THEORETICAL STUDIES OF PHOTODISSOCIATION DYNAMICS OF $BRCN^-$

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We present the results of theoretical studies of photodissociation dynamics of $BrCN^-$ following electronic excitation to states that dissociate to Br^- + CN and Br^* + CN^-. The electronic states were evaluated at the SO-MRCI level of theory with aug-cc-pVTZ basis set using MOLPRO 2010 package. Based on the 0.05 eV difference between these two asymptotic channels, we anticipate a non-adiabatic interaction similar to that observed in ICN^- will play an important role in the dynamics. In this study, we develop the diabatic models for the two relevant excited states and then study the quantum dynamics of wave packets that are excited to these two states. In the $BrCN^-$ geometry, the two surfaces cross and contain wells that are at least 0.1 eV deep. In contrast, in the $BrNC^-$ geometry, the curves do not cross and only the lower energy diabatic potential contains a well. The overall shape of the excited state potential energy surfaces is expected to play a significant role in the distribution of the photofragments.