Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information for

Mechanism and Kinetic Properties for the Complete Series Reactions of Chloro(thio)phenols with O(^{3}P) in High Temperature Conditions

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Keywords

Chlorophenols, Chlorothiophenols, O(^{3}P), Formation mechanism, Rate constants

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Contains four figures and ten tables and thirty-one pages

Figure S1. MPWB1K/6-31+G(d,p) optimized geometries for phenol and 19 chlorophenols (provided by reference 44). Distances are in angstroms. Gray sphere, C; White sphere, H; Green sphere, Cl; Red sphere, O.

Figure S2. MPWB1K/6-31+G(d,p) optimized geometries for phenoxy radical and 19 chlorophenoxy radicals (provided by reference 44). Distances are in angstroms. Gray sphere, C; White sphere, H; Green sphere, Cl; Red sphere, O.

Figure S3. MPWB1K/6-31+G(d,p) optimized geometries for thiophenol and 19 chlorothiophenols (provided by reference 43). Distances are in angstroms. Gray sphere, C; White sphere, H; Green sphere, Cl; Yellow sphere, S.

Figure S4. MPWB1K/6-31+G(d,p) optimized geometries for thiophenoxy and 19 chlorothiophenoxy radicals (provided by reference 43). Distances are in angstroms. Gray spher, C; White sphere, H; Green sphere, Cl; Yellow sphere, S.

Table S1. Imaginary frequencies (in cm^{-1}), zero-point energies (ZPE, in a.u.) and total energies (in a.u.) for the transition states involved in the phenoxyl-hydrogen abstraction from chlorophenols by $O(^3P)$.

Table S2. Imaginary frequencies (in cm^{-1}), zero-point energies (ZPE, in a.u.) and total energies (in a.u.) for the transition states involved in the thiophenoxyl-hydrogen abstraction from chlorothiophenols by $O(^3P)$.

Table S3. Bond length parameters (*L*) of C-O and O-H bonds in chlorophenols and transition states, the bond length change values (*C*) and the bond length change ratio (*R*) of the transition states with respect to the chlorophenols. Distance are in angstroms.

Table S4. Bond length parameters (*L*) of C-S and S-H bonds in chlorothiophenols and transition states, the bond length change values (*C*) and the bond length change ratio (*R*) of the transition states with respect to the chlorothiophenols. Distance are in angstroms.

Table S5. Observed HOMO and LOMO energies, and HOMO-LOMO gap of chlorophenols calculated at MPWB1K/6-31+G(d,p) level.

Table S6. Observed HOMO and LOMO energies, and HOMO-LOMO gap of chlorothiophenols calculated at MPWB1K/6-31+G(d,p) level.

Table S7. Rate constants for the phenoxyl-hydrogen abstraction from chlorophenols by $O(^3P)$ over the temperature range of 600–1200 K.

Table S8. Rate constants for the thiophenoxyl-hydrogen abstraction from chlorothiophenols by $O(^3P)$ over the temperature range of 600–1200 K.

Table S9. Cartesian coordinates of the transition states for the phenoxyl-hydrogen abstraction from chlorophenols by $O(^3P)$.

Table S10. Cartesian coordinates for the transition states the thiophenoxyl-hydrogen abstraction from chlorothiophenols by $O(^3P)$.

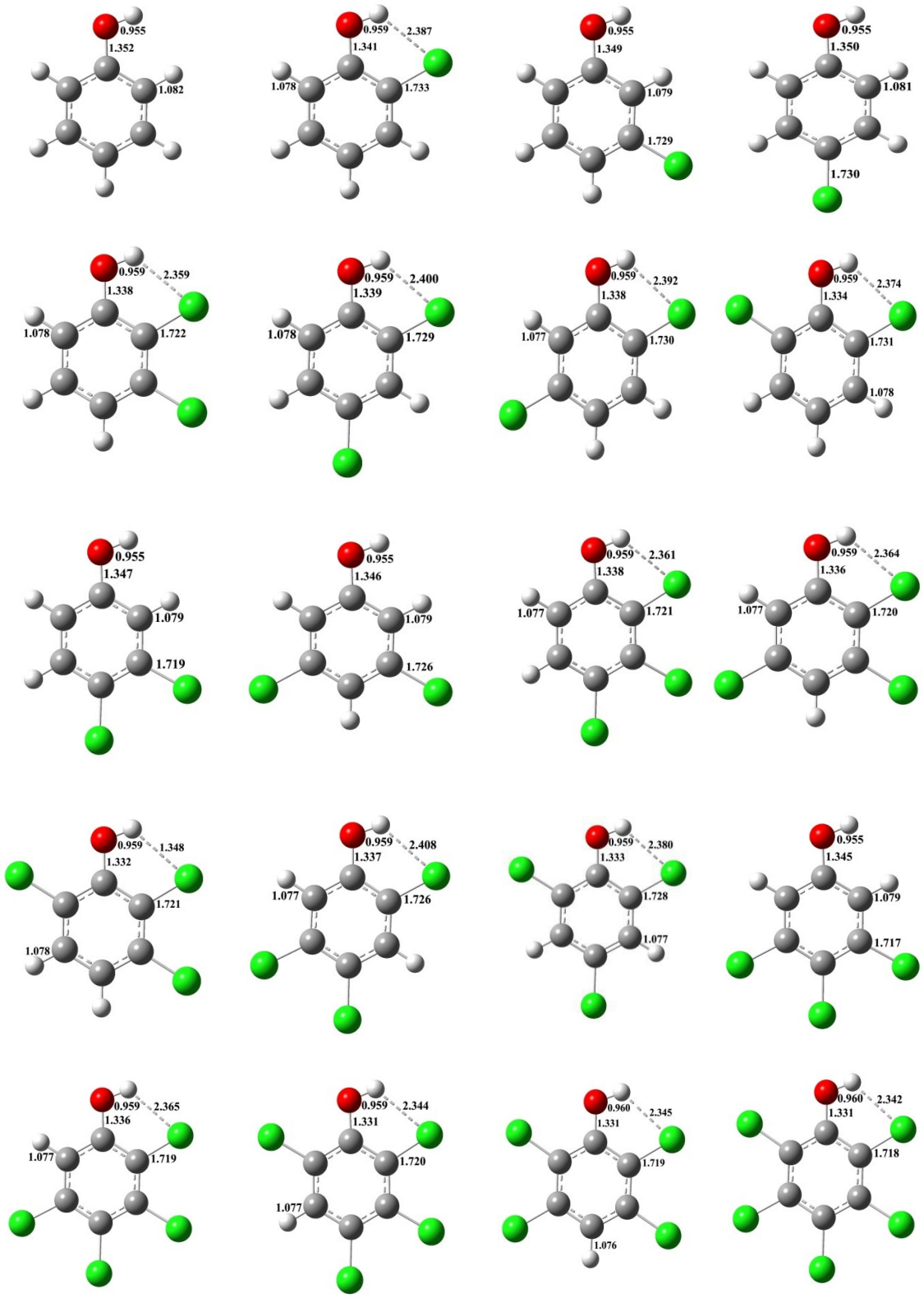
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Figure S1.

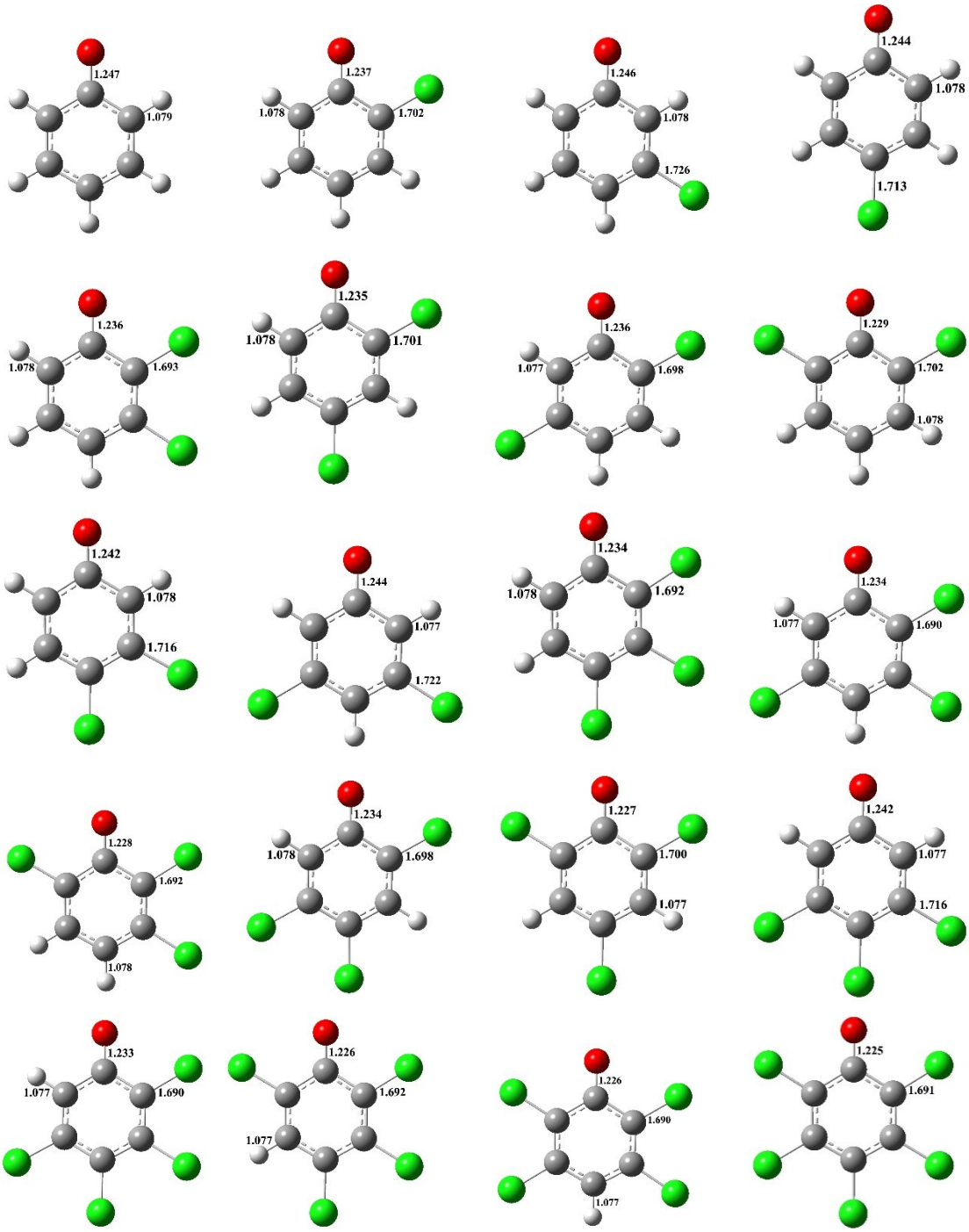
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Figure S2.

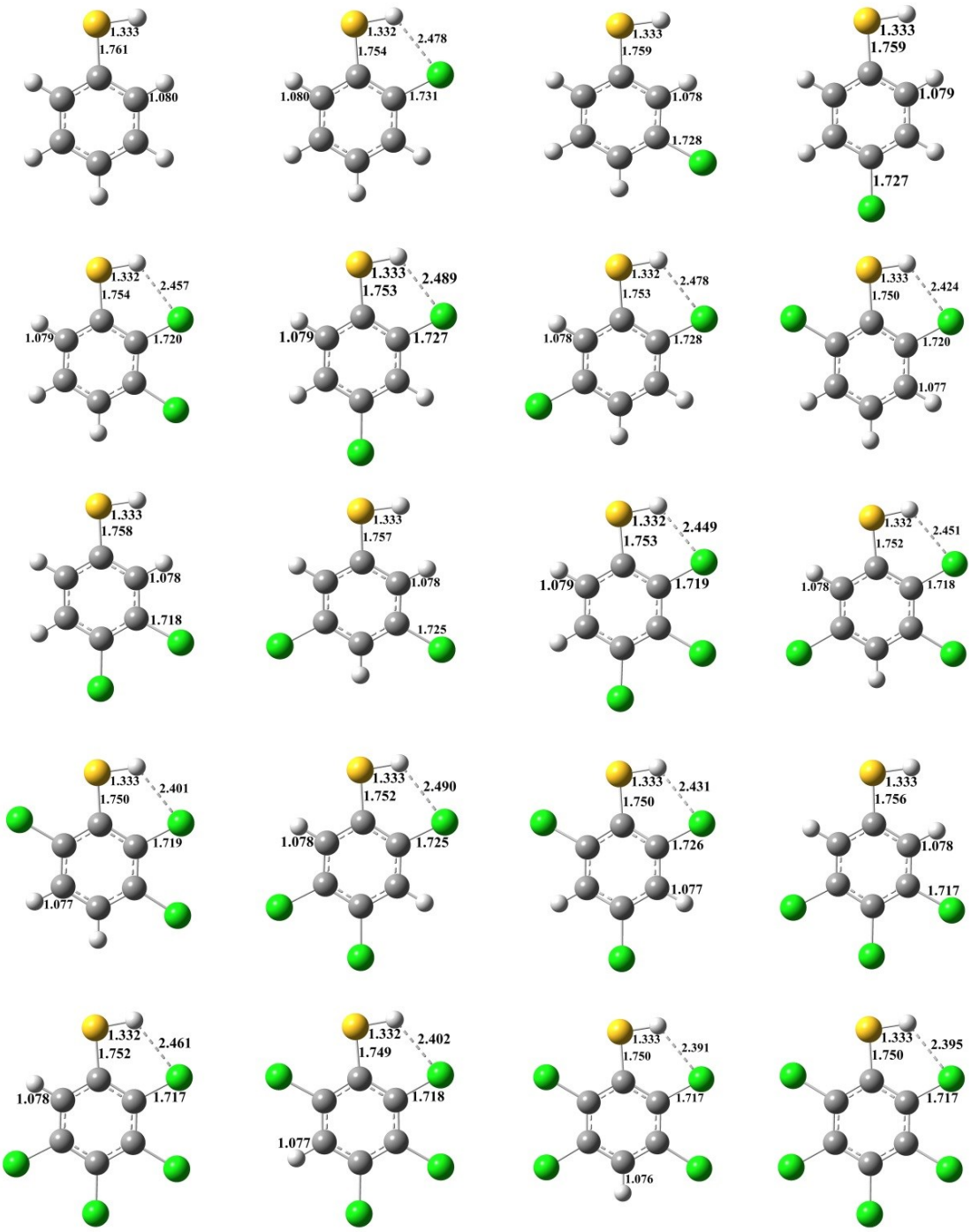
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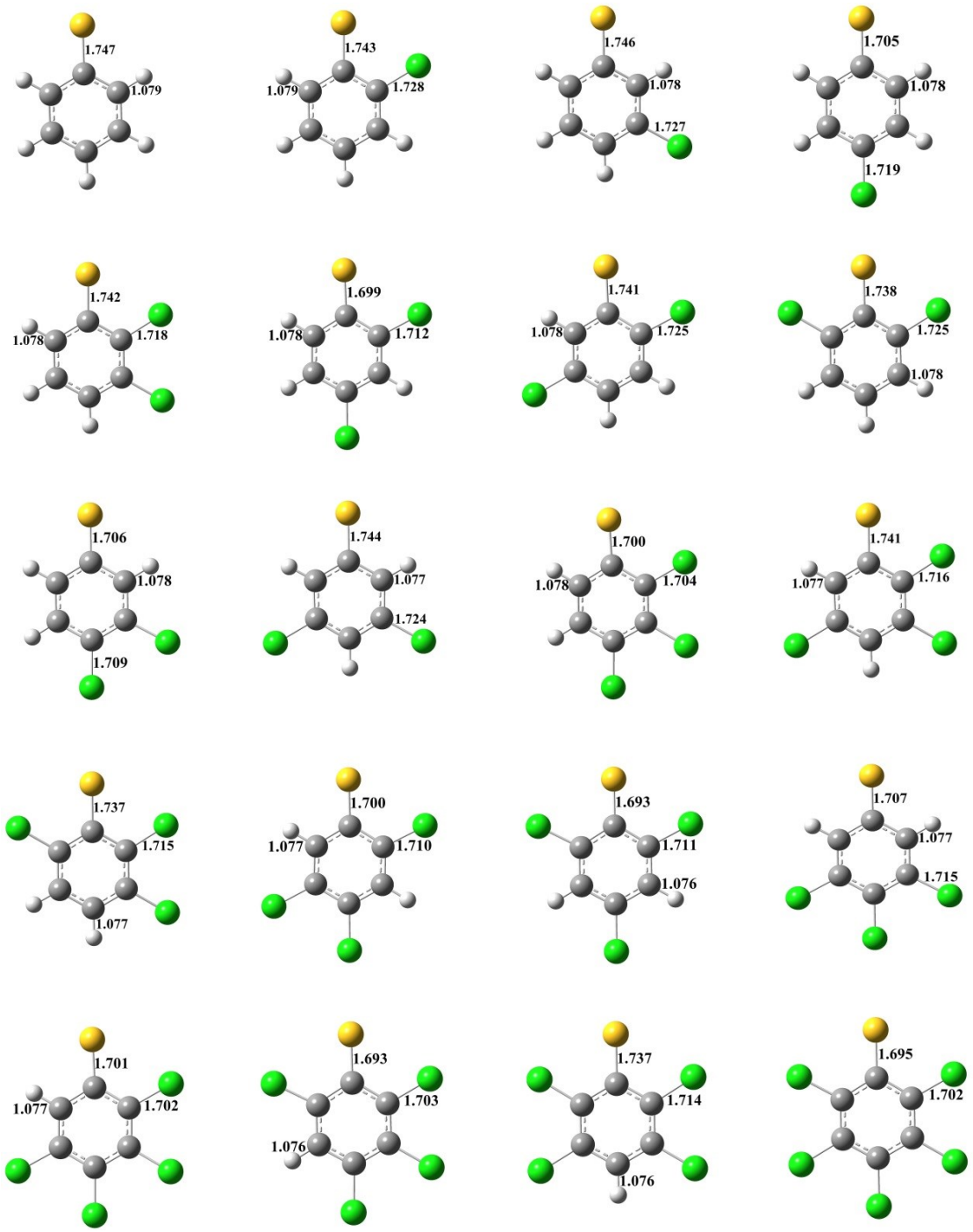
Figure S3.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1.077
1.702
1.693
1.703
1.076
1.737
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1.076
1.695
1.702

Figure S4.

Table S1. Imaginary frequencies (in cm^{-1}), zero point energies (ZPE, in a.u.) and total energies (in a.u.) for the transition states involved in the phenoxyl-hydrogen abstraction from chlorophenols by $O(^3P)$.

Transition states	Imaginary frequencies	ZPE	Total energies
TS(Phenol)	2272i	0.10227	−382.46701
TS(2-CP)	2550i	0.09211	−842.14845
TS(3-CP)	2424i	0.09205	−842.14502
TS(4-CP)	2273i	0.09248	−842.14951
TS(2,3-DCP)	2576i	0.08228	−1301.82634
TS(2,4-DCP)	2496i	0.08222	−1301.82987
TS(2,5-DCP)	2613i	0.08218	−1301.82893
TS(2,6-DCP)	2551i	0.08259	−1301.82732
TS(3,4-DCP)	2425i	0.08237	−1301.82691
TS(3,5-DCP)	2513i	0.08222	−1301.82987
TS(2,3,4-TCP)	2569i	0.07201	−1761.50443
TS(2,3,5-TCP)	2691i	0.07245	−1761.50571
TS(2,3,6-TCP)	2645i	0.07255	−1761.50465
TS(2,4,5-TCP)	2652i	0.07232	−1761.50680
TS(2,4,6-TCP)	2599i	0.07234	−1761.50773
TS(3,4,5-TCP)	2500i	0.07256	−1761.50047
TS(2,3,4,5-TeCP)	2712i	0.06260	−2221.18043
TS(2,3,4,6-TeCP)	2669i	0.06282	−2221.18188
TS(2,3,5,6-TeCP)	2710i	0.06253	−2221.18111
TS(PCP)	2700i	0.05285	−2680.85479

Table S2. Imaginary frequencies (in cm^{-1}), zero point energies (ZPE, in a.u.) and total energies (in a.u.) for the transition states involved in the thiophenoxyl-hydrogen abstraction from chlorothiophenols by $O(^3P)$.

Transition states	Imaginary frequencies	ZPE	Total energies
TS(Thiophenol)	506i	0.09920	−705.50941
TS(2-CTP)	531i	0.08915	−1165.19043
TS(3-CTP)	576i	0.08928	−1165.19089
TS(4-CTP)	523i	0.08945	−1165.19175
TS(2,3-DCTP)	1192i	0.07949	−1624.86830
TS(2,4-DCTP)	1046i	0.07928	−1624.87157
TS(2,5-DCTP)	1199i	0.07872	−1624.87115
TS(2,6-DCTP)	1292i	0.07953	−1624.86872
TS(3,4-DCTP)	586i	0.07938	−1624.85229
TS(3,5-DCTP)	651i	0.07927	−1624.87129
TS(2,3,4-TCTP)	1136i	0.06969	−2084.54587
TS(2,3,5-TCTP)	1227i	0.06945	−2084.54816
TS(2,3,6-TCTP)	1320i	0.06846	−2084.54581
TS(2,4,5-TCTP)	1053i	0.06952	−2084.54876
TS(2,4,6-TCTP)	1256i	0.06956	−2084.54884
TS(3,4,5-TCTP)	642i	0.06936	−2084.52897
TS(2,3,4,5-TeCTP)	1155i	0.06219	−2544.22227
TS(2,3,4,6-TeCTP)	1307i	0.05945	−2544.22257
TS(2,3,5,6-TeCTP)	1366i	0.05984	−2544.22228
TS(PCTP)	1327i	0.04953	−3003.37019

Table S3. Bond length parameters (*L*) of C-O and O-H bonds in chlorophenols and transition states, the bond length change values (*C*) and the bond length change ratio (*R*) of the transition states with respect to the chlorophenols. Distance are in angstroms.

	$L(\text{C-O})^{R}$	$L(\text{C-O})^{T}$	*C*(C-O)	*R*(C-O)	$L(\text{O-H})^{R}$	$L(\text{O-H})^{T}$	*C*(O-H)	*R*(O-H)
TS(Phenol)	1.352	1.314	−0.038	−2.81%	0.955	1.071	0.116	12.15%
TS(2-CP)	1.341	1.306	−0.035	−2.61%	0.959	1.088	0.129	13.45%
TS(3-CP)	1.349	1.312	−0.037	−2.74%	0.955	1.084	0.129	13.51%
TS(4-CP)	1.350	1.311	−0.039	−2.89%	0.955	1.070	0.115	12.04%
TS(2,3-DCP)	1.339	1.305	−0.034	−2.54%	0.959	1.094	0.135	14.08%
TS(2,4-DCP)	1.339	1.305	−0.034	−2.54%	0.959	1.083	0.124	12.93%
TS(2,5-DCP)	1.338	1.304	−0.034	−2.54%	0.959	1.096	0.137	14.29%
TS(2,6-DCP)	1.334	1.300	−0.034	−2.55%	0.959	1.088	0.129	13.45%
TS(3,4-DCP)	1.347	1.310	−0.037	−2.75%	0.955	1.081	0.126	13.19%
TS(3,5-DCP)	1.346	1.310	−0.036	−2.67%	0.955	1.095	0.140	14.66%
TS(2,3,4-TCP)	1.338	1.303	−0.035	−2.62%	0.959	1.090	0.131	13.66%
TS(2,3,5-TCP)	1.336	1.302	−0.034	−2.54%	0.959	1.105	0.146	15.22%
TS(2,3,6-TCP)	1.332	1.298	−0.034	−2.55%	0.959	1.095	0.136	14.18%
TS(2,4,5-TCP)	1.337	1.302	−0.035	−2.62%	0.959	1.095	0.136	14.18%
TS(2,4,6-TCP)	1.333	1.298	−0.035	−2.63%	0.959	1.088	0.129	13.45%
TS(3,4,5-TCP)	1.345	1.309	−0.036	−2.68%	0.955	1.090	0.135	14.14%
TS(2,3,4,5-TeCP)	1.336	1.301	−0.035	−2.62%	0.959	1.101	0.142	14.81%
TS(2,3,4,6-TeCP)	1.331	1.296	−0.035	−2.63%	0.959	1.094	0.135	14.08%
TS(2,3,5,6-TeCP)	1.331	1.296	−0.035	−2.63%	0.959	1.100	0.141	14.70%
TS(PCP)	1.331	1.295	−0.036	−2.70%	0.959	1.097	0.138	14.39%

Table S4. Bond length parameters (*L*) of C-S and S-H bonds in chlorothiophenols and transition states, the bond length change values (*C*) and the bond length change ratio (*R*) of the transition states with respect to the chlorothiophenols. Distance are in angstroms.

	L(C-S)^R	L(C-S)^T	C(C-S)	R(C-S)	L(S-H)^R	L(S-H)^T	C(S-H)	R(S-H)
TS(Thiophenol)	1.761	1.761	0.000	0.00%	1.333	1.400	0.067	5.03%
TS(2-CTP)	1.754	1.747	−0.007	−0.40%	1.332	1.419	0.087	6.53%
TS(3-CTP)	1.759	1.761	−0.002	−0.11%	1.333	1.404	0.071	5.33%
TS(4-CTP)	1.759	1.759	0.000	0.000	1.333	1.401	0.068	5.10%
TS(2,3-DCTP)	1.754	1.748	−0.006	−0.34%	1.332	1.424	0.092	6.91%
TS(2,4-DCTP)	1.753	1.746	−0.007	−0.40%	1.332	1.417	0.085	6.38%
TS(2,5-DCTP)	1.753	1.747	−0.006	−0.34%	1.332	1.425	0.093	6.98%
TS(2,6-DCTP)	1.750	1.745	−0.005	−0.29%	1.333	1.428	0.095	7.13%
TS(3,4-DCTP)	1.758	1.759	−0.001	−0.06%	1.333	1.404	0.071	5.33%
TS(3,5-DCTP)	1.757	1.761	−0.004	−0.23%	1.333	1.408	0.075	5.63%
TS(2,3,4-TCTP)	1.753	1.746	−0.007	−0.40%	1.332	1.421	0.089	6.68%
TS(2,3,5-TCTP)	1.752	1.748	−0.004	−0.23%	1.332	1.428	0.096	7.21%
TS(2,3,6-TCTP)	1.750	1.746	−0.004	−0.23%	1.333	1.431	0.098	7.35%
TS(2,4,5-TCTP)	1.752	1.747	−0.005	−0.29%	1.333	1.419	0.086	6.45%
TS(2,4,6-TCTP)	1.750	1.744	−0.006	−0.34%	1.333	1.427	0.094	7.05%
TS(3,4,5-TCTP)	1.756	1.759	−0.003	−0.17%	1.333	1.407	0.074	5.55%
TS(2,3,4,5-TeCTP)	1.752	1.747	−0.005	−0.29%	1.333	1.424	0.091	6.83%
TS(2,3,4,6-TeCTP)	1.749	1.744	−0.005	−0.29%	1.332	1.429	0.097	7.28%
TS(2,3,5,6-TeCTP)	1.750	1.746	−0.004	−0.23%	1.333	1.434	0.101	7.58%
TS(PCTP)	1.750	1.745	−0.005	−0.29%	1.333	1.432	0.099	7.43%

Table S5. Observed HOMO and LOMO energies, and HOMO-LOMO gap of chlorophenols calculated at MPWB1K/6-31+G(d,p) level.

	HOMO(eV)	LOMO(eV)	$E_{HOMO}-E_{LOMO}$(eV)
Phenol	−0.26580	0.01558	0.28138
2-CP	−0.27462	0.00361	0.27823
3-CP	−0.27555	0.00254	0.27809
4-CP	−0.26717	0.00169	0.26886
2,3-DCP	−0.28237	−0.00446	0.27791
2,4-DCP	−0.27550	−0.00934	0.26616
2,5-DCP	−0.28165	−0.00834	0.27331
2,6-DCP	−0.28182	−0.00680	0.27502
3,4-DCP	−0.27482	−0.00818	0.26664
3,5-DCP	−0.28754	−0.00837	0.27917
2,3,4-TCP	−0.28064	−0.01474	0.26590
2,3,5-TCP	−0.29050	−0.01530	0.27520
2,3,6-TCP	−0.28479	−0.01460	0.27019
2,4,5-TCP	−0.28171	−0.01856	0.26315
2,4,6-TCP	−0.28251	−0.01888	0.26363
3,4,5-TCP	−0.28290	−0.01698	0.26592
2,3,4,5-TeCP	−0.28715	−0.02355	0.26360
2,3,4,6-TeCP	−0.28550	−0.02419	0.26131
2,3,5,6-TeCP	−0.29308	−0.02127	0.27181
PCP	−0.29048	−0.02916	0.26132

Table S6. Observed HOMO and LOMO energies, and HOMO-LOMO gap of chlorothiophenols calculated at MPWB1K/6-31+G(d,p) level.

	HOMO(eV)	LOMO(eV)	$E_{HOMO}-E_{LOMO}$(eV)
Thiophenol	−0.25816	−0.01075	0.24741
2-CTP	−0.26557	−0.00009	0.26548
3-CTP	−0.26804	−0.00198	0.26606
4-CTP	−0.26174	−0.00231	0.25943
2,3-DCTP	−0.27259	−0.00842	0.26417
2,4-DCTP	−0.26858	−0.01228	0.25630
2,5-DCTP	−0.27477	−0.01214	0.26263
2,6-DCTP	−0.28181	−0.00679	0.27502
3,4-DCTP	−0.26923	−0.01219	0.25704
3,5-DCTP	−0.27780	−0.01201	0.26579
2,3,4-TCTP	−0.27333	−0.01685	0.25648
2,3,5-TCTP	−0.28117	−0.01957	0.26160
2,3,6-TCTP	−0.28479	−0.01460	0.27019
2,4,5-TCTP	−0.27548	−0.02168	0.25380
2,4,6-TCTP	−0.28249	−0.01886	0.26363
3,4,5-TCTP	−0.27646	−0.02012	0.25634
2,3,4,5-TeCTP	−0.27867	−0.02831	0.25036
2,3,4,6-TeCTP	−0.27911	−0.02605	0.25306
2,3,5,6-TeCTP	−0.28488	−0.02400	0.26088
PCTP	−0.28352	−0.03023	0.25329

Table S7. Rate constants for the phenoxyl-hydrogen abstraction from chlorophenols by $O(^3P)$ over the temperature range of 600–1200 K (units are cm^3 $molecule^{-1}$ s^{-1} for all reactions).

	600 K	700 K	800 K	900 K	1000 K	1100 K	1200K
TS(Phenol)	2.96E-14	7.50E-14	1.56E-13	2.58E-13	4.73E-13	2.98E-13	4.21E-13
TS(2-CP)	9.20E-16	3.19E-15	8.49E-15	1.88E-14	3.64E-14	6.39E-14	1.04E-13
TS(3-CP)	2.55E-16	8.49E-16	2.17E-15	4.63E-15	8.69E-15	1.48E-14	2.35E-14
TS(4-CP)	4.04E-15	9.79E-15	1.97E-14	3.51E-14	5.72E-14	8.69E-14	1.25E-13
TS(2,3-DCP)	1.11E-16	3.95E-16	1.07E-15	2.38E-15	4.63E-15	8.16E-15	1.33E-14
TS(2,4-DCP)	1.57E-16	4.89E-16	1.19E-15	2.46E-15	4.51E-15	7.56E-15	1.18E-14
TS(2,5-DCP)	3.62E-17	1.37E-16	3.86E-16	8.94E-16	1.80E-15	3.24E-15	5.40E-15
TS(2,6-DCP)	7.27E-16	2.30E-15	5.66E-15	1.17E-14	2.14E-14	3.58E-14	5.57E-14
TS(3,4-DCP)	1.29E-15	3.29E-15	6.90E-15	1.26E-14	2.09E-14	3.23E-14	4.70E-14
TS(3,5-DCP)	2.31E-18	6.26E-18	1.37E-17	2.59E-17	4.44E-17	7.04E-17	1.05E-16
TS(2,3,4-TCP)	6.02E-16	2.16E-15	5.94E-15	1.35E-14	2.69E-14	4.84E-14	8.05E-14
TS(2,3,5-TCP)	6.84E-18	2.71E-17	7.97E-17	1.91E-16	3.93E-16	7.25E-16	1.23E-15
TS(2,3,6-TCP)	1.34E-16	4.73E-16	1.26E-15	2.79E-15	5.39E-15	9.42E-15	1.52E-14
TS(2,4,5-TCP)	2.27E-16	8.22E-16	2.28E-15	5.23E-15	1.05E-14	1.89E-14	3.16E-14
TS(2,4,6-TCP)	6.22E-16	2.12E-15	5.60E-15	1.24E-14	2.41E-14	4.26E-14	6.97E-14
TS(3,4,5-TCP)	1.89E-16	6.46E-16	1.68E-15	3.64E-15	6.91E-15	1.19E-14	1.90E-14
TS(2,3,4,5-TeCP)	4.98E-19	1.83E-18	5.10E-18	1.17E-17	2.34E-17	4.22E-17	7.02E-17
TS(2,3,4,6-TeCP)	9.73E-17	3.23E-16	8.23E-16	1.75E-15	3.28E-15	5.58E-15	8.84E-15
TS(2,3,5,6-TeCP)	1.73E-17	5.61E-17	1.41E-16	2.96E-16	5.50E-16	9.32E-16	1.47E-15
TS(PCP)	1.16E-18	4.02E-18	1.08E-17	2.41E-17	4.74E-17	8.41E-17	1.38E-16

Table S8. Rate constants for the thiophenoxyl-hydrogen abstraction from chlorothiophenols by O(^{3}P) over the temperature range of 600–1200 K (units are cm^3 molecule^{-1} s^{-1} for all reactions).

	600 K	700 K	800 K	900 K	1000 K	1100 K	1200 K
TS(Thiophenol)	4.11E-18	4.03E-17	2.33E-16	3.15E-17	1.04E-16	2.81E-16	6.58E-16
TS(2-CTP)	3.49E-14	6.16E-14	9.82E-14	1.46E-13	2.06E-13	2.78E-13	3.65E-13
TS(3-CTP)	1.33E-16	4.29E-16	1.06E-15	2.18E-15	3.96E-15	6.51E-15	9.98E-15
TS(4-CTP)	4.56E-16	1.37E-15	3.21E-15	6.35E-15	1.11E-14	1.79E-14	2.69E-14
TS(2,3-DCTP)	9.91E-14	1.92E-13	3.27E-13	5.08E-13	7.38E-13	1.02E-12	1.35E-12
TS(2,4-DCTP)	6.56E-14	1.17E-13	1.87E-13	2.77E-13	3.86E-13	5.16E-13	6.66E-13
TS(2,5-DCTP)	1.59E-13	1.02E-12	7.72E-12	6.95E-11	6.88E-10	6.62E-09	5.81E-16
TS(2,6-DCTP)	2.08E-14	4.56E-14	8.83E-14	1.53E-13	2.46E-13	3.72E-13	5.34E-13
TS(3,4-DCTP)	2.62E-12	3.33E-12	3.99E-12	4.59E-12	5.13E-12	5.63E-12	6.08E-12
TS(3,5-DCTP)	7.20E-13	1.26E-12	1.99E-12	2.92E-12	4.06E-12	5.42E-12	7.00E-12
TS(2,3,4-TCTP)	6.99E-15	1.53E-14	2.84E-14	4.73E-14	7.29E-14	1.06E-13	1.46E-13
TS(2,3,5-TCTP)	9.61E-14	1.81E-13	3.01E-13	4.61E-13	6.64E-13	9.11E-13	1.21E-12
TS(2,3,6-TCTP)	5.36E-20	2.96E-19	1.13E-18	3.33E-18	8.14E-18	1.73E-17	3.29E-17
TS(2,4,5-TCTP)	2.75E-16	5.05E-16	8.28E-16	1.25E-15	1.77E-15	2.41E-15	3.14E-15
TS(2,4,6-TCTP)	3.56E-16	7.79E-13	1.40E-15	2.22E-15	3.19E-15	4.31E-15	5.53E-15
TS(3,4,5-TCTP)	2.83E-16	1.75E-15	7.12E-15	2.19E-14	5.49E-14	1.19E-13	2.29E-13
TS(2,3,4,5-TeCTP)	6.68E-14	1.09E-13	1.58E-13	2.10E-13	2.64E-13	3.19E-13	3.73E-13
TS(2,3,4,6-TeCTP)	1.01E-14	1.72E-14	2.65E-14	3.81E-14	7.76E-14	1.04E-13	1.33E-13
TS(2,3,5,6-TeCTP)	1.95E-14	4.27E-14	7.97E-14	1.33E-13	2.06E-13	2.99E-13	4.14E-13
TS(PCTP)	3.57E-15	7.09E-15	1.23E-14	1.95E-14	2.89E-14	4.06E-14	5.48E-14

Table S9. Cartesian coordinates of the transition states for the phenoxyl-hydrogen abstraction from chlorophenols by O(^{3}P).

TS(Phenol)

0 3

C	1.188406	-0.579710	0.000000
C	2.481419	-0.984711	-0.243660
C	2.807040	-2.347894	-0.163549
C	1.819300	-3.284522	0.169167
C	0.527097	-2.865357	0.385140
C	0.206413	-1.514100	0.307831
H	2.102423	-4.322556	0.236791
H	-0.238133	-3.586454	0.626178
H	-0.806144	-1.189536	0.489131
O	4.018916	-2.780506	-0.428747
H	4.775318	-2.100371	-0.093011
O	5.544727	-1.478539	0.757210
H	0.936247	0.467570	-0.057345
H	3.254869	-0.275654	-0.495819

TS(2-CP)

0 3

C	0.101449	-0.362319	0.000000
C	-1.051192	0.348173	-0.259261
C	-1.016484	1.747608	-0.405710
C	0.215003	2.402155	-0.270836
C	1.365100	1.686986	-0.038833
C	1.310768	0.304048	0.101099
H	0.219898	3.475260	-0.373991
H	2.309173	2.201406	0.044787
H	2.210846	-0.256902	0.296169
O	-2.074710	2.450844	-0.707879
H	-3.030348	2.176293	-0.266181
O	-3.950803	2.064288	0.606952
Cl	-2.562815	-0.448987	-0.365058
H	0.047607	-1.432397	0.117200

TS(3-CP)

0 3

C	-0.768116	0.594203	0.000000
C	-2.037957	0.146915	-0.276403
C	-3.099286	1.064637	-0.255868
C	-2.860586	2.411864	0.045024
C	-1.574159	2.833144	0.292592
C	-0.518075	1.932236	0.280539

H	-3.699017	3.088510	0.065127
H	-1.380043	3.871216	0.511226
H	0.488920	2.255641	0.486583
O	-4.321775	0.691191	-0.551026
H	-4.564048	-0.293604	-0.168077
O	-4.870736	-1.181494	0.701981
H	-2.226992	-0.888926	-0.508099
Cl	0.546593	-0.520212	-0.015159

TS(4-CP)

0 3

C	-0.028593	-1.115550	-0.029967
C	-1.377677	-0.894886	-0.173707
C	-1.901342	0.396235	-0.000178
C	-1.041161	1.453931	0.324912
C	0.309470	1.234627	0.443265
C	0.811059	-0.050576	0.270897
H	-1.465450	2.434561	0.467335
H	0.981935	2.043272	0.678440
O	-3.177432	0.648719	-0.165642
H	-3.792714	-0.157108	0.175888
O	-4.397042	-0.950252	1.025271
H	-2.046757	-1.704789	-0.419630
H	0.384346	-2.102718	-0.158109
Cl	2.498625	-0.327422	0.434186

TS(2,3-DCP)

0 3

C	0.594203	-0.724638	0.000000
C	-0.751874	-0.975281	-0.205605
C	-1.658685	0.103089	-0.266270
C	-1.183178	1.409145	-0.106625
C	0.159783	1.638858	0.070021
C	1.051304	0.578250	0.128392
H	-1.902973	2.210031	-0.145927
H	0.527114	2.646969	0.175136
H	2.104415	0.747240	0.281066
O	-2.926863	-0.073507	-0.519256
H	-3.449785	-0.917744	-0.061090
O	-4.010734	-1.614090	0.830218
Cl	1.723741	-2.012757	0.092752
Cl	-1.368622	-2.557100	-0.347641

TS(2,4-DCP)

0 3

C	0.086957	-1.028986	0.000000
C	-1.223735	-0.635359	-0.155704
C	-1.566715	0.726335	-0.240634
C	-0.540174	1.674201	-0.148870
C	0.770993	1.290116	-0.018991
C	1.077817	-0.063323	0.057587
H	-0.816567	2.714661	-0.202396
H	1.559544	2.022431	0.032975
O	-2.787552	1.137985	-0.450009
H	-3.604444	0.639249	0.057383
O	-4.400147	0.299588	1.002018
H	0.334064	-2.074856	0.071734
Cl	2.713712	-0.554565	0.237568
Cl	-2.474511	-1.800887	-0.208226

TS(2,5-DCP)

0 3

C	-0.072464	-1.101449	0.000000
C	0.879756	-2.067653	-0.248029
C	0.501668	-3.410476	-0.432452
C	-0.855222	-3.747197	-0.346774
C	-1.790084	-2.767368	-0.126265
C	-1.411533	-1.441230	0.052498
H	-1.133976	-4.779466	-0.476191
H	-2.158970	-0.687334	0.236035
O	1.356770	-4.350707	-0.725044
H	2.336138	-4.354457	-0.234175
O	3.203273	-4.490122	0.669932
Cl	2.541741	-1.670078	-0.292116
H	0.235687	-0.079282	0.147237
Cl	-3.460376	-3.180836	-0.054185

TS(2,6-DCP)

0 3

C	-0.578670	-0.478121	-0.036594
C	-0.230304	-1.785931	-0.286035
C	-1.202203	-2.800798	-0.379934
C	-2.548901	-2.430203	-0.197806
C	-2.900385	-1.118508	0.028097
C	-1.915713	-0.146366	0.111168
H	-3.940513	-0.863835	0.146781

H	-2.192924	0.878498	0.298762
O	-0.908193	-4.033560	-0.667939
H	-0.031776	-4.491295	-0.214983
O	0.716702	-5.023030	0.666656
Cl	1.413838	-2.233209	-0.451373
H	0.191372	0.271868	0.036924
Cl	-3.749577	-3.643972	-0.286170

TS(3,4-DCP)

0 3

C	-0.072464	-0.304348	0.000000
C	1.290986	-0.278555	-0.181367
C	2.024770	-1.472542	-0.169438
C	1.363725	-2.691413	0.030421
C	0.001178	-2.708676	0.184622
C	-0.729434	-1.524023	0.178396
O	3.318203	-1.477309	-0.373881
H	3.809098	-0.627849	0.078854
O	4.296151	0.116006	1.012421
H	-0.524539	-3.638848	0.325594
H	1.945018	-3.598446	0.049513
H	1.799812	0.659751	-0.333638
Cl	-0.940943	1.173755	-0.012781
Cl	-2.422890	-1.594268	0.393041

TS(3,5-DCP)

0 3

C	0.130435	-0.014493	0.000000
C	1.113440	-0.949295	-0.222780
C	0.753117	-2.303393	-0.285048
C	-0.581511	-2.693780	-0.119652
C	-1.535973	-1.724095	0.074474
C	-1.201326	-0.378523	0.145125
O	1.645241	-3.230262	-0.533524
H	2.607956	-3.045414	-0.044939
O	3.439121	-2.986242	0.901435
H	-0.831480	-3.740431	-0.157289
H	2.142915	-0.657706	-0.352043
Cl	0.545695	1.653460	0.085876
Cl	-3.186255	-2.177739	0.255187
H	-1.959694	0.368163	0.309002

TS(2,3,4-TCP)

0 3

C	-0.768116	-0.318841	0.000000
C	-2.132631	-0.117095	-0.147442
C	-2.662332	1.186475	-0.208347
C	-1.790857	2.274945	-0.106988
C	-0.440689	2.076344	0.011495
C	0.077779	0.788133	0.068826
H	-2.214843	3.264718	-0.143261
H	0.236834	2.911746	0.071729
O	-3.930146	1.415053	-0.406915
H	-4.671222	0.794019	0.096416
O	-5.393963	0.322232	1.027871
Cl	-0.138948	-1.903686	0.084073
Cl	-3.224890	-1.421846	-0.218425
Cl	1.767220	0.587525	0.235739

TS(2,3,5-TCP)

0 3

C	-0.811525	-0.782609	-0.010623
C	0.079002	-1.828095	-0.190244
C	-0.412248	-3.147229	-0.279502
C	-1.787036	-3.383243	-0.171315
C	-2.644995	-2.323309	-0.021728
C	-2.173745	-1.021115	0.063900
H	-2.138585	-4.399286	-0.228000
H	-2.855187	-0.197709	0.193793
O	0.371391	-4.161648	-0.508611
H	1.366281	-4.201737	-0.029548
O	2.227099	-4.339876	0.860947
Cl	-0.253967	0.832752	0.113509
Cl	1.761188	-1.585345	-0.263371
Cl	-4.339389	-2.601674	0.078672

TS(2,3,6-TCP)

0 3

C	0.347826	-0.855072	0.000000
C	0.997408	0.347500	-0.204859
C	2.407292	0.398352	-0.249164
C	3.125183	-0.798073	-0.067837
C	2.464665	-1.992534	0.111480
C	1.083277	-2.022456	0.148661
H	3.031492	-2.900797	0.231403
H	0.562038	-2.953032	0.300504

O	3.052664	1.496525	-0.496474
H	2.722608	2.434557	-0.038853
O	2.521971	3.315323	0.842059
Cl	-1.362553	-0.932984	0.068089
Cl	0.150610	1.816394	-0.371025
Cl	4.831347	-0.747283	-0.098698

TS(2,4,5-TCP)

0 3

C	0.391304	-0.362319	0.000000
C	1.553444	-1.082482	-0.148745
C	1.520183	-2.487076	-0.230948
C	0.279384	-3.126226	-0.143871
C	-0.883981	-2.406116	-0.023817
C	-0.831765	-1.011337	0.052825
H	0.258569	-4.202019	-0.193195
O	2.584267	-3.211299	-0.427404
H	3.524146	-2.924397	0.055079
O	4.396279	-2.762587	0.955687
H	0.426768	0.711882	0.070134
Cl	-2.252723	-0.077431	0.218461
Cl	3.065454	-0.288973	-0.190910
Cl	-2.378989	-3.240547	0.042913

TS(2,4,6-TCP)

0 3

C	-0.579710	0.173913	0.000000
C	-1.907305	0.505504	-0.136865
C	-2.340049	1.844870	-0.162591
C	-1.355039	2.843469	-0.030077
C	-0.021589	2.525148	0.082224
C	0.354901	1.191477	0.098882
H	0.716427	3.304936	0.164098
O	-3.579907	2.182951	-0.342790
H	-4.366292	1.606574	0.138418
O	-5.141691	1.155911	1.046236
H	-0.275062	-0.858434	0.025817
Cl	2.016499	0.792034	0.254190
Cl	-3.092731	-0.722686	-0.237751
Cl	-1.845689	4.478998	-0.035969

TS(3,4,5-TCP)

0 3

C	-0.304348	-0.739130	0.000000

C	0.991617	-1.158711	-0.178257
C	1.278524	-2.528400	-0.215585
C	0.246733	-3.459793	-0.067682
C	-1.047718	-3.027504	0.083328
C	-1.349883	-1.660805	0.128954
O	2.494268	-2.967221	-0.420416
H	3.254313	-2.379605	0.094327
O	3.955011	-1.952109	1.065470
H	0.481089	-4.510574	-0.084700
H	1.785048	-0.438337	-0.292371
Cl	-0.620053	0.944971	0.046263
Cl	-2.951791	-1.130025	0.333916
Cl	-2.293621	-4.194925	0.234509

TS(2,3,4,5-TeCP)

0 3

C	0.260870	1.130435	0.000000
C	1.417181	0.401739	-0.108833
C	2.654444	1.041058	-0.202445
C	2.704087	2.446715	-0.138932
C	1.536512	3.178983	0.002023
C	0.301561	2.527151	0.061174
O	3.716156	0.313556	-0.391195
H	4.664475	0.597062	0.091662
O	5.529276	0.758100	0.985494
H	1.393496	-0.674044	-0.145296
Cl	4.230181	3.195092	-0.196296
Cl	-1.136319	3.423575	0.213426
Cl	-1.233090	0.295435	0.073605
Cl	1.604496	4.881470	0.091544

TS(2,3,4,6-TeCP)

0 3

C	-0.637681	0.057971	0.000000
C	0.690773	0.425559	-0.135733
C	1.720904	-0.535971	-0.160865
C	1.361995	-1.890035	-0.033199
C	0.044749	-2.260992	0.075246
C	-0.952004	-1.298338	0.095334
H	-0.218962	-3.301920	0.154527
O	2.964189	-0.218515	-0.340805
H	3.373375	0.674380	0.139860
O	3.834693	1.439630	1.037616
Cl	-2.573173	-1.814467	0.251228

Cl	1.152295	2.061079	-0.237755
Cl	2.590637	-3.072946	-0.040292
Cl	-1.865139	1.241013	0.039751

TS(2,3,5,6-TeCP)

0 3

C	0.144481	-0.362288	0.012321
C	-0.172453	0.972644	-0.154619
C	0.852855	1.938154	-0.211407
C	2.196406	1.527631	-0.086050
C	2.486792	0.183060	0.054113
C	1.468287	-0.754691	0.105261
H	1.708455	-1.797556	0.224144
O	0.602136	3.193014	-0.417889
H	-0.250901	3.674403	0.083701
O	-0.952774	4.175528	0.992757
Cl	-1.078575	-1.556765	0.097574
Cl	-1.780961	1.518038	-0.254284
Cl	4.103579	-0.366111	0.182175
Cl	3.412888	2.712131	-0.133086

TS(PCP)

0 3

C	-0.028986	-0.275362	0.000000
C	-1.122412	0.560907	-0.129505
C	-0.963037	1.957400	-0.167585
C	0.333664	2.494302	-0.056208
C	1.430959	1.658301	0.045540
C	1.253682	0.271699	0.076572
O	-1.962006	2.762499	-0.342140
H	-2.917649	2.573293	0.163094
O	-3.785534	2.497522	1.072945
Cl	-0.251983	-1.964982	0.054794
Cl	-2.710574	-0.045817	-0.204018
Cl	3.001496	2.315685	0.144720
Cl	0.501824	4.184386	-0.077359
Cl	2.602393	-0.755545	0.214962

Table S10. Cartesian coordinates for the transition states the thiophenoxyl-hydrogen abstraction from chlorothiophenols by $O(^3P)$.

TS(Thiophenol)

0 3

C	0.0579263	-1.3478261	0.0022759

C	1.3822223	-1.4718691	-0.3752321
C	2.0157143	-2.7072221	-0.2926831
C	1.3078923	-3.8177751	0.1536209
C	-0.0186957	-3.6897571	0.5236169
C	-0.6431937	-2.4555681	0.4511119
H	1.8043563	-4.7738021	0.2072159
H	4.3082473	-2.4910181	0.3739729
H	1.9331543	-0.6175181	-0.7356791
S	3.6876553	-2.8836821	-0.8173951
H	-1.6777527	-2.3572211	0.7417109
H	-0.5639337	-4.5540441	0.8698129
H	-0.4289597	-0.3868831	-0.0581581
O	4.9193873	-2.1217001	1.6516889

TS(2-CTP)

0 3

C	-0.5215603	-0.6231884	0.0136575
C	0.7152177	-1.1850464	-0.2415805
C	0.8755247	-2.5707754	-0.2863085
C	-0.2439153	-3.3711824	-0.0711145
C	-1.4859463	-2.8134204	0.1564975
C	-1.6234273	-1.4368484	0.2038535
H	-0.1198633	-4.4425884	-0.0818235
H	-2.3398483	-3.4531024	0.3131835
H	-2.5866393	-0.9906864	0.3950045
H	3.2387267	-2.5961124	0.1675635
S	2.3872957	-3.3547754	-0.6776505
O	3.6795257	-2.0779384	1.3929365
Cl	2.0594657	-0.1370574	-0.4822725
H	-0.6131583	0.4499986	0.0545395

TS(3-CTP)

0 3

C	0.0144928	-0.3623188	0.0000000
C	-1.2108013	-0.8896228	-0.3585290
C	-2.3177773	-0.0515708	-0.4202860
C	-2.1852353	1.3020782	-0.1333650
C	-0.9516313	1.8086192	0.2299350
C	0.1560818	0.9813082	0.2982530
H	-3.0478753	1.9454082	-0.1978180
H	-0.8461523	2.8575702	0.4581630
H	1.1222728	1.3698732	0.5763530
H	-4.4077133	-0.9331148	0.3469370
H	-1.3091123	-1.9379498	-0.5875520

S	-3.8715083	-0.7058738	-0.9302790
Cl	1.3918338	-1.3998608	0.0767770
O	-4.8915793	-1.1807598	1.6856670

TS(4-CTP)

0 3

C	0.7681159	-0.3188406	0.0000000
C	-0.5914111	-0.2224206	-0.2222840
C	-1.2679461	0.9632644	0.0426330
C	-0.5596491	2.0614964	0.5174960
C	0.8013929	1.9765034	0.7377780
C	1.4539599	0.7838504	0.4795670
H	-1.0815881	2.9843004	0.7149290
H	-3.4554471	0.5944314	0.9407700
H	-1.1365431	-1.0711186	-0.6037300
S	-2.9916181	1.0969714	-0.2815470
H	1.3543109	2.8246754	1.1072200
H	1.2962789	-1.2369136	-0.1993170
Cl	3.1514629	0.6712284	0.7548120
O	-3.8767241	0.0859344	2.2439630

TS(2,3-DCTP)

0 3

C	-0.2028986	-0.4347826	0.0000000
C	-1.5246326	-0.8000086	-0.2223070
C	-2.5205516	0.1825804	-0.2160940
C	-2.1668236	1.5084554	0.0057540
C	-0.8466756	1.8626964	0.1961120
C	0.1355195	0.8926544	0.1998000
H	-2.9446006	2.2544864	0.0314740
H	-0.5822666	2.8949044	0.3605220
H	1.1694845	1.1475214	0.3642640
H	-4.3510776	-1.3187626	0.2455080
Cl	-1.9331206	-2.4417106	-0.4835140
Cl	1.0489705	-1.6103876	0.0191500
S	-4.1988626	-0.1589516	-0.5658000
O	-4.3137616	-2.0202476	1.4456530

TS(2,4-DCTP)

0 3

C	-0.0579710	-0.6521739	0.0000000
C	1.2788790	-0.9650669	-0.1532380
C	1.7161190	-2.2907009	-0.1433420
C	0.7617230	-3.2912899	0.0199880

C	-0.5799240	-2.9978189	0.1457340
C	-0.9782660	-1.6735629	0.1395680
H	1.0911770	-4.3177199	0.0506300
H	-1.3073790	-3.7835279	0.2643460
H	3.9830330	-1.8914039	0.5403130
Cl	2.3947120	0.3294001	-0.3343800
S	3.3783350	-2.7581459	-0.4042660
O	4.2209450	-1.2795119	1.7852730
H	-0.3761060	0.3766621	0.0025140
Cl	-2.6453030	-1.2828239	0.3162830

TS(2,5-DCTP)

0 3

C	-2.8550724	-0.6231884	0.0000000
C	-1.8578764	-1.5561144	-0.2116670
C	-2.1653924	-2.9138964	-0.3071060
C	-3.4954824	-3.3056024	-0.1904500
C	-4.4855284	-2.3623994	-0.0088270
C	-4.1749414	-1.0186454	0.0934940
H	-3.7463364	-4.3526564	-0.2374610
H	0.0337406	-3.7085554	0.2587520
Cl	-0.2321934	-1.0097634	-0.3338960
S	-0.9770374	-4.1499634	-0.6431830
H	-2.5939724	0.4191386	0.0830250
Cl	-6.1270324	-2.8726304	0.1165400
H	-4.9549194	-0.2917454	0.2493440
O	0.5273976	-3.3615774	1.5082150

TS(2,6-DCTP)

0 3

C	0.5072464	0.1884058	0.0000000
C	0.8857674	-1.1163842	-0.2450760
C	-0.0429816	-2.1626742	-0.2699930
C	-1.3840346	-1.8204652	-0.0666060
C	-1.7760886	-0.5154262	0.1586970
C	-0.8267136	0.4865418	0.1986670
H	1.6084694	-3.8492502	0.1596220
Cl	2.5580144	-1.4292562	-0.5098310
S	0.3962754	-3.8195222	-0.5947700
H	1.2591404	0.9594768	0.0240700
H	-1.1278986	1.5053028	0.3830040
H	-2.8208606	-0.2985122	0.3068200
Cl	-2.6042566	-3.0335272	-0.1082230
O	2.3233984	-3.7741162	1.3337880

TS(3,4-DCTP)

0 3

C	1.2173913	-0.0724638	0.0000000
C	2.5589793	0.1693932	-0.2330110
C	3.4536213	-0.8846818	-0.3480850
C	2.9917463	-2.1913948	-0.2405890
C	1.6552953	-2.4337888	-0.0058210
C	0.7619423	-1.3812008	0.1157280
H	5.6051633	-0.5375478	0.6347400
S	5.1481493	-0.5606198	-0.6925750
H	3.6823443	-3.0128768	-0.3414260
Cl	0.1451453	1.2601632	0.1387990
Cl	-0.8925797	-1.7247128	0.4010900
O	6.0041483	-0.5117088	2.0245100
H	2.9049933	1.1859122	-0.3236560
H	1.2867683	-3.4427048	0.0826160

TS(3,5-DCTP)

0 3

C	-0.4347826	-0.0579710	0.0000000
C	0.9117684	-0.1533730	-0.2905210
C	1.4889794	-1.4121250	-0.4004440
C	0.7210204	-2.5576790	-0.2379510
C	-0.6254366	-2.4272230	0.0430680
C	-1.2192276	-1.1849620	0.1684350
H	1.1700794	-3.5324420	-0.3296940
H	3.7141414	-1.3962470	0.4796040
H	1.5053184	0.7342780	-0.4314780
S	3.1934544	-1.5646110	-0.8173700
Cl	-1.1628796	1.4968360	0.1485180
Cl	-1.5892136	-3.8410290	0.2450110
H	-2.2696066	-1.0967110	0.3893870
O	4.1663964	-1.2802930	1.8295970

TS(2,3,4-TCTP)

0 3

C	-0.6811594	-0.9565217	0.0000000
C	0.7004146	-1.0373057	-0.1572940
C	1.3431236	-2.2780217	-0.1632570
C	0.5780546	-3.4289817	-0.0172930
C	-0.7904784	-3.3595467	0.1093500
C	-1.4208584	-2.1295817	0.1234610
H	3.5200226	-1.4972517	0.4989820

Cl	1.6148626	0.3989133	-0.3215560
S	3.0582986	-2.4637097	-0.4350680
H	-1.3802094	-4.2547497	0.2157260
H	1.0742836	-4.3856657	-0.0000070
Cl	-1.4655204	0.5606993	0.0260820
Cl	-3.1241134	-2.0822667	0.3067040
O	3.6495126	-0.8867937	1.7493190

TS(2,3,5-TCTP)

0 3

C	1.5072464	-0.3188406	0.0000000
C	2.5230694	-1.2488516	-0.1808210
C	2.2024364	-2.6094376	-0.2284770
C	0.8785354	-3.0098906	-0.1035810
C	-0.1151977	-2.0646696	0.0441610
C	0.1874834	-0.7201516	0.1046730
H	4.4013174	-3.3909726	0.3696370
Cl	4.1474494	-0.7351666	-0.3284060
S	3.3915024	-3.8563336	-0.5256700
H	0.6353334	-4.0592766	-0.1159020
Cl	1.8462904	1.3608054	0.0836350
Cl	-1.7545257	-2.5698396	0.1827680
H	-0.5877857	0.0151484	0.2376380
O	4.8737524	-2.9840106	1.5996090

TS(2,3,6-TCTP)

0 3

C	0.3623188	-0.6231884	0.0000000
C	1.1017678	0.5294356	-0.2249600
C	2.5039498	0.4876426	-0.2207840
C	3.1206178	-0.7493224	-0.0215860
C	2.3792188	-1.8968544	0.1803750
C	1.0041258	-1.8318864	0.1999840
H	2.7148958	2.8334546	0.2491310
Cl	0.2905328	2.0113796	-0.5003960
S	3.4868718	1.9005386	-0.5126470
Cl	-1.3530272	-0.5934464	0.0201290
H	0.4161728	-2.7188294	0.3683910
H	2.8855538	-2.8357854	0.3300370
Cl	4.8341738	-0.8853214	-0.0342070
O	2.1709678	3.2940476	1.4185430

TS(2,4,5-TCTP)

0 3

C	1.2173913	-0.4057971	0.0000000
C	1.2768693	-1.7930091	-0.0474740
C	2.5030333	-2.4152841	-0.1751130
C	3.6797633	-1.6864681	-0.2901010
C	3.5994733	-0.2933201	-0.2479950
C	2.3821963	0.3355589	-0.0921020
H	5.9446383	-1.9539941	0.4559610
H	2.5467473	-3.4920371	-0.1824790
H	2.3329983	1.4106229	-0.0501020
Cl	-0.1387087	-2.7521081	0.0717220
Cl	-0.2712017	0.4211989	0.1774850
Cl	5.0112423	0.6753459	-0.3662310
S	5.1662883	-2.5630051	-0.5623230
O	6.3024513	-1.4816341	1.7242990

TS(2,4,6-TCTP)

0 3

C	-1.6086956	-0.6231884	0.0000000
C	-2.0199656	0.6938366	0.0229730
C	-3.3661216	0.9765276	-0.0954700
C	-4.3265666	-0.0282684	-0.2521280
C	-3.8549476	-1.3446014	-0.2928250
C	-2.5168996	-1.6514964	-0.1537150
H	-6.5559916	-0.6648134	0.3526510
H	-2.1906676	-2.6771394	-0.1746310
Cl	0.0632144	-0.9889544	0.1616620
Cl	-4.9475416	-2.6545024	-0.5051300
S	-6.0096876	0.3864276	-0.4429910
O	-6.7289726	-1.3576374	1.5343910
Cl	-3.8372086	2.6289936	-0.0604950
H	-1.3081706	1.4932416	0.1380230

TS(3,4,5-TCTP)

0 3

C	1.0144058	-0.0579710	-0.0132793
C	2.3756368	-0.0568220	-0.2445543
C	3.0617128	-1.2566810	-0.3536393
C	2.3750078	-2.4561430	-0.2441763
C	1.0137608	-2.4542090	-0.0129613
C	0.3121308	-1.2558910	0.1060727
H	5.2370118	-1.2556720	0.6364927
S	4.7873138	-1.2572570	-0.6968513
H	2.8968618	-3.3936740	-0.3383383
Cl	0.2039228	1.4480360	0.1190217

Cl	-1.3697072	-1.2554100	0.3861287
Cl	0.2025028	-3.9597590	0.1197567
O	5.6178578	-1.2549070	2.0177767
H	2.8979558	0.8804110	-0.3390953

TS(2,3,4,5-TeCTP)

0 3

C	0.8840580	-0.5797101	0.0000000
C	2.1459610	-1.1440001	-0.1510050
C	2.2923180	-2.5323671	-0.1858240
C	1.1652880	-3.3314991	-0.0752520
C	-0.0905800	-2.7755931	0.0437630
C	-0.2452620	-1.3951761	0.0893220
H	4.5897400	-2.6180831	0.5159190
Cl	3.5209300	-0.1368671	-0.2757150
S	3.8238090	-3.3299081	-0.4509730
H	1.2709820	-4.4035041	-0.0778120
Cl	0.7048710	1.1171379	0.0600380
Cl	-1.7959860	-0.7077341	0.2605830
Cl	-1.4426230	-3.8220991	0.1585960
O	4.9019780	-2.1132891	1.7700340

TS(2,3,4,6-TeCTP)

0 3

C	-0.3623188	-0.3188406	0.0000000
C	-1.7095658	-0.6330516	-0.1476260
C	-2.7007008	0.3565944	-0.1257220
C	-2.2845288	1.6813444	0.0175250
C	-0.9520048	2.0084474	0.1416960
C	0.0053712	1.0153114	0.1414120
H	-4.4541448	-1.1641166	0.4835920
Cl	-2.1612008	-2.2707616	-0.3475860
S	-4.3962838	0.0055574	-0.3349540
Cl	1.6472012	1.4640564	0.3195020
Cl	0.8252222	-1.5446156	-0.0065380
H	-0.6561108	3.0379814	0.2483810
Cl	-3.4233118	2.9664754	0.0282050
O	-4.3360998	-1.8412986	1.6732840

TS(2,3,5,6-TeCTP)

0 3

C	-0.2028986	-0.8115942	0.0000000
C	0.2054845	-2.1270902	-0.1694890
C	-0.7402536	-3.1592242	-0.1814660

C	-2.0967466	-2.8371652	-0.0575380
C	-2.4877126	-1.5131892	0.0903260
C	-1.5430576	-0.5088152	0.1261230
H	0.8984475	-4.8264942	0.3908100
Cl	1.8697085	-2.4744332	-0.3588130
S	-0.2917726	-4.8314912	-0.4089470
Cl	0.9260875	0.4772448	0.0390510
Cl	-3.2771876	-4.0734762	-0.1017720
O	1.5560005	-4.6980072	1.5749640
Cl	-4.1390646	-1.0844492	0.2460540
H	-1.8524966	0.5150518	0.2489240

TS(PCTP)

0 3

C	-1.1449275	-0.0289855	0.0000000
C	-2.3852015	0.5814095	-0.1344700
C	-2.5081135	1.9733905	-0.1228890
C	-1.3462035	2.7411735	-0.0150300
C	-0.0988105	2.1394835	0.0959760
C	0.0013885	0.7519825	0.1142360
H	-4.8199805	1.9086615	0.5253770
Cl	-3.7788555	-0.3940465	-0.3066560
S	-4.0440855	2.7819125	-0.3031480
Cl	-1.0210525	-1.7306425	0.0087800
Cl	-1.4508645	4.4472385	-0.0356600
Cl	1.3102465	3.0933575	0.2207400
Cl	1.5265425	0.0075335	0.2707000
O	-5.1275175	1.3160235	1.7169700