Theoretical and experimental studies on concerted elimination of 1, 2-bromochloroethane monocation to C2H4+ and BrCl

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Abstract

We calculate the concerted pathway of 1, 2-bromochloroethane monocation to C2H4+ and BrCl using the Minnesota density functional M06-2X and the def2-TZVP basis set. We also calculate the elimination channel of 1, 2-bromochloroethane monocation to C2H4 and BrCl+ for the reason that positive charge can be assigned to either moiety in the fragmentation process of 1,2-C2H4BrCl+. Our results demonstrate that the elimination channel of 1, 2-bromochloroethane monocation to C2H4+ and BrCl is preferred, and the singly charged 1,2-bromochloroethane ions surpass two energy barriers and then separate into C2H4+ + BrCl by an asynchronous concerted process. Experimentally, we confirm that this elimination channel is from the dissociative ionization process of 1,2-bromochloroethane monocation by dc-slice imaging technique. Besides, we can see in laser-induced time-of-flight mass spectra of 1,2-bromochloroethane that fragment ion C2H4+ occur at the laser intensity of 6.0×1013 W/cm2 while BrCl+ occur at a higher laser intensity, which is consistent with the theoretical results that appearance energy of ion C2H4+ should be lower than that of BrCl+, and this is the reason why the low-velocity component of ion BrCl+ is absent from our sliced images.

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