ELECTRON ATTACHMENT AND DETACHMENT IN THE WATER HEXAMER ANION

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AIMD simulations have been performed on isomers of the water hexamer anion at temperatures comparable to those found in molecular beams. Electron detachment from these species has been simulated using a sudden approximation where the anion geometry at a selected time is propagated using ordinary MD with a neutral water potential. The resulting distribution of conformers and the relationship between the electron attachment and detachment pathways will be discussed.