

Supplementary Information

for

Theoretical Study on the Photochemical Reaction Mechanism of HOSO Radical with CO

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Table S1. Benchmark calculation results for the active space and basis set. Comparison of the vertical excitation energies (E) by MS-CASPT2 methods with two active spaces, (19,13) and (13,10), and two basis sets, ANO-S-VDZP and cc-pVTZ, at the HOSO structure optimized by MS-CASPT2(13,10)/cc-pVTZ. Previous reported calculation results with MRCI+Q and MS-CASPT2 methods are also provided.

States	MS-CASPT2(13,10)		MS-CASPT2(19,13)		MRCI+Q	MS-CASPT2(13,10)
	cc-pVTZ	ANO-S-VDZP	cc-pVTZ	ANO-S-VDZP	aug-cc-pV(Q+d)Z ^a	ANO-S-VDZP ^b
D ₀	0.00	0.00	0.00	0.00	0.00	0.00
D ₁	3.55	3.59	3.48	3.52	3.63	3.83
D ₂	3.73	3.71	3.73	3.64	4.38	3.94
D ₃	4.53	4.61	4.51	4.58	4.97	4.87

^a Extracted from Table 1 of T. Trabelsi, J. M. Anglada, M. F. Ruiz-López and J. S. Francisco, *J. Chem. Phys.*, 2019, 151, 111103–111108.

^b Extracted from Table S1 of J. Carmona-García, A. Francés-Monerris, C. A. Cuevas, T. Trabelsi, A. Saiz-Lopez, J. S. Francisco and D. Roca-Sanjuán, *J. Am. Chem. Soc.*, 2021, 143, 10836–10841.

Table S2. Absolute and relative MS-CASPT2 energies of the critical points in the PES.

Structure	State	Absolute energy (Hartree)	Relative energy (eV)	Zero-point energy (ZPE, kcal mol ⁻¹)	Relative energy with ZPE	Active space Zero point
HOSO-D ₀	D ₀	-548.51754796	0.00	10.443	0.00	(13,10) HOSO-D ₀
	D ₁	-548.37059770	4.00		3.55	
	D ₂	-548.36388998	4.18		3.73	
	D ₃	-548.33445909	4.98		4.53	
	D ₄	-548.32750651	5.17		4.72	
HOSO-(D ₃ /D ₂) _X	D ₀	-548.47756124	1.09	-----	-	(13,10) HOSO-D ₀
	D ₁	-548.39718325	3.28			
	D ₂	-548.37228154	3.95			
	D ₃	-548.37228023	3.95			
	D ₄	-548.31209381	5.59			
HOSO-D ₂	D ₀	-548.48542973	0.87	11.956	0.42	(13,10) HOSO-D ₀
	D ₁	-548.39128955	3.44		2.98	
	D ₂	-548.38972157	3.48		3.54	
	D ₃	-548.36646395	4.11		3.66	
	D ₄	-548.32132875	5.34		4.89	
HOSO-(D ₂ /D ₁) _X	D ₀	-548.44948364	1.85	-----	-	(13,10) HOSO-D ₀
	D ₁	-548.38435027	3.62			
	D ₂	-548.38434879	3.62			
	D ₃	-548.36235900	4.22			
	D ₄	-548.35180264	4.51			
HOSO-D ₁	D ₀	-548.47498557	1.16	10.447	0.71	(13,10) HOSO-D ₀
	D ₁	-548.41293936	2.85		2.85	
	D ₂	-548.35701701	4.37		3.92	
	D ₃	-548.35126348	4.52		4.07	
	D ₄	-548.34724685	4.63		4.18	
HO+SO	D ₀	-548.41856041	2.69	-----	-	(13,10) HOSO-D ₀
	D ₁	-548.41824534	2.70			
	D ₂	-548.39164463	3.43			
	D ₃	-548.39092827	3.45			
	D ₄	-548.39024689	3.46			
CO-S ₀	S ₀	-113.13472227	0.00	3.116	0.00	(6,6) CO-S ₀
	S ₁	-112.82129560	8.53		8.39	
	S ₂	-112.82129560	8.53		8.39	

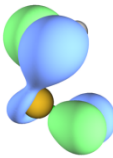
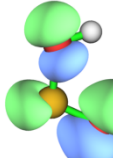
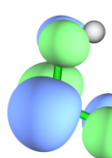
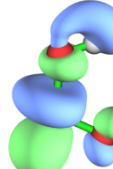
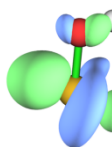
	S ₃	-112.77795167	9.71		9.57	
	S ₄	-112.77238433	9.86		9.72	
Path 1: HOSO+CO→HCO+SO ₂						
[OSOH···CO]-R-D ₀	D ₀	-661.66592379	0.00	14.822	0.00	(9,9) [OSOH···CO]-R-D ₀
	D ₁	-661.51499984	4.11		3.47	
	D ₂	-661.51211819	4.19		3.55	
	D ₃	-661.47188786	5.28		4.64	
	D ₄	-661.42471768	6.56		5.92	
[OSO···H···CO]-TS-D ₀	D ₀	-661.60294560	1.71	12.244	1.58	(9,9) [OSOH···CO]-R-D ₀
	D ₁	-661.53697019	3.51		2.87	
	D ₂	-661.51132348	4.21		3.57	
	D ₃	-661.48726051	4.86		4.22	
	D ₄	-661.45571165	5.72		5.08	
[OSOH···CO]-R-D ₁	D ₀	-661.62237201	1.19	14.371	0.55	(9,9) [OSOH···CO]-R-D ₀
	D ₁	-661.56049435	2.87		2.85	
	D ₂	-661.50408584	4.40		3.76	
	D ₃	-661.48723576	4.86		4.22	
	D ₄	-661.46584055	5.44		4.81	
[OSO···H···CO]-TS-D ₁	D ₀	-661.56206515	2.83	12.268	2.19	(9,9) [OSOH···CO]-R-D ₀
	D ₁	-661.51905696	4.00		3.89	
	D ₂	-661.46707747	5.41		4.77	
	D ₃	-661.45573490	5.72		5.08	
	D ₄	-661.42001564	6.69		6.05	
[SO ₂ -HCO]-(D ₁ /D ₀) _x	D ₀	-661.55364761	3.06	-----	-	(9,9) [OSOH···CO]-R- D ₀
	D ₁	-661.55364551	3.06			
	D ₂	-661.51309286	4.16			
	D ₃	-661.49541772	4.64			
	D ₄	-661.40487807	7.10			
[SO ₂ ···HCO]-D ₀	D ₀	-661.61919056	1.27	13.141	1.20	(9,9) [OSOH···CO]-R- D ₀
	D ₁	-661.53316401	3.61		2.97	
	D ₂	-661.51266528	4.17		3.53	
	D ₃	-661.47489908	5.20		4.56	
	D ₄	-661.46796058	5.39		4.75	
Path 2: HOSO+OC→HOC+SO ₂ (step 1)						
[OSOH···OC]-R-D ₀	D ₀	-661.66208358	0.10	14.117	0.08	(9,9) [OSOH···CO]-R-D ₀
	D ₁	-661.50997881	4.24		3.60	

	D ₂	-661.50796612	4.30		3.66	
	D ₃	-661.46766623	5.39		4.76	
	D ₄	-661.43130035	6.38		5.75	
[OSO \cdots OC]-R-D ₁	D ₀	-661.62034861	1.24	13.956	0.60	(9,9)
	D ₁	-661.55743706	2.95		2.92	[OSO \cdots CO]-R-D ₀
	D ₂	-661.50234413	4.45		3.81	
	D ₃	-661.48648726	4.88		4.24	
	D ₄	-661.46262550	5.53		4.89	
[OSO \cdots H \cdots OC]-TS-D ₁	D ₀	-661.57665015	2.43	11.092	1.79	(9,9)
	D ₁	-661.48764543	4.85		4.69	[OSO \cdots CO]-R-D ₀
	D ₂	-661.45689892	5.69		5.05	
	D ₃	-661.41643305	6.79		6.15	
	D ₄	-661.39127129	7.47		6.83	
[OSO \cdots H \cdots OC]- (D ₁ /D ₀) _x	D ₀	-661.53606732	3.53	-----	-	(9,9)
	D ₁	-661.53606657	3.53			[OSO \cdots CO]-R-D ₀
	D ₂	-661.49827268	4.56			
	D ₃	-661.41667008	6.78			
	D ₄	-661.39583959	7.35			
[SO ₂ \cdots HOC]-D ₀	D ₀	-661.54800092	3.21	16.016	2.18	(9,9)
	D ₁	-661.51462124	4.12		3.48	[OSO \cdots CO]-R-D ₀
	D ₂	-661.47134228	5.29		4.66	
	D ₃	-661.40785074	7.02		6.38	
	D ₄	-661.39717693	7.31		6.67	
Path 2: HOC \rightarrow HCO (step 2)						
HOC-D ₀	D ₀	-113.60367252	0.00	8.541	0.00	(3,5)
	D ₁	-113.57037083	0.91		0.54	HOC-D ₀
	D ₂	-113.42476189	4.87		4.50	
	D ₃	-113.39187145	5.76		5.39	
	D ₄	-113.38489199	5.95		5.58	
HOC-TS-D ₀	D ₀	-113.56742436	0.99	5.808	0.87	(3,5)
	D ₁	-113.53893794	1.76		1.39	HOC-D ₀
	D ₂	-113.42451507	4.88		4.50	
	D ₃	-113.35467532	6.78		6.41	
	D ₄	-113.35192268	6.85		6.48	
HCO-D ₀	D ₀	-113.65992079	-1.53	8.238	-1.60	(3,5)
	D ₁	-113.58597310	0.48		0.11	HOC-D ₀

	D ₂	-113.44274113	4.38		4.01	
	D ₃	-113.42157222	4.96		4.58	
	D ₄	-113.38561082	5.93		5.56	
Path 3: HOCO+CO→HCO+CO ₂						
[OCOH…CO]-D ₀	D ₀	-301.95287976	0.00	17.136	0.00	(7,7)
	D ₁	-301.81041765	3.88		3.13	[OCOH…CO]-D ₀
	D ₂	-301.74635499	5.62		4.88	
	D ₃	-301.74112572	5.76		5.02	
	D ₄	-301.71451819	6.49		5.74	
[OCOH…CO]-(D ₁ /D ₀) _x	D ₀	-301.86296103	2.45	-----	-	(7,7)
	D ₁	-301.86295749	2.45			[OCOH…CO]-D ₀
	D ₂	-301.78185529	4.65			
	D ₃	-301.60873144	9.36			
	D ₄	-301.59401473	9.77			
[CO ₂ …HCO]-D ₀	D ₀	-301.98067143	-0.76	16.765	0.10	(7,7)
	D ₁	-301.89578334	1.55		1.55	[OCOH…CO]-D ₀
	D ₂	-301.69253037	7.08		7.08	
	D ₃	-301.67211083	7.64		7.64	
	D ₄	-301.67203498	7.64		7.64	
Path 3: OSOS+CO→SO ₂ +SCO						
[OSOS…CO]-S ₀	S ₀	-1058.74133601	0.00	8.102	0.00	(10,10)
	S ₁	-1058.70530732	0.98		0.63	[OSOS…CO]-S ₀
	S ₂	-1058.61705491	3.38		3.03	
	S ₃	-1058.56398537	4.83		4.47	
	S ₄	-1058.53752239	5.55		5.19	
[OSO…S…CO]-TS-S ₀	S ₀	-1058.73658448	0.13	11.900	0.18	(10,10)
	S ₁	-1058.68964725	1.41		1.05	[OSOS…CO]-S ₀
	S ₂	-1058.63186043	2.98		2.63	
	S ₃	-1058.55012036	5.20		4.85	
	S ₄	-1058.51881668	6.06		5.70	
[SO ₂ …SCO]-S ₀	S ₀	-1058.83065690	-2.43	10.218	-2.23	(10,10)
	S ₁	-1058.68689447	1.48		1.13	[OSOS-CO]-S ₀
	S ₂	-1058.68000742	1.67		1.32	
	S ₃	-1058.63696993	2.84		2.49	
	S ₄	-1058.63289443	2.95		2.60	

Table S3. Relative TD-B3LYP vertical excitation energy (E) and wavelength (λ) at HOSO-D₀ together with the electronic configuration (weight in the parenthesis, related orbitals in the lower part of the Table) and oscillation strength (f).

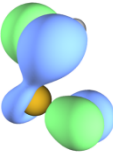
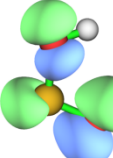
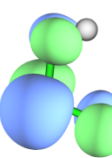
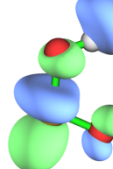
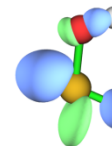
State	Configuration (weight)	E/eV	λ/nm	f
D ₀	SOMO	0.00	-	-
D ₁	SOMO-1 \rightarrow SOMO (0.99)	3.44	360	0.0012
D ₂	SOMO \rightarrow SOMO+1 (0.96)	3.89	319	0.0000
D ₃	SOMO-2 \rightarrow SOMO (0.92)	4.44	279	0.0263
D ₄	SOMO \rightarrow SOMO+2 (0.90)	4.91	252	0.0006

SOMO-2
SOMO-1
SOMO
SOMO+1
SOMO+2

Table S4. Relative TD-CAM-B3LYP vertical excitation energy (ΔE) and wavelength (λ) at HOSO-D₀ together with the electronic configuration (weight in the parenthesis, related orbitals in the lower part of the Table) and oscillation strength (f).

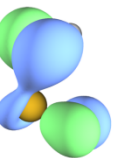
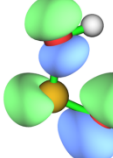
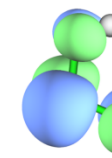
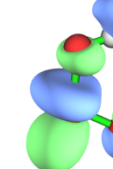
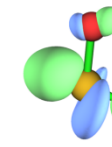
State	Configuration (weight)	E/eV	λ/nm	f
D ₀	SOMO	0.00	-	-
D ₁	SOMO-1 \rightarrow SOMO (0.98)	3.55	350	0.0014
D ₂	SOMO \rightarrow SOMO+1 (0.80)	4.09	303	0.0001
D ₃	SOMO-2 \rightarrow SOMO (0.91)	4.65	266	0.0321
D ₄	SOMO \rightarrow SOMO+2 (0.68)	5.07	245	0.0009

SOMO-2
SOMO-1
SOMO
SOMO+1
SOMO+2

Table S5. Relative TD- ω B97XD vertical excitation energy (ΔE) and wavelength (λ) at HOSO-D₀ together with the electronic configuration (weight in the parenthesis, related orbitals in the lower part of the Table) and oscillation strength (f).

State	Configuration (weight)	E/eV	λ/nm	f
D ₀	SOMO	0.00	-	-
D ₁	SOMO-1 \rightarrow SOMO (0.98)	3.53	351	0.0015
D ₂	SOMO \rightarrow SOMO+1 (0.84)	4.16	298	0.0001
D ₃	SOMO-2 \rightarrow SOMO (0.91)	4.70	264	0.0321
D ₄	SOMO \rightarrow SOMO+2 (0.71)	5.16	240	0.0010

SOMO-2
SOMO-1
SOMO
SOMO+1
SOMO+2

Table S6. Relative TD-B3LYP vertical excitation energy (E) and wavelength (λ) at CO-S₀ together with the electronic configuration (weight in the parenthesis, related orbitals in the lower part of the Table) and oscillation strength (f).

State	Configuration (weight)	E/eV	λ/nm	f
S ₀	-	0.00	-	-
S ₁	HOMO → LUMO (0.98)	8.36	148	0.0905
S ₂	HOMO → LUMO + 1 (0.98)	8.36	148	0.0905
S ₃	HOMO-1 → LUMO (0.49)	9.57	130	0.0000
S ₄	HOMO-2 → LUMO (0.46)	9.91	125	0.0000
	HOMO-1 → LUMO (0.46)			

HOMO-2 HOMO-1 HOMO LUMO LUMO+1

Table S7. Relative TD-CAM-B3LYP vertical excitation energy (E) and wavelength (λ) at CO-S₀ together with the electronic configuration (weight in the parenthesis, related orbitals in the lower part of the Table) and oscillation strength (f).

State	Configuration (weight)	E/eV	λ/nm	f
S ₀	-	0.00	-	-
S ₁	HOMO → LUMO (0.95)	8.48	146	0.0938
S ₂	HOMO → LUMO + 1 (0.95)	8.48	146	0.0938
S ₃	HOMO-1 → LUMO (0.46)	9.64	129	0.0000
S ₄	HOMO-2 → LUMO (0.46)	10.04	123	0.0000
	HOMO-1 → LUMO (0.46)			

HOMO-2 HOMO-1 HOMO LUMO LUMO+1

Table S8. Relative MS-CASPT2(6,6) vertical excitation energy with ZPE (E) and wavelength (λ) at CO-S₀ together with the electronic configuration (weight in the parenthesis, active orbitals in the lower part of the Table) and oscillation strength (f).

State	Configuration (weight)	E/eV	λ/nm	f
S ₀	222000 (0.94)	0.00	-	-
S ₁	22ud00 (0.71)	8.39	148	0.1651
S ₂	22u0d0 (0.71)	8.39	148	0.1651
S ₃	2u20d0 (0.47) u22d00 (0.47)	9.57	130	0.0003
S ₄	2u2d00 (0.45) u220d0 (0.45)	9.72	127	0.0003

1 2 3 4 5 6

“u” and “d” stand for singly occupied orbitals with electrons of spin up (u) or spin down (d)

Table S9. Relative MS-CASPT2 vertical excitation energy with ZPE (E) and wavelength (λ) at [OSOH \cdots CO]-R-D₀ together with the electronic configuration (weight in the parenthesis, active orbitals in the lower part of the Table), and oscillation strength (f).

State	Configuration (weight)	E/eV	λ/nm	f
D ₀	2222u0000(0.91)	0.00	-	-
D ₁	2u2220000(0.60)	3.47	357	0.0021
D ₂	2222000u0(0.59)	3.55	349	0.0050
D ₃	u22220000(0.81)	4.64	267	0.0388
D ₄	222u20000(0.93)	5.92	209	0.0009

“u” and “d” stand for singly occupied orbitals with electrons of spin up (u) or spin down (d)

Table S10. Relative MS-CASPT2 vertical excitation energy with ZPE (E) and wavelength (λ) at [OSOH \cdots OC]-R-D₀ together with the electronic configuration (weight in the parenthesis, active space below the Table) and oscillation strength (f).

State	Configuration (weight)	E/eV	λ/nm	f
D ₀	2222u0000(0.92)	0.00	-	-
D ₁	2u2220000(0.64)	3.53	352	0.0020
D ₂	2222000u0(0.62)	3.58	346	0.0044
D ₃	u22220000(0.81)	4.68	265	0.0401
D ₄	222u20000(0.60)	5.67	219	0.0001

“u” and “d” stand for singly occupied orbitals with electrons of spin up (u) or spin down (d)

Table S11. Relative MS-CASPT2 vertical excitation energy with ZPE (E) and wavelength (λ) at [OCOH \cdots CO]-D₀ together with the electronic configuration (weight in the parenthesis, active orbitals in the lower part of the Table) and oscillation strength (f).

State	Configuration (weight)	E/eV	λ/nm	f
D ₀	222u000 (0.90)	0.00	-	-
D ₁	222000u (0.86)	3.13	396	0.0098
D ₂	2u22000 (0.51)	4.88	254	0.0084
D ₃	u222000 (0.90)	5.02	247	0.0290
D ₄	22ud0u0 (0.43)	5.74	216	0.0009

“u” and “d” stand for singly occupied orbitals with electrons of spin up (u) or spin down (d)

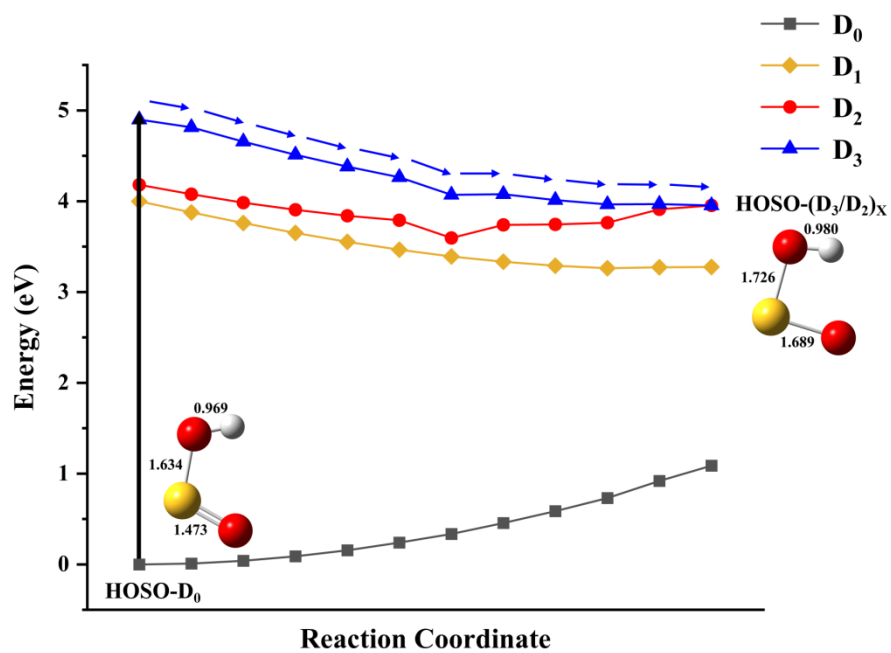


Figure S1. Energy plot from HOSO-D₀ to HOSO-(D₃/D₂)_x. Bond lengths are given in Å.

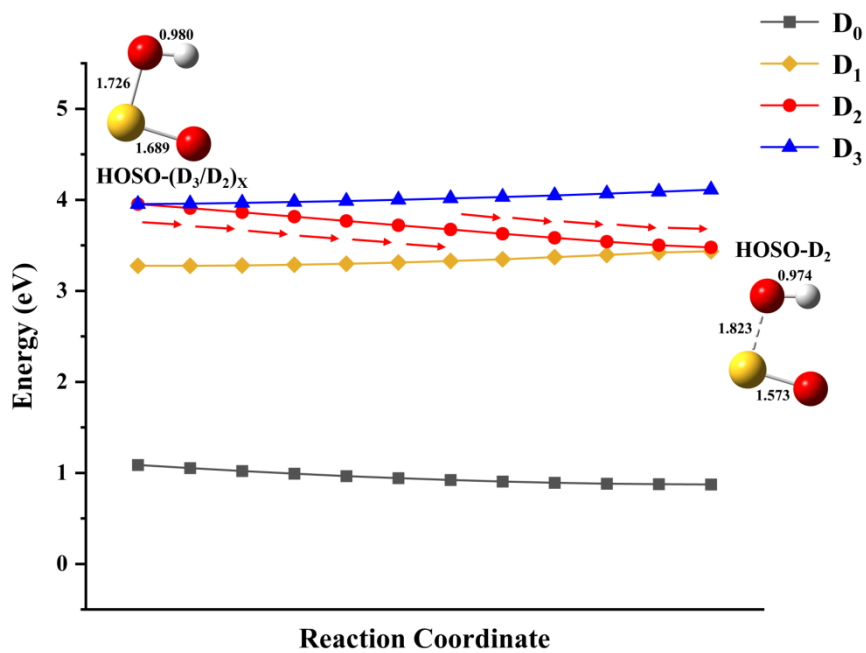


Figure S2. Energy plot from HOSO-(D₃/D₂)_x to HOSO-D₂. Bond lengths are given in Å.

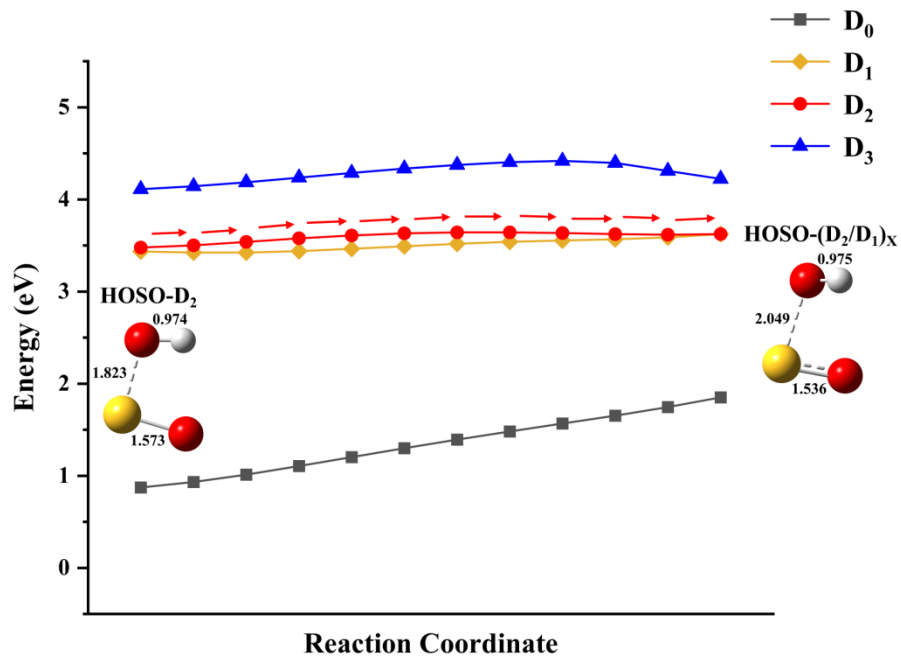


Figure S3. Energy plot from HOSO-D₂ to HOSO-(D₂/D₁)_x. Bond lengths are given in Å.

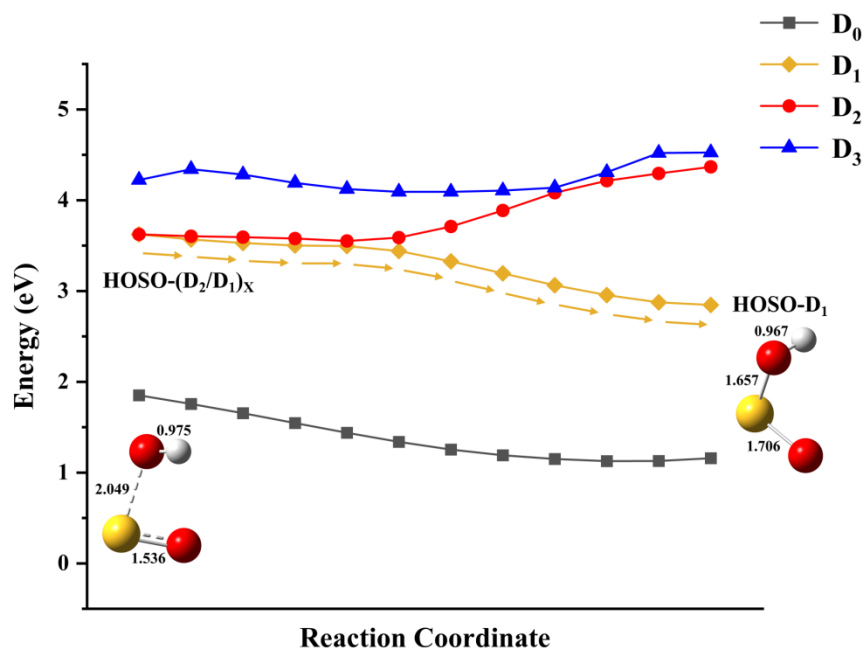


Figure S4. Energy plot from HOSO-(D₂/D₁)_x to HOSO-D₁. Bond lengths are given in Å.

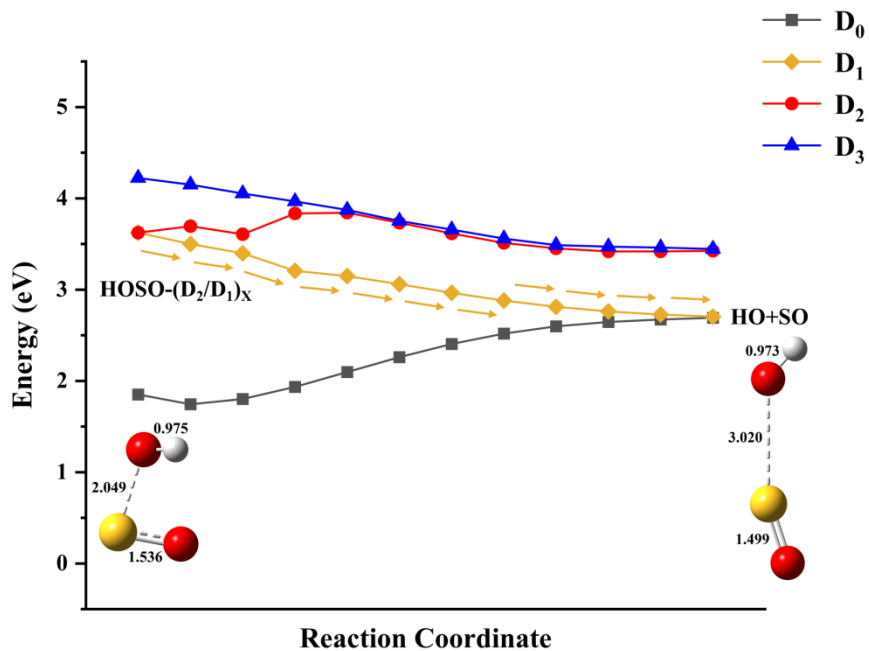


Figure S5. Energy plot from HOSO-(D₂/D₁)_x to HO+SO. Bond lengths are given in Å.

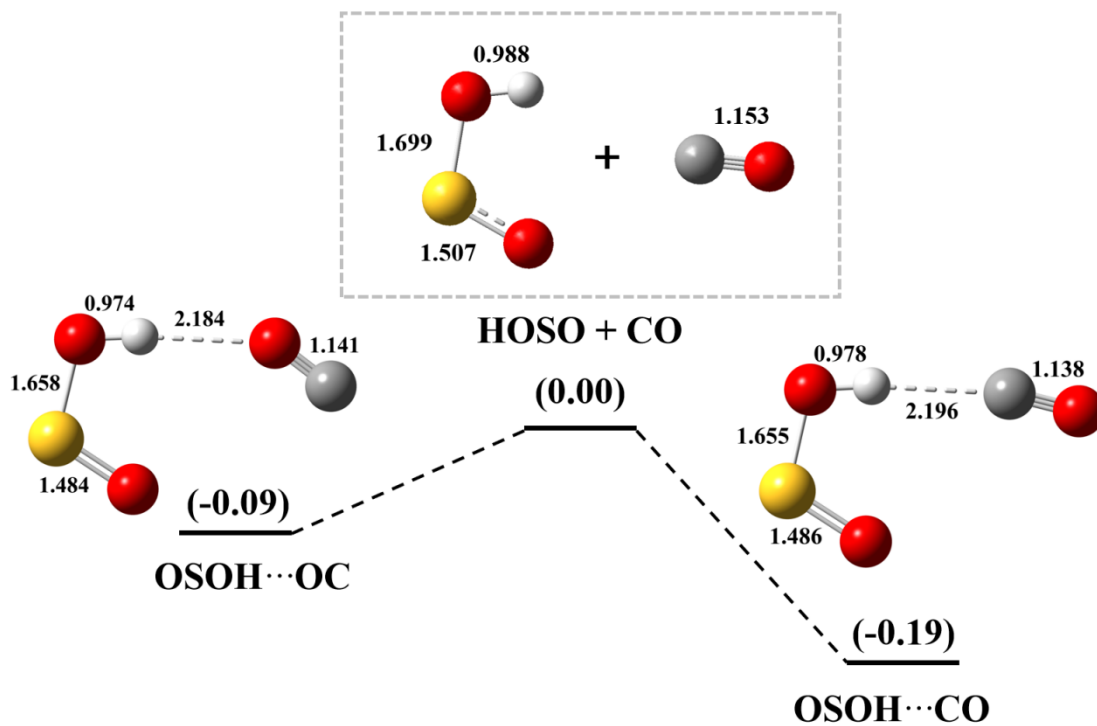


Figure S6. MS-CASPT2 energy profile (energy in eV) and key structures (distance in Å) from HOSO + CO to OSOH...CO and OSOH...OC.

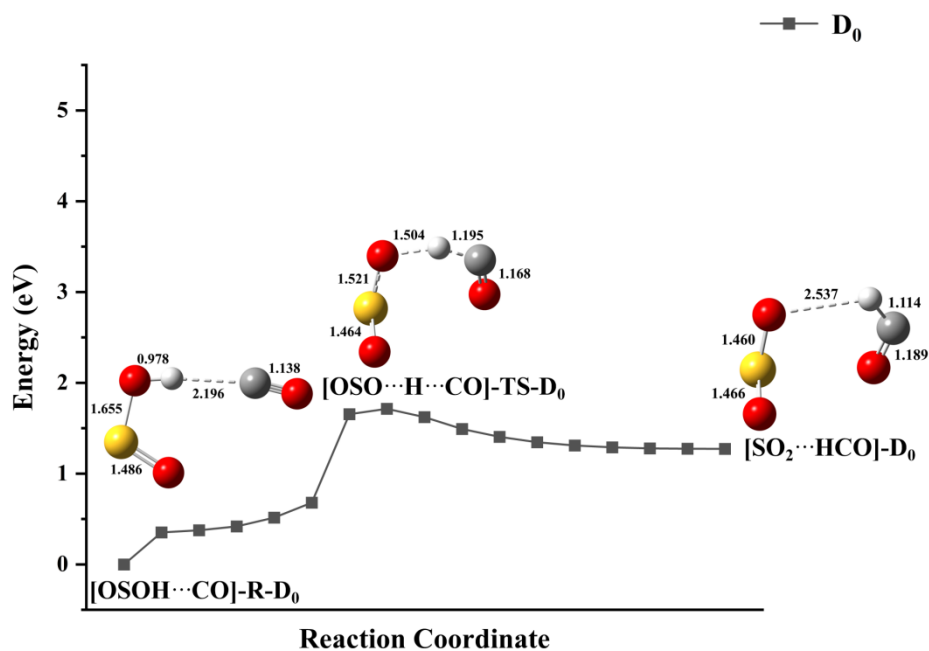


Figure S7. Energy plot from [OSOH...CO]-R-D₀ to [SO₂...HCO]-D₀ via [OSO...H...CO]-TS-D₀. Bond lengths are given in Å.

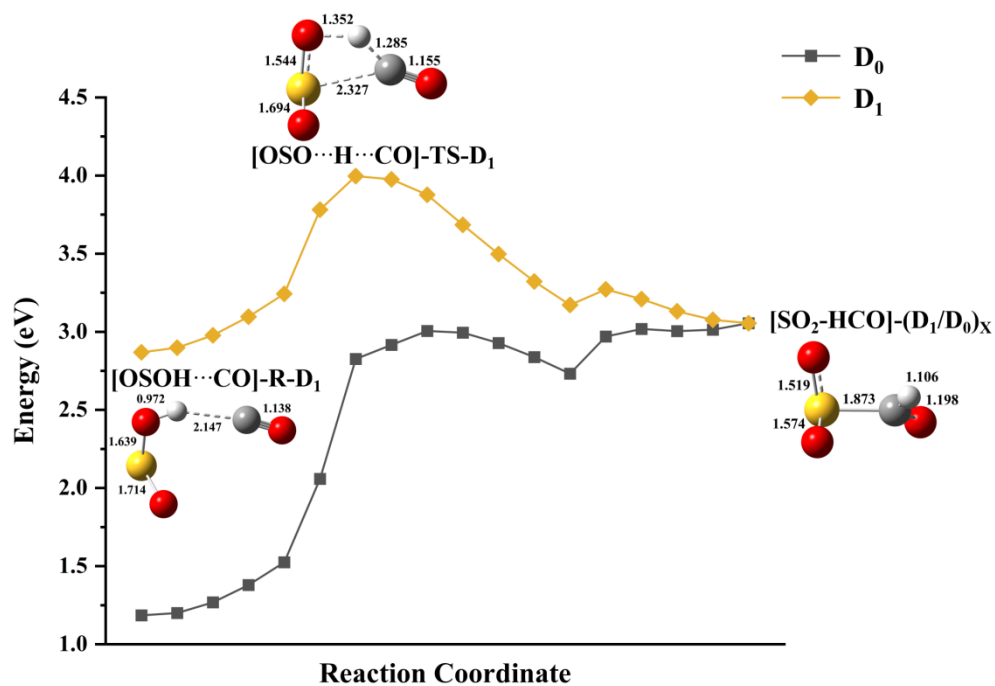


Figure S8. Energy plot from [OSOH...CO]-R-D₁ to [SO₂-HCO]-(D₁/D₀)_x via [OSO...H...CO]-TS-D₁. Bond lengths are given in Å.

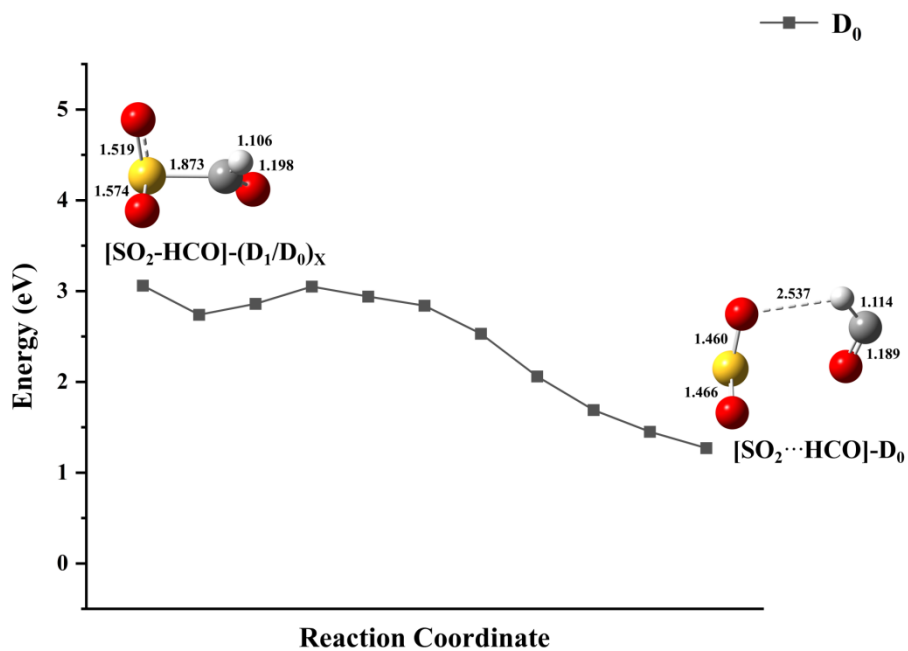


Figure S9. Energy plot from $[\text{SO}_2\text{-HCO}]-(\text{D}_1/\text{D}_0)_x$ to $[\text{SO}_2\cdots\text{HCO}]-\text{D}_0$. Bond lengths are given in Å.

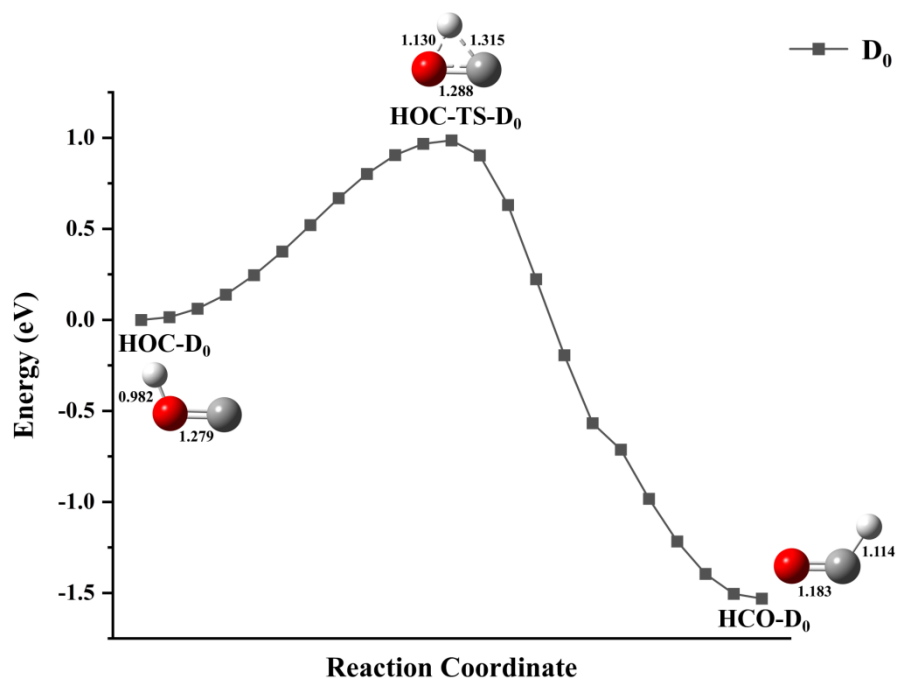


Figure S10. Energy plot from $\text{HOC}-\text{D}_0$ to $\text{HCO}-\text{D}_0$ via $\text{HOC-TS}-\text{D}_0$. Bond lengths are given in Å.

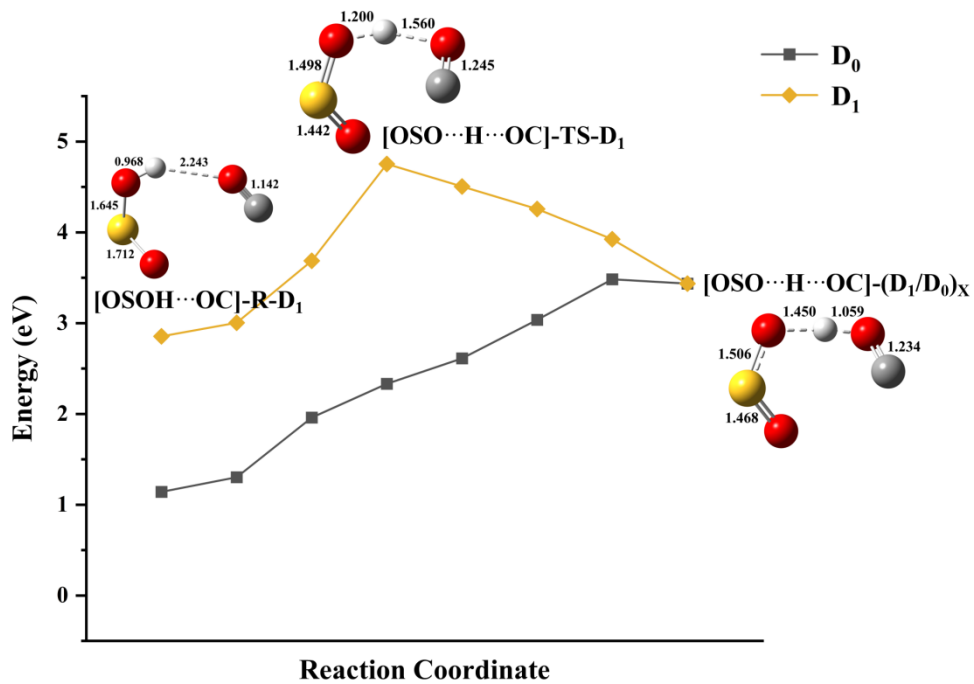


Figure S11. Energy plot from $[\text{OSOH}\cdots\text{OC}]\text{-R-D}_1$ to $[\text{OSO}\cdots\text{H}\cdots\text{OC}]\text{-(D}_1/\text{D}_0)_\text{X}$ via $[\text{OSO}\cdots\text{H}\cdots\text{OC}]\text{-TS-D}_1$. Bond lengths are given in Å.

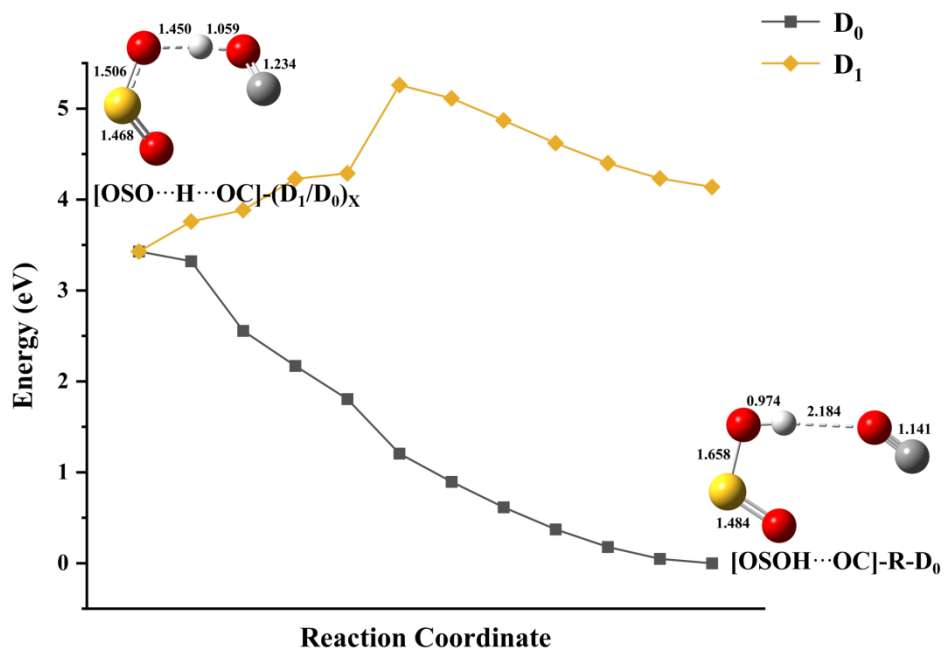


Figure S12. Energy plot from $[\text{OSO}\cdots\text{H}\cdots\text{OC}]\text{-(D}_1/\text{D}_0)_\text{X}$ to $[\text{OSOH}\cdots\text{OC}]\text{-R-D}_0$. Bond lengths are given in Å.

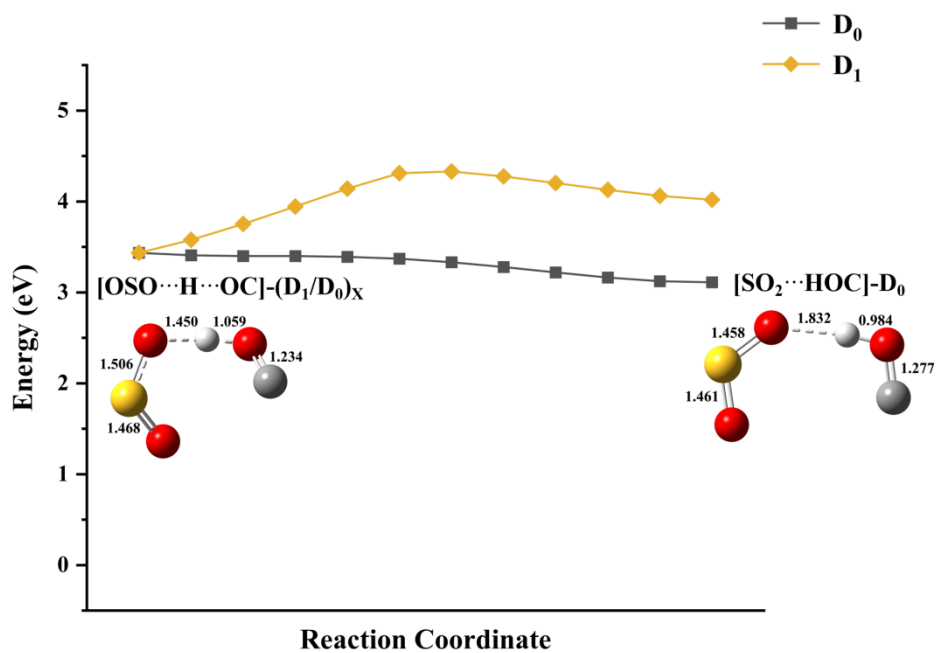


Figure S13. Energy plot from $[\text{OSO}\cdots\text{H}\cdots\text{OC}]-(\text{D}_1/\text{D}_0)_x$ to $[\text{SO}_2\cdots\text{HOC}]-\text{D}_0$. Bond lengths are given in Å.

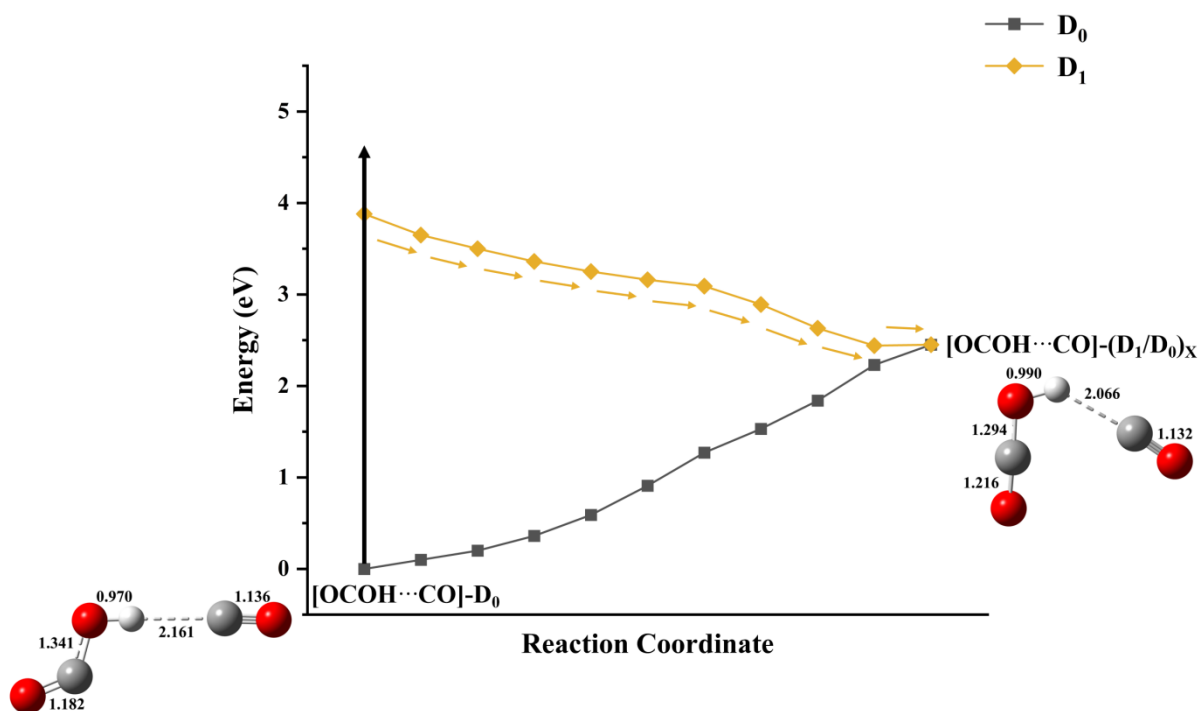


Figure S14. Energy plot from $[\text{OCOH}\cdots\text{CO}]-\text{D}_0$ to $[\text{OCOH}\cdots\text{CO}]-(\text{D}_1/\text{D}_0)_x$. Bond lengths are given in Å.

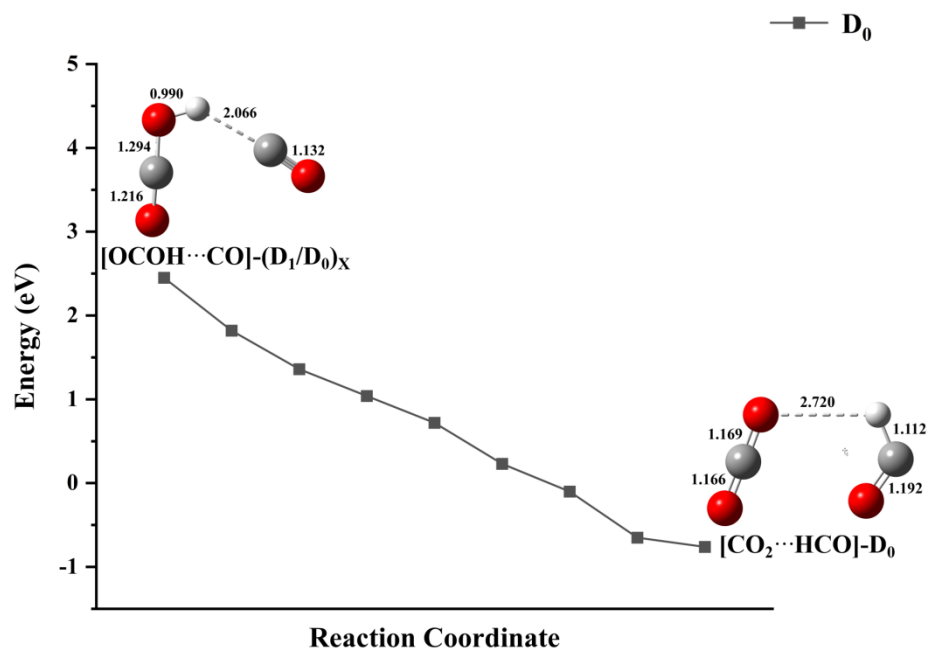


Figure S15. Energy plot from $[OCOH \cdots CO]-(D_1/D_0)_x$ to $[CO_2 \cdots HCO]-D_0$. Bond lengths are given in Å.

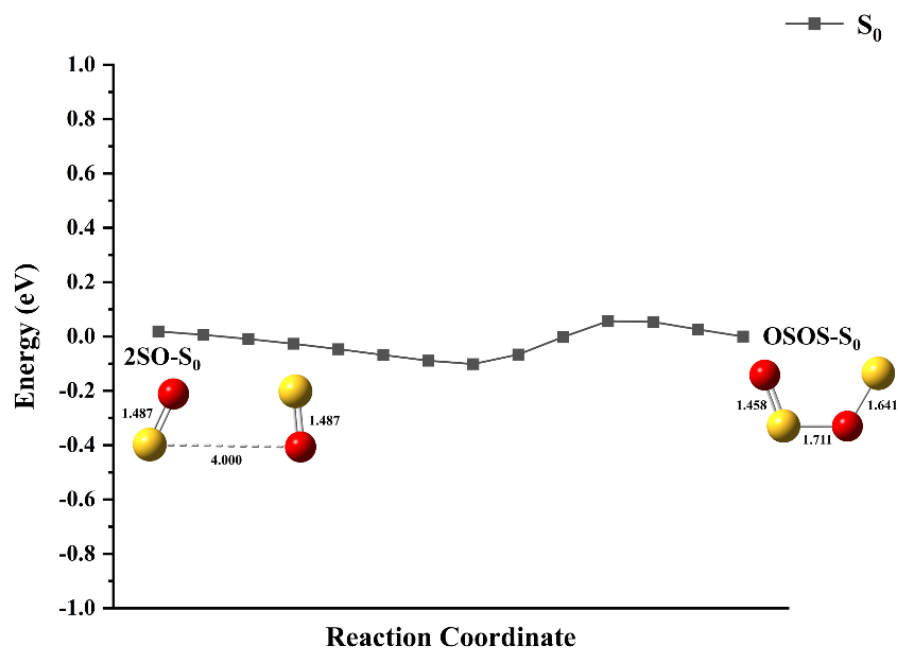


Figure S16. Energy plot from $2SO-S_0$ to $OSOS-S_0$. Bond lengths are given in Å.

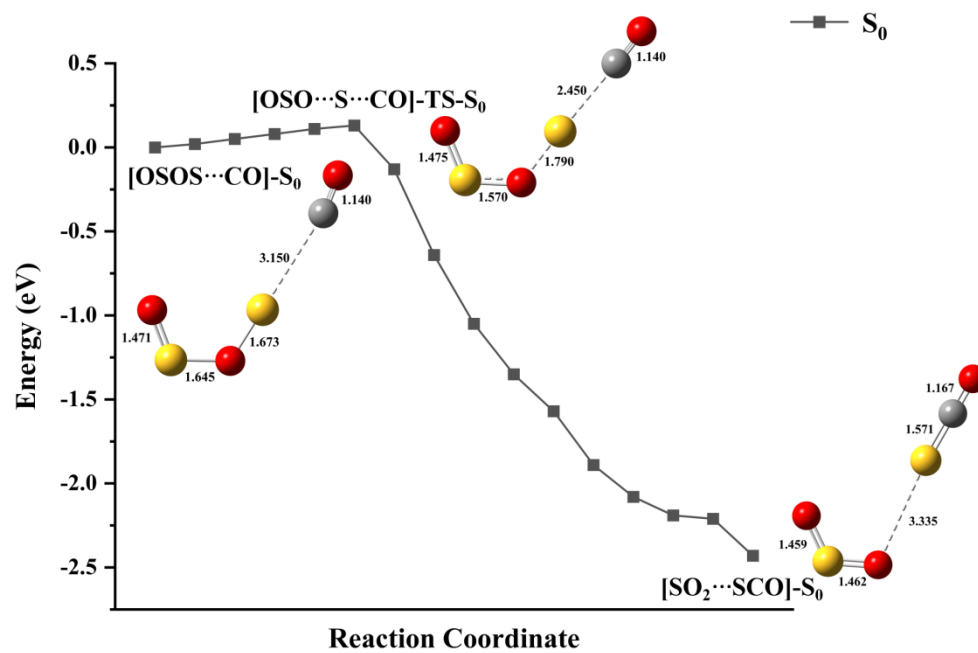


Figure S17. Energy plot from [OSOS...CO]-S₀ to [SO₂...SCO]-S₀ via [OSO...S...CO]-TS-S₀. Bond lengths are given in Å.

Cartesian coordinates of the optimized structures by MS-CASPT2 method

HOSO→HO+SO							
HOSO-D ₀				HOSO-(D ₃ /D ₂) _X			
S1	-0.131294	-0.476905	0.031254	S1	-0.094205	-0.621327	-0.090182
O2	1.318574	0.267414	-0.086701	O2	1.357964	0.300355	0.055880
H3	1.231710	1.159512	0.281844	H3	0.987600	1.199574	0.174212
O4	-1.183963	0.552467	-0.011230	O4	-1.064161	0.750214	0.084834
HOSO-D ₂				HOSO-(D ₂ /D ₁) _X			
S1	-0.191287	-0.648247	-0.064431	S1	-0.254080	-0.686441	-0.270337
O2	1.374704	0.279271	0.044790	O2	1.314594	0.401756	0.474980
H3	1.095367	1.205415	0.157032	H3	1.208417	1.199031	-0.076817
O4	-1.043758	0.666048	0.077776	O4	-1.033903	0.588142	0.087341
HOSO-D ₁				HO+SO			
S1	-0.054948	-0.545964	0.212595	S1	-0.832988	-0.424002	-0.042743
O2	1.173572	0.445079	-0.290819	O2	2.021201	0.554404	0.079189
H3	1.391816	1.017809	0.457698	H3	2.489049	1.400485	0.179793
O4	-1.275413	0.585564	-0.164308	O4	-2.331709	-0.456716	-0.051027
Path 1: HOSO+CO→HCO+SO ₂							
[OSOH⋯CO]-R-D ₀				[OSOH⋯CO]-R-D ₁			
O1	-0.775341	1.335034	0.180032	O1	-0.751487	1.117336	0.542012
S2	-1.638652	-0.075117	0.103479	S2	-1.206185	0.073752	-0.637099
O3	-0.717419	-1.236613	0.005046	O3	-1.023462	-1.327895	0.331902
C4	2.202675	0.265974	-0.010772	C4	2.121418	0.304060	-0.044361
O5	3.156715	-0.348772	-0.092111	O5	3.034142	-0.278050	-0.394722
H6	0.166905	1.077741	0.128036	H6	0.220456	1.129043	0.515978
[OSO⋯H⋯CO]-TS-D ₀				[OSO⋯H⋯CO]-TS-D ₁			
O1	-0.848536	1.101389	-0.006118	O1	-0.880004	1.125695	0.109112
S2	-1.580031	-0.172472	-0.399947	S2	-0.833558	-0.346234	-0.355337
O3	-1.718302	-1.188156	0.644995	O3	-0.737655	-1.107542	1.155071
C4	1.538926	0.247550	-0.303714	C4	1.366796	0.408733	-0.285011
O5	1.335376	-0.711919	-0.937914	O5	2.469416	0.134965	-0.494339
H6	0.635860	0.898588	0.129577	H6	0.466843	1.236979	0.110153

[SO ₂ -HCO]-(D ₁ /D ₀) _x				[SO ₂ ···HCO]-D ₀			
O1	-1.369282	0.889673	-0.250091	O1	-2.029851	1.207399	-0.220601
S2	-0.513966	-0.360558	-0.361553	S2	-2.527992	-0.135019	-0.469626
O3	-0.695924	-0.762672	1.149274	O3	-2.771514	-1.027852	0.668800
C4	1.182922	0.405772	-0.154070	C4	1.013542	0.236186	-0.379705
O5	2.139562	0.161154	-0.831623	O5	0.463059	-0.747250	-0.768670
H6	1.108526	1.119228	0.687710	H6	0.470503	1.122423	0.015707

Path 2: HOSO+OC→HOC+SO₂ (step 1)

[OSOH···OC]-R-D ₀				[OSOH···OC]-R-D ₁			
S1	-0.149058	-0.392401	-0.110840	S1	-0.167363	-0.063937	0.657914
O2	1.326997	0.305691	0.175893	O2	1.190379	0.323157	-0.185499
H3	1.161344	1.261727	0.257288	H3	1.416458	1.231422	0.059481
O4	-1.206522	0.648859	-0.130085	O4	-1.243181	0.640370	-0.473116
O5	0.598185	3.367971	0.388124	O5	0.623947	3.312539	0.326977
C6	-0.266398	4.111146	0.342750	C6	-0.355691	3.859440	0.537372

[OSO···H···OC]-TS-D ₁				[OSO···H···OC]-(D ₁ /D ₀) _x			
S1	-0.204754	0.131847	-0.395858	S1	-0.126263	-0.099941	-0.288256
O2	1.155154	0.722836	-0.186064	O2	1.197586	0.592106	-0.096195
H3	1.167864	1.722823	0.477159	H3	1.037985	1.943103	0.406840
O4	-1.281741	0.523932	0.479020	O4	-1.267636	0.562662	0.355482
O5	0.695764	3.189326	0.722292	O5	0.795336	2.955503	0.600853
C6	-0.164681	3.281290	-0.172288	C6	-0.172459	3.349560	-0.055595

[SO ₂ ···HOC]-D ₀			
S1	-0.072031	-0.237014	-0.083745
O2	0.958345	0.785226	0.053311
H3	1.032479	2.607387	0.222589
O4	-1.473991	0.173988	-0.111461
O5	0.932274	3.582796	0.307934
C6	-0.300332	3.914554	0.286067

Path 2: HOC→HCO (step 2)

HOC-D ₀				HOC-TS-D ₀			
H1	1.046852	2.603294	0.222824	H1	0.214849	2.675314	0.070262
O2	0.923388	3.574400	0.306786	O2	0.927100	3.523402	0.295418
C3	-0.305819	3.927043	0.286982	C3	-0.315195	3.861397	0.274121

HCO-D ₀			
H1	1.084884	2.594278	0.215986
O2	-0.256364	4.092463	0.381562
C3	0.843943	3.681208	0.243315

Path 3: HOCO+CO→HCO+CO₂

[OCOH…CO]-D ₀			[OCOH…CO]-(D ₁ /D ₀) _x				
O1	1.032747	0.560723	0.208955	O1	1.021549	0.089347	0.068004
H2	0.681515	0.970259	-0.597635	H2	1.334934	0.725961	-0.622198
O3	0.553427	0.907386	2.396098	O3	-1.102897	0.959721	1.054756
C4	0.403469	1.134193	1.245559	C4	-0.135044	0.486582	0.489915
C5	-0.138427	1.923588	-2.355319	C5	0.570988	2.450476	-1.464253
O6	-0.591365	2.447140	-3.255479	O6	0.084329	3.399141	-1.845087

[CO ₂ …HCO]-D ₀			
O1	0.651764	0.021212	0.385482
H2	1.702147	1.554583	-1.599946
O3	-1.351166	0.932443	1.168186
C4	-0.349793	0.486148	0.769894
C5	1.068287	2.443729	-1.811616
O6	0.052620	2.673112	-1.230863

Path 3: OSOS+CO→SO₂+SCO

[OSOS…CO]-S ₀			[OSO…S…CO]-TS-S ₀				
O1	0.456435	-0.566954	0.601705	O1	0.339878	-0.675844	0.559116
S2	0.782001	-0.322272	-0.812071	S2	0.906324	-0.533266	-0.795369
S3	2.345088	-2.731446	-0.449902	S3	2.513935	-2.943192	-0.106014
O4	1.799927	-1.470611	-1.405023	O4	1.976427	-1.615433	-1.179438
C5	3.424995	-5.062540	1.374374	C5	3.326117	-4.777660	1.300254
O6	3.828232	-5.709756	2.221876	O6	3.699227	-5.610683	1.984224

[SO ₂ …SCO]-S ₀			
O1	0.688231	-1.047753	0.542228
S2	0.911294	-0.571537	-0.821454
S3	2.560380	-3.730849	1.187200
O4	1.850180	-1.286397	-1.679198
C5	3.390256	-4.989272	1.627970
O6	4.006553	-5.924588	1.957093