So, why is water biologically important?

Terence H. Lilley

School of Clinical Dentistry, The University of Sheffield, Sheffield S10 2TA and Faculty of Health, Natural and Social Sciences, University of Sunderland, Sunderland SR1 3SD, UK (thlilley@aol.com)

Some brief impressionistic and necessarily subjectively based comments on the content of the Discussion Meeting are made. It is pointed out that the principal thrust of most of the presentations was directed towards structural aspects of proteins in various media. Comments are also made on the necessary interplay between the medium in which biomolecules occur and the interatomic forces between the atoms comprising the biomolecules. Some speculation is made on the possibility of life-forms existing in extreme environments.

Keywords: life; water; aqueous; biopolymers; inter-atomic and intermolecular forces

The thing we call life on Earth can be identified as having three necessary and sufficient processes, namely synthesis, metabolism and reproduction. (As a physical chemist, I have interests in two of these but I do have some friends who are organic and inorganic chemists who are interested in all three.)

The conference has purposely not addressed any of these issues from the viewpoint of hydration or from the more generic stance of solvation. It is, however, clear that even a cursory glance at any metabolic-pathway diagram indicates that to keep a ‘life engine’ running, any changes (equilibrium and/or kinetic) induced by a change in the surrounding ‘solvent’ medium must lead to a continued synchrony of the whole.

It is, I believe, fair to say that most of the work that has been presented during the conference has addressed issues from the ‘structural’ level, and there has been rather less concern about kinetic phenomena, although there has of course been some attention given to kinetic effects. Again, the majority of the work presented has been directed towards proteins, and fairly easily isolatable ones at that. It is certainly true that proteins can exist in various environments and in frozen aqueous media; much important information has been obtained over many years, which relates to, and sometimes explains, aspects of some life processes. There has been a bow towards nucleic acids but almost no mention has been made of the carbohydrates (other than peripherally in some of the discussion) or of the lipids. These are important not only to those forms of animal life that exist in a ‘watery’ environment but also to the contiguous plant life. Our attention during the meeting has been directed only to fauna and not to flora.

Life, even as we know it, consists of more than the 20 primary mammalian protein amino acids and the polymers thus formed. Many hundreds of structurally different amino acids exist in what we call ‘Nature’ and it is worth remembering that, for example, fungi also use amino acids that exhibit a wide range of molecular embroidery. Mushrooms are just as alive as we are (they synthesize, metabolize and reproduce) and have as a species been around a lot longer. There is a tendency for us humans to consider all things associated with us and our living to be the most important of all things on Earth or even the universe: this may not be true.

One of the more transparent features associated with life is that, at least at the molecular level, there must be movement, and molecular movement implies that interactions between atoms or chemical groups of atoms must be relatively small compared with thermal energies, or at least not too far in magnitude from such energies. It is worth remembering that most of the ‘chemistry’, i.e. covalent bond rearrangements (excluding photosynthesis) that occurs in our world is ground-state electronic and ground-state vibrational transformations. Molecular flexibility and fluctuation arise from non-covalent interactions, for example, electrostatic forces, van der Waals forces and hydrogen bonds.

Most of the atoms involved in our aqueous-based life processes are bound into molecules that comprise hydrogen and atoms from groups 4, 5 and 6 of the Periodic Table, namely carbon, nitrogen, oxygen, phosphorus and sulphur. There are also of course enormous amounts of ionic species (e.g. Na⁺, Mg²⁺, Ca²⁺, Cl⁻) also present in the environment in which we humans survive. The variety of molecular compounds that can be formed from carbon, nitrogen, oxygen, phosphorus and sulphur seems to be limitless (see, for example, Chemical Abstracts for any year) and the changes of behaviour and properties that can be induced by subtle changes in bonding patterns are remarkable. On a personal note, one of the things that attracted me, as a youth, to study chemistry was the fact that the two isoelectronic molecules di-nitrogen (N₂) and carbon monoxide (CO) had such widely different properties. The latter can kill you whereas the former acts as a moderator to prevent oxygen from killing you.

If we accept that life necessitates using molecules of some complexity such as proteins, nucleic acids,
The importance of water

carbohydrates and lipids, then we can ask the question ‘could life forms as we know them exist in a liquid medium other than water?’ It seems apparent from information presented at this meeting, as well as a large body of other information, that some biomolecular polymers can retain their structure and perhaps their function, in a variety of non-aqueous media, including frozen ice-media. There are, however, aspects of this that disturb me if one tries to extend this onwards using the laws of physics. If we just stay with protein structures, it seems to be established that protein structures depend on a delicate balance between what might be termed intra-tactic and inter-tactic intermolecular forces, i.e. forces between atoms and groups within the protein chain and those between the chain and its molecular environment (its solvation region).

Now, given the nature and importance of charged residues on protein surfaces in aqueous environments and given that water has a high relative permittivity (also known as dielectric constant) of ca. 80 at ambient temperatures, it seems to be inescapable that the intra-tactic and inter-tactic balance must be significantly disturbed if the solvent medium has a different dielectric constant. The balance could be tipped one way if the solvent environment had a dielectric constant less than that of water (e.g. methanol, ethanol, ethane-diol) and in the other direction if the permittivity was greater than that of water (e.g. N-methylacetamide). Of course, the interplay between atoms and chemical molecular functionalities is not only a matter of electrostatics, in that other forces come into play including the repulsive van der Waals which reflect the sizes of the molecular species involved including those of the solvent.

One of the nice and surprising things that came from John Finney’s talk was that water molecules, as well as being small, also do not show clear evidence of the presence of lone pairs of electrons. Rather, what we appear to have is a ‘slippery’ surface to which the hydrogens of an adjacent water molecule can ‘slide’. This necessarily gives flexibility and consequently some orientational compatibility in any water–water interactions. It also suggests that hydrogen bonds from solvent water to peptide groups are only a little stronger than water–water hydrogen bonds; there must also be some orientational tolerance here.

One aspect of the findings regarding the water solvent situation that I find encouraging is that the experimental results from the neutron-scattering studies are qualitatively what one would expect and predict from chemical knowledge. The findings are important since they buttress chemical intuition based on much other experimental data and give a firmer foundation on which to discuss, at least from a structural viewpoint, systems that are more complex.

If it is accepted that the bio-macromolecules of any life form that is different from those that currently exist on Earth must have (as well as having an abundance of the requisite atoms present), among other features, flexibility and robustness, then if we stay on the Earth, there is for example lots of aluminium and silicon present. A question that has not been addressed during the meeting is ‘Could we have a life form on Earth based on say aluminium and silicon plus some other elements?’ From the known properties of these elements and their compounds, the minimum requirement of molecular flexibility or possible atomic movement within molecules would be possible only at very high temperatures since the ‘bonds’ would need to ‘move’, i.e. would have enough energy from their thermal environment to allow flexibility. (Perhaps in such systems the natural solvent would need to be an appropriate fused salt.) This is not to imply that a life form could be based on aluminium–silicon chemistry, or even that substitute proteins could be formed under appropriate conditions based on these and other elements, but these and other possibilities do merit consideration and further discussion. We live in a water-based environment and it is fair to ask if our thinking is overly distorted by our immediate experience.

Support from University College Northampton is acknowledged.