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

Electronic Supporting Information for

Climbing up Conical Intersections: A Direct Dynamics Study of the Exotic Photochemistry of Criegee Intermediates

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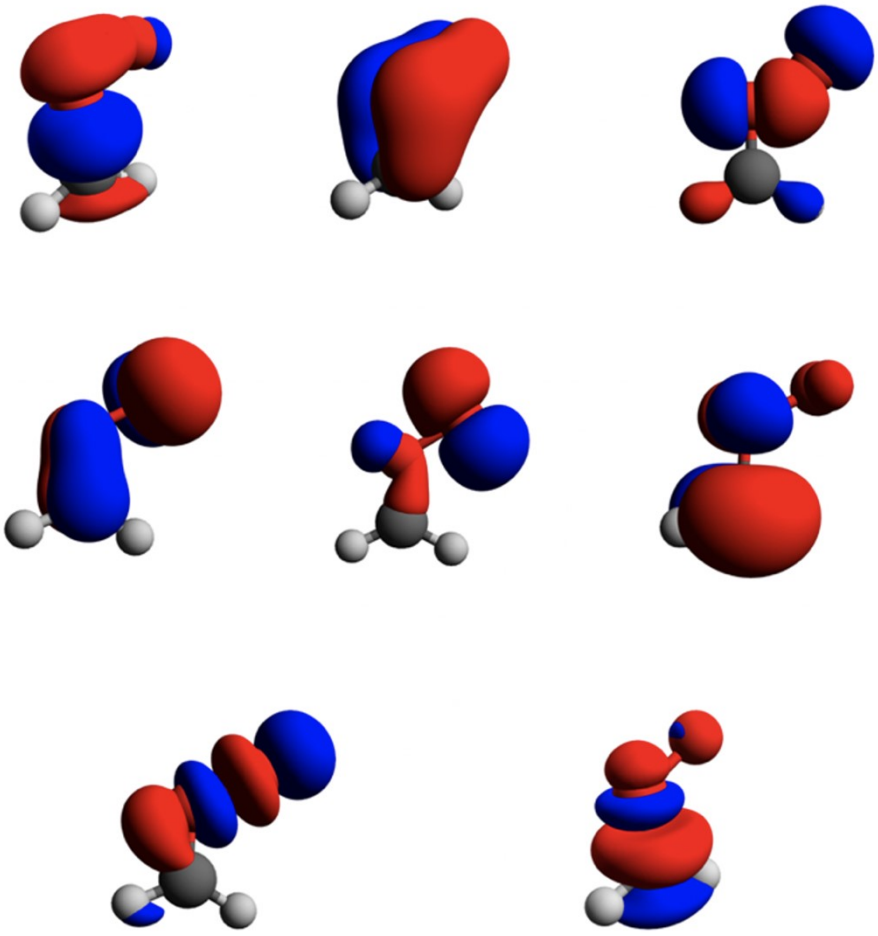

Figure S1: Molecular orbitals that make up the 10 electrons in 8 orbitals active space of CH_2OO.

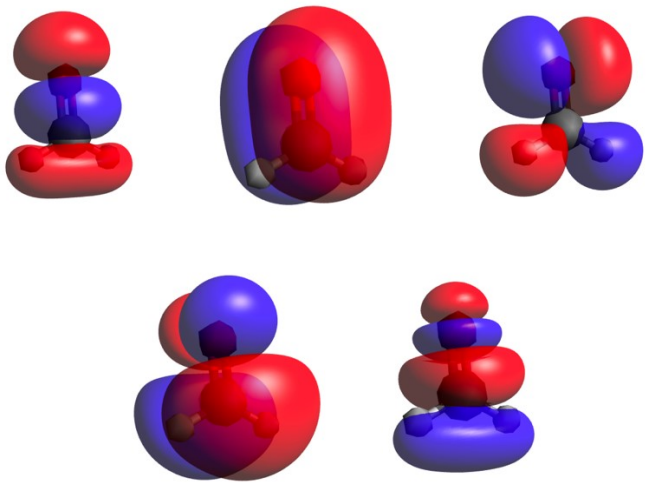

Figure S2: Molecular orbitals that make up the 6 electrons in 5 orbitals active space of formaldehyde.

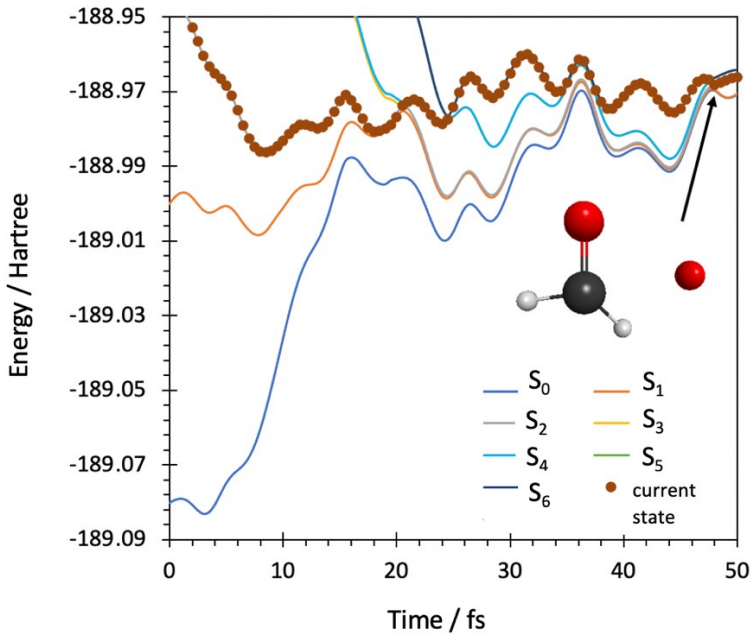

Figure S3: Energy vs. Time for a representative trajectory that undergoes hopping at long R_{OO}

Figure S4: Comparison between the Relaxed PE profiles along A_{HCO} of formaldehyde, calculated at the SS-CASPT2/aug-cc-pVTZ//B3LYP/cc-pVTZ and SS-SR-CASPT2/aug-cc-pVTZ//B3LYP/cc-pVTZ levels of theory.

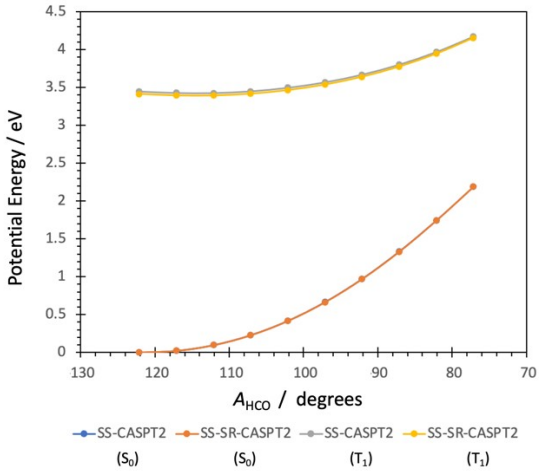

Table S1: Comparison between the S_0 and T_1 optimized A_{HCO} and R_{CO} values, optimized at the B3LYP/cc-pVTZ and SS-SR-CASPT2/aug-cc-pVTZ levels of theory.

Parameter	S_0 opt B3LYP/VTZ	S_0 opt SS-SR-CASPT2 /AVTZ	T_1 opt B3LYP/VTZ	T_1 opt SS-SR-CASPT2 /AVTZ
R_{CO} / Å	1.19904	1.21006	1.30240	1.31584
A_{HCO} / deg.	122.12062	121.71083	114.02247	113.94501