CUBIC HYDRATION OF DNA

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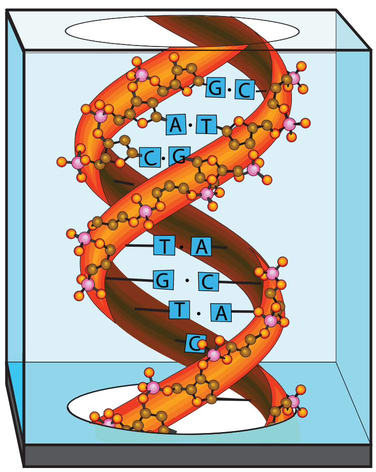
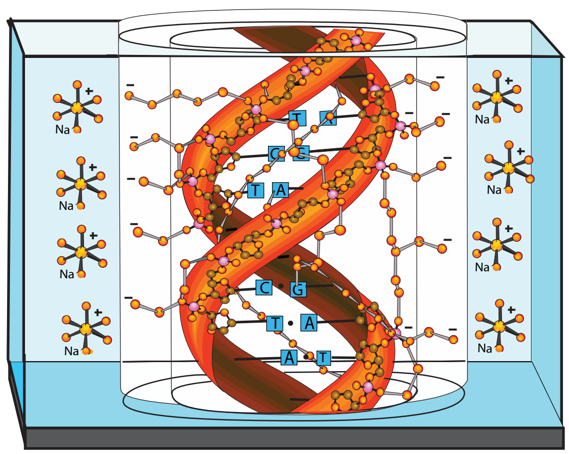
Dedicated to the late Professors Carl Djerassi and William S. Johnson of Stanford University.

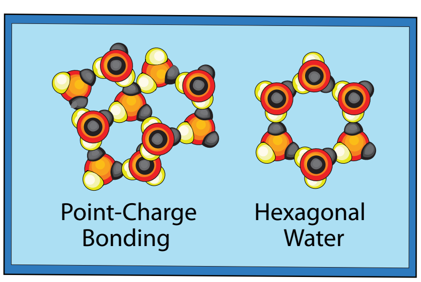
Although it is assumed that the uniformity in structure of DNA is due to the base-pairing of the nucleotides across the double helix, it may also be due primarily to hydration within and around the[1] helix.

When Watson and Crick were searching for an interpretable X-ray diffraction pattern for DNA, it was Roselind Franklin at Kings College in London who sprayed a crystalline sample with water and obtained the diffraction pattern which was used by the two men to complete their model and publish their classical paper.[2] Unfortunately, Roselind received almost no credit for her contribution [3] and so little attention was directed to the fact that water was required to produce the proper X-ray diffraction pattern, that water is never displayed around the helix. In fact, at least 13 water molecules per base pair are required to provide stability,[4] as water forms a linear element in the narrow groove around the helix[5] and forms bridging between the base pairs.[6]



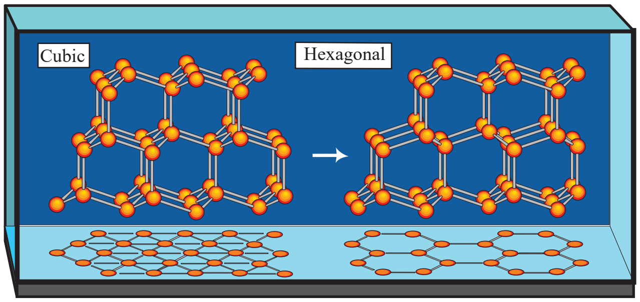


However, much of the stability comes from ice-like linear elements of hydration which continually extend out from the negatively-charged phosphates to the positively-charged sodium (or calcium) ions which surround the the helix.[7] One might expect that the cations would be extremely close helix but, in fact, they are held out away from the helix by the linear elements[8] which display the spectral properties of ice rather than liquid water.[9] Before we discuss more about the helix, it is important to understand that there are two basic types of bonding between water molecules.



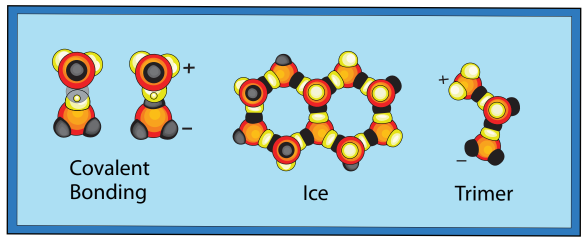
Most molecules in liquid water are held together at multiple angles and distances which range from 2.5 to 3.0 Angstroms. They are extremely dynamic with bonds which last about 10^{-11} seconds [10] and cluster so closely together that they cannot aline their electron orbitals properly to form ice-bonding at 0 °C. Only if water is on a surface where atoms or ions are in the hexagonal positions of water molecules in the surface of ice, will it crystallize at 0°.[10]

In fact, surfaces with random or the pentagonal rings of atoms depress the freezing temperature of water[11] and pure water, in a clean glass container, can be cooled to -30°C without crystallizing.[10] Viscosity increases as the temperature is lowered,[12] but only at -40 °C does freezing occur. But the ice produced is not "normal" - it has cubic (diamond) structure composed of linear elements of hydration.[13]

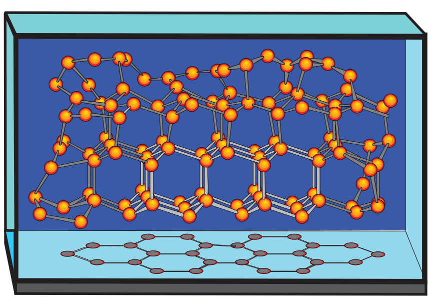


The cubic structure forms as water freezes because electrons of adjacent molecules aline in a linear fashion to form the bond.[14] But, the cubic form is unstable and rapidly isomerizes into the normal hexagonal ice with hexagonal units above each other.

But, bonds in ice are entirely different from most of those in liquid water. In both forms of ice, the bonds are relatively ridged and covalent,[16] like those that hold carbon atoms together, except that the electron orbitals which form the bond circle a central proton.[16] In cubic ice the molecules are 2.75 A apart.[15]



The most unique feature of the bond is that, by moving only a fraction of an Angstrom, the proton can move into the adjacent water molecules and produced charged molecules which can either produce ions or ,in linear elements, be tunnelled through at extremely high speeds.[17] In 2004, the trimer shown above, with bond-length of 2.76 Å, was identified in liquid water by neutron bombardment[18] and, in the same year, Professor Zewail and his group at CalTech, using 4D ultrafast X-ray crystallography, reported that, at subzero temperatires, water on graphite and a poly-ionic surface produced several layers of linear elements of hydration in cubic conformations with a bond length of 2.76 Angstroms.[19]



By choosing solid surfaces which simulate the hydration-ordering properties of the lipid regions of proteins and the surfaces of nucleic acids and lowering temperature to increase stability of the cubic form, Professor Zewail was able to reveal what happens as water molecules approach the dynamic ordering surfaces of molecules in living cells.

As double helix DNA approaches a polymerase enzyme, surface hydration is swept away as cationic sites on the enzyme match positions of phosphates on the helix. Without stabilizing hydration the helix relaxes, strands separate and prepare to be read or or stored. If there is a mismatch in reading the code, the diameter of the double helix will be altered, uniform structuring will be altered and a scanning enzyme will install the correct nucleotide. Millions of years of evolution have produced an incredible variety of enzymes to provide genetic and structural order in the living cell.[20]

In molecular biology today, the emphasis is on genetics and enzyme performance; the role of surface water is rarely addressed. However, as pointed out by Thales of Miletus in 600 BC: "Water is the basis of all things" and as pointed out in *The Matrix of Life*, the molecules of life function so smoothly and spontaneously in living cells to give us life because they are all spatial homologs of the ionic aqueous environment in which they formed and evolved.[7] Enjoy reading.

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