Supporting Information

Phenylsulfinyl Radical: Gas-phase Generation, Photoisomerization, and Oxidation

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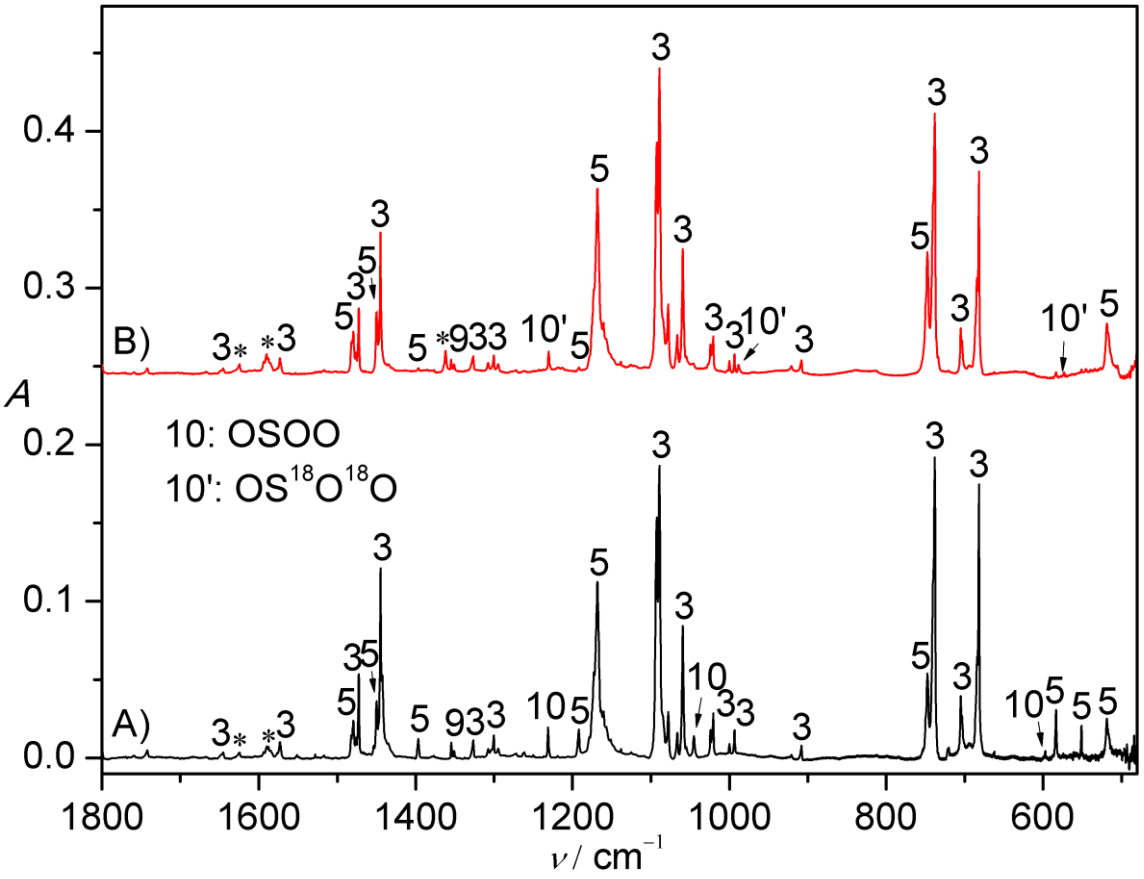


Figure S1. (A) IR spectrum of Ar-matrix isolated HVFP products of a mixture of PhS(O)Cl (**5**), O_2, and Ar (1:50:1000). (B) IR spectrum of Ar-matrix isolated HVFP products of a mixture of PhS(O)Cl (**5**), $^{18}O_2$ (97 atom %), and Ar (1:50:1000). The IR bands of PhSO• (**3**), SO_2 (**9**), and OSOO (**10**) are labeled.

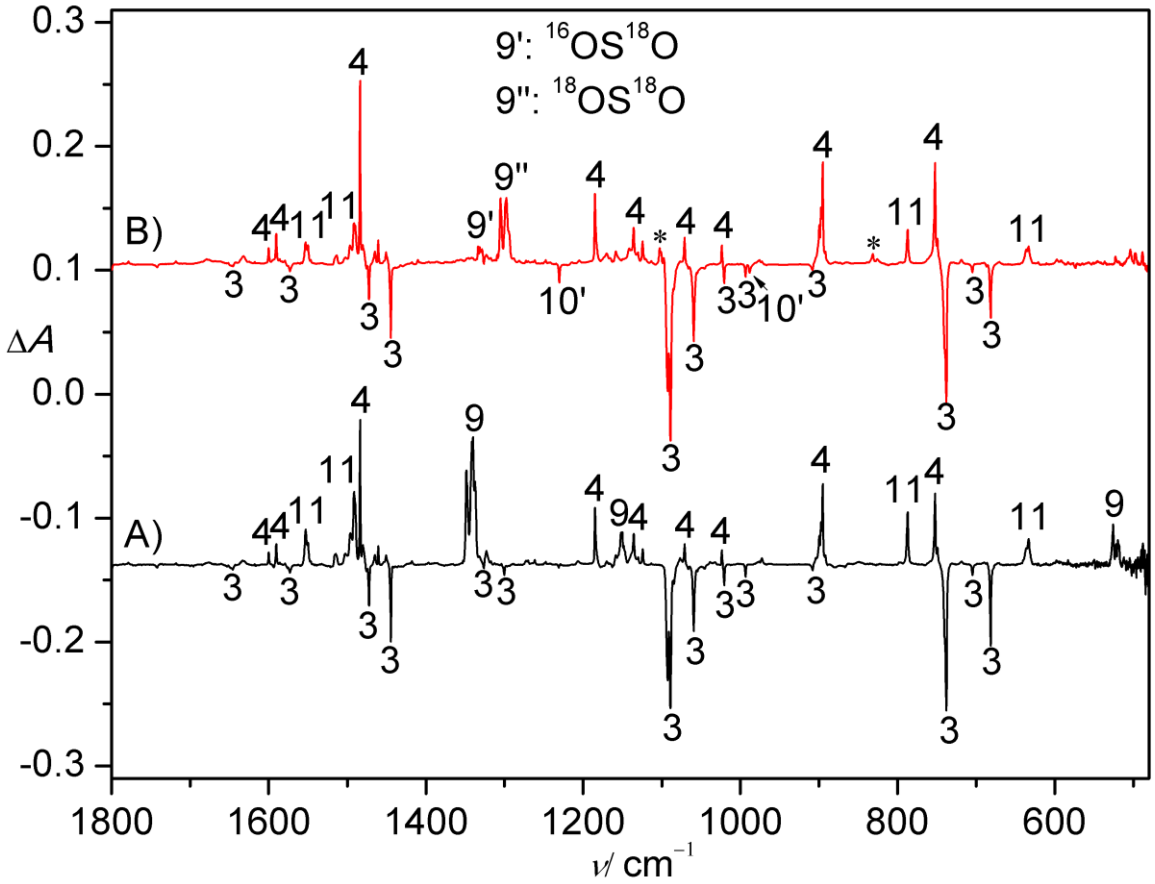


Figure S2. (A) IR difference spectrum reflecting the change of the Ar-matrix isolated HVFP products of a mixture of PhS(O)Cl (**5**), $^{18}O_2$ (97 atom %), and Ar (1:50:1000) upon 130 min UV light irradiation (365 nm). (B) IR difference spectrum reflecting the change of the Ar-matrix isolated HVFP products of a mixture of PhS(O)Cl (**5**) and $^{18}O_2$ (1:50) upon 130 min UV light irradiation (365 nm). IR bands of PhSO• (**3**), PhOS• (**4**), SO_2 (**9**), $OS^{18}O^{18}O$ (**10'**), and PhO• (**11**) are labeled.

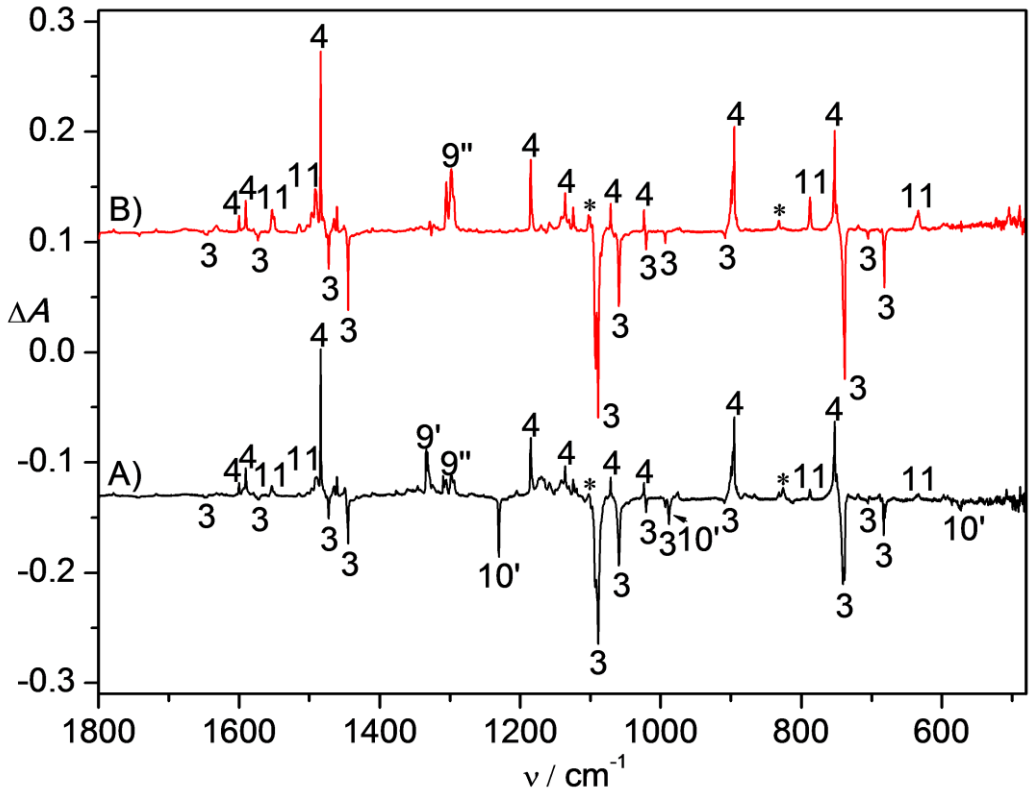


Figure S3. (A) IR difference spectrum reflecting the change of the Ar-matrix isolated HVFP products of a mixture of PhS(O)Cl (**5**), $^{18}O_2$ (97 atom %), and Ar (1:50:1000) upon 20min UV light irradiation (365 nm). (B) IR difference spectrum reflecting the change of the Ar-matrix isolated HVFP products of a mixture of PhS(O)Cl (**5**) and $^{18}O_2$ (1:50) upon further 30min UV light irradiation (365 nm). IR bands of PhSO• (**3**), PhOS• (**4**), SO_2 (**9**), $OS^{18}O^{18}O$ (**10'**), and PhO• (**11**) are labeled.

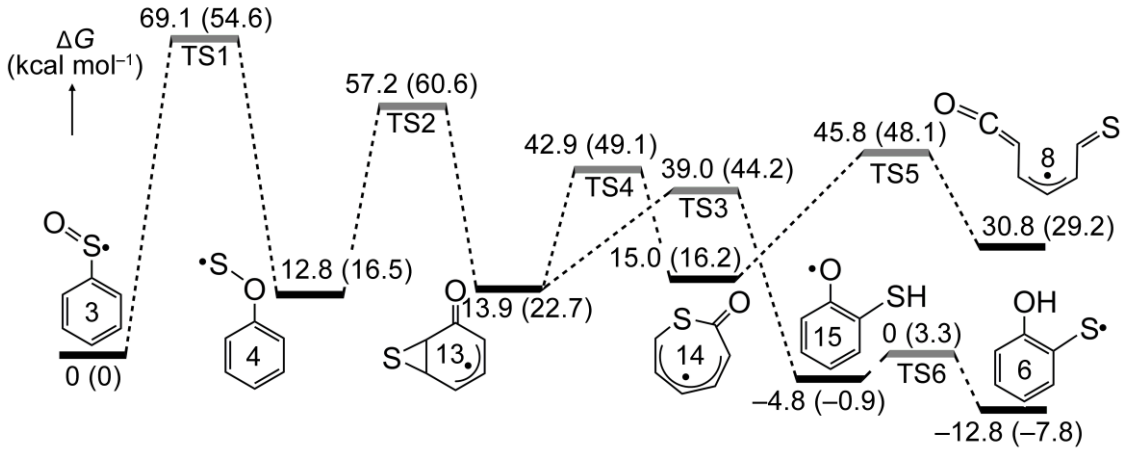


Figure S4. Computed potential energy profile for the isomerization of PhSO• (**3**) at the CCSD(T)/cc-pVTZ//B3LYP/def2-TZVPP and B3LYP/def2-TZVPP (in parentheses) levels.

Table S1. Computed vertical transitions for **3**, **4**, **6**, and **8** at TD-B3LYP/def2-TZVPP level.

PhSO• (**3**)		PhOS• (**4**)		*ortho*-HOPhS• (**6**)		thioketoketene (**8**)		thiirane (**13**)		seven-membered ring (**14**)	
energy (nm)	oscillator strength (*f*)	energy (nm)	oscillator strength (*f*)	energy (nm)	oscillator strength (*f*)	energy (nm)	oscillator strength (*f*)	energy (nm)	oscillator strength (*f*)	energy (nm)	oscillator strength (*f*)
521	0.0006	2097	0.0000	794	0.0000	1695	0.0001	759	0.0001	599	0.0023
395	0.0179	522	0.0775	703	0.0197	570	0.0127	589	0.0010	477	0.0293
377	0.0086	500	0.0131	352	0.0282	529	0.0015	408	0.0044	432	0.0001
311	0.0554	344	0.0000	333	0.0061	419	0.0000	329	0.0406	363	0.0022
295	0.0432	315	0.0109	313	0.0612	385	0.3037	324	0.0018	328	0.0000
277	0.0756	283	0.0001	288	0.0233	375	0.0281	309	0.0103	311	0.0081
265	0.0002	278	0.0035	281	0.0004	364	0.0318	298	0.0027	300	0.0000
240	0.0032	267	0.0098	258	0.0550	354	0.0868	289	0.0114	264	0.0007
236	0.0226	264	0.0091	252	0.0000	344	0.0083	287	0.0117	261	0.0009
234	0.0003	263	0.0007	244	0.0000	338	0.0116	283	0.0409	257	0.0556
			EOM-CCSD/aug-cc-pV(D+d)Z								
479	0.0015	2244	0.0000	1229	0.0000	1242	0.0000				
343	0.0927	408	0.0010	509	0.1053	494	0.0000				
299	0.0121	335	0.0001	384	0.0704	426	0.0077				
277	0.0016	316	0.0247	292	0.0361	335	0.4342				
269	0.0012	301	0.0067	281	0.0331	295	0.0019				

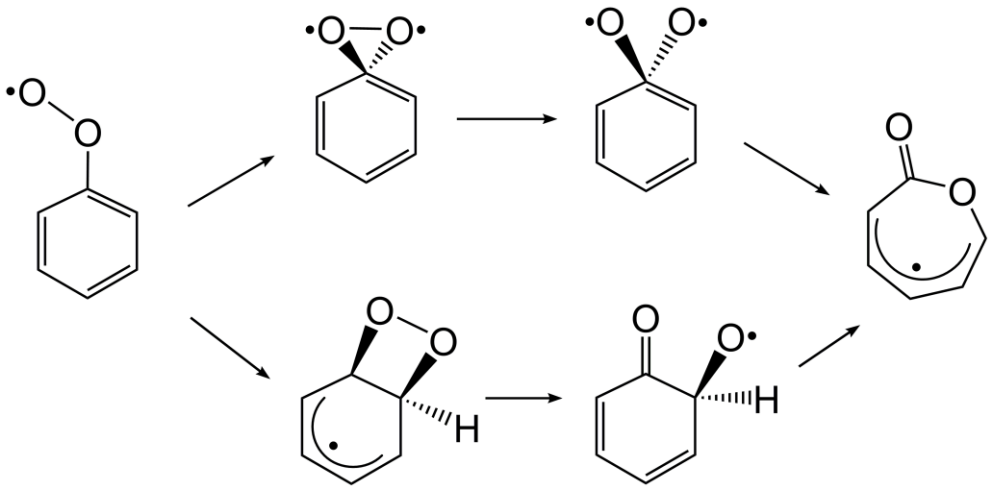
Table S2. Computed IR frequencies (cm^{-1}) and intensity (km mol^{-1}, in parentheses) of **3**, **4**, and **6** at the UB3LYP/def2-TZVPP and UCCSD(T)/aug-cc-pV(D+d)Z levels.

PhSO• (**3**)			PhOS• (**4**)			*ortho*-HOPhS• (**6**)		
UB3LYP	UCCS	Assignment	UB3LYP	UCCS	Assignment	UB3LYP	UCCSD(T)	Assignment
3203 (9)	3202.8	ν(CH)	3213 (2)	3216.1	ν(CH)	3487 (56)	3557	ν(OH)
3197 (9)	3191.7	ν(CH)	3205 (6)	3202.9	ν(CH)	3206 (7)	3219	ν(CH)
3186 (12)	3184.6	ν(CH)	3197 (13)	3194.6	ν(CH)	3202 (6)	3214	ν(CH)
3176 (<1)	3176.5	ν(CH)	3184 (10)	3181.3	ν(CH)	3191 (4)	3200	ν(CH)
3166 (1)	3162.7	ν(CH)	3175 (<1)	3171.9	ν(CH)	3178 (2)	3188	ν(CH)
1616 (<1)	1599.8	ν(CC)	1634 (4)	1623.4	ν(CC)	1621 (55)	1633	ν(CC)
1610 (1)	1595.0	ν(CC)	1625 (3)	1611.3	ν(CC)	1583 (37)	1595	ν(CC)
1508 (5)	1462.6	ρ(CH)	1516 (30)	1476.0	ρ(CH)	1484 (139)	1486	ν(CC) + ρ(CH)
1477 (10)	1431.7	ρ(CH)	1493 (4)	1448.2	ρ(CH)	1477 (46)	1473	ν(CO) + ρ(CH)
1354 (2)	1333.4	ρ(CH)	1351 (<1)	1337.0	ρ(CH)	1386 (45)	1389	ρ(OH) + ρ(CH)
1325 (1)	1296.7	ν(CC) + ρ(CH)	1333 (<1)	1298.6	ν(CC) + ρ(CH)	1341 (43)	1338	ν(CO) + ρ(CH)
1201 (<1)	1178.1	ρ(CH)	1207 (12)	1184.7	ρ(CH)	1270 (59)	1279	ν(CC) + ρ(CH)
1184 (<1)	1162.2	ρ(CH)	1182 (<1)	1153.7	ρ(CH)	1213 (83)	1205	ρ(OH) + ρ(CH)
1104 (3)	1136.9	ρ(CH)	1147 (10)	1142.0	ν(CO) + ρ(CH)	1185 (3)	1162	ρ(CH)
1097 (64)	1082.8	ν_{as}(CSO)	1101 (8)	1078.9	ρ(CH)	1142 (11)	1125	ρ(CH)
1069 (13)	1070.5	ν_{s}(CSO)	1044 (5)	1024.3	ρ(CH)	1085 (8)	1062	ν(CS) + ring distortion
1044 (4)	1021.8	ν(CS) + ring distortion	1021 (<1)	987.2	Ring distortion	1038 (6)	1027	Ring breathing
1023 (<1)	975.8	ω(CH)	1010 (<1)	921.9	ω(CH)	997 (<1)	938	ω(CH)
1014 (1)	937.1	ω(CH)	994 (<1)	903.4	ω(CH)	978 (2)	931	ω(CH)
1000 (<1)	914.0	ω(CH)	940 (6)	876.5	ω(CH)	878 (2)	842	ω(CH)
945 (2)	883.1	ω(CH)	906 (29)	861.0	ν_{as}(COS)	851 (5)	833	ν(CO) +
865 (<1)	832.4	ω(CH)	849 (<1)	811.1	ω(CH)	774 (47)	755	ω(CH)
767 (47)	720.3	ω(CH)	780 (56)	737.0	ω(CH)	752 (8)	694	Ring breath
711 (1)	690.7	ν(CS) + ring distortion	760 (6)	730.9	ν_{s}(COS)	707 (7)	661	ν(CS) + ring distortion

707 (32)	604.5	Ring breathing	703 (26)	600.4	ω(CH)	678 (72)	626	ω(CH)
628 (<1)	560.2	Ring distortion	627 (<1)	583.0	Ring distortion	560 (6)	547	Ring distortion
475 (23)	460.7	δ(CSO)	555 (3)	540.4	δ(COS)	524 (5)	503	δ(CCO)
466 (6)	430.9	Ring breathing	505 (7)	470.6	Ring breathing	512 (4)	495	Ring breathing
409 (<1)	388.5	Ring breathing	423 (<1)	396.3	Ring breathing	455 (2)	429	Ring breathing
343 (<1)	340.1		382 (<1)	370.2		389 (5)	376	
180 (5)	185.1		230 (<1)	213.4		275 (4)	263	
175 (1)	174.8		205 (<1)	209.8		254 (<1)	246	
91 (3)	90.2		45 (<1)	39.2		140 (<1)	141	

Table S3. Computed IR frequencies (cm^{-1}) and intensity (km mol^{-1}, in parentheses) of thioketoketene (**8**) and 2-thiepinoxy (**12**) at the UB3LYP/def2-TZVPP level.

thioketoketene (**8**)	2-thiepinoxy (**12**)
3195 (11)	3487 (56)
3171 (11)	3206 (7)
3159 (5)	3202(6)
3145 (3)	3191 (4)
3125 (10)	3178 (2)
2198 (1880)	1621 (55)
1575 (210)	1583 (37)
1494 (5)	1484 (139)
1454 (57)	1477 (46)
1346 (12)	1386 (45)
1315 (47)	1341 (43)
1287 (17)	1270 (59)
1255 (10)	1213 (83)
1145 (8)	1185 (3)
1103 (12)	1142 (11)
1008 (9)	1085 (8)
990 (15)	1038 (6)
948 (2)	997 (<1)
928 (9)	978 (2)
890 (15)	878 (2)
766 (32)	851 (5)
708 (5)	774 (47)
681 (33)	752 (8)
625 (26)	707 (7)
520 (9)	678 (72)
440 (4)	560 (6)
388 (<1)	524 (5)
267 (<1)	512 (4)
198 (<1)	455 (2)
153 (<1)	389 (5)
146 (1)	275 (4)
93 (1)	254 (<1)
56 (3)	140 (<1)



Scheme S1. Generation of 2-oxepinoxy radical. See reference: Fadden, M. J.; Hadad, C. M. *J. Phys. Chem. A* **2000**, *104*, 8121.

Computed atomic coordinates (in Angstroms) and energies (in Hartrees) for all optimized radicals.

PhSO• (**3**)
UB3LYP/def2-TZVPP

C	-1.69062600	1.33544100	-0.00001900
C	-0.31941600	1.12556000	-0.00002600
C	0.17043200	-0.18129300	0.00002700
C	-0.70553200	-1.27143400	0.00001700
C	-2.07423600	-1.04782400	-0.00000700
C	-2.56911300	0.25415800	-0.00000200
H	-2.07747400	2.34589700	-0.00002700
H	0.37865200	1.95119200	-0.00003100
H	-0.31652400	-2.28244200	0.00003600
H	-2.75609200	-1.88768100	-0.00000400
H	-3.63711000	0.42546100	-0.00000500
S	1.90387700	-0.51218400	0.00004400
O	2.63468300	0.79436000	-0.00007600

Zero-point correction=	0.094128
Thermal correction to Energy=	0.100912
Thermal correction to Enthalpy=	0.101856
Thermal correction to Gibbs Free Energy=	0.061751
Sum of electronic and zero-point Energies=	-705.087411
Sum of electronic and thermal Energies=	-705.080626
Sum of electronic and thermal Enthalpies=	-705.079682
Sum of electronic and thermal Free Energies=	-705.119787

UCCSD(T)/aug-cc-pV(D+d)Z ENERGY=-703.75070424

S	-0.0303667972	0.0000000000	0.0083009352
O	0.0058254396	0.0000000000	1.5355958398
C	1.6582618766	0.0000000000	-0.5576125737
C	1.8928178410	0.0000000000	-1.9548254754
C	2.7295074863	0.0000000000	0.3649385605
C	3.2191988667	0.0000000000	-2.4308764415
H	1.0484813261	0.0000000000	-2.6566474450
C	4.0515114758	0.0000000000	-0.1242821614
H	2.5107029561	0.0000000000	1.4387514541
C	4.2981728507	0.0000000000	-1.5168905742
H	3.4119351753	0.0000000000	-3.5100105984
H	4.8913177644	0.0000000000	0.5805063268
H	5.3291037385	0.0000000000	-1.8896048467

PhOS• (**4**)
UB3LYP/def2-TZVPP

C	-2.23368000	-0.95050300	-0.00011900
C	-0.89128200	-1.30137000	-0.00003700
C	0.07344900	-0.29782000	0.00003400
C	-0.28056000	1.04476700	0.00006700
C	-1.62924100	1.37882800	-0.00001500

C	-2.60783200	0.38975100	-0.00012000
H	-2.98742000	-1.72639000	-0.00019400
H	-0.57525900	-2.33507600	-0.00002500
H	0.48685700	1.80427900	0.00015400
H	-1.91517100	2.42228700	0.00000800
H	-3.65442400	0.66185500	-0.00018700
S	2.68727200	0.22901100	0.00000200
O	1.38299300	-0.75913200	0.00017000

Zero-point correction= 0.094638
Thermal correction to Energy= 0.101255
Thermal correction to Enthalpy= 0.102199
Thermal correction to Gibbs Free Energy= 0.061973
Sum of electronic and zero-point Energies= -705.060874
Sum of electronic and thermal Energies= -705.054256
Sum of electronic and thermal Enthalpies= -705.053312
Sum of electronic and thermal Free Energies= -705.093539

UCCSD(T)/aug-cc-pV(D+d)Z ENERGY=-703.72880649

O	0.2958386754	0.0000000000	-0.1468879043
S	-0.1450144436	0.0000000000	1.4636699793
C	1.6583966839	0.0000000000	-0.5188761072
C	1.8652197437	0.0000000000	-1.9136322664
C	2.7315934834	0.0000000000	0.3908984876
C	3.1847566897	0.0000000000	-2.4087596258
H	0.9982001802	0.0000000000	-2.5832126917
C	4.0469174113	0.0000000000	-0.1251546043
H	2.5471152319	0.0000000000	1.4687584668
C	4.2806380069	0.0000000000	-1.5169528209
H	3.3542525243	0.0000000000	-3.4918206921
H	4.8924940547	0.0000000000	0.5727931463
H	5.3060617581	0.0000000000	-1.9034803671

ortho-HOPhS• (**6**)
UB3LYP/def2-TZVPP

C	-2.31334600	0.04915700	0.00008500
C	-1.46552900	1.14094500	0.00001300
C	-0.08555500	0.94147100	-0.00003300
C	0.45818300	-0.38634500	-0.00000600
C	-0.45195500	-1.47445300	0.00007100
C	-1.80896300	-1.26425500	0.00011400
H	-3.38334400	0.21025400	0.00012000
H	-1.84695000	2.15235100	-0.00001000
H	-0.04297700	-2.47514000	0.00009300
H	-2.49059500	-2.10343100	0.00017200
O	0.72216600	2.00319300	-0.00010800
S	2.14686500	-0.59425100	-0.00005200
H	1.63968100	1.65931700	-0.00013400

Zero-point correction= 0.095258

Thermal correction to Energy=	0.101643
Thermal correction to Enthalpy=	0.102587
Thermal correction to Gibbs Free Energy=	0.063661
Sum of electronic and zero-point Energies=	-705.100554
Sum of electronic and thermal Energies=	-705.094169
Sum of electronic and thermal Enthalpies=	-705.093225
Sum of electronic and thermal Free Energies=	-705.132151

UCCSD(T)/ aug-cc-pV(D+d)Z ENERGY=-703.69648567

C	2.1220400643	-0.0042343003	-0.0000120599
C	1.2032420744	1.0540597180	0.0000629485
C	-0.1841826415	0.7793955084	0.0001092136
C	-0.6545683141	-0.5840436975	0.0000792246
C	0.3177289753	-1.6412450024	0.0000016900
C	1.6829794125	-1.3596987450	-0.0000434417
H	3.1969375580	0.2187666335	-0.0000474184
H	1.5311440626	2.1000659852	0.0000873562
H	-0.0486006246	-2.6751329747	-0.0000209375
H	2.4167645513	-2.1746752623	-0.0001028832
O	-1.0465087663	1.8136591881	0.0001810474
S	-2.3535067509	-0.8882988749	0.0001328735
H	-1.9376046009	1.3988278238	0.0002013869

thioketokene (**8**)
UB3LYP/def2-TZVPP

C	-1.25225100	1.08551700	-0.05320600
C	0.02637600	1.68618600	0.01924200
C	1.28901100	1.14430800	0.03910400
C	-1.60909700	-0.24908900	0.13648900
C	1.66894300	-0.22688100	-0.12382000
C	2.93073500	-0.63227500	-0.03562700
H	-2.07882500	1.76072200	-0.24492100
H	0.00967500	2.76990600	0.03994400
H	2.10726400	1.84450400	0.15475100
H	0.95990700	-1.00639300	-0.36617600
H	-0.84009400	-0.95298700	0.43799700
O	4.02177400	-0.99785800	0.04578600
S	-3.16590100	-0.82996800	-0.01756100

Zero-point correction=	0.090612
Thermal correction to Energy=	0.098927
Thermal correction to Enthalpy=	0.099872
Thermal correction to Gibbs Free Energy=	0.055482
Sum of electronic and zero-point Energies=	-705.038195
Sum of electronic and thermal Energies=	-705.029880
Sum of electronic and thermal Enthalpies=	-705.028935
Sum of electronic and thermal Free Energies=	-705.073325

2-thiepinoxy (**12**)
UB3LYP/def2-TZVPP

C	0.03517900	-2.09427900	0.00000000
C	1.37572500	-1.65727100	0.00000000
C	1.91510100	-0.36105800	0.00000000
C	-1.13265100	-1.38468100	0.00000000
C	1.36611400	0.90296500	0.00000000
C	0.00000000	1.38685100	0.00000000
H	-0.09642400	-3.17288600	0.00000000
H	2.11268800	-2.45315900	0.00000000
H	3.00227100	-0.34984500	0.00000000
H	-2.06362100	-1.94402400	0.00000000
H	2.05494800	1.74177300	0.00000000
S	-1.50256900	0.30944100	0.00000000
O	-0.29069600	2.55899000	0.00000000

Zero-point correction=	0.092410
Thermal correction to Energy=	0.099469
Thermal correction to Enthalpy=	0.100413
Thermal correction to Gibbs Free Energy=	0.059735
Sum of electronic and zero-point Energies=	-705.061255
Sum of electronic and thermal Energies=	-705.054196
Sum of electronic and thermal Enthalpies=	-705.053252
Sum of electronic and thermal Free Energies=	-705.093930

thiirane (**13**)
UB3LYP/def2-TZVPP

C	0.65606900	1.82360800	-0.27404600
C	1.51729100	0.74454800	-0.40756000
C	1.18692900	-0.57634700	0.10322800
C	-0.20487300	-0.77196000	0.63851600
C	-1.10007000	0.40993200	0.74270600
C	-0.59730300	1.70052600	0.29893100
H	0.97565400	2.79716400	-0.62425800
H	2.49957400	0.85951500	-0.84461500
H	-0.27931900	-1.54949000	1.38786200
H	-1.84262900	0.41172800	1.52947200
H	-1.23610500	2.56576200	0.41062600
S	-1.55383800	-0.82210400	-0.60121800
O	1.99949700	-1.48910700	0.14371800

Zero-point correction=	0.093167
Thermal correction to Energy=	0.099737
Thermal correction to Enthalpy=	0.100681
Thermal correction to Gibbs Free Energy=	0.061408
Sum of electronic and zero-point Energies=	-705.051881
Sum of electronic and thermal Energies=	-705.045311
Sum of electronic and thermal Enthalpies=	-705.044366
Sum of electronic and thermal Free Energies=	-705.083639

2-thiolphenoxy (**14**)
UB3LYP/def2-TZVPP

C	-2.34551700	-0.01539700	-0.00004400
C	-1.56111300	1.09939200	-0.00005400
C	-0.11694400	1.00625500	-0.00013200
C	0.45345700	-0.35453000	0.00004000
C	-0.38608900	-1.46578900	0.00007400
C	-1.76097800	-1.30492200	0.00000100
H	-3.42364000	0.07693200	-0.00002700
H	-1.97887700	2.09674600	-0.00000500
H	0.03864500	-2.46105000	0.00013900
H	-2.39834300	-2.17882000	0.00003200
O	0.61208500	2.01370700	0.00017900
S	2.17505900	-0.51600300	-0.00000800
H	2.36769000	0.82252500	-0.00075600

Zero-point correction= 0.091284
Thermal correction to Energy= 0.097995
Thermal correction to Enthalpy= 0.098939
Thermal correction to Gibbs Free Energy= 0.059427
Sum of electronic and zero-point Energies= -705.089385
Sum of electronic and thermal Energies= -705.082674
Sum of electronic and thermal Enthalpies= -705.081730
Sum of electronic and thermal Free Energies= -705.121242

TS1
UB3LYP/def2-TZVPP

C	-1.75343100	1.21515600	-0.02256500
C	-0.37914700	1.23169000	-0.07895600
C	0.34146500	-0.00000100	-0.10845300
C	-0.37914800	-1.23169100	-0.07895800
C	-1.75343300	-1.21515500	-0.02256600
C	-2.45057400	0.00000100	0.00455600
H	-2.29892600	2.14908700	-0.00283800
H	0.17941800	2.15567000	-0.09853900
H	0.17941500	-2.15567200	-0.09854300
H	-2.29892900	-2.14908400	-0.00284000
H	-3.53101700	0.00000200	0.04907600
S	2.08004900	0.00000200	-0.45135700
O	1.59185900	-0.00000300	1.15213100

Zero-point correction= 0.091472
Thermal correction to Energy= 0.097913
Thermal correction to Enthalpy= 0.098857
Thermal correction to Gibbs Free Energy= 0.059807
Sum of electronic and zero-point Energies= -705.001105
Sum of electronic and thermal Energies= -704.994664
Sum of electronic and thermal Enthalpies= -704.993720
Sum of electronic and thermal Free Energies= -705.032770

TS2
UB3LYP/def2-TZVPP

H	0.67158500	-0.87798800	1.41585800
C	0.18689200	-0.65307100	0.46584500
C	0.06774900	0.76342900	0.23511000
C	-1.19034900	1.37127200	0.06893300
C	-2.24532600	0.52664900	-0.19887100
C	-0.92665400	-1.48808000	0.12080600
C	-2.11023500	-0.89103300	-0.21123500
H	-1.27883200	2.44573800	-0.00306900
H	-3.20664100	0.95492800	-0.45233800
H	-0.84465500	-2.56352500	0.20059600
H	-2.97634400	-1.49492500	-0.44459900
O	1.21475000	1.31226600	0.05590800
S	2.20152700	-0.42108500	-0.25295200

Zero-point correction= 0.091879
Thermal correction to Energy= 0.097983
Thermal correction to Enthalpy= 0.098927
Thermal correction to Gibbs Free Energy= 0.060659
Sum of electronic and zero-point Energies= -704.989709
Sum of electronic and thermal Energies= -704.983605
Sum of electronic and thermal Enthalpies= -704.982661
Sum of electronic and thermal Free Energies= -705.020929

TS3
UB3LYP/def2-TZVPP

H	1.26884700	-0.30198600	1.09563200
C	0.49368400	-0.29671200	0.08466200
C	-0.17444600	1.05278900	0.02558100
C	-1.63202900	1.03504200	-0.05605500
C	-2.33452300	-0.12230600	-0.06794200
C	-0.31726400	-1.47680700	0.07288800
C	-1.67545800	-1.39142800	-0.00342900
H	-2.11466000	2.00181100	-0.09998400
H	-3.41528000	-0.09961400	-0.12621900
H	0.17875800	-2.43690800	0.10869200
H	-2.26799700	-2.29601300	-0.02721800
O	0.46471300	2.09643600	0.05542000
S	2.27955300	-0.40264100	-0.10803100

Zero-point correction= 0.087876
Thermal correction to Energy= 0.094589
Thermal correction to Enthalpy= 0.095533
Thermal correction to Gibbs Free Energy= 0.055678
Sum of electronic and zero-point Energies= -705.017096
Sum of electronic and thermal Energies= -705.010383
Sum of electronic and thermal Enthalpies= -705.009439
Sum of electronic and thermal Free Energies= -705.049294

TS4
UB3LYP/def2-TZVPP

H	0.81920100	-1.41316800	1.46734100
C	0.27613000	-1.02005400	0.61524700
C	0.69692100	0.73360100	0.23980400
C	-0.45818900	1.43564500	-0.33519200
C	-1.69256000	0.91380800	-0.47068700
C	-1.15175900	-1.21112500	0.61335600
C	-2.04825800	-0.38582900	0.02296400
H	-0.25949400	2.47232500	-0.57599900
H	-2.47736400	1.53585400	-0.88063100
H	-1.50813400	-2.05518300	1.19473000
H	-3.09605100	-0.65565500	0.03392000
O	1.54119600	1.25701100	0.95927300
S	1.27866000	-0.79603400	-0.81415600

Zero-point correction= 0.090306
Thermal correction to Energy= 0.096985
Thermal correction to Enthalpy= 0.097929
Thermal correction to Gibbs Free Energy= 0.058621
Sum of electronic and zero-point Energies= -705.009871
Sum of electronic and thermal Energies= -705.003192
Sum of electronic and thermal Enthalpies= -705.002248
Sum of electronic and thermal Free Energies= -705.041556

TS5
UB3LYP/def2-TZVPP

C	-1.42867400	-1.24430200	0.07884200
C	-1.96116100	-0.19069700	-0.52934500
O	-1.02893900	-2.20116800	0.59454700
C	-1.64916900	1.20033200	-0.42442600
C	-0.57130700	1.87536900	0.16938200
C	0.63025500	1.44140700	0.66791900
C	1.22404800	0.09741500	0.63436500
H	-2.81081400	-0.47581900	-1.14204300
H	-2.40154800	1.83485200	-0.87229500
H	-0.71292200	2.94943000	0.21822500
H	1.28368200	2.19307600	1.10168000
H	1.07327400	-0.53062800	1.51559800
S	2.14599300	-0.46491900	-0.57237300

Zero-point correction= 0.088172
Thermal correction to Energy= 0.096091
Thermal correction to Enthalpy= 0.097035
Thermal correction to Gibbs Free Energy= 0.053731
Sum of electronic and zero-point Energies= -705.008732
Sum of electronic and thermal Energies= -705.000813
Sum of electronic and thermal Enthalpies= -704.999868
Sum of electronic and thermal Free Energies= -705.043173

TS6

UB3LYP/def2-TZVPP

C	2.31750800	0.15818100	-0.00005700
C	1.44097600	1.20665800	-0.00001100
C	0.03934200	0.95185000	0.00001400
C	-0.41748600	-0.44921400	-0.00003000
C	0.52437900	-1.48991400	-0.00010500
C	1.86592000	-1.19026000	-0.00009900
H	3.38239700	0.35098100	-0.00010900
H	1.77582300	2.23421500	-0.00000800
H	0.18828800	-2.51741900	-0.00017400
H	2.59485400	-1.98919000	-0.00010800
O	-0.85195400	1.85218800	0.00000000
S	-2.11398800	-0.56167900	0.00010800
H	-1.92575000	0.96696100	0.00039500

Zero-point correction=	0.089600
Thermal correction to Energy=	0.095660
Thermal correction to Enthalpy=	0.096604
Thermal correction to Gibbs Free Energy=	0.058299
Sum of electronic and zero-point Energies=	-705.083153
Sum of electronic and thermal Energies=	-705.077093
Sum of electronic and thermal Enthalpies=	-705.076149
Sum of electronic and thermal Free Energies=	-705.114454