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

Supporting Information

Spectroscopic Identification of the Phenyltelluryl Radical and its Reactivity Towards Molecular Oxygen

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1 Spectroscopic Data

1.1 Phenyltelluryl radical **1**

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]	Symm.	Assignment (approx.)
25	1603(7.8)	1643 (0.1)	1577 (m)	a_1	C=C str
24	1596 (0.5)	1636 (0.3)		b_2	C=C str
23	1499 (1.2)	1513 (4.0)	1483 (w)	a_1	C–H def
22	1466 (11.6)	1477 (12.4)	1434 (s)	b_2	C–H def
21	1349 (6.8)	1348 (4.9)	1323 (m)	b_2	C–H def
20	1304 (0.0)	1296 (0.2)		b_2	C=C str + CH def
19	1207 (3.7)	1210 (1.6)	1183 (w)	a_1	C–H def
18	1184 (0.2)	1179 (0.3)		b_2	C–H def
17	1095 (2.8)	1106 (2.7)	1085 (w)	b_2	ring distortion
16	1070 (9.3)	1096 (4.4)	1056 (m)	a_1	C–Te str. + ring distortion
15	1034 (0.1)	1051 (0.4)		a_1	ring distortion
14	1018 (0.0)	1037 (0.0)		b_1	C–H o.o.p. def
13	1016 (4.4)	1018 (5.4)	997 (m)	a_1	ring distortion
12	1001 (0.0)	1015 (0)		a_2	C–H o.o.p. def
11	947 (0.6)	960 (0.5)		b_1	C–H o.o.p. def
10	859 (0)	871 (0)		a_2	C–H o.o.p. def
9	756 (39.5)	762 (39.3)	730 (s)	b_1	C–H o.o.p. def
8	703 (31.3)	715 (32.2)	686 (s)	b_1	C–H o.o.p. def.
7	675 (0.4)	678 (0.2)	659 (w)	a_1	C–Te str. + ring distortion
6	628 (0.0)	629 (0.0)		b_2	ring distortion
5	453 (4.2)	454 (4.5)	440 (m)	b_1	ring breathing
4	391 (0)	392 (0)		a_2	ring breathing

[a] UB3LYP/Def2QZVPP, anharmonic approximation, unscaled frequencies, intensities (in parentheses) in km mol^{-1}. [b] UM062X/Def2QZVPP harmonic approximation, unscaled frequencies, intensities (in parentheses) in km mol^{-1}. [c] Experiment: argon matrix, 10 K.; approximate relative intensities (w: weak, m: medium, s: strong).

1.2 Phenyltelluro peroxy radical **8**

Table S2: Experimental (Ar matrix, 10 K) and computed IR frequencies of **8c** and **8t** and $^{18}O_2$-**8c** and $^{18}O_2$-**8t**, band origins in cm^{-1}, computed intensities (km mol^{-1}) in parentheses.

Mode	$C_6H_5Te^{16}O^{16}O$			$C_6H_5Te^{18}O^{18}O$			Assignment (approx.)
	Computed[a]		Ar, 10 K[b]	Computed[a]		Ar, 10 K[b]	
	8c	**8t**		^{18}O-**8c**	^{18}O-**8t**		
31	1615 (0.1)	1613 (1.2)	-	1613 (2.9)	1613 (1.3)	-	C=C str
30	1611 (0.4)	1608 (0.5)	-	1608 (0.4)	1608 (0.5)	-	C=C str
29	1507 (1.9)	1507 (2.6)	1474 (w)	1507 (1.7)	1507 (2.6)	1475 (w)	C–H def
28	1471 (13.2)	1470 (11.7)	1437 (s)	1470 (12.4)	1470 (11.7)	1437 (s)	C–H def
27	1351 (7.0)	1351 (6.5)	1325 (w)	1352 (7.1)	1351 (6.5)	1326 (w)	C–H def
26	1315 (0.2)	1309 (0.3)	-	1312 (0.4)	1309 (0.3)	-	C=C str +CH def
25	1215 (256)	1209 (3)	-	1210 (3.3)	1209 (3.6)	-	C–H def
24	1209 (28.0)	1187 (0.2)	-	1187 (0.3)	1187 (0.2)	-	C–H def
23	1187 (0.3)	1177 (232)	1125 (s)	1139 (233)	1110 (206)	1065 (s)	O–O str
22	1098 (2.8)	1097 (3)	1074 (w)	1098 (2.9)	1097 (3)	1073 (w)	C–H def
21	1081 (9.1)	1080 (8.6)	1064 (w)	1080 (9.0)	1080 (7.9)	1065 (w)	C–Te str
20	1038 (0.6)	1037 (1.2)	1023 (m)	1037 (1.0)	1037 (1.4)	1022 (m)	ring distortion
19	1020 (5.0)	1023 (0.0)	-	1022 (0.3)	1023 (0.0)	-	C–H o.o.p. def
18	1018 (0.9)	1019 (6.1)	999 (s)	1020 (5.6)	1019 (6.2)	999 (s)	ring distortion
17	996 (0.0)	1003 (0.0)	-	1002 (0.0)	1003 (0.0)	-	C–H o.o.p. def
16	951 (0.1)	951 (0.2)	-	951 (0.0)	951 (0.2)	-	C–H o.o.p. def
15	864 (0.0)	865 (0.0)	-	864 (0.0)	865 (0.0)	-	C–H o.o.p. def
14	758 (40.0)	758 (40.1)	735 (s)	757 (38.0)	758 (40.0)	735 (s)	C–H o.o.p. def + dist.
13	706 (26.0)	707 (26.5)	686 (s)	705 (25.0)	707 (26.5)	686 (s)	C–H o.o.p. def + dist.
12	678 (0.3)	677 (0.2)	-	678 (0.3)	676 (0.3)	-	C–Te str +ring dist.
11	630 (0.0)	630 (0.0)	-	630 (0.0)	630 (0.0)	-	ring distortion
10	480 (23.3)	494 (7.3)	-	471 (16.2)	480 (5.9)	-	ring dist. + Te–O str
9	433 (7.6)	443 (9.8)	460(w)	418 (11.4)	431 (10.3)	454 (w)	ring breathing
8	410 (0.0)	411 (0.0)	-	410 (0.0)	411 (0.0)	-	ring breathing

[a] UB3LYP/Def2QZVPP, anharmonic 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 **8c** and **8t** and $^{18}O_2$-**8c** and $^{18}O_2$-**8t**, band origins in cm^{-1}, computed intensities (km mol^{-1}) in parentheses.

Mode	$C_6H_5Te^{16}O^{16}O$			$C_6H_5Te^{18}O^{18}O$			Assignment (approx.)
	Computed[a]		Ar, 10 K[b]	Computed[a]		Ar, 10 K[b]	
	8c	**8t**		^{18}O-**8c**	^{18}O-**8t**		
31	1648 (0.5)	1649 (1.0)	-	1648 (0.5)	1649 (1.0)	-	C=C str
30	1642 (0.1)	1642 (0.2)	-	1642 (0.19	1642 (0.2)	-	C=C str
29	1518 (3.1)	1520 (2.5)	1474 (w)	1518 (3.1)	1520 (2.5)	1475 (w)	C–H def
28	1480 (14.2)	1480 (13.3)	1437 (s)	1480 (14.2)	1480 (13.3)	1437 (s)	C–H def
27	1352 (5.8)	1352 (5.4)	1325 (w)	1352 (5.8)	1352 (5.4)	1326 (w)	C–H def
26	1302 (1.2)	1301 (1.1)	-	1302 (1.0)	1301 (1.1)	-	C=C str +CH def
25	1238 (47.1)	1256 (36.7)	-	1213 (2.5)	1214 (3.2)	-	C–H def
24	1213 (2.4)	1214 (3.3)	-	1181 (0.8)	1184 (32.2)	-	C–H def
23	1181 (0.7)	1182 (0.6)	1125 (s)	1167 (41.9)	1182 (1.0)	1065 (s)	O–O str
22	1109 (2.8)	1108 (2.8)	1074 (w)	1109 (2.8)	1108 (2.8)	1073 (w)	C–H def
21	1103 (6.0)	1105 (9.4)	1064 (w)	1103 (5.9)	1105 (9.4)	1065 (w)	C–Te str
20	1053 (0.4)	1053 (0.1)	1023 (m)	1053 (0.4)	1053 (0.1)	1022 (m)	ring distortion
19	1042 (0.1)	1044 (0.0)	-	1042 (0.1)	1044 (0.0)	-	C–H o.o.p. def
18	1020 (1.8)	1023 (0.3)	999 (s)	1020 (1.8)	1023 (0.3)	999 (s)	ring distortion
17	1019 (4.1)	1019 (5.8)	-	1019 (4.1)	1019 (5.8)	-	C–H o.o.p. def
16	965 (0.2)	969 (0.4)	-	965 (0.2)	969 (0.4)	-	C–H o.o.p. def
15	880 (0.3)	883 (0.0)	-	880 (0.3)	883 (0.0)	-	C–H o.o.p. def
14	768 (37.4)	769 (36.2)	735 (s)	768 (37.4)	769 (36.5)	735 (s)	C–H o.o.p. def + dist.
13	716 (28.2)	717 (31.0)	686 (s)	716 (28.2)	717 (30.8)	686 (s)	C–H o.o.p. def + dist.
12	682 (0.0)	682 (0.1)	-	682 (0.0)	682 (0.19	-	C–Te str +ring dist.
11	628 (0.0)	628 (0.0)	-	628 (0.0)	629 (0.0)	-	ring distortion
10	526 (5.5)	551 (8.3)	-	499 (5.3)	524 (8.9)	-	ring dist. + Te–O str
9	466 (7.4)	461 (4.7)	460(w)	464 (7.0)	459 (3.79	454 (w)	ring breathing
8	411 (0.1)	410 (0.0)	-	411 (0.1)	410 (0.0)	-	ring breathing

[a] UM062X/Def2QZVPP, 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).

1.3 Phenyltelluroyl radical **9**

Table S4: Experimental (Ar matrix, 10 K) and computed IR frequencies of **9** and $^{18}O_2$-**9**, band origins in cm^{-1}, computed intensities (km mol^{-1}) in parentheses.

Mode	$C_6H_5Te(^{16}O)^{16}O$			$C_6H_5Te(^{18}O)^{18}O$			Assignment
	Computed[a]	Computed[b]	Ar, 10 K	Computed[a]	Computed[b]	Ar, 10 K	(approx.)
31	1615 (2.2)	1649 (0.6)	-	1615 (2.2)	1649 (0.6)	-	C=C str
30	1603 (4.6)	1644 (0.3)	1594 (m)	1603 (4.6)	1644 (0.3)	1592 (w)	C=C str
29	1508 (7.6)	1520 (4.2)	1487 (s)	1508 (7.6)	1520 (4.2)	1486 (s)	C–H def
28	1473 (9.1)	1485 (13.6)	1441 (m)	1473 (9.1)	1485 (13.6)	1441 (s)	C–H def
27	1354 (5.7)	1354 (5.7)	-	1354 (5.7)	1354 (5.7)	-	C–H def
26	1318 (1.0)	1313 (0.7)	-	1318 (1.0)	1313 (0.7)	-	C=C str + CH def
25	1204 (3.6)	1207 (3.3)	1200 (m)	1204 (3.6)	1207 (3.3)	1200 (w)	C–H def
24	1187 (0.0)	1183 (0.2)	-	1187 (0.0)	1183 (0.2)	-	C–H def
23	1097 (6.4)	1109 (4.5)	1087 (w)	1097 (6.4)	1109 (4.5)	1087 (w)	ring dist.
22	1065 (6.1)	1092 (10.2)	1045 (w)	1065 (6.1)	1092 (10.3)	1045 (w)	C-Te str. / ring dist.
21	1028 (1.2)	1051 (0.2)	-	1028 (1.2)	1051 (0.2)	-	ring distortion
20	1023 (1.4)	1044 (0.5)	-	1023 (1.4)	1044 (0.4)	-	C–H o.o.p. def
19	1010 (13.6)	1020 (0.5)	990 (m)	1010 (13.6)	1021 (0.5)	990 (m)	ring distortion
18	1003 (0.6)	1012 (7.1)	-	1003 (0.6)	1012 (7.2)	-	C–H o.o.p. def
17	948 (0.8)	967 (1.0)	-	948 (0.8)	966 (1.0)	-	C–H o.o.p. def
16	861 (0.5)	881 (0.5)	-	861 (0.5)	881 (0.5)	-	C–H o.o.p. def
15	761 (27.3)	829 (23.5)	758 (m)	720 (13.5)	785 (23.9)	725 (w)	OTeO symm. str
14	752 (41.8)	815 (10.0)	731 (s)	754 (56.1)	776 (9.2)	732 (s)	C–H o.o.p. def
13	701 (20.0)	763 (50.1)	681 (s)	701 (18.6)	763 (48.0)	681 (s)	ring breathing
12	696 (0.4)	714 (24.4)	-	662 (0.4)	714 (24.4)	-	OTeO asymm. str
11	663 (0.6)	677 (0.3)	-	663 (0.5)	677 (0.2)	-	ring distortion
10	624 (0.0)	624 (0.0)	-	624 (0.0)	624 (0.0)	-	ring distortion
9	455 (8.1)	456 (8.6)	438 (w)	455 (7.8)	456 (8.1)	438 (w)	ring breathing
8	405 (0.2)	404 (0.1)	-	405 (0.2)	404 (0.1)	-	ring breathing

[a]UB3LYP/Def2QZVPP; anharmonic approximation, unscaled frequencies, intensities (in parentheses) in km mol^{-1}. [b] UM062X/Def2QZVPP 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).

2 UV/Vis spectra

2.1 Phenyltelluryl radical **1**

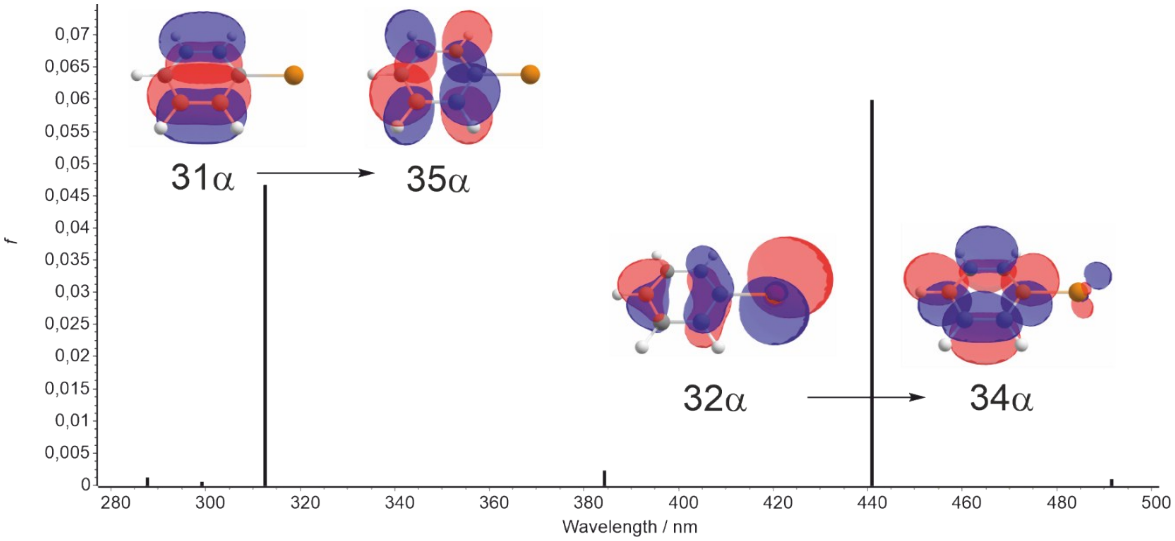

Figure S1: Computed UV/Vis spectrum of phenyltelluryl radical **1** at the UB3LYP/Def2QZVPP level of theory.

2.2 Phenyltelluryl peroxy radical **8** and phenyltelluroyl radical **9**

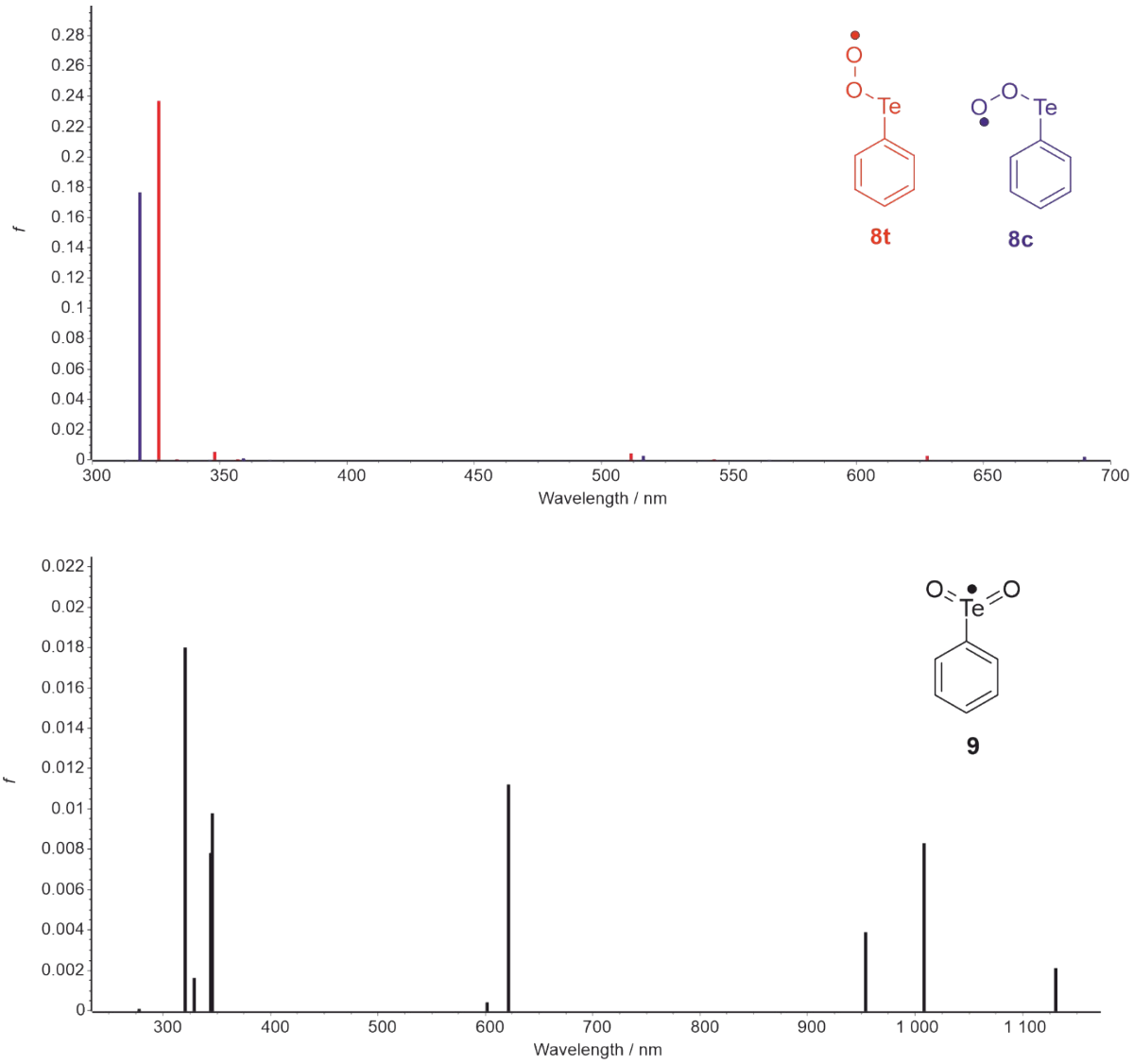

Figure S2: Computed UV/Vis spectra of **8t** (red) and **8c** (blue) (top) and **9** at the UB3LYP/Def2QZVPP level of theory.

3 Geometric Structure and Electronic Energies

3.1 UB3LYP/Def2QZVPP

3.1.1 Tellurium containing compounds

3.1.1.1 Phenyltelluryl radical **1** – $^2B_1$ (C_{2v})

52	0.000000000	0.000000000	1.569673000
6	0.000000000	0.000000000	-0.530046000
6	0.000000000	1.208932000	-1.238866000
6	0.000000000	1.205332000	-2.626128000
6	0.000000000	0.000000000	-3.321794000
6	0.000000000	-1.205332000	-2.626128000
6	0.000000000	-1.208932000	-1.238866000
1	0.000000000	2.144727000	-0.698534000
1	0.000000000	2.142843000	-3.165788000
1	0.000000000	0.000000000	-4.403402000
1	0.000000000	-2.142843000	-3.165788000
1	0.000000000	-2.144727000	-0.698534000

E(UB3LYP) = –499.746061
ZVPE(UB3LYP) = 0.089719

3.1.1.2 Phenyltellenyl peroxy radical **8t** – ^2A (C_s)

6	2.967037000	0.194106000	-1.218396000
6	3.641505000	0.429850000	-0.025619000
6	2.960486000	0.370796000	1.185164000
6	1.603556000	0.074662000	1.207183000
6	0.921503000	-0.160893000	0.010419000
6	1.609895000	-0.101643000	-1.204287000
8	-1.672499000	1.462197000	-0.091589000
8	-2.932565000	1.709237000	-0.107387000
1	1.086778000	-0.282504000	-2.131891000
1	3.495957000	0.241218000	-2.160081000
1	4.697875000	0.659655000	-0.039648000
1	3.484320000	0.555412000	2.112668000
1	1.075718000	0.029683000	2.148553000
52	-1.138924000	-0.604158000	0.037220000

E(UB3LYP) = – 650.139552
ZVPE(UB3LYP) = 0.094675

3.1.1.3 Phenyltellenyl peroxy radical **8c** – ^2A (C_s)

6	-2.822177000	0.017705000	1.205321000
6	-3.508613000	0.114214000	-0.000003000
6	-2.822174000	0.017700000	-1.205325000
6	-1.447326000	-0.177513000	-1.209272000
6	-0.754122000	-0.276832000	0.000001000
6	-1.447329000	-0.177506000	1.209272000
8	1.797585000	1.573292000	-0.000044000
8	0.817588000	2.387741000	0.000028000
1	-0.914191000	-0.249024000	2.145899000
1	-3.355747000	0.096532000	2.142221000

1	-4.579062000	0.266405000	-0.000005000
1	-3.355741000	0.096523000	-2.142227000
1	-0.914187000	-0.249040000	-2.145898000
52	1.327077000	-0.553005000	0.000003000

E(UB3LYP) = – 650.139540
ZVPE(UB3LYP) = 0.094668

3.1.1.4 **TS1** – ^{2}A (C_s)

8	1.796688000	1.217040000	0.865120000
8	1.796418000	1.216425000	-0.866363000
52	1.241440000	-0.439782000	0.000131000
6	-0.849015000	-0.132314000	0.000478000
6	-1.711520000	-1.227324000	-0.000021000
6	-3.085452000	-1.015091000	-0.000367000
6	-3.588290000	0.281641000	-0.000298000
6	-2.718681000	1.369299000	0.000193000
6	-1.344176000	1.169325000	0.000583000
1	-1.327606000	-2.240781000	-0.000068000
1	-3.760078000	-1.860857000	-0.000734000
1	-4.657618000	0.445288000	-0.000649000
1	-3.112036000	2.377230000	0.000291000
1	-0.659596000	2.006873000	0.000877000

E(UB3LYP) = – 650.088613
ZVPE(UB3LYP) = 0.093201

3.1.1.5 Phenyltellunoyl radical **9** – ^{2}A' (C_s)

8	0.764240000	-1.669637000	1.544251000
52	-0.127809000	-1.288775000	0.000000000
6	-0.131387000	0.857201000	0.000000000
6	-0.137953000	1.527974000	1.215903000
6	-0.137953000	2.918696000	1.207204000
6	-0.140886000	3.609207000	0.000000000
6	-0.137953000	2.918696000	-1.207204000
6	-0.137953000	1.527974000	-1.215903000
8	0.764240000	-1.669637000	-1.544251000
1	-0.116725000	0.981599000	2.148477000
1	-0.130883000	3.459277000	2.143285000
1	-0.142033000	4.690222000	0.000000000
1	-0.130883000	3.459277000	-2.143285000
1	-0.116725000	0.981599000	-2.148477000

E(UB3LYP) = – 650.174411
ZVPE(UB3LYP) = 0.094470

3.1.1.6 Phenyltellenol – ^{1}A (C_s)

52	1.566223000	0.000000000	-0.032743000
1	1.719875000	0.000003000	1.623951000
6	-0.573217000	0.000000000	0.008403000
6	-1.272924000	-1.205121000	0.001540000
6	-2.664036000	-1.202367000	0.000742000

6	-3.360566000	0.000000000	0.001060000
6	-2.664036000	1.202367000	0.000741000
6	-1.272924000	1.205121000	0.001540000
1	-0.737186000	-2.143229000	-0.000907000
1	-3.200551000	-2.141320000	-0.001416000
1	-4.441759000	0.000000000	-0.000836000
1	-3.200551000	2.141320000	-0.001416000
1	-0.737186000	2.143229000	-0.000907000

E(UB3LYP) = – 500.350372
ZVPE(UB3LYP) = 0.096291

3.1.2 Selenium containing compounds

3.1.2.1 Phenylselenyl radical – $^2B_2$ (C_{2v})

34	0.000000000	0.000000000	1.842045000
6	0.000000000	0.000000000	-0.073031000
6	0.000000000	1.207110000	-0.772073000
6	0.000000000	1.200058000	-2.161488000
6	0.000000000	0.000000000	-2.862366000
6	0.000000000	-1.200058000	-2.161488000
6	0.000000000	-1.207110000	-0.772073000
1	0.000000000	2.148587000	-0.240723000
1	0.000000000	2.140701000	-2.695009000
1	0.000000000	0.000000000	-3.942963000
1	0.000000000	-2.140701000	-2.695009000
1	0.000000000	-2.148587000	-0.240723000

E(UB3LYP) = – 2633.257391
ZVPE(UB3LYP) = 0.089892

3.1.2.2 Phenylselenol – ^1A (C_s)

34	-1.820724000	-0.043513000	0.000261000
6	0.103798000	0.018384000	-0.000009000
6	0.816281000	1.215297000	-0.000107000
6	2.205853000	1.193839000	-0.000313000
6	2.893734000	-0.013577000	-0.000429000
6	2.179570000	-1.205946000	-0.000335000
6	0.790613000	-1.194367000	-0.000122000
1	-2.004885000	1.413976000	0.000500000
1	0.296172000	2.162622000	-0.000027000
1	2.749860000	2.128498000	-0.000384000
1	3.974327000	-0.025237000	-0.000591000
1	2.702536000	-2.152422000	-0.000422000
1	0.247518000	-2.129777000	-0.000041000

E(UB3LYP) = – 2633.882144
ZVPE(UB3LYP) = 0.097597

3.1.3 Sulfur containing compounds

3.1.3.1 Phenylthiyl radical – $^2B_2$ (C_{2v})

16	0.000000000	0.000000000	2.312085000
6	0.000000000	0.000000000	0.556144000

6	0.000000000	1.208108000	-0.148078000
6	0.000000000	1.199292000	-1.536360000
6	0.000000000	0.000000000	-2.238507000
6	0.000000000	-1.199292000	-1.536360000
6	0.000000000	-1.208108000	-0.148078000
1	0.000000000	2.148011000	0.385537000
1	0.000000000	2.140390000	-2.069021000
1	0.000000000	0.000000000	-3.318953000
1	0.000000000	-2.140390000	-2.069021000
1	0.000000000	-2.148011000	0.385537000

E(UB3LYP) = – 629.842471
ZVPE(UB3LYP) = 0.090375

3.1.3.2 Phenylthiol – ^{1}A (C_s)

16	-2.279655000	-0.083243000	-0.000013000
6	-0.507629000	0.000817000	-0.000004000
6	0.194474000	1.206014000	0.000002000
6	1.583329000	1.202230000	0.000011000
6	2.287073000	0.003968000	0.000015000
6	1.586639000	-1.196753000	0.000010000
6	0.198637000	-1.203179000	0.000000000
1	-2.508962000	1.237259000	-0.000029000
1	-0.339035000	2.146367000	0.000000000
1	2.114992000	2.143897000	0.000014000
1	3.367633000	0.005742000	0.000022000
1	2.120965000	-2.136801000	0.000013000
1	-0.336248000	-2.143167000	-0.000005000

E(UB3LYP) = – 630.479853
ZVPE(UB3LYP) = 0.099191

3.1.4 Oxygen containing compounds

3.1.4.1 Phenyloxy radical – ^{2}B$_1$ (C_2)

8	0.000000000	0.000000000	2.294344000
6	0.000000000	0.000000000	1.044361000
6	0.000000000	1.235796000	0.288466000
6	0.000000000	1.220434000	-1.082417000
6	0.000000000	0.000000000	-1.777194000
6	0.000000000	-1.220434000	-1.082417000
6	0.000000000	-1.235796000	0.288466000
1	0.000000000	2.158015000	0.851974000
1	0.000000000	2.148236000	-1.638053000
1	0.000000000	0.000000000	-2.858170000
1	0.000000000	-2.148236000	-1.638053000
1	0.000000000	-2.158015000	0.851974000

E(UB3LYP) = – 306.905638
ZVPE(UB3LYP) = 0.091348

3.1.4.2 Phenol – ^{1}A (C_s)

8	-2.299937000	-0.110506000	0.000000000
6	-0.935676000	-0.025483000	0.000000000
6	-0.262938000	1.193389000	0.000000000
6	1.126896000	1.214624000	0.000000000
6	1.850114000	0.028754000	0.000000000
6	1.168318000	-1.184431000	0.000000000
6	-0.218561000	-1.218849000	0.000000000
1	-2.681330000	0.771414000	0.000000000
1	-0.823390000	2.120492000	0.000000000
1	1.642349000	2.165150000	0.000000000
1	2.930303000	0.048380000	0.000000000
1	1.720389000	-2.114231000	0.000000000
1	-0.757748000	-2.155180000	0.000000000

E(B3LYP) = – 307.539887
ZVPE(B3LYP) = 0.104494

3.1.5 Carbon containing compounds

3.1.5.1 Benzyl radical – $^2B_1$ (C_{2v})

6	0.000000000	0.000000000	2.391949000
6	0.000000000	0.000000000	0.991652000
6	0.000000000	1.213546000	0.250641000
6	0.000000000	1.206960000	-1.128710000
6	0.000000000	0.000000000	-1.831665000
6	0.000000000	-1.206960000	-1.128710000
6	0.000000000	-1.213546000	0.250641000
1	0.000000000	0.924525000	2.949675000
1	0.000000000	-0.924525000	2.949675000
1	0.000000000	2.152151000	0.788739000
1	0.000000000	2.143529000	-1.669624000
1	0.000000000	0.000000000	-2.912370000
1	0.000000000	-2.143529000	-1.669624000
1	0.000000000	-2.152151000	0.788739000

E(UB3LYP) = – 270.951541
ZVPE(UB3LYP) = 0.114443

3.1.5.2 Toluene – ^1A (C_s)

6	-2.417341000	0.000001000	0.009458000
6	-0.910850000	0.000001000	-0.010952000
6	-0.193469000	1.197365000	-0.008695000
6	1.196649000	1.200323000	0.001744000
6	1.897988000	-0.000001000	0.008124000
6	1.196647000	-1.200324000	0.001743000
6	-0.193470000	-1.197364000	-0.008696000
1	-2.822406000	0.882709000	-0.485746000
1	-2.795773000	-0.000072000	1.035156000
1	-2.822408000	-0.882639000	-0.485869000
1	-0.730048000	2.138536000	-0.017794000
1	1.731921000	2.141092000	0.001165000
1	2.979925000	-0.000002000	0.013354000
1	1.731918000	-2.141094000	0.001163000
1	-0.730051000	-2.138535000	-0.017796000

E(B3LYP) = – 271.575573
ZVPE(B3LYP) = 0.127598

3.2 UM06-2X/Def2QZVPP

3.2.1 Tellurium containing compounds

3.2.1.1 Phenyltelluryl radical **1** – $^2B_1$ (C_{2v})

52	0.000000000	0.000000000	1.566676000
6	0.000000000	0.000000000	-0.530279000
6	0.000000000	1.204659000	-1.235173000
6	0.000000000	1.201873000	-2.621661000
6	0.000000000	0.000000000	-3.315975000
6	0.000000000	-1.201873000	-2.621661000
6	0.000000000	-1.204659000	-1.235173000
1	0.000000000	2.140768000	-0.696000000
1	0.000000000	2.139103000	-3.159548000
1	0.000000000	0.000000000	-4.396542000
1	0.000000000	-2.139103000	-3.159548000
1	0.000000000	-2.140768000	-0.696000000

E(UM062X) = – 499.480813
ZVPE(UM062X) = 0.090663

3.2.1.2 Phenyltellenyl peroxy radical **8t** – ^2A (C_s)

6	2.923456000	1.045169000	-0.722775000
6	3.634007000	0.328678000	0.230218000
6	2.989797000	-0.612776000	1.019861000
6	1.630473000	-0.837797000	0.861284000
6	0.913722000	-0.123279000	-0.097259000
6	1.566387000	0.817203000	-0.892876000
8	-1.641629000	1.130148000	0.860352000
8	-2.922322000	1.261336000	0.944393000
1	1.013940000	1.369617000	-1.639136000
1	3.425623000	1.779075000	-1.336233000
1	4.692446000	0.505016000	0.357708000
1	3.543008000	-1.168878000	1.762717000
1	1.125761000	-1.562966000	1.482948000
52	-1.139158000	-0.456864000	-0.335705000

E(UM062X) = – 649.803488
ZVPE(UM062X) = 0.096100

3.2.1.3 Phenyltellenyl peroxy radical **8c** – ^2A (C_s)

6	-2.927430000	-0.849099000	0.775920000
6	-3.520803000	0.188276000	0.070907000
6	-2.748796000	1.026266000	-0.721518000
6	-1.380813000	0.822726000	-0.822493000
6	-0.781577000	-0.212565000	-0.107282000
6	-1.556979000	-1.046300000	0.696319000
8	1.748524000	1.084748000	0.986864000
8	1.238529000	2.205600000	0.607106000
1	-1.090471000	-1.840160000	1.261459000

1	-3.528371000	-1.498707000	1.395651000
1	-4.587782000	0.344788000	0.139942000
1	-3.211781000	1.835503000	-1.267304000
1	-0.778577000	1.468483000	-1.444071000
52	1.284595000	-0.504010000	-0.234395000

E(UM062X) = – 649.804024
ZVPE(UM062X) = 0.096194

3.2.1.4 **TS1** – ^{2}A (C_s)

8	1.738359000	1.186826000	0.880436000
8	1.738374000	1.186834000	-0.880411000
52	1.238396000	-0.424191000	-0.000002000
6	-0.829708000	-0.149777000	-0.000016000
6	-1.695194000	-1.236951000	-0.000001000
6	-3.064915000	-1.016148000	0.000010000
6	-3.555755000	0.281762000	0.000004000
6	-2.682304000	1.362703000	-0.000003000
6	-1.312416000	1.153381000	-0.000012000
1	-1.314786000	-2.250879000	0.000011000
1	-3.745651000	-1.854955000	0.000012000
1	-4.622605000	0.452318000	0.000002000
1	-3.070138000	2.371089000	0.000004000
1	-0.615514000	1.981264000	-0.000017000

E(UM062X) = – 649.777708
ZVPE(UM062X) = 0.094675

3.2.1.5 Phenyltellunoyl radical **9** – ^{2}A' (C_s)

8	0.712485000	-1.684469000	1.536151000
52	-0.115213000	-1.265546000	0.000000000
6	-0.129769000	0.836226000	0.000000000
6	-0.133416000	1.506730000	1.214670000
6	-0.133416000	2.894025000	1.206492000
6	-0.136834000	3.581492000	0.000000000
6	-0.133416000	2.894025000	-1.206492000
6	-0.133416000	1.506730000	-1.214670000
8	0.712485000	-1.684469000	-1.536151000
1	-0.109666000	0.954820000	2.144857000
1	-0.125323000	3.436469000	2.140542000
1	-0.137074000	4.661954000	0.000000000
1	-0.125323000	3.436469000	-2.140542000
1	-0.109666000	0.954820000	-2.144857000

E(UM062X) = – 649.838454
ZVPE(UM062X) = 0.096018