CALIFORNIA STATE SCIENCE FAIR
2009 PROJECT SUMMARY

Name(s)

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Project Number

S0505

Project Title

The Nonhomogeneous Intermolecular Bonding Structure of Liquid Water: An X-ray Study

Abstract

Objectives/Goals

A detailed understanding of the bonding structure of ambient liquid water is of high importance and interest. The intention of this project is to probe the bulk structure of ambient water with a novel X-ray technique to determine the details of its intermolecular structure.

Methods/Materials

X-ray Raman based X-ray Absorption Near-Edge Spectroscopy is a novel X-ray technique that uses hard X-rays to probe for absorption information that lies in the soft X-ray region. Experiments were performed at a high-brightness synchrotron lightsource with incident energy ranges of ~6-7 KeV. Using a 14-crystal analyzer spectrometer, the energy losses (~500 eV) necessary to observe the oxygen K-edge were detectable with high energy resolution. Spectra were analyzed by comparison with hexagonal ice spectra and by application of a model based on Density Functional Theory.

Conclusions/Discussion

The spectral analysis suggests that liquid water is not a near-homogeneous distribution of tetrahedrally bonded molecules, as has been generally thought. Instead, a nonhomogeneous bonding model is presented, wherein about 80% of water molecules are bonded to only two neighbors while about 20% are bonded to four neighboring molecules. This finding is supported by some studies, but is disputed by others.

Summary Statement

The application of novel X-ray spectroscopic techniques to investigate the bonding structure of water seems to indicate that water structure is more complex than generally assumed.

Help Received

I was part of a 3-person reserach team; I worked full-time on the experiment, and completed data processing and preliminary analysis myself. The project presentation was developed independently. Dad helped proofread.