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

Supporting Information

Generation and Characterization of the Phenylthiyl Radical and its Oxidation to the Phenylthiylperoxy and Phenylsulfonyl Radical

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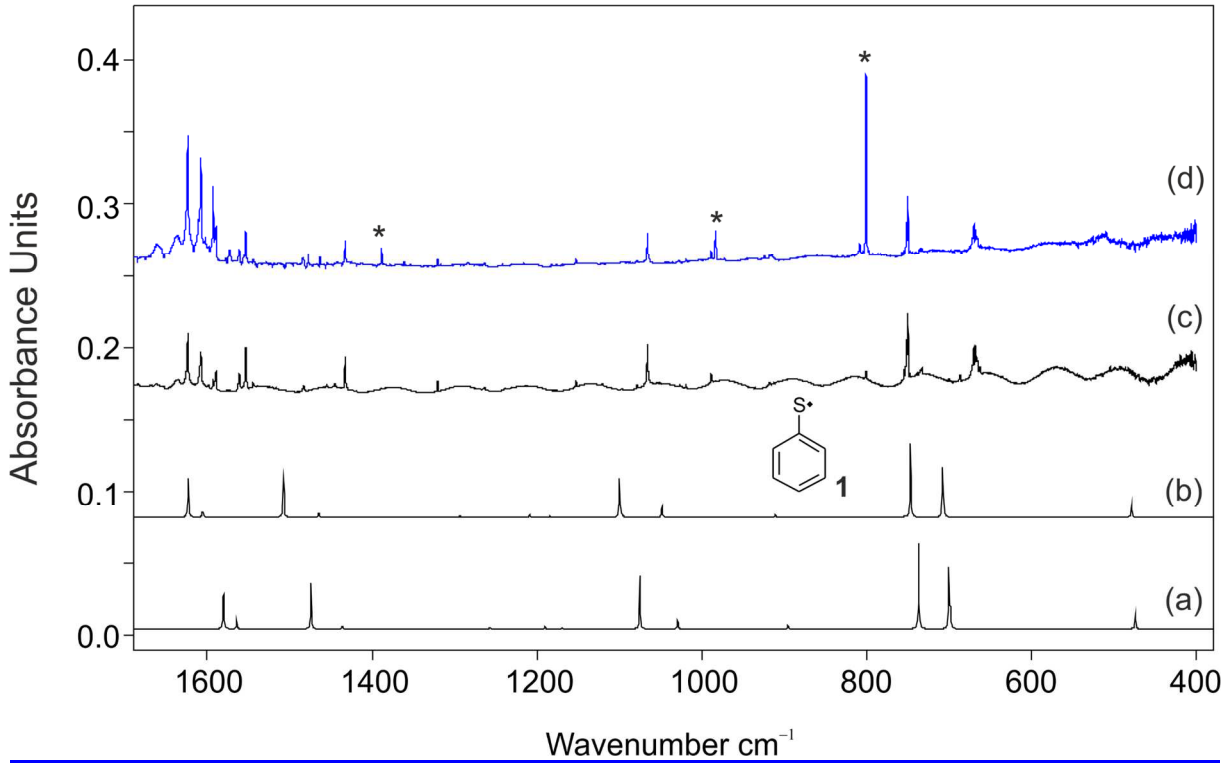

Figure S1 (a) IR spectrum of **1** computed at B3LYP/cc-pVTZ (unscaled, anharmonic). (b) IR spectrum of **1** computed at B3LYP/cc-pVTZ (unscaled, harmonic). (c) IR spectrum of the matrix-isolated pyrolysis products of diphenyl sulfide (**3**) in Ar at 10 K; pyrolysis temperature: 850 °C. (d) IR spectrum of the matrix-isolated pyrolysis products of allylphenyl sulfide (**2**) in Ar at 10 K; pyrolysis temperature: 850 °C. Bands attributed to the allyl radical are marked with an asterisk (*).

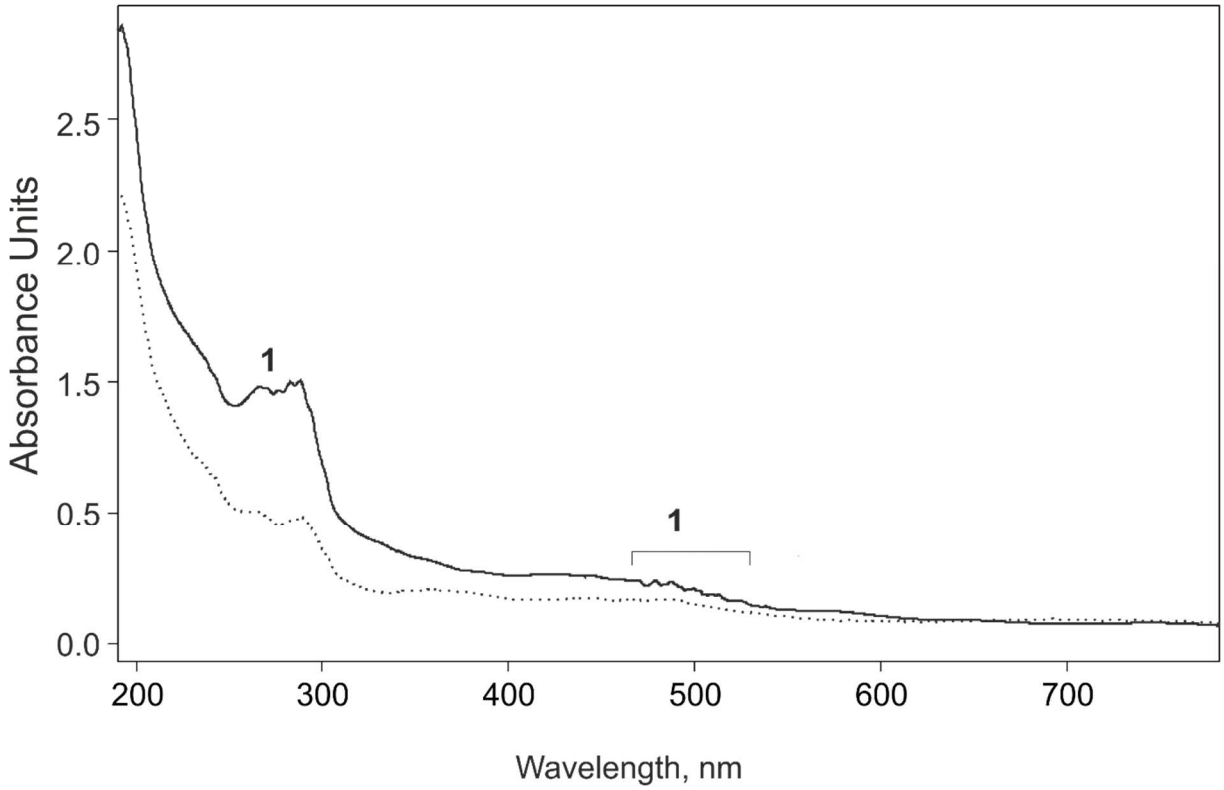

Figure S2. Solid line: UV/Vis spectrum of pyrolysis of **3** at 850 °C, isolated at 10 K in Ar, indicative for **1**. Dashed line: UV/Vis spectrum of **3** at 10 K, Ar.

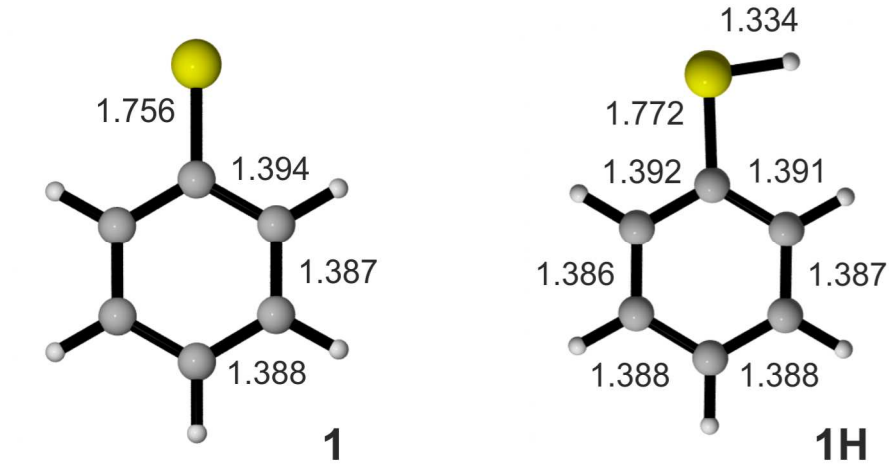

Figure S3. M06-2X/6-311++G(2d,2p) bond lengths (Å) of phenylthiyl radical (**1**) and thiophenol (**1H**).

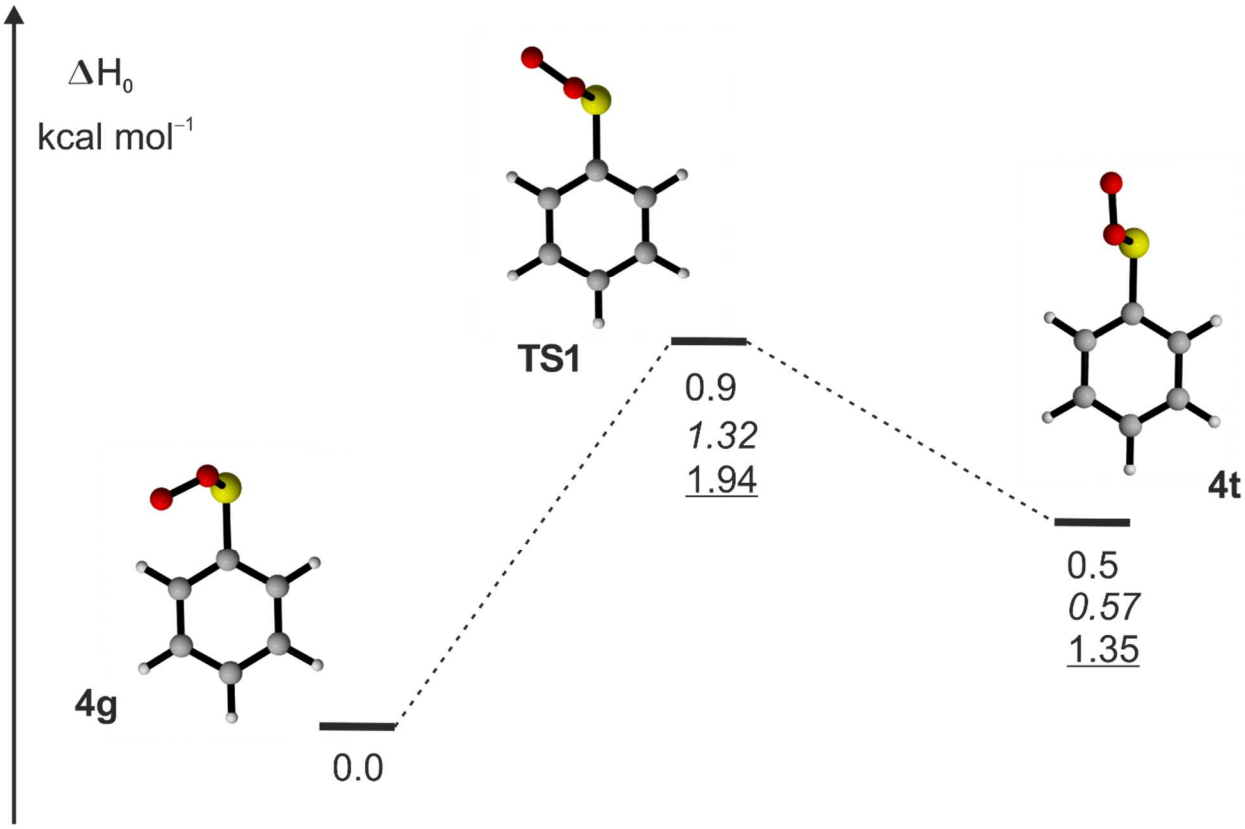

Figure S4. Theoretical isomerization partway between two isomers of phenylthiyl peroxy radical (**4g** and **4t**). Stationary points and transition state were computed by use M06-2X/6-311++G(2d,2p), *B3LYP/cc-pVTZ*, and B3LYP-D3/cc-pVTZ methods.

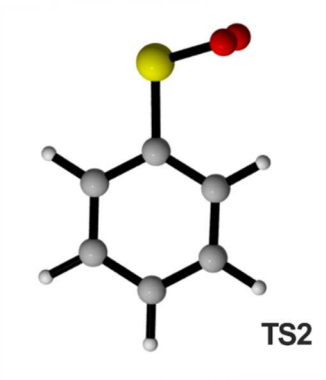

Figure S5. TS2 calculated at the M06-2X/6-311++G(2d,2p) level of theory.

Table S1. Experimental (Ar matrix, 10 K) and computed IR frequencies of **1**, band origins in cm^{-1}, computed intensities (km mol^{-1}) in parentheses.

Mode	Computed[a]	Computed[b]	Ar, 10 K[c]	Sym.	Assignment (approx.)
25	1623 (25)	1662 (31)	1553 (s)	a_1	C=C str
24	1606 (4)	1645 (3)	1544 (w)	b_2	C=C str
23	1508 (26)	1523 (29)	1433 (m)	a_1	C–H def
22	1465 (3)	1482 (3)	1419 (w)	b_2	C–H def
21	1357 (0)	1353 (0)	-	b_2	C–H def
20	1294 (0.8)	1297 (0.6)	1263 (w)	b_2	C=C str + C–H def
19	1209 (1)	1212 (1)	1152 (w)	a_1	C–H def
18	1184 (0.5)	1180 (0.4)	-	b_2	C–H def
17	1101 (22)	1116 (22)	1066 (m)	a_1	C–S str + ring distortion
16	1099 (5)	1111 (5)	-	b_2	ring distortion
15	1049 (7)	1062 (8)	1019 (m)	a_1	ring distortion
14	1013 (0)	1021 (0.1)	-	b_1	C–H o.o.p. def
13	1001 (1)	1019 (1)	989 (w)	a_1	ring breathing
12	980 (0)	1002 (0)	-	a_2	C–H o.o.p. def
11	911 (2)	928 (1.5)	908 (w)	b_1	C–H o.o.p. def
10	848 (0.0)	862 (0)	-	a_2	C–H o.o.p. def
9	747 (47)	761 (47)	750 (s)	b_1	C–H o.o.p. def
8	710 (34)	716 (34)	670 (s)	b_1	C–H o.o.p. def.
7	708 (9)	711 (8)	662 (w)	a_1	C–S str. + ring distortion
6	630 (0.1)	629 (0.1)	-	b_2	ring distortion
5	479 (8)	483 (10)	451(w)	b_1	ring breathing
4	423 (0.0)	421 (0)	-	a_2	ring breathing
3	410 (0.2)	413 (0.2)	415 (w)	a_1	ring breathing

[a]UB3LYP/cc-pVTZ, harmonic approximation, unscaled frequencies, intensities (in parentheses) in km mol^{-1}. [b]UM06-2X/6-311++G(2d,2p), harmonic approximation, unscaled frequencies, intensities (in parentheses) in km mol^{-1} [c] Experiment: argon matrix, 10 K.; approximate relative intensities (v. w: very weak, w: weak, s: strong).

Table S2. Experimental (Ar matrix, 10 K) and computed IR frequencies of **4g** and $^{18}O_2$-**4g**, band origins in cm^{-1}, computed intensities (km mol^{-1}) in parentheses.

	$C_6H_5S^{16}O^{16}O$		$C_6H_5S^{18}O^{18}O$		
Mode	Computed[a]	Ar, 10 K[b]	Computed[a]	Ar, 10 K[b]	Assignment
31	1652 (3.8)	-	1648 (3.0)		C=C str
30	1645 (0.1)	-	1641 (0.2)		C=C str
29	1521 (3.7)	-	1521 (3.8)		C–H def
28	1487 (13.0)	1442 (m)	1486 (12.7)	1442 (m)	C–H def
27	1347 (5.3)	1310 (w)	1346 (5.4)	1310 (w)	C–H def
26	1308 (3.1)	1279 (w)	1306 (2.9)	1278 (w)	C=C str +CH def
25	1239 (35)	1173 (m)	1156 (20)	1109 (m)	O–O str
24	1204 (1.7)	1142 (w)	1184 (3.0)		C–H def
23	1182 (1.1)	-	1170 (1.3)		C–H def
22	1122 (8.0)	1090 (m)	1116 (12)	1089 (m)	C–S str
21	1107 (2.6)	-	1102 (3.0)		C–H def
20	1055 (1.4)	-	1046 (1.0)		ring distortion
19	1035 (0.01)	-	1035 (0.01)		C–H o.o.p. def
18	1024 (1.6)	-	1014 (0.2)		ring distortion
17	1013 (0.2)	-	1005 (2.6)		C–H o.o.p. def
16	967 (0.7)	-	966 (0.6)		C–H o.o.p. def
15	872 (0.1)	-	872 (0.2)		C–H o.o.p. def
14	780 (33.9)	751 (s)	780 (34.3)	751 (s)	C–H o.o. p. def + ring distortion
13	729 (2.7)	719 (w)	699 (0.8)	-	C–S str +ring distortion
12	711 (37.5)	686 (s)	711 (38.9)	685 (s)	ring distortion
11	629 (0.04)	-	599 (0.7)		ring distortion
10	605 (11)	-	561 (11.8)		S–O str
9	519(12)	475 (m)	511 (8.9)	477 (m)	ring breathing
8	433 (3.4)	-	402 (2.2)		ring breathing
7	418 (0.3)	-	417 (0.2)		ring breathing

[a] UM062X/6-311++G(2d,2p), harmonic approximation, unscaled frequencies, intensities (in parentheses) in km mol^{-1}. [b] Experiment: argon matrix, 10 K.; approximate relative intensities (v. w: very weak, w: weak, s: strong).

Table S3. Experimental (Ar matrix, 10 K) and computed IR frequencies of **5** and $^{18}O_2$-**5**, band origins in cm^{-1}, computed intensities (km mol^{-1}) in parentheses.

	$C_6H_5S(^{16}O)^{16}O$		$C_6H_5S(^{18}O)^{18}O$		
Mode	Computed	Ar, 10 K	Computed	Ar, 10 K	Assignment
31	1667 (0.2)	-	1667 (0.2)		C=C str
30	1656 (0.4)	-	1656 (0.4)		C=C str
29	1524 (5.8)	-	1524 (5.7)		C–H def
28	1499 (12.2)	1436 (w)	1499 (12.4)		C–H def
27	1353 (0.3)	-	1352 (1.8)		C–H def
26	1336 (0.4)	-	1336 (0.6)	-	C=C str + CH def
25	1304 (139.2)	1271 (s)	1263 (127.6)	1232 (s)	OSO asym. str
24	1205 (0.8)	-	1205 (1.0)	-	C–H def
23	1185 (0.6)	-	1185 (0.7)	-	C–H def
22	1120 (115.7)	1093 (s)	1106 (52.7)	1082 (m)	C–S str +OSO symm. str
21	1112 (6.2)	-	1112 (7.0)		C–H def
20	1090 (10.7)	1049 (w)	1062 (19.5)	1027 (w)	C–H def + OSO sym. str
19	1056 (4.3)	1021 (w)	1051 (44.6)	1012 (m)	ring distortion
18	1041 (0.2)	-	1041 (0.4)	-	C–H o.o.p. def
17	1022 (0.1)	-	1022 (0.1)	-	C–H o.o.p. def.
16	1019 (4.2)	997 (w)	1019 (12.9)	996 (m)	ring distortion
15	972 (2.3)	-	972 (2.3)	-	C–H o.o.p. def
14	878 (0.2)	-	878 (0.2)	-	C–H o.o.p. def
13	780 (46.8)	747 (s)	780 (47.1)	747 (s)	C–H o.o.p. def
12	714 (31.3)	681 (s)	714 (31.4)	681 (s)	C–H o.o.p. def
11	706 (3.6)	668 (w)	705 (2.7)	668 (w)	ring distortion
10	626 (0.01)	-	625 (0.01)	-	ring distortion
9	530 (38.4)	518 (s)	526 (36.7)	514 (s)	ring breathing
8	491 (45.2)	487 (s)	476 (41.0)	471 (s)	OSO def
7	416 (0.004)	-	416 (0.005)	-	ring breathing
6	402 (13.4)	-	398 (12.3)	-	ring breathing

[a] UM062X/6-311++G(2d,2p), harmonic approximation, unscaled frequencies, intensities (in parentheses) in km mol^{-1}. [b] Experiment: argon matrix, 10 K.; approximate relative intensities (v. w: very weak, w: weak, s: strong).

Geometric Structures and Electronic energies

1: Phenylthiyl radical $-^2B_1$ (C_{2v} point group)

0 2

C	0.00000000	0.00000000	-2.23444000
C	0.00000000	1.19889300	-1.53397600
C	0.00000000	1.20639000	-0.14693000
C	0.00000000	0.00000000	0.55168600
C	0.00000000	-1.20639000	-0.14693000
C	0.00000000	-1.19889300	-1.53397600
H	0.00000000	0.00000000	-3.31471100
H	0.00000000	2.13927000	-2.06736500
H	0.00000000	2.14436200	0.39120800
H	0.00000000	-2.14436200	0.39120800
H	0.00000000	-2.13927000	-2.06736500
S	0.00000000	0.00000000	2.30840100

E[UM062X] = -629.75382104
ZPVE[UM062X] = 0.0912123

C	0.000000000	0.000000000	-2.240288000
C	0.000000000	1.199543000	-1.538236000
C	0.000000000	1.208332000	-0.149665000
C	0.000000000	0.000000000	0.553509000
C	0.000000000	-1.208332000	-0.149665000
C	0.000000000	-1.199543000	-1.538236000
H	0.000000000	0.000000000	-3.321376000
H	0.000000000	2.141147000	-2.071299000
H	0.000000000	2.148472000	0.384708000
H	0.000000000	-2.148472000	0.384708000
H	0.000000000	-2.141147000	-2.071299000
S	0.000000000	0.000000000	2.316878000

E[UB3LYP] = -629.9104751
ZPVE[UB3LYP] = 0.090403

C	0.000000000	0.000000000	-2.218252000
C	0.000000000	1.205144000	-1.529089000
C	0.000000000	1.206727000	-0.154662000
C	0.000000000	0.000000000	0.559727000
C	0.000000000	-1.206727000	-0.154662000
C	0.000000000	-1.205144000	-1.529089000
H	0.000000000	0.000000000	-3.312667000
H	0.000000000	2.150524000	-2.079493000

H	0.000000000	2.146906000	0.404122000
H	0.000000000	-2.146906000	0.404122000
H	0.000000000	-2.150524000	-2.079493000
S	0.000000000	0.000000000	2.301223000

E[UMP2] = -628.509978
ZPVE[UPM2] = 0.094067

2: allylphenylsulfide (C_1 point group)

0 1

C	-3.10263600	-0.82146200	-0.06472000
C	-1.78032000	-1.22818500	-0.01021100
C	-0.75480300	-0.28384900	0.06801100
C	-1.07676700	1.07034600	0.08822700
C	-2.40659400	1.46992300	0.02130400
C	-3.42419100	0.53139400	-0.05324300
H	-3.88531000	-1.56485900	-0.12572700
H	-1.53453500	-2.28148200	-0.03498100
H	-0.30391900	1.82046500	0.16461900
H	-4.45611400	0.84763700	-0.10284700
C	1.91220600	0.55687000	-0.20067200
H	1.90357900	1.24303600	0.64391800
H	1.47311600	1.04317400	-1.07154900
C	3.30446100	0.09664200	-0.49442200
H	3.43199100	-0.49567500	-1.39333100
C	4.34391700	0.35908800	0.28312400
H	4.23340500	0.93685100	1.19219400
H	5.33498200	0.00651800	0.03574700
H	-2.64238300	2.52511700	0.03451700
S	0.89709600	-0.91158600	0.17706500

E[UM062X] = -747.08313381
ZPVE[UM062X] = 0.1642029

C	-3.114329000	-0.831619000	-0.082438000
C	-1.787397000	-1.228508000	-0.019764000
C	-0.767273000	-0.275694000	0.073018000
C	-1.104168000	1.078144000	0.097918000
C	-2.437850000	1.466862000	0.021677000
C	-3.448474000	0.519312000	-0.066166000
H	-3.890422000	-1.582222000	-0.153985000
H	-1.535449000	-2.280504000	-0.049255000
H	-0.339807000	1.835928000	0.184732000
H	-4.483489000	0.827213000	-0.122214000
C	1.945574000	0.563908000	-0.178440000

H	1.953537000	1.242989000	0.672613000
H	1.501260000	1.069411000	-1.036570000
C	3.327079000	0.093413000	-0.499969000
H	3.428387000	-0.492989000	-1.406808000
C	4.393954000	0.342103000	0.248253000
H	4.323925000	0.913555000	1.165889000
H	5.375539000	-0.015041000	-0.031795000
H	-2.682467000	2.520918000	0.038692000
S	0.894143000	-0.900424000	0.198385000

E[UB3LYP] = -747.3028377

ZPVE[UB3LYP] = 0. 1623324

3: Biphenyldisulfide (C_1 point group)

0 1

C	4.096281000	0.565250000	0.419027000
C	3.155188000	-0.399665000	0.743992000
C	1.895917000	-0.367638000	0.148771000
C	1.583835000	0.623780000	-0.771361000
C	2.537030000	1.580742000	-1.096170000
C	3.791617000	1.558602000	-0.503363000
H	5.072491000	0.533798000	0.882318000
H	3.399049000	-1.180313000	1.452678000
H	0.609002000	0.645290000	-1.237492000
H	2.290719000	2.349112000	-1.815663000
H	4.527804000	2.306862000	-0.759625000
C	-1.895917000	-0.367638000	-0.148771000
C	-3.155186000	-0.399663000	-0.743997000
C	-1.583837000	0.623777000	0.771365000
C	-4.096280000	0.565250000	-0.419031000
H	-3.399044000	-1.180309000	-1.452686000
C	-2.537034000	1.580737000	1.096175000
H	-0.609006000	0.645286000	1.237499000
C	-3.791619000	1.558599000	0.503364000
H	-5.072488000	0.533800000	-0.882324000
H	-2.290725000	2.349105000	1.815671000
H	-4.527807000	2.306857000	0.759627000
S	0.750969000	-1.626322000	0.693355000
S	-0.750967000	-1.626322000	-0.693355000

E[UM062X] = -1259.61418364
ZPVE[UM062X] = 0.1856807

C	4.176284000	0.546673000	0.513472000
C	3.182695000	-0.366665000	0.838577000
C	1.966145000	-0.342282000	0.155007000

C	1.752070000	0.591073000	-0.852213000
C	2.756667000	1.497118000	-1.174139000
C	3.968399000	1.481934000	-0.494652000
H	5.117372000	0.520795000	1.046545000
H	3.353855000	-1.098814000	1.617447000
H	0.813831000	0.604622000	-1.387868000
H	2.584926000	2.219631000	-1.961016000
H	4.745082000	2.189972000	-0.749125000
C	-1.966142000	-0.342290000	-0.155012000
C	-3.182662000	-0.366618000	-0.838638000
C	-1.752104000	0.590999000	0.852277000
C	-4.176258000	0.546707000	-0.513518000
H	-3.353792000	-1.098714000	-1.617564000
C	-2.756708000	1.497033000	1.174216000
H	-0.813888000	0.604505000	1.387973000
C	-3.968410000	1.481902000	0.494675000
H	-5.117322000	0.520872000	-1.046635000
H	-2.584994000	2.219494000	1.961146000
H	-4.745098000	2.189930000	0.749158000
S	0.753468000	-1.555185000	0.698579000
S	-0.753457000	-1.555177000	-0.698602000

E[UB3LYP] = -1259.9137855

ZPVE[UB3LYP] = 0.183486

4g: phenylthiylperoxy radical (C_1 point group)

0 2

C	-2.22925800	-0.95341200	0.57211600
C	-2.74298900	0.29871900	0.25469800
C	-1.94206700	1.25319000	-0.35993400
C	-0.62221200	0.95674400	-0.66659500
C	-0.10510900	-0.29580700	-0.34072900
C	-0.90778300	-1.25252600	0.27941800
S	1.57191500	-0.67460300	-0.72077100
O	2.34175500	0.01427200	0.71354800
O	2.10764200	1.26366200	0.88498000
H	-0.48922600	-2.21764200	0.52636000
H	-2.85617500	-1.69273000	1.04976000
H	-3.77311900	0.53076900	0.48689800
H	-2.34600800	2.22523600	-0.60417100
H	0.01521800	1.68309500	-1.14857300

E[UM062X] = -780.07978623

ZPVE[UM062X] = 0.097748

C	-2.048019000	-1.214871000	0.066852000
C	-2.711227000	-0.022372000	0.340225000
C	-2.054117000	1.196371000	0.200323000
C	-0.731701000	1.226326000	-0.215491000
C	-0.061102000	0.030896000	-0.501184000
C	-0.725745000	-1.192072000	-0.349934000
S	1.606639000	0.064280000	-1.027177000
O	2.474868000	-0.037729000	0.669516000
O	1.721128000	-0.105598000	1.682573000
H	-0.197953000	-2.110218000	-0.564046000
H	-2.561249000	-2.159917000	0.181052000
H	-3.743079000	-0.042934000	0.664696000
H	-2.572102000	2.120459000	0.417839000
H	-0.208347000	2.165086000	-0.326155000

E[UB3LYP] = -780.3055236

ZPVE[UB3LYP] = 0.096254

C	-2.780126000	0.356477000	0.242692000
C	-1.924402000	1.304875000	-0.345605000
C	-0.593222000	0.968763000	-0.639957000
C	-0.114739000	-0.320615000	-0.319463000
C	-0.970413000	-1.273001000	0.276559000
C	-2.303975000	-0.931496000	0.549648000
H	-3.820110000	0.620441000	0.461567000
H	-2.297445000	2.306127000	-0.584797000
H	0.084054000	1.691519000	-1.102546000
H	-0.582655000	-2.266354000	0.522803000
H	-2.971584000	-1.668371000	1.008130000
S	1.563661000	-0.746479000	-0.688205000
O	2.342000000	0.022656000	0.758323000
O	2.244305000	1.306130000	0.757037000

E[UMP2] = -778.489613
ZPVE[UPM2] = 0.097153

4t: phenylthiylperoxy radical $-^2A''$ (C_s point group)

0 2

C	-0.42106700	2.90516800	0.00000000
C	-0.42072700	2.21485600	1.20612000
C	-0.42072700	0.82828000	1.20925600
C	-0.41856400	0.13521000	0.00000000
C	-0.42072700	0.82828000	-1.20925600
C	-0.42072700	2.21485600	-1.20612000
H	-0.42289900	3.98629200	0.00000000
H	-0.42152200	2.75570900	2.14161800
H	-0.42199100	0.27521400	2.13755000
H	-0.42199100	0.27521400	-2.13755000
H	-0.42152200	2.75570900	-2.14161800
S	-0.42539500	-1.62659300	0.00000000
O	1.32787000	-1.80716900	0.00000000
O	1.67856400	-3.04065000	0.00000000

E[UM062X] = -780.07872621
ZPVE[UM062X] = 0.0976035

C	-0.430503000	2.922735000	0.000000000
C	-0.430375000	2.230339000	1.206963000
C	-0.430375000	0.842899000	1.210698000
C	-0.430444000	0.142486000	0.000000000
C	-0.430375000	0.842899000	-1.210698000
C	-0.430375000	2.230339000	-1.206963000
H	-0.431874000	4.004521000	0.000000000
H	-0.430239000	2.771435000	2.143334000
H	-0.430784000	0.293066000	2.140944000
H	-0.430784000	0.293066000	-2.140944000
H	-0.430239000	2.771435000	-2.143334000
S	-0.449693000	-1.619857000	0.000000000
O	1.373052000	-1.853188000	0.000000000
O	1.732408000	-3.082562000	0.000000000

E[UB3LYP] = -780.304575

ZPVE[UB3LYP] = 0.096216

5: phenylsulfonyl radical $-^2A'$ (C_s point group)

0 2

C	-0.10257200	2.82951500	0.00000000
C	-0.10063200	2.14075000	1.20715000

C	-0.10063200	0.75334400	1.21626900
C	-0.08944200	0.08864900	0.00000000
C	-0.10063200	0.75334400	-1.21626900
C	-0.10063200	2.14075000	-1.20715000
H	-0.10330400	3.91040400	0.00000000
H	-0.09583400	2.68280300	2.14186700
H	-0.08844300	0.19177400	2.13914300
H	-0.08844300	0.19177400	-2.13914300
H	-0.09583400	2.68280300	-2.14186700
S	-0.13934500	-1.70348800	0.00000000
O	0.39179000	-2.16511600	1.27453000
O	0.39179000	-2.16511600	-1.27453000

E[UM062X] = -780.17109834

ZPVE[UM062X] = 0.099906

C	-0.104393000	2.846316000	0.000000000
C	-0.102548000	2.155145000	1.207564000
C	-0.102548000	0.766057000	1.216793000
C	-0.089813000	0.095911000	0.000000000
C	-0.102548000	0.766057000	-1.216793000
C	-0.102548000	2.155145000	-1.207564000
H	-0.106446000	3.927872000	0.000000000
H	-0.097882000	2.696248000	2.143775000
H	-0.090522000	0.209354000	2.142287000
H	-0.090522000	0.209354000	-2.142287000
H	-0.097882000	2.696248000	-2.143775000
S	-0.144997000	-1.716473000	0.000000000
O	0.401850000	-2.186456000	1.285327000
O	0.401850000	-2.186456000	-1.285327000

E[UB3LYP] = -780.3920749

ZPVE[UB3LYP] = 0.098527

C	-0.114181000	2.865660000	0.000000000
C	-0.110571000	2.164938000	1.220271000
C	-0.110571000	0.759057000	1.231926000
C	-0.108792000	0.087316000	0.000000000
C	-0.110571000	0.759057000	-1.231926000
C	-0.110571000	2.164938000	-1.220271000
H	-0.115519000	3.960402000	0.000000000
H	-0.105540000	2.713512000	2.167822000
H	-0.093146000	0.191541000	2.166579000
H	-0.093146000	0.191541000	-2.166579000
H	-0.105540000	2.713512000	-2.167822000

S	-0.132558000	-1.731866000	0.000000000
O	0.414085000	-2.179153000	1.320607000
O	0.414085000	-2.179153000	-1.320607000

E[UMP2] = -778.5667093
ZPVE[UPM2] = 0.0991069

Allyl radical: $^2A_2$ (C_{2v} point group)

0 2

C	1.21865900	0.19714400	0.00000000
H	1.27159100	1.27703300	0.00000200
H	2.14714100	-0.35201600	-0.00000100
C	-0.00000200	-0.44737300	0.00000000
H	-0.00000500	-1.53154800	0.00000000
C	-1.21865800	0.19714800	0.00000000
H	-1.27158600	1.27703600	-0.00000100
H	-2.14713500	-0.35202200	0.00000000

E[UM062X] = -117.22914959

ZPVE[UM062X] = 0.066396

C	-1.224600000	-0.195272000	0.000000000
H	-1.293044000	-1.275365000	0.000000000
H	-2.149488000	0.362369000	0.000000000
C	0.000000000	0.440492000	0.000000000
H	0.000002000	1.526319000	0.000000000
C	1.224600000	-0.195274000	0.000000000
H	2.149490000	0.362364000	0.000000000
H	1.293042000	-1.275367000	0.000000000

E[UB3LYP] = -117.3092686

ZPVE[UB3LYP] = 0.065982

1H: Thiophenol $-^1A'$ (C_s point group)

0 1

C	2.28316000	0.00454200	-0.00000100
C	1.58004600	1.20157300	-0.00000100
C	0.19245200	1.20409600	0.00000000
C	-0.50523600	-0.00000400	0.00000100
C	0.19784400	-1.20228400	0.00000000
C	1.58456400	-1.19571300	-0.00000100
H	3.36352500	0.00689700	-0.00000200
H	2.11130900	2.14319100	-0.00000100

H	-0.34419400	2.14287200	0.00000000
H	-0.34006800	-2.14078600	0.00000000
H	2.11946000	-2.13519000	-0.00000200
S	-2.27591700	-0.08277700	0.00000100
H	-2.49234500	1.23419100	0.00000700

E[UM062X] = -630.39732916

ZPVE[UM062X] = 0.0999427

C	-2.288861000	0.003926000	0.000002000
C	-1.585286000	1.202399000	0.000001000
C	-0.196104000	1.206255000	0.000000000
C	0.505131000	0.000786000	0.000000000
C	-0.200203000	-1.203519000	0.000000000
C	-1.588404000	-1.197034000	0.000002000
H	-3.370062000	0.005656000	0.000003000
H	-2.117356000	2.144579000	0.000001000
H	0.337963000	2.146986000	-0.000001000
H	0.335702000	-2.143527000	0.000000000
H	-2.123090000	-2.137620000	0.000002000
S	2.284251000	-0.083376000	-0.000002000
H	2.511190000	1.241065000	-0.000005000

E[UB3LYP] = -630.5561367
ZPVE[UB3LYP] = 0.099165

Oxygen: ($D_{\infty h}$ point group)

0 3

O	0.000000000	0.000000000	0.596021000
O	0.000000000	0.000000000	-0.596021000

E[UM062X] = -150.31387522

ZPVE[UM062X] = 0.004014

O	0.000000000	0.000000000	0.602914000
O	0.000000000	0.000000000	-0.602914000

E[UB3LYP] = - -150.38094430
ZPVE[UB3LYP] = 0.003710

8	0.000000000	0.000000000	0.616028000
8	0.000000000	0.000000000	-0.616028000

E[UMP2] = -149.97318254
ZPVE[UPM2] = 0.003242

TS1: 4g → 4t (C_1 point group)

0 2

C	2.41673000	-0.91445400	-0.43438500
C	2.85790000	0.39123100	-0.26609500
C	1.98343100	1.37728300	0.17872500
C	0.66723200	1.05595100	0.46784100
C	0.22129700	-0.25277200	0.28649400
C	1.09366600	-1.23836800	-0.16757100
S	-1.45225400	-0.66933400	0.65773900
O	-2.16636100	0.03860800	-0.78399700
O	-3.11233900	0.87113400	-0.52591800
H	0.72947600	-2.24557100	-0.31051100
H	3.09791000	-1.67779400	-0.78231100
H	3.88683800	0.64314600	-0.48182000
H	2.33116500	2.39199800	0.30995700
H	-0.02125800	1.80640800	0.83013000

E[UM062X] = -780.07798176

ZPVE[UM062X] = 0.0975212

C	-2.353829000	-0.950062000	0.505119000
C	-2.852847000	0.336485000	0.329582000
C	-2.036829000	1.342779000	-0.179243000
C	-0.720405000	1.064805000	-0.516805000
C	-0.213315000	-0.226487000	-0.337007000
C	-1.035755000	-1.234153000	0.175645000
S	1.456441000	-0.588695000	-0.784517000
O	2.262656000	-0.116474000	0.789861000
O	2.985477000	0.947029000	0.725462000
H	-0.634257000	-2.228219000	0.310898000
H	-2.990193000	-1.730176000	0.900256000
H	-3.880250000	0.555575000	0.587861000
H	-2.428191000	2.341662000	-0.316176000
H	-0.077360000	1.835636000	-0.916898000

E[UB3LYP] = -780.303185
ZPVE[UB3LYP] = 0.096017

TS2: 4g → 5 (C_1 point group)

0 2

C	-2.80574700	0.36187300	0.01860300
C	-1.85731800	1.37883900	-0.03926600
C	-0.50611200	1.07719100	-0.05936400
C	-0.11942500	-0.25858700	-0.02817100
C	-1.05594800	-1.28732300	0.02807000
C	-2.40430400	-0.96831300	0.05397300
H	-3.85802100	0.60711800	0.03625200
H	-2.17385900	2.41185100	-0.06475300
H	0.25037800	1.84797900	-0.09452700
H	-0.73340500	-2.32017900	0.04802800
H	-3.14059300	-1.75788200	0.09805700
S	1.57160000	-0.70448800	-0.05256500
O	2.30778700	0.49374300	-0.76336500
O	2.31759100	0.58886200	0.88522800

E[UM062X] = -780.03126204

ZPVE[UM062X] = 0.0955588

C	-2.827521000	0.367165000	0.044317000
C	-1.879676000	1.382687000	-0.066328000
C	-0.527970000	1.080338000	-0.114779000
C	-0.135281000	-0.255863000	-0.057525000
C	-1.074311000	-1.282158000	0.053418000
C	-2.423864000	-0.962523000	0.105791000
H	-3.879766000	0.613490000	0.083160000
H	-2.197109000	2.415662000	-0.110176000
H	0.222709000	1.853158000	-0.187520000
H	-0.754404000	-2.315650000	0.094879000
H	-3.158718000	-1.751180000	0.190978000
S	1.564694000	-0.725101000	-0.113443000
O	2.336159000	0.487408000	-0.724582000
O	2.406832000	0.613623000	0.968881000

E[UB3LYP] = -780.2637574
ZPVE[UB3LYP] = 0.094752