Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Dissociative Photoionization of CF_3Cl with Threshold Photoelectron-photoion Coincidence Velocity Map Imaging

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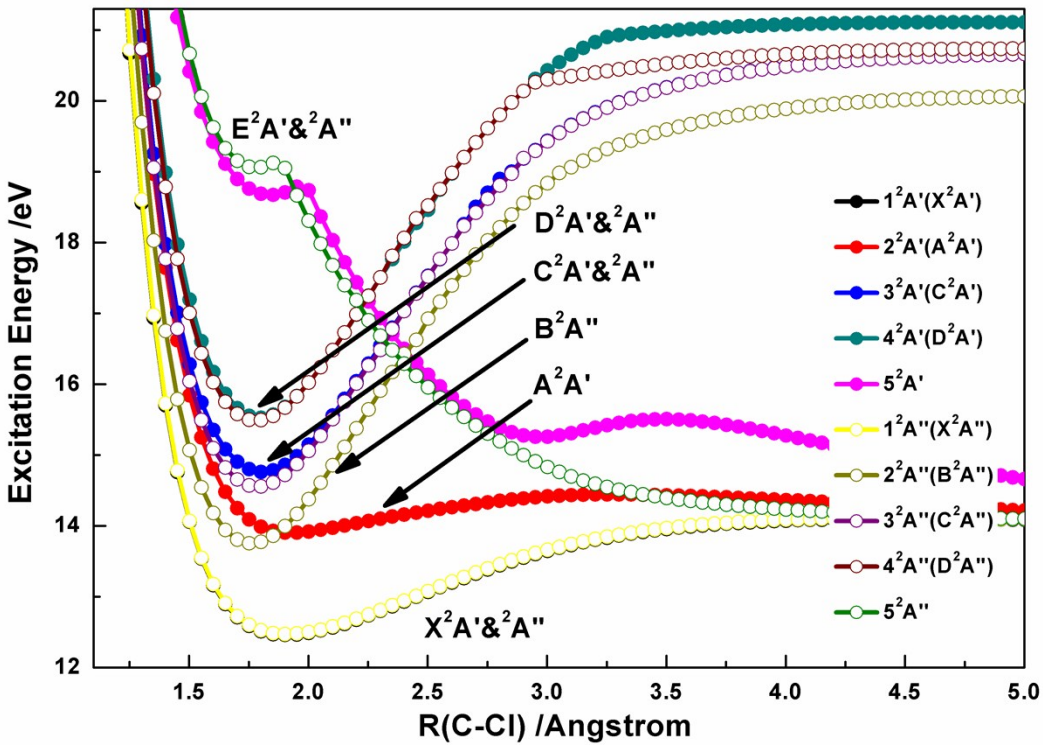

Figure S1. Cl-loss potential energy curves of the low-lying electronic states of CF_3Cl^+ at TD-B3LYP/6-311+G(d) level, where the geometric parameters are fixed at the optimized values of the neutral molecule.

These potential energy curves show the Franck-Condon region when being ionized. As suggested in Figure S1, the higher electronic states than the D^2E ionic state are repulsive, but the cross points are much higher than the band origin of D^2E state. Thus, the crosses of the higher repulsive electronic states are not taken into account in the present dissociative photoionization mechanism via A^2A_1, B^2A_2, C^2E and D^2E ionic states.