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Cold cluster snapshots of the Grotthuss proton relay mechanism in water

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The Grotthuss mechanism explains the anomalously high proton mobility in water as a sequence of proton transfers along a hydrogen-bonded network. However, the vibrational spectroscopic signatures of this process are masked by the diffuse nature of the key bands in bulk water. Here we report how the much simpler vibrational spectra of cold, composition-selected heavy water clusters, $D^+(D_2O)_n$, can be exploited to capture clear markers that encode the collective reaction coordinate along the proton transfer event. By complexing the solvated hydronium "Eigen" cluster, $D_3O^+(D_2O)_3$, with increasingly strong H-bond acceptor molecules (H_2, N_2, CO, H_2O), we are able to track the frequency of every O-D stretch in the complex as the transferring hydron is incrementally pulled from the central hydronium to a neighboring water molecule.