

Abstract Submitted
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Isomers and the correlation between excess electron binding and the local H-bonding motif in hydrated electron clusters.¹ MARK JOHNSON², Yale University — We describe a series of experimental results that address the origin of the isomeric classes of negatively charged water clusters that differ according to their electron binding energies. The molecular structure of the local electron binding site is revealed through the isomer-specific vibrational spectra in the intramolecular HOH bending and OH stretching regions for both H and D isotopomers. Isomer selection is accomplished with a photochemical population modulation scheme in which low electron binding isomers are sequentially and systematically removed from the mixed isomer ensembles created in free jet ion sources. The class of clusters (type I) that most strongly binds an excess electron exhibits a characteristic red-shifted band in the bending region that is assigned, based on the behavior of very small clusters, to electron attachment to a single water molecule held to the supporting network by a double H-bond acceptor (AA) motif. Isomers that bind the electron more weakly do not display this spectral signature, indicating that local H-bonding topology is a significant factor in controlling the overall work functions of the clusters. Isomer interconversion and growth mechanisms will also be addressed using Ar-mediated incorporation of hetero-isotopes and surface electron scavenging by reactive charge-transfer collisions.

¹Department of Chemistry, Yale University

²submitted to chemical physics electron and ion solvation (Rossky)

Mark Johnson
Yale University

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