

Abstract Submitted
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Dynamics of electron solvation in $\text{I}^-(\text{CH}_3\text{OH})_n$ clusters ($4 \leq n \leq 11$) RYAN YOUNG, University of California, Berkeley — The dynamics of electron solvation following excitation of the charge-transfer-to-solvent (CTTS) precursor state in iodide-doped methanol clusters, $\text{I}^-(\text{CH}_3\text{OH})_{n=4-11}$ are studied with time-resolved photoelectron imaging (TRPEI). This excitation produces a $\text{I}^{\cdot-}(\text{CH}_3\text{OH})_n^-$ cluster that is unstable with respect to electron autodetachment, and whose autodetachment lifetime increases monotonically from ~ 800 fs to 85 ps as n increases from 4-11. The vertical detachment energy (VDE) and width of the excited state feature in the photoelectron spectrum show complex time dependences during the lifetime of this state. The VDE decreases over the first 100-400 fs, then rises exponentially to a maximum with a ~ 1 ps time constant, decreasing by as much as 180 meV with timescales from 4-10 ps. The early dynamics are assigned to electron transfer from the iodide to a localized portion of the methanol cluster, while the longer-time changes in VDE are attributed to solvent reordering, possibly in conjunction with ejection of neutral iodine from the cluster. Changes in the observed width of the spectrum largely follow those of the VDEs; the dynamics of both are attributed to the major rearrangement of the solvent cluster during relaxation. The relaxation dynamics are interpreted as a reorientation of at least one methanol molecule and the disruption and formation of the solvent network in order to accommodate the excess charge.

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