

Supplementary Information
for
Theoretical Insights into Photo-induced Isomerization Mechanisms
of Phenylsulfinyl Radical PhSO·

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Table S1. Relative TD-CAM-B3LYP vertical excitation energy (ΔE), wavelength (λ), configuration and oscillator strength (f) with electron transition for D₁, D₂, and D₃ states by NTO analysis at 1-D₀.

State	Configuration	E/eV	λ/nm	f
D ₀	$\pi^*(SOMO)$	0.00	-	-
D ₁	$n_O \rightarrow \pi^*$	2.22	560	0.0006
D ₂	$\pi_1 \rightarrow \pi^*$	3.38	375	0.0187
D ₃	$\pi_2 \rightarrow \pi^*$	3.96	313	0.0022
D ₄	-	4.12	301	0.0765

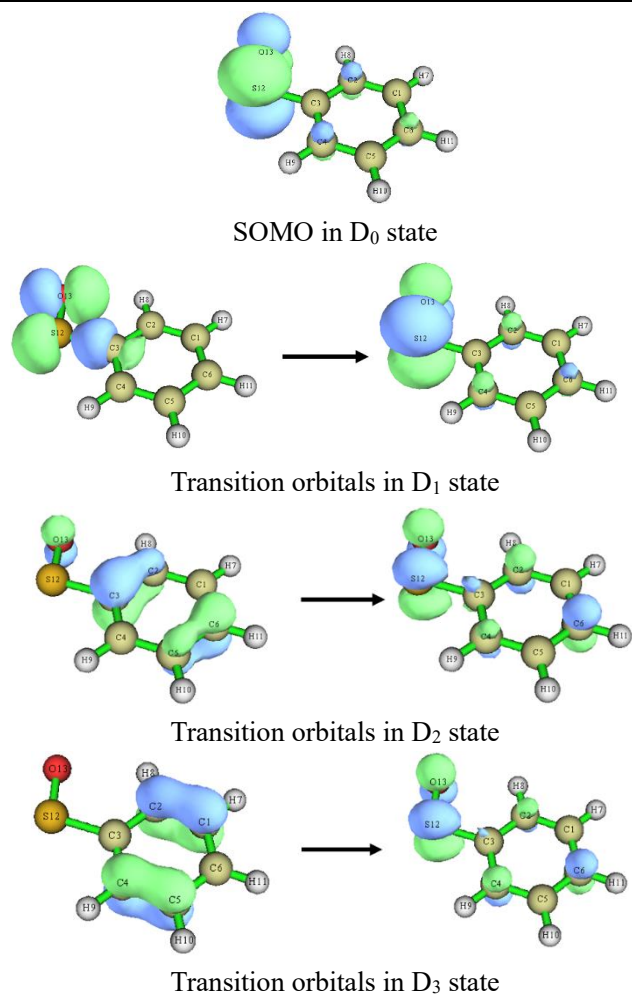
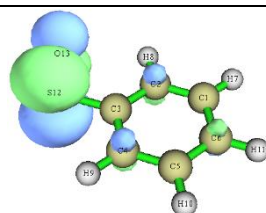
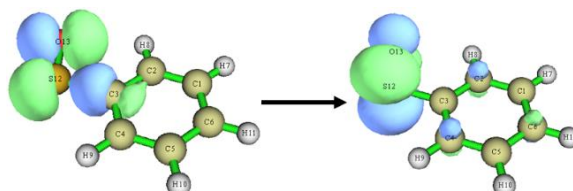


Table S2. Relative TD- ω B97XD vertical excitation energy (ΔE), wavelength (λ), configuration and oscillator strength (f) with electron transition for D₁, D₂, and D₃ states by NTO analysis at 1-D₀.

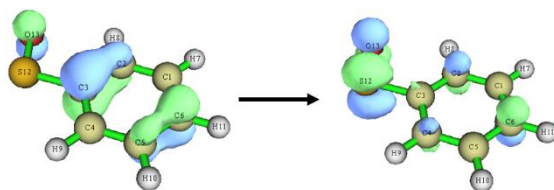
State	Configuration	E/eV	λ/nm	f
D ₀	$\pi^*(SOMO)$	0.00	-	-
D ₁	$n_O \rightarrow \pi^*$	2.19	567	0.0006
D ₂	$\pi_1 \rightarrow \pi^*$	3.38	367	0.0237
D ₃	$\pi_2 \rightarrow \pi^*$	3.94	314	0.0033
D ₄	-	4.20	295	0.0760



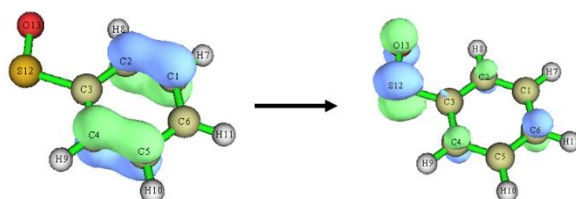
SOMO in D₀ state



Transition orbitals in D₁ state



Transition orbitals in D₂ state



Transition orbitals in D₃ state

Table S3. Selected bond lengths (in Å), angles (in °), dihedral angles (in °), and fuzzy bond order of radicals **1** and **2** at D₀, D₁, and D₂ states.

	Bond length					Angle	Dihedral angle	Fuzzy bond order		
	C1-C2	C1-C6	C1-S12	C1-O12	S12-O13	C1-S12-O13	C2-C1-S21-O13	S12-O13	C1-S12	C1-O13
1-D₀	1.39	1.39	1.79	-	1.54	108	180	2.22	1.14	-
1-D₁	1.40	1.39	1.82	-	1.75	94	91	1.79	1.13	-
1-D₂	1.47	1.46	1.72	-	1.55	109	180	2.05	1.34	-
2-D₀	1.40	1.37	-	1.41	1.67	121	179	1.16	-	1.14
2-D₁	1.40	1.37	-	1.39	1.70	120	179	1.12	-	1.17
2-D₂	1.44	1.43	-	1.29	1.94	117	180	0.90	-	1.35

Table S4. MS-CASPT2 vertical excitation energy (E) and wavelength (λ) at 2-D₀, together with the oscillator strength (f), the main electronic configuration with weight in parentheses and the relative orbitals.

State	Configuration (weight)	E/eV	λ/nm	f
D ₀	π_1^* (SOMO)	0.00	-	-
D ₁	$n_s \rightarrow \pi_1^*$ (0.84)	0.53	2327	0.0000
D ₂	$\pi_1 \rightarrow \pi_1^*$ (0.50)	2.49	497	0.0535
D ₃	$\pi_2 \rightarrow \pi_1^*$ (0.42)	3.47	358	0.0272
D ₄	$\pi_2 \rightarrow \pi_2^*$ (0.30)	4.29	289	0.0220

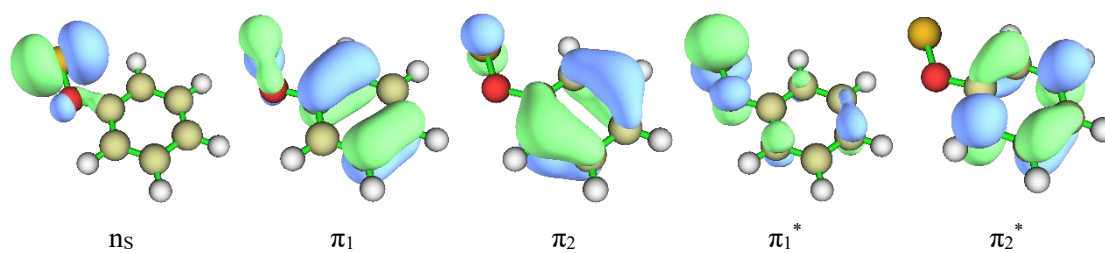


Table S5. MS-CASPT2 vertical excitation energy (E) and wavelength (λ) at **Int1-D₀**, together with the oscillator strength (f), the main electronic configuration with weight in parentheses and the relative orbitals.

State	Configuration (weight)	E/eV	λ/nm	f
D ₀	n's (SOMO)	0.00	-	-
D ₁	n _s →n's (0.76)	0.10	12430	0.0000
D ₂	π_1 →n's (0.27)	1.75	709	0.0012
D ₃	n _s → π_1^* (0.69)	2.74	452	0.0000
D ₄	π_2 →n's (0.27)	3.04	408	0.0026

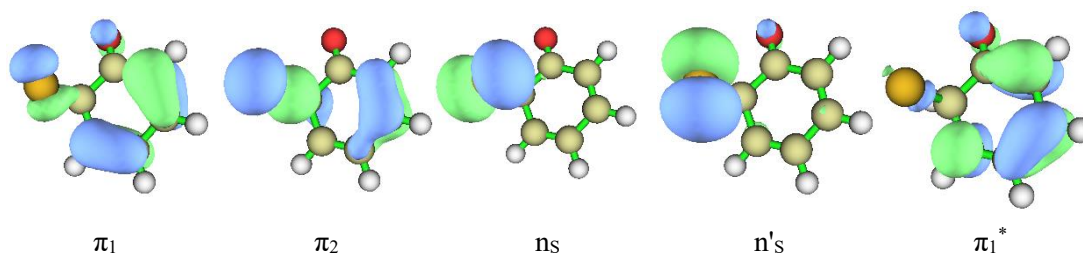
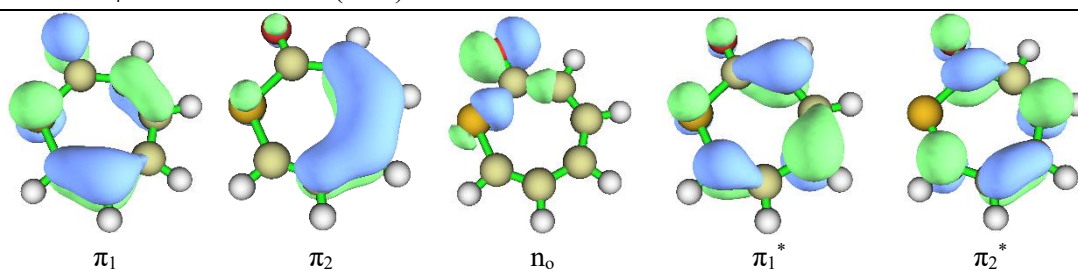
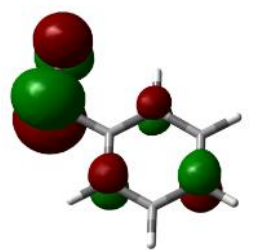


Table S6. MS-CASPT2 vertical excitation energy (E) and wavelength (λ) at **Int3-D₀**, together with the oscillator strength (f), the main electronic configuration with weight in parentheses and the relative orbitals.

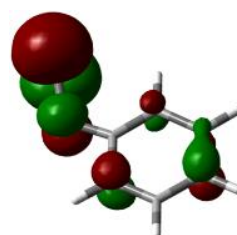
State	Configuration (weight)	E/eV	λ/nm	f
D ₀	π_1^* (SOMO)	0.00	-	-
D ₁	$\pi_1 \rightarrow \pi_1^*$ (0.31) $\pi_1^* \rightarrow \pi_2^*$ (0.34)	2.07	599	0.0009
D ₂	$n_o \rightarrow \pi_1^*$ (0.62)	2.58	480	0.0002
D ₃	$\pi_1 \rightarrow \pi_1^*$ (0.36)	3.05	406	0.0276
D ₄	$\pi_2 \rightarrow \pi_1^*$ (0.34)	3.88	319	0.0091





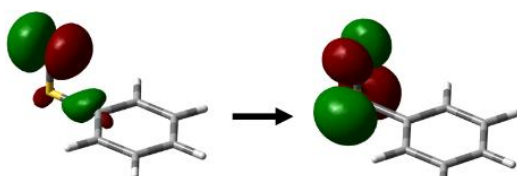
π_{SO}^*

SOMO of 1-D₀



π_{SO}^*

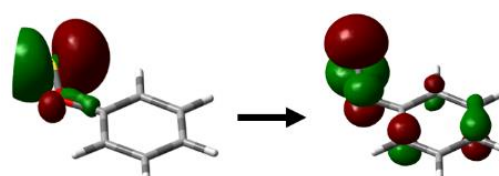
SOMO of 2-D₀



n_O

π_{SO}^*

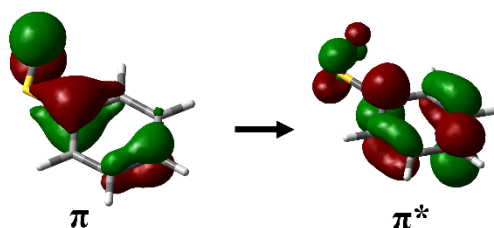
Related orbitals of 1-D₁



n_S

π_{SO}^*

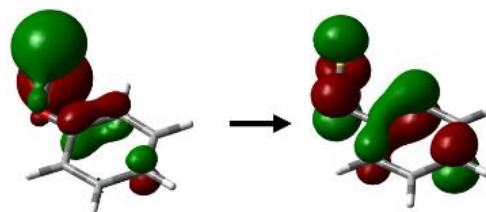
Related orbitals of 2-D₁



π

π^*

Related orbitals of 1-D₂

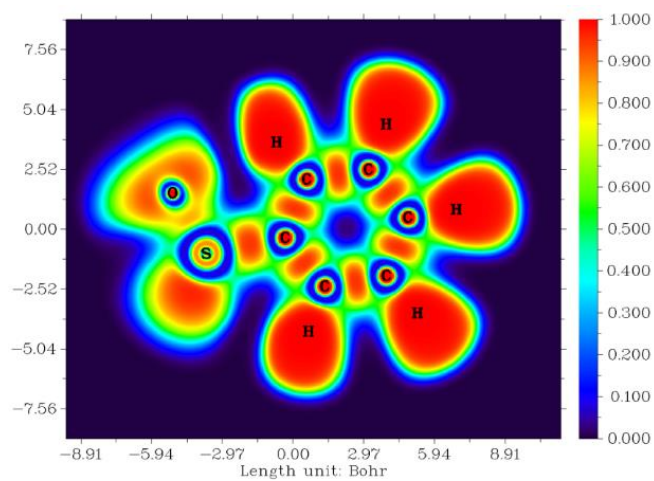


π_{SO}

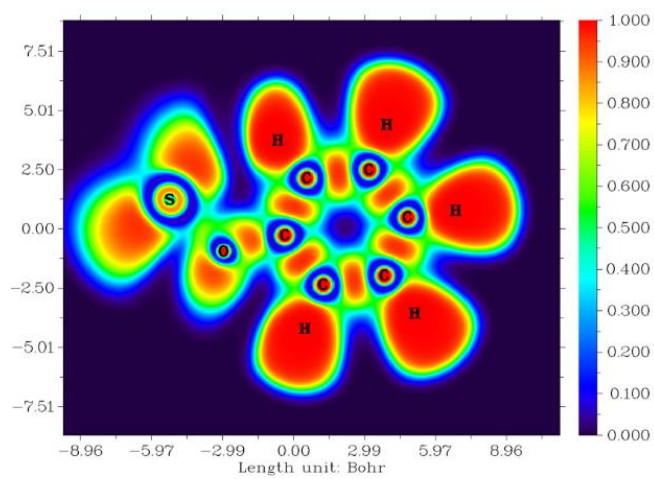
π_{SO}^*

Related orbitals of 2-D₂

Figure S1. Related orbitals of radicals **1** and **2** at D₀, D₁, and D₂ states.



(a)



(b)

Figure S2. Electron localization of radicals (a) 1-D₀ and (b) 2-D₀.

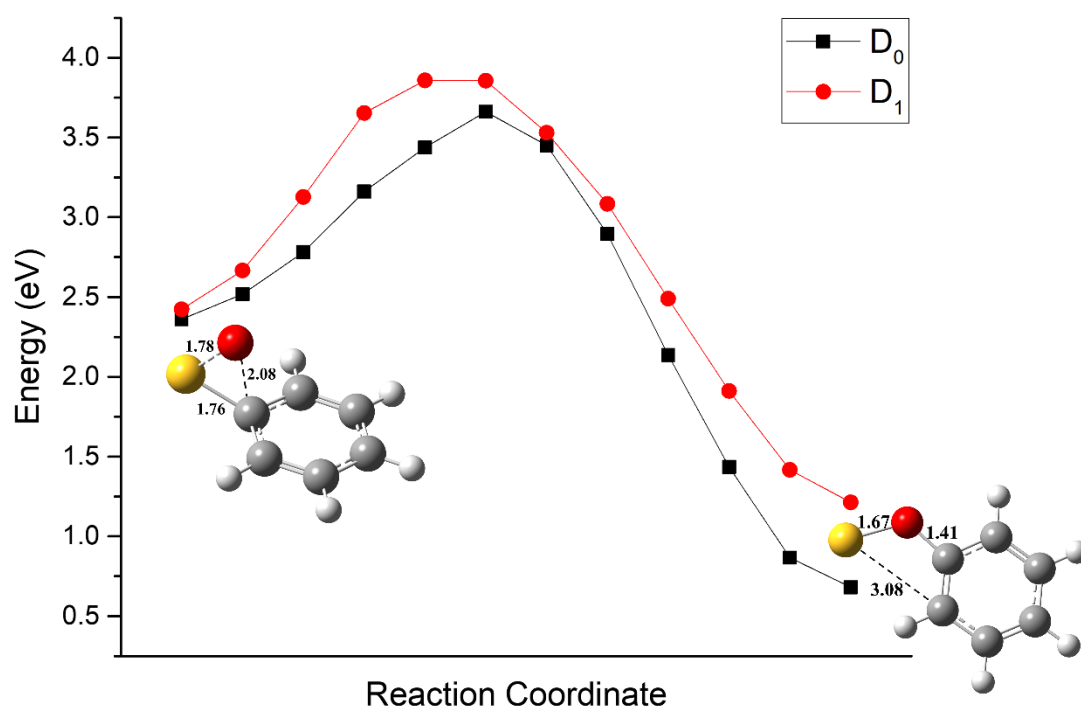


Figure S3. MS-CASPT2 energy plot from $1-(D_0/D_1)_x$ to $2-D_0$. Bond lengths are given in Å.

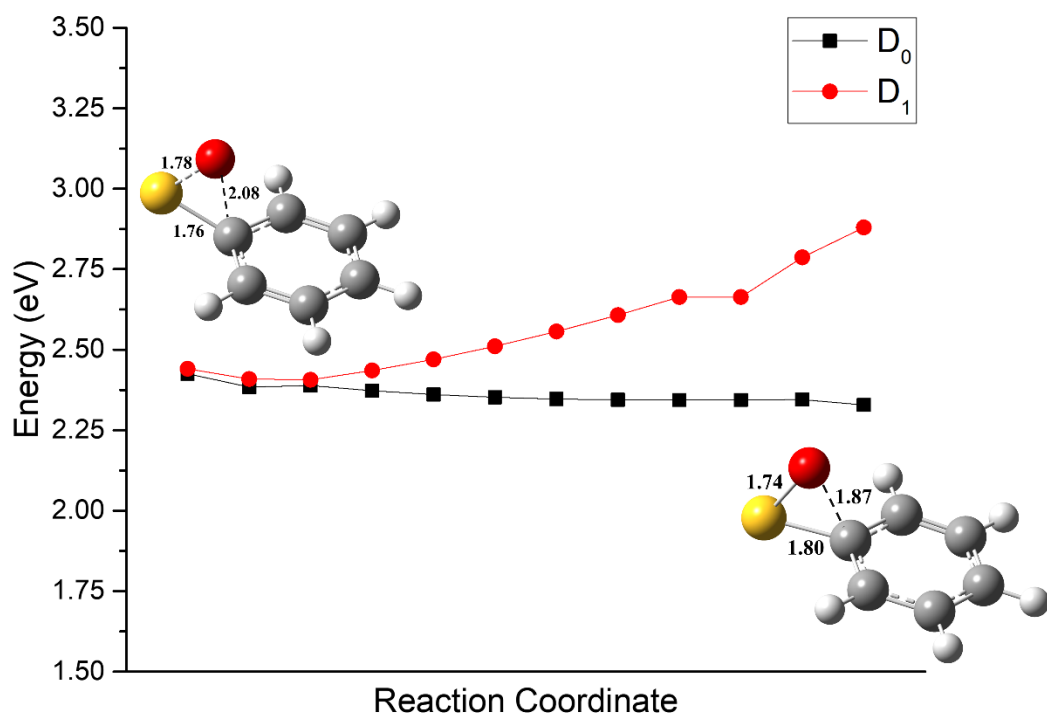
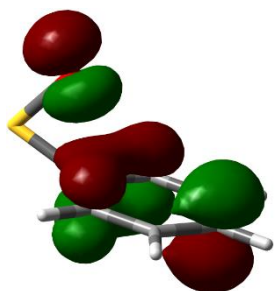
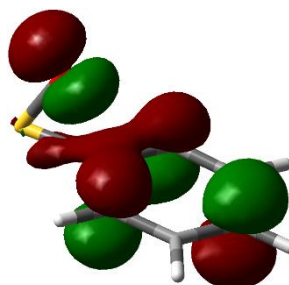


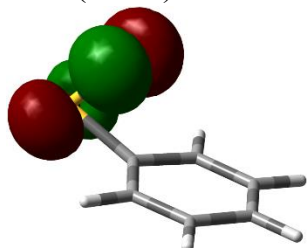
Figure S4. MS-CASPT2 energy plot from $1-(D_0/D_1)_x$ to $TS1-D_0$. Bond lengths are given in Å.



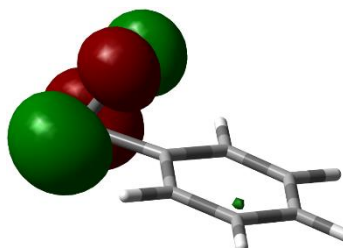
Orbital-1 of $1-(D_0/D_1)_x$



Orbital-1 of **TS1-D₀**



Orbital-2 of $1-(D_0/D_1)_x$



Orbital-2 of **TS1-D₀**

Figure S5. Related orbitals of $1-(D_0/D_1)_x$ and **TS1-D₀**.

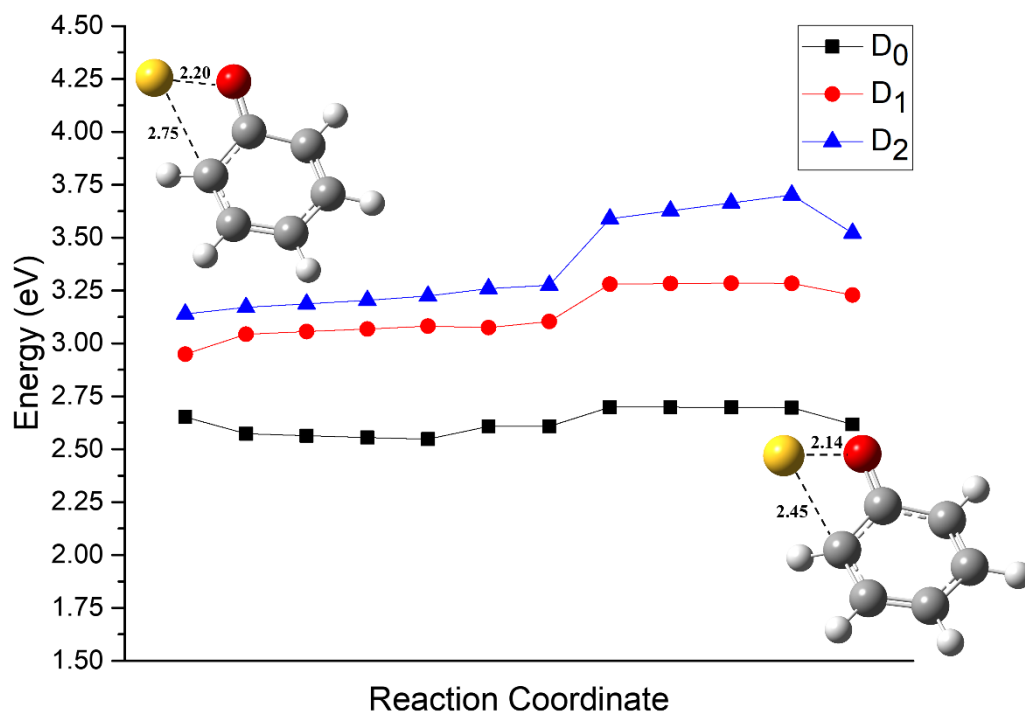


Figure S6. MS-CASPT2 energy plot from $2-(D_0/D_1/D_2)_x$ to $TS2-D_0$. Bond lengths are given in Å.

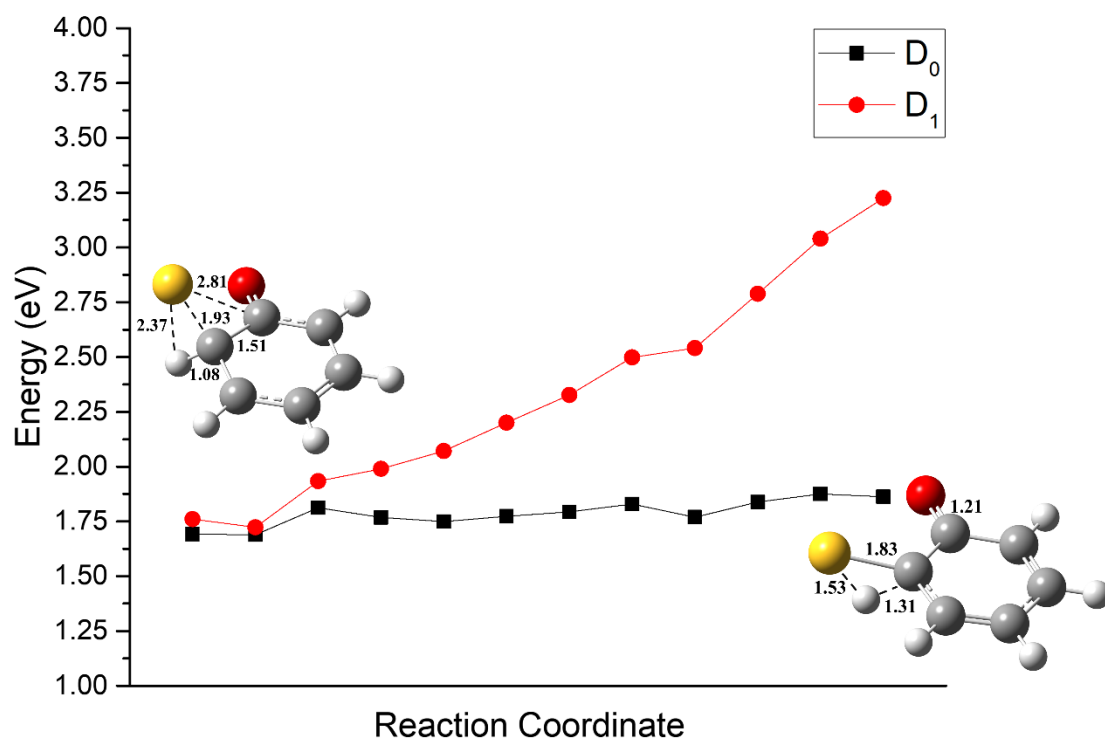


Figure S7. MS-CASPT2 energy plot from **Int1**-(D_0/D_1)_x to **TS3**- D_0 . Bond lengths are given in Å.

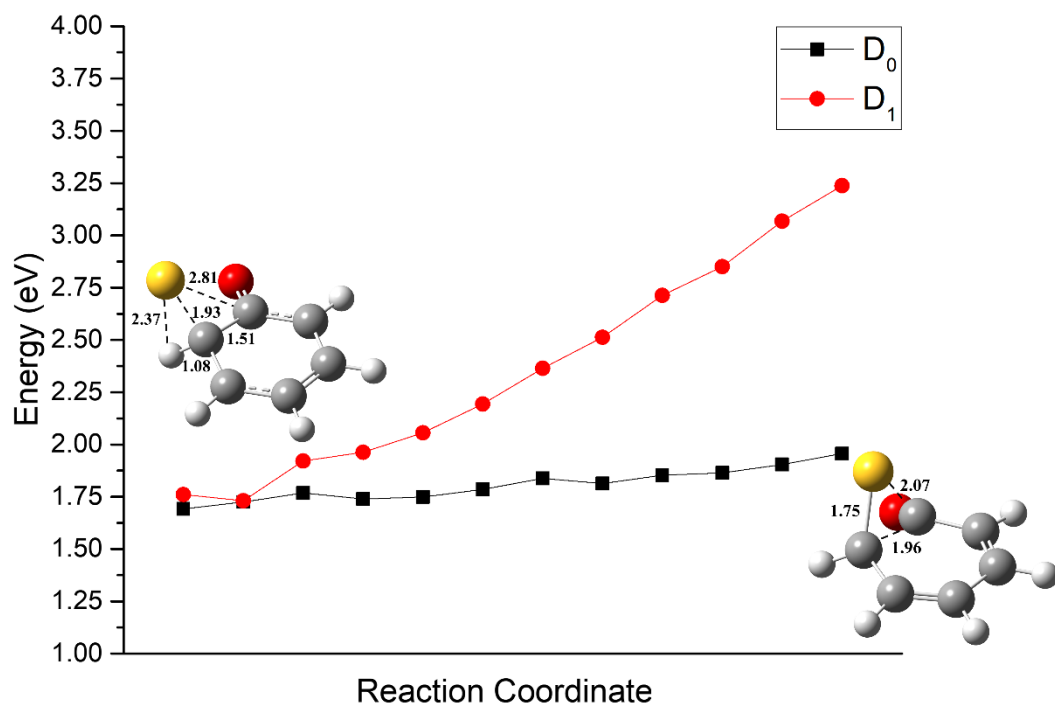


Figure S8. MS-CASPT2 energy plot from **Int1**-(D_0/D_1)_x to **TS4**- D_0 . Bond lengths are given in Å.

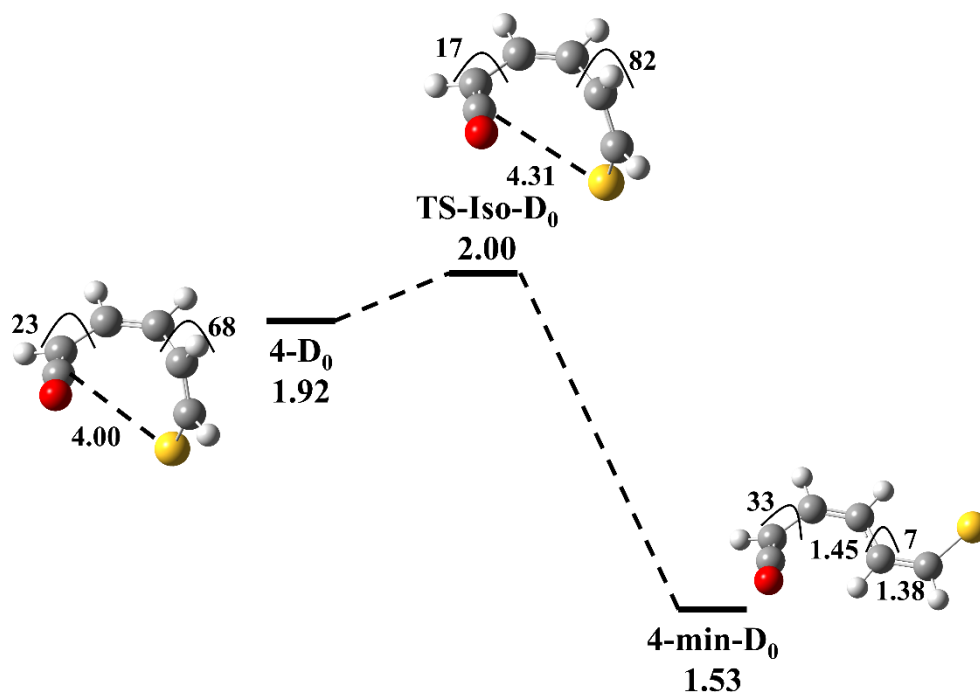
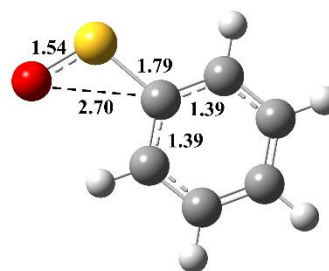


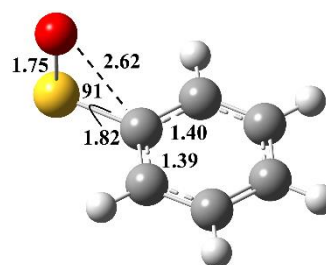
Figure S9. MS-CASPT2//CASSCF energy profile for isomerization of 4-D₀. Energies are given in eV. Bond lengths are given in Å. Dihedral angles are given in °.

Molecular structures, Cartesian coordinates, MS-CASPT2 absolute energies (in Hartree) and relative energies in parentheses (in eV) of critical points relative to 1-D₀

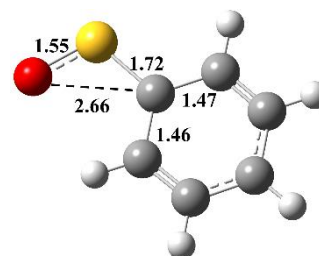
1-D ₀	-703.9357090 (0.00)		
C	1.693910	1.332507	0.000017
C	0.321445	1.117741	0.000015
C	-0.159315	-0.186540	-0.000003
C	0.719939	-1.266914	-0.000019
C	2.088261	-1.032434	-0.000016
C	2.570435	0.263198	0.000002
H	2.072490	2.337703	0.000031
H	-0.366170	1.940991	0.000026
H	0.345779	-2.275118	-0.000032
H	2.770239	-1.862194	-0.000028
H	3.630083	0.439638	0.000004
S	-1.915531	-0.533965	-0.000008
O	-2.663557	0.809654	0.000018



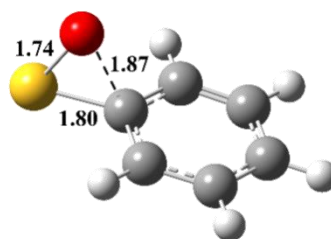
1-D ₁	-703.8597261 (2.07)		
C	1.749360	1.372818	0.133565
C	0.381078	1.220878	0.334616
C	-0.178182	-0.050808	0.291530
C	0.622253	-1.168010	0.049694
C	1.983945	-0.999419	-0.149895
C	2.540985	0.274183	-0.107522
H	2.184043	2.354517	0.165739
H	-0.242064	2.074563	0.519581
H	0.180675	-2.145529	0.019242
H	2.606739	-1.853922	-0.337159
H	3.596678	0.398927	-0.263915
S	-1.972298	-0.257419	0.524582
O	-2.345205	-0.136509	-1.180052



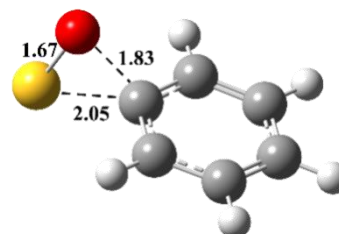
1-D₂	-703.8359657 (2.71)		
C	1.811195	1.426491	0.306585
C	0.479036	1.395223	0.333242
C	-0.230811	0.147731	0.043795
C	0.549655	-1.059515	-0.271211
C	1.902543	-0.993483	-0.290734
C	2.588027	0.248575	-0.004281
H	2.328788	2.343918	0.519696
H	-0.087801	2.278194	0.565694
H	0.021595	-1.968303	-0.479855
H	2.479959	-1.868840	-0.520126
H	3.657157	0.295117	-0.022132
S	-1.950390	0.134505	0.079633
O	-2.440946	-1.295344	-0.260301



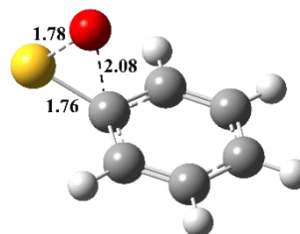
TS1-D₀	-703.8501445 (2.33)		
C	-1.765485	1.214598	-0.020672
C	-0.381113	1.228532	-0.122211
C	0.332904	0.004058	-0.140785
C	-0.396929	-1.232538	-0.112759
C	-1.740721	-1.215346	-0.027783
C	-2.454290	0.008218	0.021490
H	-2.303956	2.143102	0.009509
H	0.165568	2.149815	-0.155217
H	0.152630	-2.152517	-0.145236
H	-2.285149	-2.141215	-0.002865
H	-3.525071	-0.001935	0.090240
S	2.109484	-0.004220	-0.413815
O	1.585114	-0.000486	1.250293



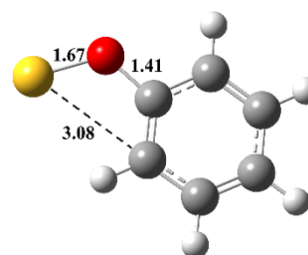
TS1-D₁	-703.8122369 (3.36)		
C	-1.791197	1.189181	-0.028180
C	-0.405123	1.213564	-0.021184
C	0.273903	0.005054	-0.012273
C	-0.400619	-1.212043	-0.017481
C	-1.784344	-1.196807	-0.024863
C	-2.488112	0.004397	-0.034165
H	-2.321519	2.123746	-0.031787
H	0.127683	2.141500	-0.011247
H	0.139846	-2.135786	-0.001909
H	-2.314840	-2.131030	-0.025211
H	-3.560168	0.003383	-0.038412
S	2.245988	0.001100	-0.567639
O	1.771487	-0.006193	1.044540



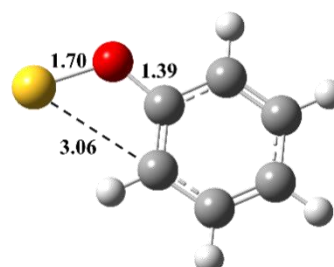
1-(D₀/D₁)_x	-703.8463087 (2.07)		
C	0.009674	-0.027035	0.051858
C	0.001716	0.133888	1.422066
C	1.218509	0.194154	2.174348
C	2.431045	0.148519	1.414549
C	2.421127	-0.011244	0.045549
C	1.214466	-0.115047	-0.656356
H	-0.928552	-0.076514	-0.472459
H	-0.948331	0.227510	1.936167
H	3.382396	0.259132	1.922709
H	3.357436	-0.049762	-0.483150
H	1.213694	-0.234985	-1.727433
S	1.235328	-0.140848	3.905124
O	1.230792	-1.703025	3.039941



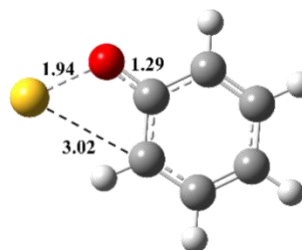
2-D₀	-703.9106872 (0.68)		
C	1.696025	1.325411	-0.000675
C	0.308777	1.138133	-0.004588
C	-0.178823	-0.137753	-0.004744
C	0.674924	-1.243113	-0.001955
C	2.037151	-1.039519	0.001740
C	2.553741	0.260935	0.002469
H	2.080664	2.328418	-0.000626
H	-0.349249	1.982354	-0.007135
H	0.252670	-2.229368	-0.002604
H	2.701130	-1.883538	0.004222
H	3.615814	0.418728	0.005276
S	-2.743288	0.660327	0.020309
O	-1.541526	-0.496748	-0.011684



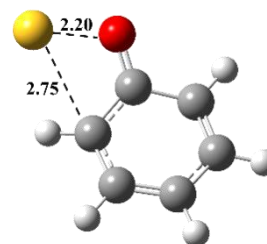
2-D₁	-703.8911529 (1.21)		
C	1.689551	1.321582	-0.000107
C	0.301067	1.126205	-0.003831
C	-0.187577	-0.150872	-0.004664
C	0.679198	-1.251805	-0.001716
C	2.037573	-1.039630	0.000684
C	2.551976	0.264872	0.001670
H	2.066992	2.327397	0.000986
H	-0.350354	1.977580	-0.008041
H	0.264164	-2.240976	-0.001203
H	2.705283	-1.880915	0.003242
H	3.613119	0.426496	0.004943
S	-2.730654	0.703917	0.018700
O	-1.532328	-0.499582	-0.010658



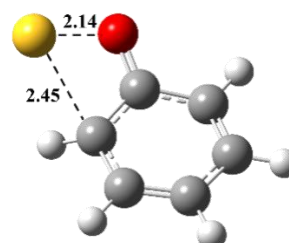
2-D₂	-703.8387102 (2.64)		
C	1.664105	1.336563	0.000603
C	0.288281	1.124991	0.002240
C	-0.212626	-0.219717	-0.001259
C	0.712233	-1.325932	0.001183
C	2.051221	-1.068193	0.001039
C	2.532233	0.276746	-0.002265
H	2.039245	2.343112	0.001519
H	-0.424102	1.926740	0.005682
H	0.310308	-2.322898	0.000588
H	2.757384	-1.877544	0.001155
H	3.595389	0.451332	-0.004199
S	-2.733515	0.956634	-0.002984
O	-1.472147	-0.517563	-0.003298



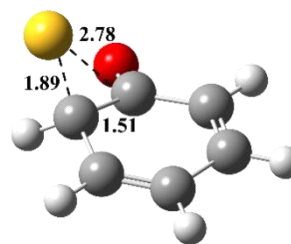
2-(D₀/D₁/D₂)_x	-703.8286474 (2.91)		
C	-1.036057	-1.486906	0.221058
C	0.094705	-0.715104	0.563048
C	0.081691	0.696151	0.255463
C	-1.202006	1.328463	0.016865
C	-2.278774	0.551243	-0.256445
C	-2.191989	-0.880755	-0.220694
H	-1.000675	-2.550942	0.354848
H	0.842096	-1.092731	1.226954
H	-1.241307	2.399500	-0.035017
H	-3.217215	1.011454	-0.505938
H	-3.05706	-1.465427	-0.465460
S	2.662053	-0.170334	-0.259650
O	1.123616	1.364354	0.110044



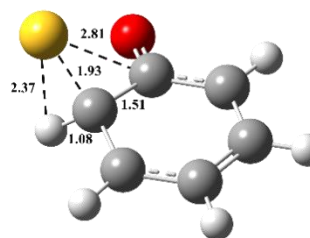
TS2-D₀	-703.8379542 (2.66)		
C	-0.991996	-1.488324	0.183461
C	0.143979	-0.686226	0.528000
C	0.078277	0.720540	0.271684
C	-1.196752	1.349094	0.051384
C	-2.252318	0.546835	-0.251653
C	-2.147153	-0.890023	-0.220098
H	-0.935985	-2.553622	0.302340
H	0.768612	-0.991267	1.344119
H	-1.246896	2.418682	-0.011224
H	-3.189987	0.990086	-0.531014
H	-3.011562	-1.478451	-0.461769
S	2.410811	-0.309083	-0.333701
O	1.150040	1.360722	0.133549



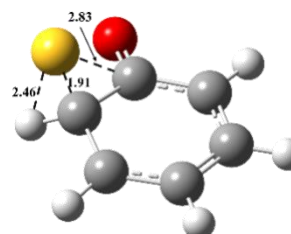
Int1-D₀	-703.8959854 (1.08)		
C	-0.654250	-1.403154	0.227548
C	0.475513	-0.440809	0.449726
C	0.054123	1.014858	0.533260
C	-1.243292	1.386356	-0.068827
C	-2.141254	0.440705	-0.392220
C	-1.857811	-0.984958	-0.190179
H	-0.445940	-2.447384	0.366427
H	1.047736	-0.693078	1.329345
H	-1.446283	2.434845	-0.175803
H	-3.098396	0.717618	-0.793501
H	-2.645130	-1.692964	-0.369338
S	1.641859	-0.655893	-1.018852
O	0.763420	1.828288	1.068045



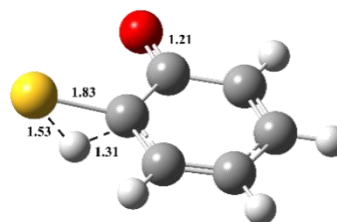
Int1-D₁	-703.8741756 (1.67)		
C	-0.518031	-1.271574	0.319357
C	0.517626	-0.261875	0.556442
C	0.048140	1.170330	0.525750
C	-1.255738	1.450085	-0.032921
C	-2.153028	0.390368	-0.393858
C	-1.805446	-0.919876	-0.219040
H	-0.291607	-2.294505	0.547442
H	1.143979	-0.449657	1.411892
H	-1.540330	2.478686	-0.132751
H	-3.115816	0.643064	-0.794995
H	-2.488995	-1.704842	-0.477643
S	1.533018	-0.681997	-1.005300
O	0.769486	2.054422	0.946865



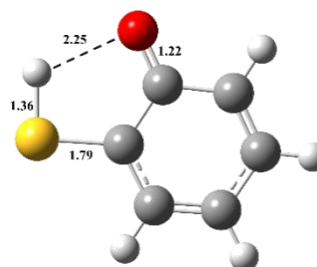
Int1-(D₀/D₁)_x	-703.8722776 (1.73)		
C	-0.559892	-1.303468	0.264968
C	0.518012	-0.310627	0.458790
C	0.048858	1.127391	0.472925
C	-1.234404	1.433691	-0.107662
C	-2.205938	0.379570	-0.374891
C	-1.886415	-0.916650	-0.149966
H	-0.338244	-2.334334	0.443871
H	1.056436	-0.513463	1.373564
H	-1.492562	2.466528	-0.229046
H	-3.189562	0.653049	-0.701899
H	-2.621215	-1.688736	-0.281346
S	1.978621	-0.394032	-0.831213
O	0.769561	2.003709	0.913144



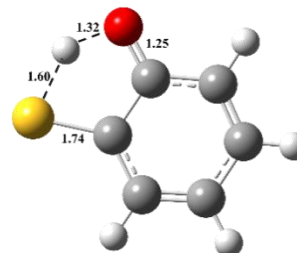
TS3-D₀	-703.8672622 (1.86)		
C	-0.561790	-1.272417	0.011768
C	0.445641	-0.272146	0.222624
C	0.056632	1.164429	0.205349
C	-1.368835	1.450874	-0.012774
C	-2.270181	0.462582	-0.199296
C	-1.864249	-0.925379	-0.187411
H	-0.259013	-2.301317	0.012080
H	1.139083	-0.525393	1.304174
H	-1.645807	2.487722	-0.019979
H	-3.305670	0.698347	-0.358819
H	-2.601686	-1.688167	-0.348856
S	2.220612	-0.733863	0.245432
O	0.858519	2.057355	0.376947



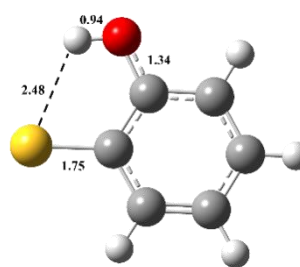
Int2-D₀	-703.9333160 (0.07)		
C	-0.391213	-1.460212	0.000028
C	0.443931	-0.338849	-0.000069
C	-0.130167	1.005905	0.000203
C	-1.591705	1.096363	-0.000083
C	-2.352584	0.002040	0.000027
C	-1.763113	-1.312456	0.000102
H	0.041149	-2.443231	-0.000002
H	2.462522	0.801156	-0.000282
H	-2.009286	2.085217	-0.000240
H	-3.423721	0.086626	-0.000014
H	-2.398621	-2.176544	0.000159
S	2.219234	-0.537082	-0.000357
O	0.569010	2.010114	-0.000032



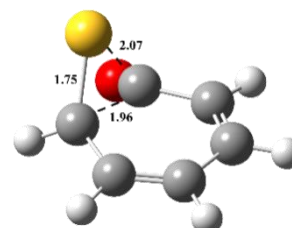
TS5-D₀	-703.9327145 (0.08)		
C	0.534803	-1.499144	-0.000193
C	-0.419379	-0.452527	-0.000345
C	0.030473	0.924852	0.000014
C	1.444194	1.198708	-0.000159
C	2.307266	0.174735	-0.000219
C	1.866163	-1.198450	-0.000016
H	0.199142	-2.517838	0.000257
H	-1.881397	1.013428	0.000216
H	1.764570	2.222365	-0.000208
H	3.363853	0.370850	-0.000057
H	2.601576	-1.979591	0.000222
S	-2.155361	-0.559016	-0.000435
O	-0.835593	1.824987	0.000740



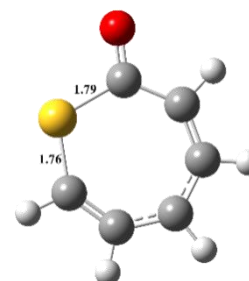
3-D₀	-703.9560899 (-0.55)		
C	-0.458486	-1.477591	0.000074
C	0.447657	-0.386636	-0.000003
C	-0.075006	0.925925	-0.000031
C	-1.453703	1.128833	0.000013
C	-2.318250	0.045444	0.000085
C	-1.819276	-1.266734	0.000117
H	-0.055904	-2.471627	0.000095
H	1.620550	1.758440	-0.000132
H	-1.822454	2.136409	-0.000014
H	-3.378556	0.214964	0.000116
H	-2.494495	-2.101206	0.000173
S	2.175977	-0.660925	-0.000062
O	0.709627	2.013516	-0.000105



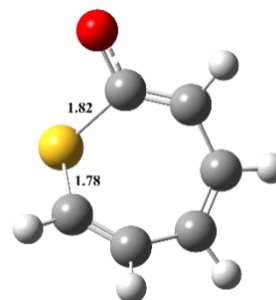
TS4-D₀	-703.8638149 (1.96)		
C	-1.172722	-1.256380	0.609729
C	0.276168	-1.047960	0.639054
C	0.731887	0.812591	0.245306
C	-0.450043	1.474191	-0.334269
C	-1.671500	0.925511	-0.439643
C	-2.043337	-0.396054	0.050655
H	-1.537045	-2.150488	1.085796
H	0.801498	-1.370169	1.519923
H	-0.278640	2.496660	-0.614970
H	-2.457110	1.531929	-0.851042
H	-3.089255	-0.640202	0.045590
S	1.246417	-0.894624	-0.809566
O	1.563980	1.326193	0.923406



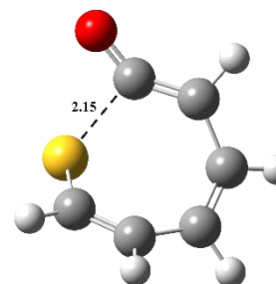
Int3-D₀	-703.9090995 (0.72)		
C	1.995418	-0.617150	-0.000075
C	0.961737	-1.498722	-0.000070
C	-1.292202	0.386485	0.000105
C	-0.421881	1.571149	0.000105
C	0.936811	1.723522	0.000067
C	2.007320	0.799553	0.000021
H	2.968762	-1.075619	-0.000156
H	1.196259	-2.546916	-0.000160
H	-1.016512	2.465728	0.000090
H	1.255224	2.751265	0.000080
H	2.984690	1.244220	0.000019
S	-0.788028	-1.335504	0.000039
O	-2.502228	0.537661	-0.000219



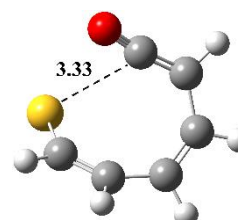
Int3-D₁	-703.8462028 (2.44)		
C	-3.199869	0.139019	0.743764
C	-2.879696	-0.614584	-0.314420
C	-0.168075	-0.509772	0.019054
C	-0.118259	0.273561	1.095392
C	-1.133677	0.318442	2.147698
C	-2.450403	0.254973	2.003265
H	-4.093754	0.737265	0.673385
H	-3.481553	-0.606917	-1.202635
H	0.735783	0.913684	1.210479
H	-0.752431	0.478235	3.141400
H	-3.055455	0.361597	2.886590
S	-1.479900	-1.716485	-0.353948
O	0.746249	-0.545244	-0.954957



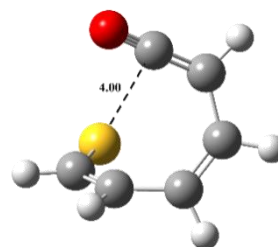
TS6-D₁	-703.8432896 (2.51)		
C	-3.166761	0.158857	0.697631
C	-2.856938	-0.620917	-0.358680
C	0.025953	-0.384211	0.039360
C	-0.087610	0.339484	1.162478
C	-1.142207	0.273103	2.168508
C	-2.453393	0.199298	1.984833
H	-4.019479	0.814474	0.607592
H	-3.419534	-0.553660	-1.270508
H	0.767344	0.939061	1.402995
H	-0.799793	0.372858	3.183797
H	-3.083466	0.231415	2.856332
S	-1.560589	-1.794640	-0.303957
O	0.659240	-0.488622	-0.980516



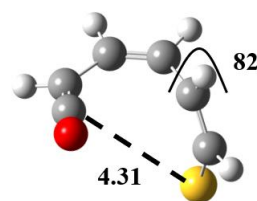
TS6-(D₀/D₁)_x	-703.8538703 (2.23)		
C	-3.041974	-0.015176	0.790759
C	-2.976328	-0.828621	-0.278592
C	0.038478	0.091301	0.141429
C	0.085868	0.068711	1.464124
C	-1.072555	0.138287	2.339546
C	-2.360242	0.139483	2.073657
H	-3.744162	0.783479	0.613205
H	-3.543714	-0.545877	-1.145239
H	1.081650	0.124054	1.855464
H	-0.807058	0.299438	3.368965
H	-3.019078	0.371908	2.894517
S	-2.115123	-2.366537	-0.493225
O	0.144411	0.172853	-1.006652



4-D₀	-703.8650847 (1.92)		
C	-3.074119	-0.208890	0.636144
C	-3.177857	-1.486341	0.187388
C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.315101
C	-1.145542	0.340088	2.172750
C	-2.453423	0.258166	1.894900
H	-3.545689	0.564463	0.009974
H	-3.674429	-1.652460	-0.751170
H	0.948707	-0.227617	1.762588
H	-0.865473	0.711704	3.141592
H	-3.142162	0.615475	2.641596
S	-2.583337	-2.888275	1.008367
O	0.024997	0.000000	-1.139005



TS-Iso-D₀	-703.8623462 (2.00)		
C	-0.651653	-0.412162	0.444694
C	-0.147186	0.845494	-0.098239
C	1.113809	1.243558	-0.039967
C	-1.969531	-0.848095	0.388943
C	2.230947	0.500011	0.612042
C	3.049454	-0.262422	-0.055084
H	0.054688	-1.060424	0.928796
H	-0.863470	1.488906	-0.572972
H	1.360782	2.199901	-0.467588
H	2.447642	0.622411	1.657558
H	-2.194973	-1.820831	0.842845
O	3.760788	-0.934540	-0.631390
S	-3.300319	0.005130	-0.336939



4-min-D₀	-703.8796453 (1.53)		
C	-0.221733	2.184075	1.860004
C	0.162468	1.043975	2.388428
C	-0.545918	3.179688	1.407599
C	-0.531801	-0.243455	2.211334
C	-1.127212	-0.740547	1.084363
C	-1.134135	-0.111044	-0.217903
H	-1.796895	-0.564787	-1.333947
H	0.996235	1.114377	3.061514
H	-0.561938	-0.855268	3.094311
H	-1.619988	-1.689491	1.170182
H	-0.549137	0.781603	-0.347809
O	-1.681556	0.002993	-2.239286
S	-2.794039	-1.950937	-1.419418

