CI-LOSS DYNAMICS OF VINYL CHLORIDE CATION IN B STATE: ROLE OF C STATE

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Dissociative photoionization of vinyl chloride (C2H3Cl) in the 11.0-14.2 eV photon energy range was investigated with the method of threshold photoelectron photoion coincidence (TPEPICO) velocity map imaging. Three electronic states, A2A’, B2A” and C2A’, of C2H3Cl+ cation were prepared and their dissociation dynamics were investigated respectively. A unique fragment ion, C2H3+, was observed within the present excitation energy range. From the TPEPICO 3-dimensional time-sliced velocity map images of C2H3+, kinetic energy release distributions (KERD) and anisotropy parameters in dissociation of internal energy-selected C2H3Cl+ cation were obtained. At 13.14 eV, the total KERD showed a bimodal distribution consisting of a Boltzmann and a Gaussian-type component, indicating competing statistical and non-statistical dissociation mechanisms. An additional component of Gaussian-type was found in KERD at 13.65 eV with a center located at lower kinetic energy. With the aid of re-calculated Cl-loss potential energy curves with time-dependent density functional theory, the overall dissociative photoionization mechanisms of C2H3Cl+ cation in the B2A” and C2A’ states are proposed. The inconsistency of the previous conclusions on dissociation mechanism of C2H3Cl+ is stated.