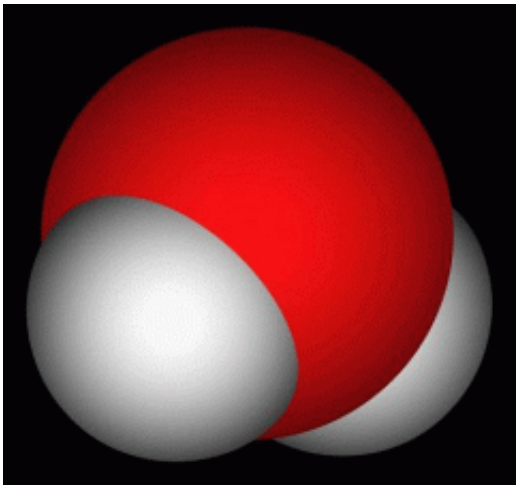
Scientists identify quantum differences between light and heavy water

August 26 2008, By Lisa Zyga



A molecule of water: the red atom is oxygen, and the gray atoms are either hydrogen (light water) or deuterium (heavy water). Physicists have investigated the underlying mechanisms for why heavy water is more structured than light water.

Scientists know that light water (H_2O) and heavy water (D_2O) have similar but not identical structures. Using quantum mechanics, researchers have recently identified several differences between the two water isotopes that previous research had not predicted.

Alan Soper from the Rutherford Appleton Laboratory in Oxfordshire, UK, and Chris Benmore from Argonne National Laboratory in Argonne, Illinois, have published their results in a recent issue of *Physical Review*

Letters.

Chemically speaking, D_2O is an isotope of normal H_2O, with each of the deuterium atoms having one neutron while the normal hydrogen atoms have no neutrons. The extra neutrons make heavy water about 10% denser than H_2O, which can be seen when heavy water ice cubes sink in a glass of normal water. Biologically, this difference means that large amounts of heavy water can have harmful effects on animals, although it would take about two weeks of consuming only D_2O and no H_2O to kill a human.

In their study, Soper and Benmore investigated the differences between light and heavy water on the quantum level. They used a combination of techniques – x-ray diffraction, neutron diffraction, and computer simulation – to discover the underlying mechanisms for why heavy water is more structured than light water, as previous research has indicated.

"The task of understanding the structure and properties of any material is immense, and, in the case of water, is doubly difficult because of (a) the very keen interest in its properties, which are actually rather amazing and complicated compared to many common liquids, and (b) the difficulty of getting really reliable data on its properties," Soper told *PhysOrg.com*. "The significance of our results is that they will challenge the theoreticians to come up with better models for water, something that has often eluded them and which even today is a subject of much study and endeavor."

Soper explained that some of their results could be controversial, since they contrast with predictions. First, the scientists found that H_2O has a longer intramolecular OH bond than D_2O's corresponding OD bond length. Specifically, the OH bond is longer by about 0.03 angstroms, or 3%.

Second, the intermolecular hydrogen bond (which connects two separate molecules) is shorter in H_2O than in D_2O. Here, the difference is about 0.07 angstroms, or 4%. Neither of these differences in bond length had been predicted in previous studies.

Further, because the OH/OD bond length difference and the hydrogen bond length difference are not equivalent (3% and 4%), there also exist geometrical differences between the structures of light and heavy water. While previous research had predicted an overall broadening of the H_2O structure compared to the D2O structure, Soper and Benmore have pinpointed three specific differences, some of which are in opposition to earlier predictions.

For one thing, the intermolecular OH peak is more asymmetric in H_2O than D_2O. Also, the distance between the hydrogen atoms on neighboring molecules is about 2% larger for H_2O than in D_2O. Finally, the number of hydrogen bonds per water molecule is less in H_2O than in D_2O (3.62 vs. 3.76). Together, these structural differences give light water a broader structure, and heavy water a narrower, more tetrahedral shape.

Soper said that some of these unexpected results (such as the large degree of asymmetry in the hydrogen bond in H_2O compared to D_2O and the OH/OD bond length difference) may be contested by computer simulators.

He also explained that the hydrogen bond length is caused by small electron movements that impact the proton (in hydrogen) or deuteron positions. Since the proton has a smaller mass than the deuteron, it sits higher in the quantum potential well (that holds the hydrogen atom) compared with the deuteron's lower position in its potential well.

"If that potential well is now perturbed by an approaching water

molecule forming a hydrogen bond, then because the proton is higher in the well, it is more likely to be influenced by the approaching water molecule, drawing it away from the parent oxygen, more so than the deuteron, which is deeper in the well, and therefore less sensitive to perturbations from neighboring water molecules," Soper said. This effect may play a role in the difference between the OH and OD bond lengths.

The researchers also explained that understanding the structures of light and heavy water might not have any immediate applications, but could help researchers in a variety of fields down the road.

"There is no obvious immediate impact from understanding these structures, apart from the obvious point that it will no doubt spur theoreticians to greater efforts to see if they can understand our findings," Soper said. "Water is arguably the most important material in the human environment. Though there are lots of other materials we can and do study, somehow water captures major interest because of its fundamental importance to us.

"Ultimately, if we understand water better, we will become better at predicting its properties, such as its ability to form crystals and water droplets in the atmosphere which in turn can cause immensely damaging storms as a consequence, its ability to act as the medium in which life has evolved, as the medium in which proteins will fold to their native structures, as the material used by our industry to both heat and cool, as the material used as a solvent and as a cleaner. The list is rather endless!"

More information: Soper, A.K. and Benmore, C.J. "Quantum Differences between Heavy and Light Water." *Physical Review Letters* 101 065502 (2008).