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

Supplementary Information: Role of conical intersection seam topography in the chemiexcitation of 1,2-dioxetanes

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Figures S-1 to S-3 are a complement to Figures 8, 11, and 14. They show, for each of the reference trajectories, the magnitude of the transition dipole moment between the ground state and the excited states. Given that the ground seems to be well separated from the excited states in all three trajectories, this offers another view at the wave function changes that occur along the trajectories.

In fig. S-1 the most significant features are exchanges between S_1 and S_2 at ~50°, ~63°, and ~70°, confirming the crossings observed in fig. 8.

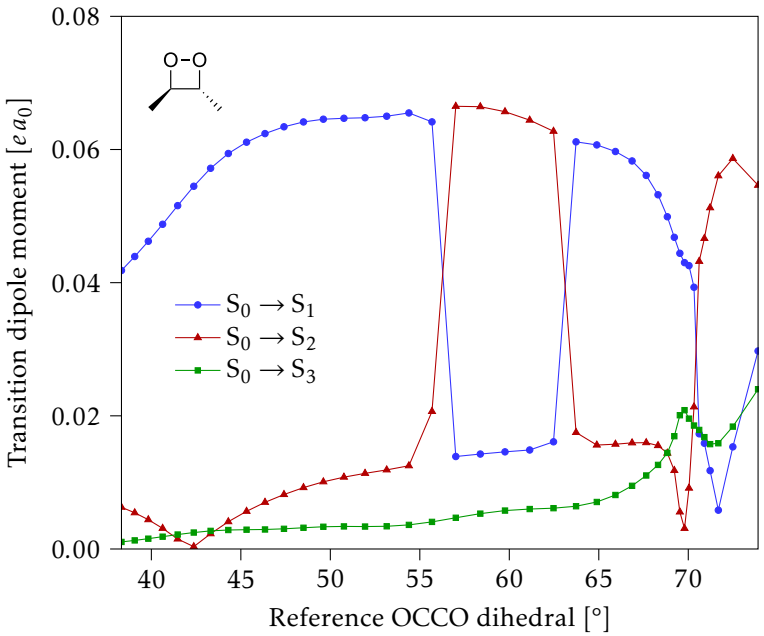

Figure S-1: Transition dipoles for the reference trajectory of 2Me.

In fig. S-2 there is an evident crossing between S_1 and S_2 at ~90°, but it is not clear that the lines crossing at ~75° corresponds to a crossing between the states, as the changes are rather gradual. Comparing with fig. 11, it seems clear some interaction occurs between these states in the range 70° to 75°.

In fig. S-3 a clear crossing between S_1 and S_2 can be observed at ~90° too. The energy crossings between S_2 and S_3 that are seen in fig. 11 at ~50° and ~70° are not as obvious, but an interaction between these states can also be deduced.

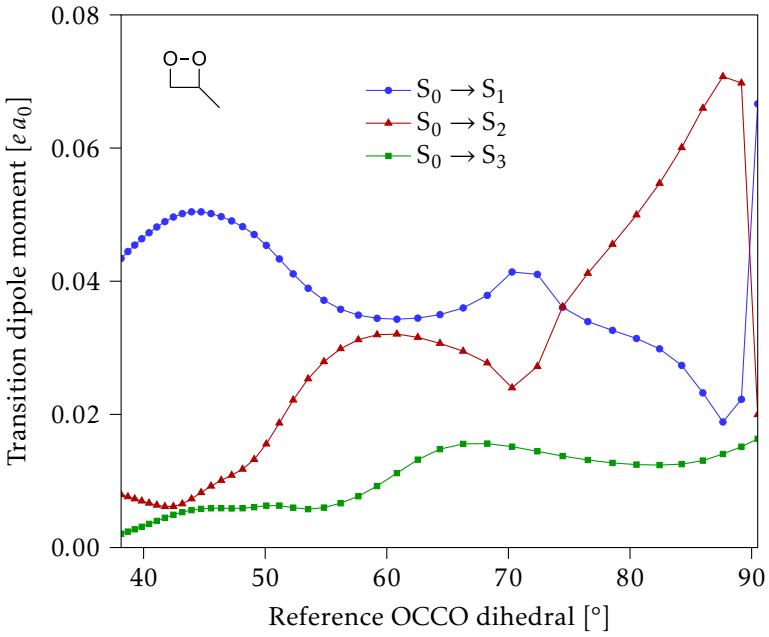

Figure S-2: Transition dipoles for the reference trajectory of 1Me.

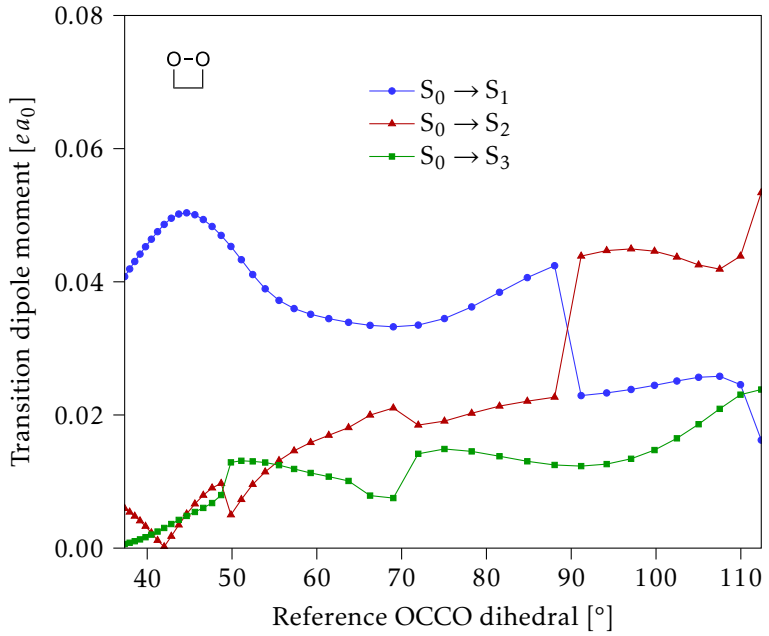

Figure S-3: Transition dipoles for the reference trajectory of 0Me.