Supporting Information for
Excited State Proton Transfer and Three-State Intersection Dynamics in Malonaldehyde

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This document contains a figure comparing SA-3-CAS(4/4) and SA-3-CAS(4/4)*SDCI potential energy surfaces along the center of a representative AIMS trajectory basis function and geometries in Cartesian coordinates (Angstroms) for structures depicted and/or discussed in the text.

Figure S1. Potential energy traces (on S_2) for the center of a representative trajectory basis function along path given by dynamics using SA-3-CAS(4/4) electronic wavefunction. Traces using both SA-3-CAS(4/4) (black) and SA-3-CAS(4/4)*SDCI (grey) are shown. In both cases, the 6-31G* basis set is used and the zero of energy is taken as the potential energy on S_2 at time t=0. The agreement demonstrates that the CAS and MRSDCI surfaces are very nearly parallel.

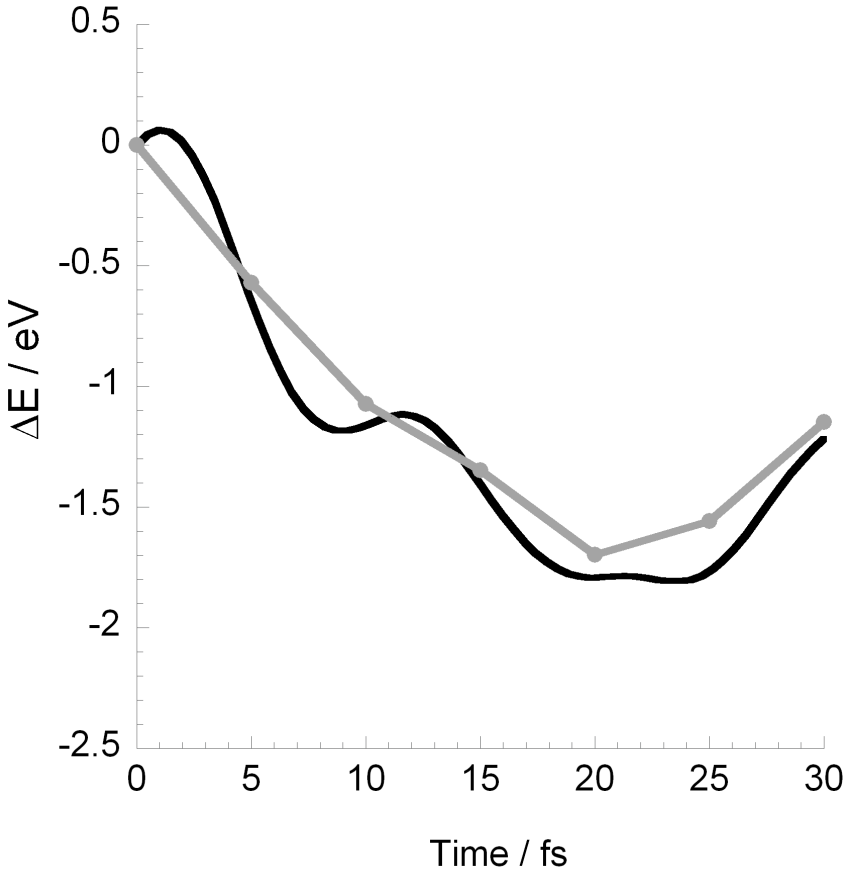

Table S2. Geometry of S_0 transition state, shown in the lower left of Figure 3 in the text.

	X	Y	Z
C_1	-1.178	0.811	0.000
C_2	0.000	0.059	0.000
C_3	1.178	0.811	0.000
O_4	-1.168	2.064	0.000
O_5	1.168	2.064	0.000
H_6	0.000	2.321	0.000
H_7	-2.143	0.321	0.000
H_8	0.000	-1.011	0.000
H_9	2.143	0.321	0.000

Table S3. Geometry of S_1 minimum, shown in top middle of Figure 3 in the text.

	X	Y	Z
C_1	-0.007	0.001	-0.007
C_2	0.083	0.000	1.394
C_3	1.192	-0.002	2.160
O_4	1.023	0.000	-0.873
O_5	2.447	-0.004	1.683
H_6	1.865	0.007	-0.440
H_7	-0.953	0.001	-0.505
H_8	-0.851	0.001	1.923
H_9	1.175	-0.002	3.234

Table S4. Geometry of S_1 transition state, shown in bottom middle of Figure 3 in the text.

	X	Y	Z
C_1	-1.181	0.748	0.000
C_2	0.000	0.022	0.000
C_3	1.181	0.748	0.000
O_4	-1.121	2.100	0.000
O_5	1.121	2.100	0.000
H_6	0.000	2.389	0.000
H_7	-2.177	0.353	0.000
H_8	0.000	-1.050	0.000
H_9	2.177	0.353	0.000

Table S5. Geometry of S_2 minimum, shown on the right of Figure 3 in the text. The minimum is also the transition state for hydrogen transfer.

	X	Y	Z
C_1	0.000	0.037	0.000
C_2	1.260	0.816	0.000
C_3	-1.260	0.816	0.000
O_4	1.180	2.078	0.000
O_5	-1.180	2.078	0.000
H_6	0.000	2.302	0.000
H_7	2.222	0.335	0.000
H_8	0.000	-1.034	0.000
H_9	-2.222	0.335	0.000

Table S6. Geometry of S_1/S_0 MECI, shown on the right in Figure 5 of the text.

	X	Y	Z
C_1	0.000	0.000	0.000
C_2	1.475	0.000	0.000
C_3	2.217	1.108	0.000
O_4	-0.647	-0.273	-1.165
O_5	1.677	2.311	-0.009
H_6	-0.223	0.175	-1.885
H_7	-0.524	-0.405	0.844
H_8	1.993	-0.949	-0.010
H_9	3.295	1.063	-0.001

Table S7. Geometry of S_0 minimum optimized at the 6-31g*, SA3-CAS(4/4) level.

	X	Y	Z
C_1	-0.004	0.000	0.012
C_2	0.032	0.000	1.367
C_3	1.293	0.000	2.094
O_4	1.044	0.000	-0.794
O_5	2.375	0.000	1.583
H_6	1.847	0.000	-0.273
H_7	-0.934	0.000	-0.524
H_8	-0.888	0.000	1.919
H_9	1.209	0.000	3.185