorough bibliography of publications on the structure and physical properties of pure liquid water, published between 1957 and 1968, has been compiled by TURNER (1969). It contains 1643 entries.