# 1.4. THE STRUCTURE OF WATER IN BIOLOGICAL SYSTEMS

Water differs from analogous molecules (CH_4, H_2S, H_2Te), it has unusually high melting and boiling points, dielectric constant, density, surface tension, specific heat and heat of vaporization. Only its viscosity and solute diffusion behaviour resemble those of other low molecular weight substances. Water exhibits the unusual behaviour of having a maximum density at 4ºC. Water has a high boiling and melting point, which is due to the dipole moment that contributes an additional force to the existing van der Waals attraction. These intermolecular forces make it difficult for water to escape into the vapour phase and give an almost crystalline structure to the liquid. Water has a high heat capacity. This means that a large amount of heat is necessary to raise its temperature. The relative permittivity of water is higher than that for most liquids. This property makes water a good solvent for ionic compounds. These physical properties suggest that water has a specific structure which is maintained by the intermolecular forces.

The water has a tetrahedral structure, with the oxygen atom in the centre and the two hydrogen atoms in two corners of the tetrahedron (Figure 1.4.1).
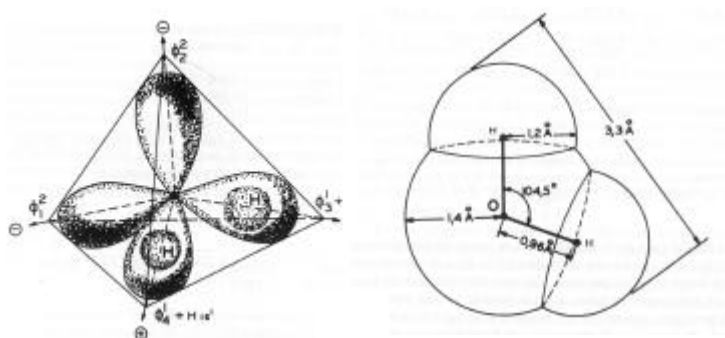

Figure 1.4.1 Schematic representation of the water molecule (Fennema, 1993)

The water molecules have a large dipole moment. This is because in the water molecule the electronic charge density is shifted towards the more electro-negative oxygen atom. Due to this polarity each molecule of water can associate with four other molecules of water. These dipole-dipole attractions are referred to as hydrogen bonds. Hydrogen bonds are very common in liquid water and ice (but not in vapour) .

The introduction of solutes into a water medium perturbs the existing organization of the water structure. The overall effect depends on the type of chemical groups that are introduced. The chemical groups can be classified into hydrophilic groups and hydrophobic groups.

The hydrophilic groups have a strong tendency to associate with water. They can be neutral (non electrolytes) and ionic (electrolytes). Neutral groups associate with water through hydrogen bonds (Figure 1.4.2 (A)). Electrolytes associate with water through ionic bonds like in Figure 1.4.2 (B). As ions tend to form a pair, the result is a hydrated ion pair.
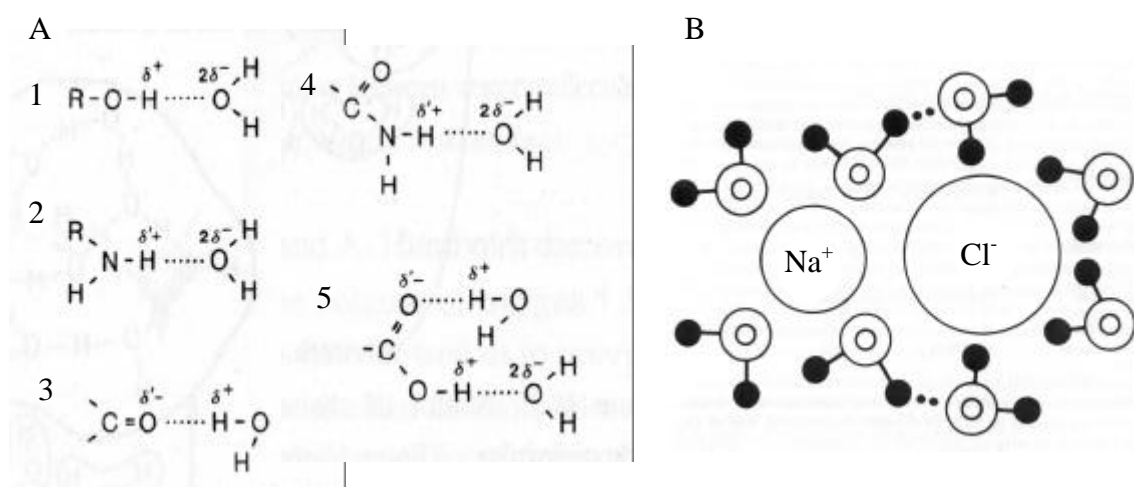

Figure 1.4.2 A. Neutral groups. 1. Hydroxyl groups. 2. Imino groups. 3. Carbonyl groups. 4. Amide groups. 5. Carboxylic groups (Motarjemi, 1988). B. Electrolytes associated with water (Fennema, 1993).

Anions are called "structure formers" because they associate with the hydrogen atoms which are externally located in the tetrahedral structure of water and are readily accessible. The anion-water association affects the water structure to a much smaller extent than the cations

which associate with the less accessible oxygen and therefore they perturb the structure of the water. The relative strength of water-anions bonds is higher than in water-cations and water-dipole.

The water molecule can be hydrogen bonded at two (or more) different loci, placed on the same or different biopolymers. This is termed a "water bridge". A molecule of water involved in a water bridge possesses a lower degree of randomness than a molecule of water attached at one single site. Also, the liberation of such a molecule requires an amount of energy equal to that necessary to rupture the bonds at two sites. Water bridging is common in, protein systems and affects to the conformation of the proteins (Figure 1.4.3).
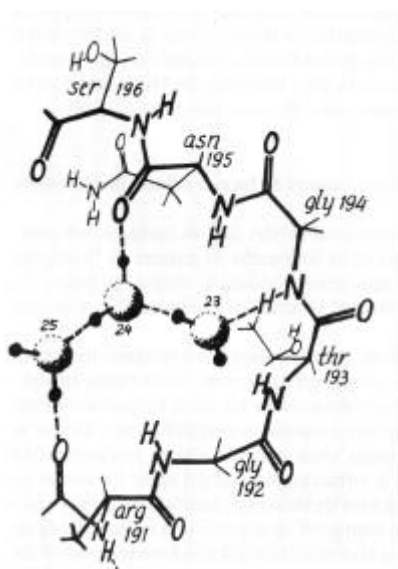
Figure 1.4.3 Example of hydrogen binding in a protein molecule (papain) illustrating water bridging (Fennema, 1993).

Hydrofobic groups have a repulsion to water, and therefore their introduction into the system interferes with the structure of the water molecules. Hydrophobic groups possess hardly any hydrogen bonding and have very low polarity, yet it is belived that they can interact with water or other hydrophobic groups. The latter interactions play an important role in the stabilization of the conformation of the proteins. The study of thermodynamic parameters (entropy, enthalpy, etc.) has shown that the water adjoining hydrophobic groups of biological molecules in aqueous solution possesses a more organized structure than that of the bulk water (i.e. a lower degree of entropy). In the presence of hydrophobic groups,

the solubility of a substance is decreased. Also, the availability of water surrounding a hydrophobic group to participate in acid and base ionization is reduced. Another consequence is the decreased interfacial tension between water and hydrophobic groups. The adherence of hydrophobic groups with each other results in the extrusion of the surrounding organized water into the bulk where they adopt a less organized structure. This happens often in the chains of protein molecules and is of great importance for the stability of the configuration of the protein chain. Denaturation of proteins causes the splitting of the hydrophobic groups, and thereby exposes increasing areas, originally masked by hydrophobic interaction, to contact with water. It therefore enhances the formation of an organized structure in the nearby water. This may result in a rise in the pH and the isoelectric point of the solution (Fennema, 1993).

The addition of electrolites to meat can affect its water structure, and the strong tendency of the electrolites to associate with water may influence the mass transfer of the meat. During drying water is removed from the meat, and being aware of the changes that reduction of water may cause to the protein conformation, the meat properties may change during the drying process. Dry-cured ham has a higher pH (Arnau *et al*., 1995) than raw meat, this is in concordance with the increasing pH due to denaturation of proteins as stated before.