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THE STRUCTURE OF WATER IN CAPSULE OF THE BOVINE CRYSTALLINE LENS

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Indexing Words

water; water structure; crystalline lens; lens capsule

Yoshimasa ISAYAMA, Akio YAMANAKA and Yukio KANAJI *The Structure of Water in Capsule of the Bovine Crystalline Lens.* Kobe J. Med. Sci. 17, 185-190, December 1971——It has been reported that water is highly oriented in the optic and sciatic nerve, and also in the aqueous region of the membrane system inside the nervous tissue. In the present experiment using the bovine lens capsule, the molecular structure of water in the membrane was studied by means of differential radial distribution function. The results obtained are reasonably explained, assuming that the molecules of water in the lens capsule are arranged octahedrally, although in the ordinary water tetrahedrally.

INTRODUCTION

In the previous report[3], the behavior and the role of water in the living body, particularly in the nervous tissue have been investigated by means of high-resolution nuclear magnetic spectroscopy. The results suggest that the high viscosity of water inside the optic and sciatic nerve is attributed to the oriented states of the molecules.

Generally, cells in the nervous tissue are divided into discrete compartments by a membrane system. It may be deduced from our previous observation[4] on the proton resonance signal of water in the lens capsule that water molecules within or at the surface of the membrane are highly oriented in relation to the ordered polar groups such as protein.

In the present paper, attention was focused on the molecular structure of water in the aqueous region of the membrane, and an X-ray study was made to illustrate the water structure with the radial distribution function.

METHODS

The radial distribution function (RDF) obtained experimentally by X-ray diffraction is available for acquiring information about the molecular structure of liquids, the method of which was utilized in the present experiment and all calculations were performed by OKITAK 5090 computer.

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MATERIALS

The anterior capsule of the bovine lens was removed without lens epithelium and sticked on a glass sample holder.

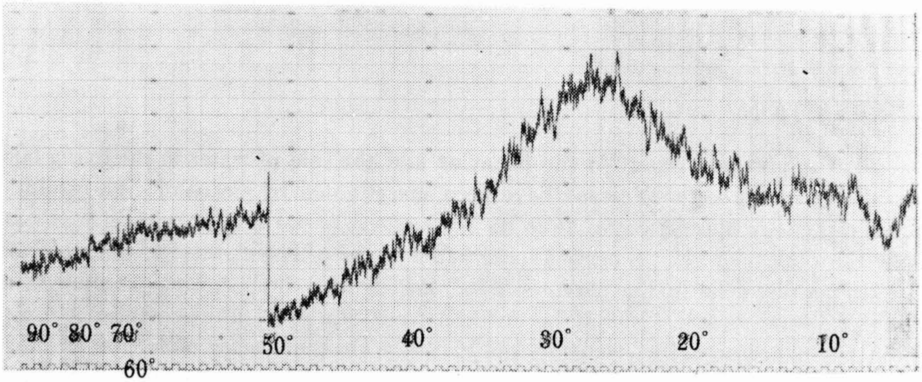
Cukα radiation (wave length: 1. 54 Å, apparatus is D-3F Geiger-Flex type made by Rigaku-Denki Co.) was filtrated through Ni filter. Reflection of X-ray from the surface of the sample applying a wide range diffractometer was counted with Geiger-Müller's tube. The diffracted intensity was measured in angle 2θ from 3° to 90°.

The same pattern of the scattering curve was observed by diffraction from either single or double membrane, which proved no appreciable effect was given from the surface of the holder glass.

RESULTS

The experimental scattering curve of the bovine capsule is illustrated in Fig. 1.

Fig. 1. Experimental scattering curve for lens capsule.



An outline of calculation procedure is described as follows. First, the experimental scattered intensity at each diffracted angle—$I_{obs}(\theta)$—is corrected.

$$I'_{obs}(\theta) = \frac{I_{obs}(\theta)}{P(\theta)} \quad \cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots (1)$$

where $P(\theta)$ is the poralization factor $(1+\cos^2 2\theta)$.

Next, co-ordinates of $I'_{obs}(\theta)$ are transformed to $I'(S)$, employing $S=2\sin\theta/\lambda$.

For normalizing the experimental function $I'_{obs}(S)$, the equation of coherent and incoherent scattering calculated from each atomic ratio in the sample is used. The ratio of each main atom in the lens capsule calculated from the analytical data by Kause:

O: 4.7893 H: 10.4595 C: 0.6260 N: 0.1605 Na: 0.0375 Cl: 0.0222

Then, function $i(S)$ expressed on the arrangement of atoms for S-coordinates is evaluated.

$$i(S)=\frac{I'_{obs}(S)-\sum_{m}\left[f_m^2+\left(Z_m-\sum_{j}f_{mj}^2\right)\right]}{f_e^2} \quad \cdots\cdots(2)$$

In this expression, f_m is the atomic scattering factor of type m atom. f_{mj} is the electron scattering factor of the jth electron in the type m atom. Z_m is the atomic number of the type m atom. f_e is the scattering factor of a single electron.

The following differential RDF is computed applying numerical values of i(S).

$$4\pi r^2 \Delta\rho(r)=8\pi r \sum_{S=0}^{S=max} Si(S)\ \sin\ (2\pi rS)\exp^{(-2.844S^2)}\Delta S \quad \cdots\cdots(3)$$

Now, $\exp^{(-2.844S^2)}$ refers to an "artificial temperature factor", wherein value 2.844 is obtained from the following equation $\exp(^{-b^2S^2max})=0.1$.

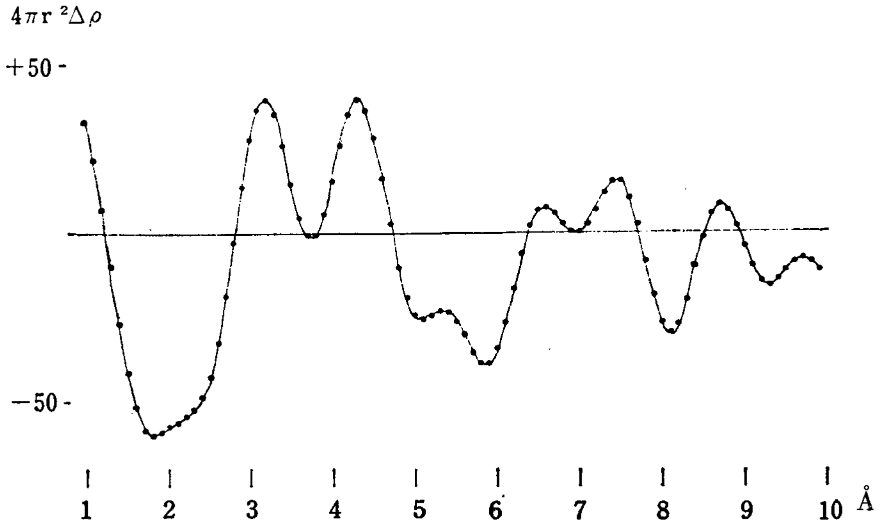
In RDF's equation (3);

$$\Delta\rho(r)=\rho(r)-\rho_0$$

where lettering $\rho(r)$ is the average atomic density at a radius r from any one atom; ρ_0 is the average density of atoms in the sample.

The results from numerical computation of differential RDF is illustrated in Fig. 2.

Fig. 2. Differencial radial distribution function of lens.



Since the radiation is scattered by electrons in an atom, the scattered intensity obtained for H atoms having only one electron can be considered to be extremely low and to be not participating in an appearance of peaks in the RDF's curve.

H_2O is a major component of the sample, comprising about 80% of total mass. Thus the following assumption can be accepted that the scattering of X-ray is due to oxygen atoms in H_2O. Peaks appeared in the radial distribution curve arise at the positions occupied by the oxygen atom.

DISCUSSION

In lattice structure of ice, the two covalent and two hydrogen bonds surrounding each oxygen atom are tetrahedrally oriented, so that an extensive three dimensional structure is built up. In the formation of ordinary water the original ice structure persists to a considerable degree[1].

Molecules of water in ordinary electrolytic solution are supposed to have a tetrahedral geometry; however, it has been suggested that there is a possibility that water molecules may be oriented octahedrally in some concentrated aqueous solution of electrolytes[6].

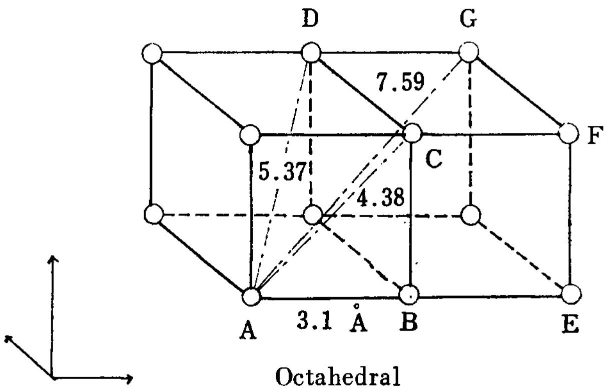
Fernández-Morán[2] has emphasized that water in living body, particularly in the aqueous region of membrane may be organized in ice-like or crystal-hydrated lattice.

In ice-like structure supposed to be ordered tetrahedrally, in ordinary water or aqueous solution; the shortest 0-0 distance (O-H---O) is calculated as about 2.8Å, while in another possible octahedral structure this distance is reported about 3.1 Å[6].

The position of peaks in RDF's curve was described in theoretical values as follows, when H_2O molecules arranged octahedrally[5]. These values almost corresponded to the positions experimentally obtained.

Fig. 3. Calculated values of significant 0-0 distance for tetrahedral and octahedral structure.

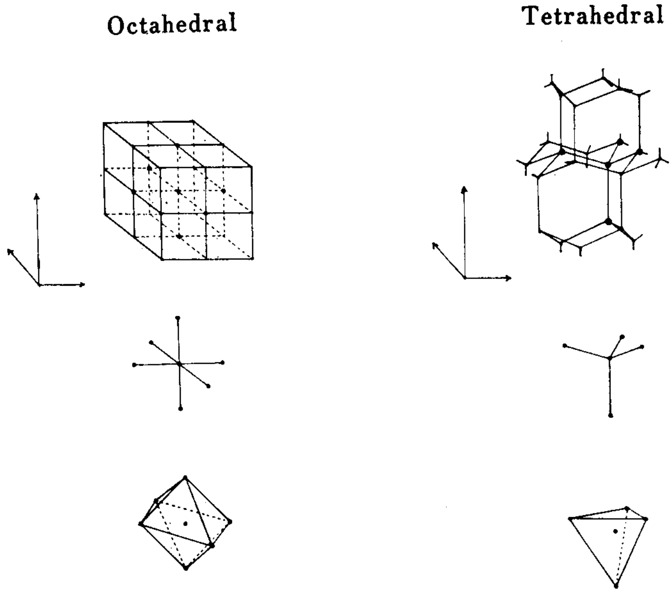
Tetrahedral	Octahedral
2.69	
	3.10
4.40	4.38
5.15	
	5.37
6.12	(6.30)
	6.93
7.61	7.59



Two structures, tetrahedron and octahedron, are shown in Fig. 4.

The results reported in this paper may propose a new concept of the water structure of the living membrane.

Fig. 4. Ideal models of two structures.



SUMMARY

Molecular structure of water in the lens capsule was investigated with the differential radial distribution function obtained by X-ray diffraction. Although ordinary ice-like structure of water is represented by tetrahedron, the possibility that the molecular geometry of water in the lens capsule is an octahedral arrangement is emphasized from the result of above experiments.

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