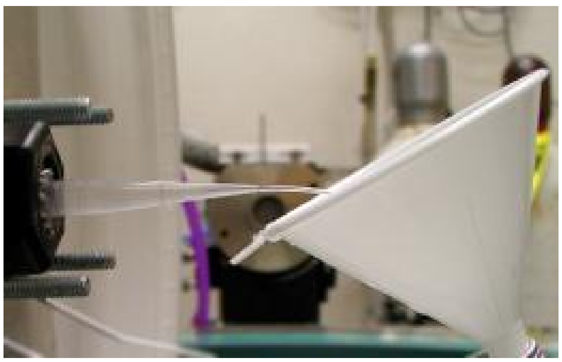
Researchers Rediscover the Structure of Water

February 26 2010, by Kelen Tuttle



Researchers at SSRL recently determined the distances between the molecules in this jet of flowing water. (Image courtesy the research team)

(PhysOrg.com) -- A team of researchers at the Stanford Synchrotron Radiation Lightsource has found the molecular structure of water to be more complex than recently thought, suggesting that molecular models that went out of fashion decades ago may be in fact more accurate than recent ones.

"The study of water has a very long history," said lead author Ling Fu, who is a postdoc at the Centre National de la Recherche Scientifique in France and who wrote her PhD thesis on these results. "Other researchers have done a very good job in their measurements; I hope that this work helps advance the field."

By recording how SSRL's X-ray beam scattered off a flowing jet of water, Fu and colleagues Arthur Bienenstock and Sean Brennan were able to determine the distances between the water molecules in the jet. As recent models predicted, they saw molecules 0.28 and 0.45 nanometers apart. These measurements confirm the current commonly accepted model, which describes liquid water as a group of water molecules held together in tetrahedral shapes, with the molecule at the center of the tetrahedron separated from four others at the shorter distance and each of these four molecules separated from one another at the longer distance.

Yet the researchers saw some molecules at a third distance as well: 0.34 nanometers. The existence of this third separation length, though not included in the current model, was first seen in 1938. Additional experiments in the 1960s and 1970s first confirmed, but later rejected, that this length exists, concluding that its detection was due to shortcomings in the analysis. As a result, models including this intermediate distance fell out of favor—until now.

That the SSRL researchers have now observed this intermediate separation length using modern-day technology suggests that "there's something more going on here" beyond the currently accepted model, Fu said.

These results suggest that liquid water's structure is not completely tetrahedral, but rather has some added complexity. But they do not fully solve the mystery of water's structure because the data taken at SSRL only reveal the distances between water molecules, not the angles of the bonds. "More research is needed to see the complete picture," said Brennan.

Fully understanding the structure of water is a surprisingly difficult task. In water's solid form, ice, the molecules are known to form a tight tetrahedral lattice. The current model holds that liquid water should be similar to ice but less structured since heat creates disorder and breaks bonds. In liquid water, then, the tetrahedral structures would loosen their grip, breaking apart as the temperature rises, but still inclined to remain as tetrahedral as possible. This new research adds a kink in this theory, requiring some sort of secondary structure. The greater density of liquid water implies that the molecules are more closely packed than the simple tetrahedra seen in ice. These data help explain how that can happen.

The baton, Brennan said, is now in the hands of the theorists. "I think of this type of research as a relay race: The experimentalists run for a while until they can't explain something they've seen, and then the theorists run for a while until they can't go any farther without more data, and then it's back to the experimentalists," he said. "So, this time, we're saying that it's time for the theorists to run their leg."

Provided by Stanford Synchrotron Radiation Lightsource