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Isomer morphology and vibrational mode dependence of the coupling between an excess electron and small water networks. MARK JOHNSON, Yale University — Negatively charged water clusters are presently the subject of intense study because of their promise to unravel the surprisingly complex dynamics of the hydrated electron. We focus on the use of vibrational spectroscopy to establish the morphologies and local binding motifs of the water networks that bind an electron. Here we will discuss the rearrangement pathways of the H-bond network in the elementary act of free electron accommodation, where we use argon-mediated population modulation to isolate the geometries of the neutral cluster precursors. We then obtain isomer-selective vibrational spectra of the anions that produced, where we correlate the local binding motifs with the overall electron binding energies. Finally, in the small cluster limit, we reveal how different intramolecular vibrational motions interact with the diffuse electron cloud by analysis of the resulting "Fano" lineshapes when vibrations are embedded in the electron continuum. These interactions vary by over an order of magnitude for various "free OH" bands. The implications of these observations on the extrapolation to bulk behavior will be considered in light of the trends displayed by the cluster properties up n=30 or so.

Mark Johnson
Yale University

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