Nonadiabatic MD simulations of IBr\textsuperscript{−}(CO\textsubscript{2})\textsubscript{n} photodissociation
MATTHEW A. THOMPSON, JOSHUA MARTIN, JOSHUA DARR, JACK BARBERA, VLADIMIR DRIBINSKI, W. CARL LINEBERGER, ROBERT PARSON, JILA and Department of Chemistry, University of Colorado at Boulder — Potential energy curves for the ground and valence excited states of IBr\textsuperscript{−} have been calculated at the MRCI level using the MOLPRO \textit{ab initio} package. Spin-orbit coupling was calculated via a spin-orbit ECP. Charge densities, transition moments, and nonadiabatic coupling matrix elements constructed from a distributed multipole analysis of the \textit{ab initio} wavefunctions \textsuperscript{1} were then used to carry out nonadiabatic molecular dynamics simulations of the photodissociation of IBr\textsuperscript{−} in CO\textsubscript{2} clusters. Experimental studies have demonstrated a large variation in ground-state recombination times which are supported by our simulations. We propose a mechanism of excited-state trapping and a configurational transition state which leads to recombination times on the order of 10-20 ps for $n=5,13$ up to 1 ns for $n=8,10$.

\textsuperscript{1}Maslen, Faeder and Parson, Molecular Physics, 1998