Supporting Information

Dissociative Photoionization of CF₃Cl with Threshold

Photoelectron-photoion Coincidence Velocity Map Imaging

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Figure S1. Cl-loss potential energy curves of the low-lying electronic states of CF₃Cl⁺ at TD-B3LYP/6-311+G(d) level, where the geometric parameters are fixed at the optimized values of the neutral molecule.

These potential energy curves show the Franck-Condon region when being ionized. As suggested in Figure S1, the higher electronic states than the D²E ionic state are repulsive, but the cross points are much higher than the band origin of D²E state. Thus, the crosses of the higher repulsive electronic states are not taken into account in the present dissociative photoionization mechanism via A²A₁, B²A₂, C²E and D²E ionic states.