Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting Information

Auto-Catalytic Mechanism and Radical/Ion Pair Formation in the Electrochemical Reduction of Arene Sulfonyl Chlorides

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I- Chemicals

Synthesis of diphenyl disulfone (**3c**):

120 mg of sodium phenyl sulfinate, dissolved in minimum amount of methanol, and 100 mg of phenyl sulfonyl chloride were mixed in 5 ml of freshly distilled acetonitrile. The solution was stirred at room temperature and the reaction was monitored by HPLC. After completion, the solvent was evaporated under reduced pressure, the residue was washed several times with chloroform, and then filtered. The combined mother liquor was dried under reduced pressure to afford a solid. The obtained solid was washed several times with minimum amounts of methanol, and then left to dry to give white solid, mp =191-193 ºC. m/z (%): 282 (M^+, 9.0), 250 (20), 141 (30), 125 (80), 109 (46), 77 (100). ^{1}H- NMR (CD_3CN, 400 MHz); δ 7.89 (2H, *tt*, *J*= 1.2, 7.6 Hz); 7.78 (4H, *dt*, *J*= 1.2, 7.2 Hz); 7.66 (4H, *td*, *J*= 1.2, 7.6 Hz). ^{13}C NMR (CD_3CN, 600 MHz); 131.14, 131.96, 132.11, 138.06.

II- Electrochemical data

I-1. Cyclic voltammetry of 4-methoxyphenyl sulfonyl chloride (**1a**):

This is a typical cyclic voltammorgam of the studied substituted sulfonyl chlorides showing the oxidation of the generated sulfinate anion (4-methoxyphenyl sulfinate in this example at Ep = 0.43 V/SCE) and of the chloride anion at Ep = 1.16 V/SCE.

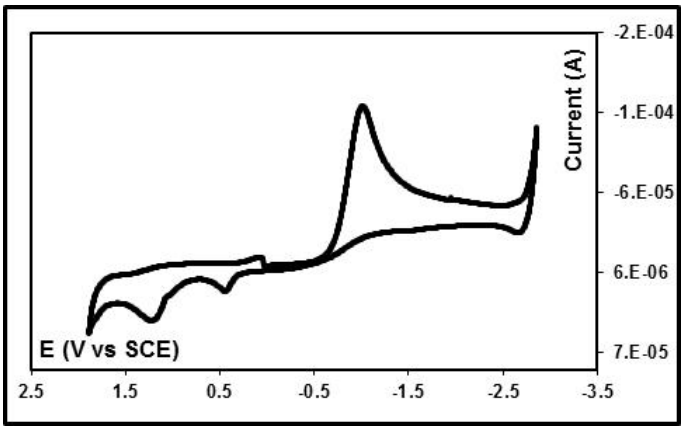

Figure S1. Cyclic voltammogram of 4-methoxyphenyl sulfonyl chloride, **1a**, (6.0 mM), in acetonitrile containing 0.10 M Bu_4NPF_6.

II-2. Cyclic voltammetry of 4-cynaophenyl sulfonyl chloride (**1f**):

Figure S2 shows the complete cyclic voltammograms of 4-cyanophenyl sulfonyl chloride at three different scan rates 0.2, 1.2 and 5V/s. At low scan rate two reversible reduction peaks are observed at E^0_1 = -2.185 V and = E^0_2 = -2.3 V vs SCE corresponding to the sulfinic acid and sulfinate anion, respectively. The sulfinic acid is obtained through protonation of the anion and/or hydrogen abstraction by the sulfinyl radical. Increasing the scan rate, the first reversible peak gradually decreases at the expense of the second one as seen on Figure S2b, at 1.2 V/s. At 5V/s only one reversible peak corresponding to the reversible reduction of the sulfinate anion is observed, as at this time scale the sulfinic acid is not formed.

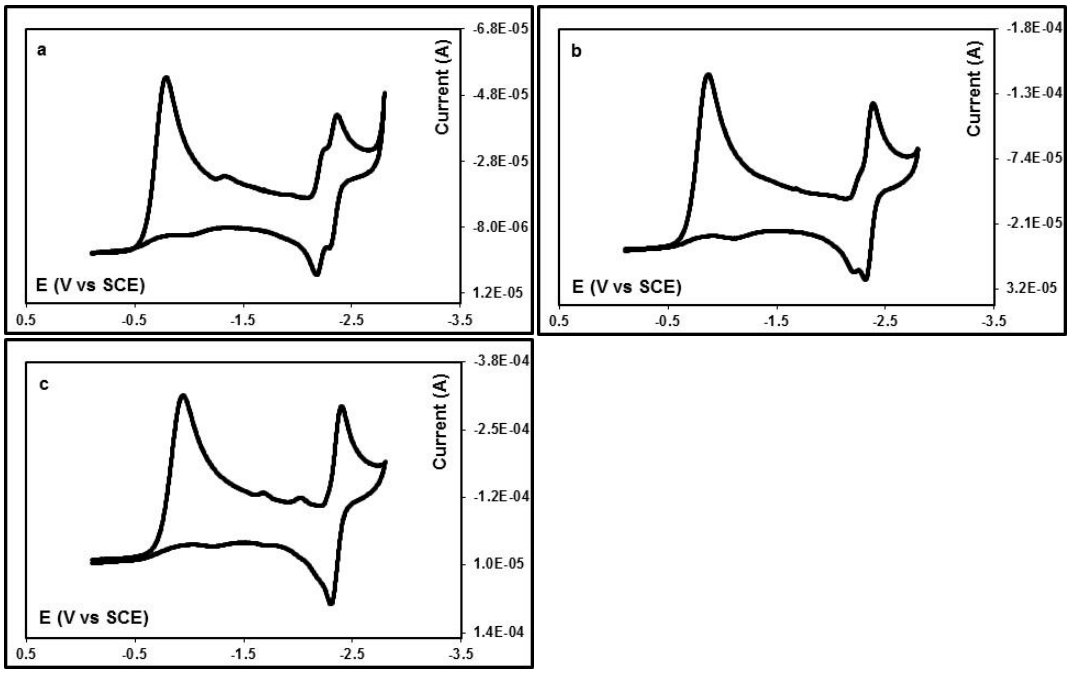

Figure S2. Cyclic voltammogram of 4-cyanophenyl sulfonyl chloride, **1f**, (2.03 mM) in CH_3CN/ Bu_4NPF_6 (0.1M) at (a) v = 0.2 V/s; (b) v = 1.2 V/s; and (c) v = 5.0 V/s.

II-3. Cyclic voltammetry of compounds **1c-3c.**

Figure S3a shows the cyclic voltammetry of $PhSO_2Cl$ (**1c**) in acetonitrile in the presence of Bu_4NPF_6 (0.1 M). This cyclic voltammogram shows one reduction peak at -1.00 V vs SCE corresponding to the reductive cleavage of the S-Cl bond of the initial compound, and two oxidation peaks at 0.46 and 1.16 V vs SCE corresponding to the oxidation of the phenyl sulfinate and chloride anions, respectively. Figure S3b shows the cyclic voltammetry of diphenyl disulfone (**3c**) as one reduction peak is observed at -1.05 V vs SCE corresponding to the reductive cleavage of the S-S chemical bond, and an oxidation peak at 0.46 V vs SCE corresponding to the oxidation of the phenyl sulfinate anion. Figure S3c shows the cyclic voltammetry of s-phenyl benzenethiosulfonate, $PhSO_2SPh$, (**2c**). Two reduction peaks are observed at –1.00 and -1.65 V vs SCE corresponding to the reduction of the initial compound and diphenyl disulfide, respectively. The disulfide is generated through reduction at the first peak of $PhSO_2SPh$. Upon reversing the scan, two oxidation peaks are observed at -0.18 and 0.46 V vs SCE corresponding to the oxidation of the phenyl thiolate and the phenyl sulfinate anions, respectively. It is important to note that the reduction of all three compounds produce an anodic peak at 0.46 V vs SCE corresponding to the oxidation of the phenyl sulfinate anion (Figure S3).

II-4. Cyclic voltammetry of the phenyl sulfinate in the absence and presence of **1c**.

Figure S4a shows the cyclic voltammetry of sodium phenyl sullfinate. It shows a single anodic peak at 0.46 V vs SCE corresponding to the oxidation of this anion. Figure S4b shows the cyclic voltammetry of $PhSO_2Cl$ (**1c**) before adding the phenyl sulfinate salt. When a mixture of $PhSO_2Cl$ and $PhSO_2Na$ are mixed in a 1:1 mole ratio, the homogenous electron transfer reaction takes place to afford the diphenyl disulfone and its peak is observed on the cyclic voltammogram (Figure S4c).

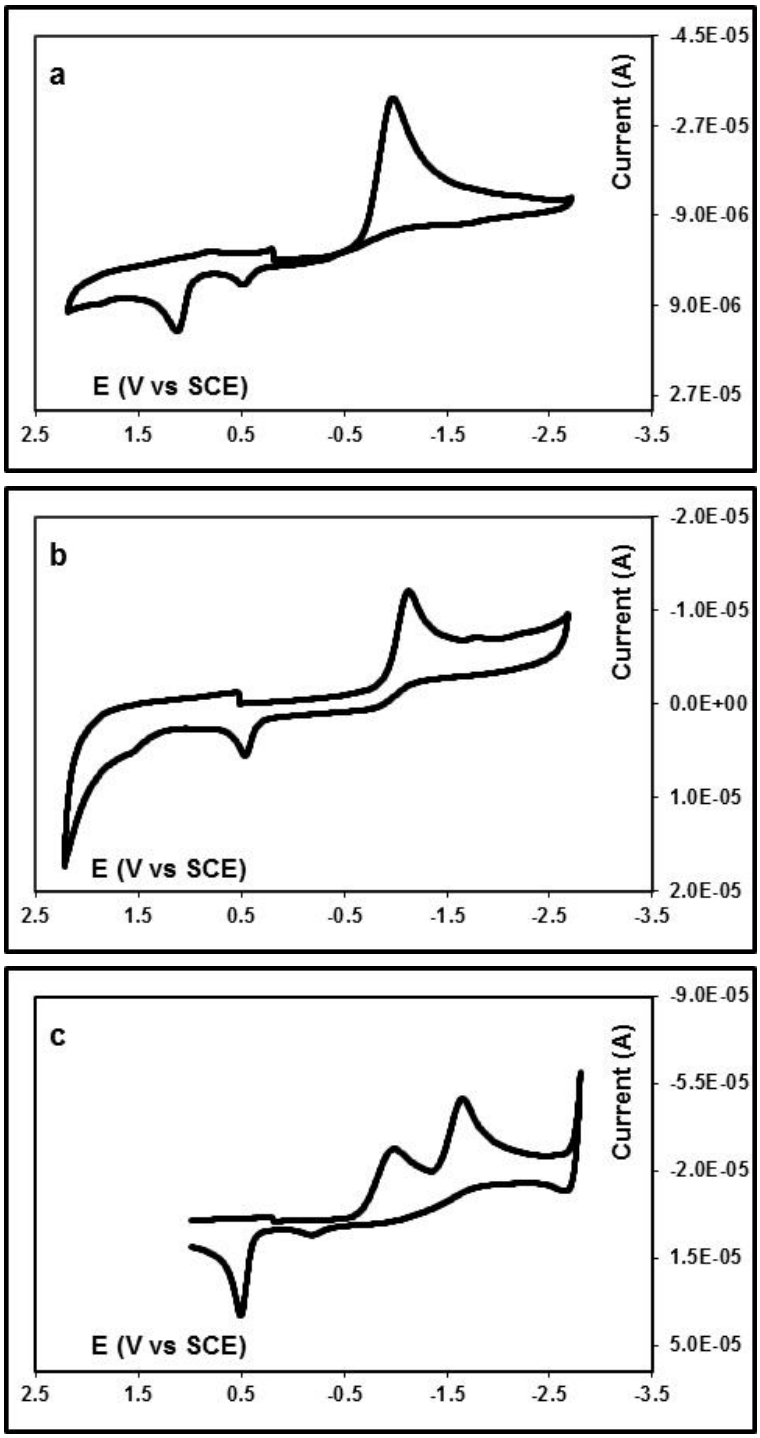

Figure S3. Cyclic voltammetry in CH_3CN/ Bu_4NPF_6 (0.1 M) at a glassy carbon electrode and at v = 200 mV/s of (a) $PhSO_2Cl$ (1.53 mM); (b) $PhSO_2SO_2Ph$ (1.48 mM); and (c) $PhSO_2SPh$ (2.36 mM).

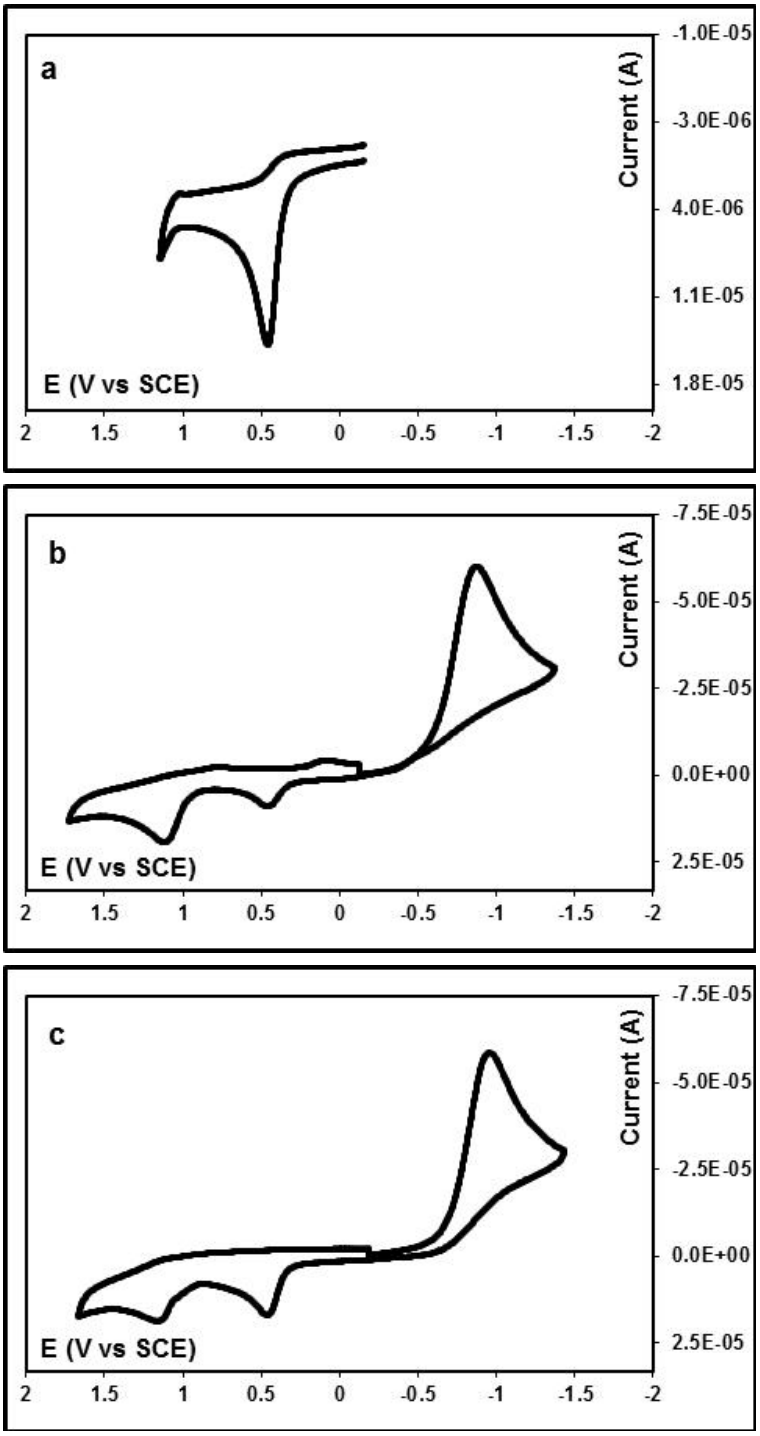

Figure S4. Cyclic voltammetry in CH_3CN/Bu_4NPF_6 (0.1 M) at a glassy carbon electrode and at v = 200 mV/s of (a) $PhSO_2Na$ (1.34 mM); (b) $PhSO_2Cl$ (2.32 mM); and (c) a mixture of $PhSO_2Cl$ (2.32mM) and $PhSO_2Na$ (2.50 mM).

II-5. Variation of the reduction peak potential with the scan rate for compounds **1a-g**:

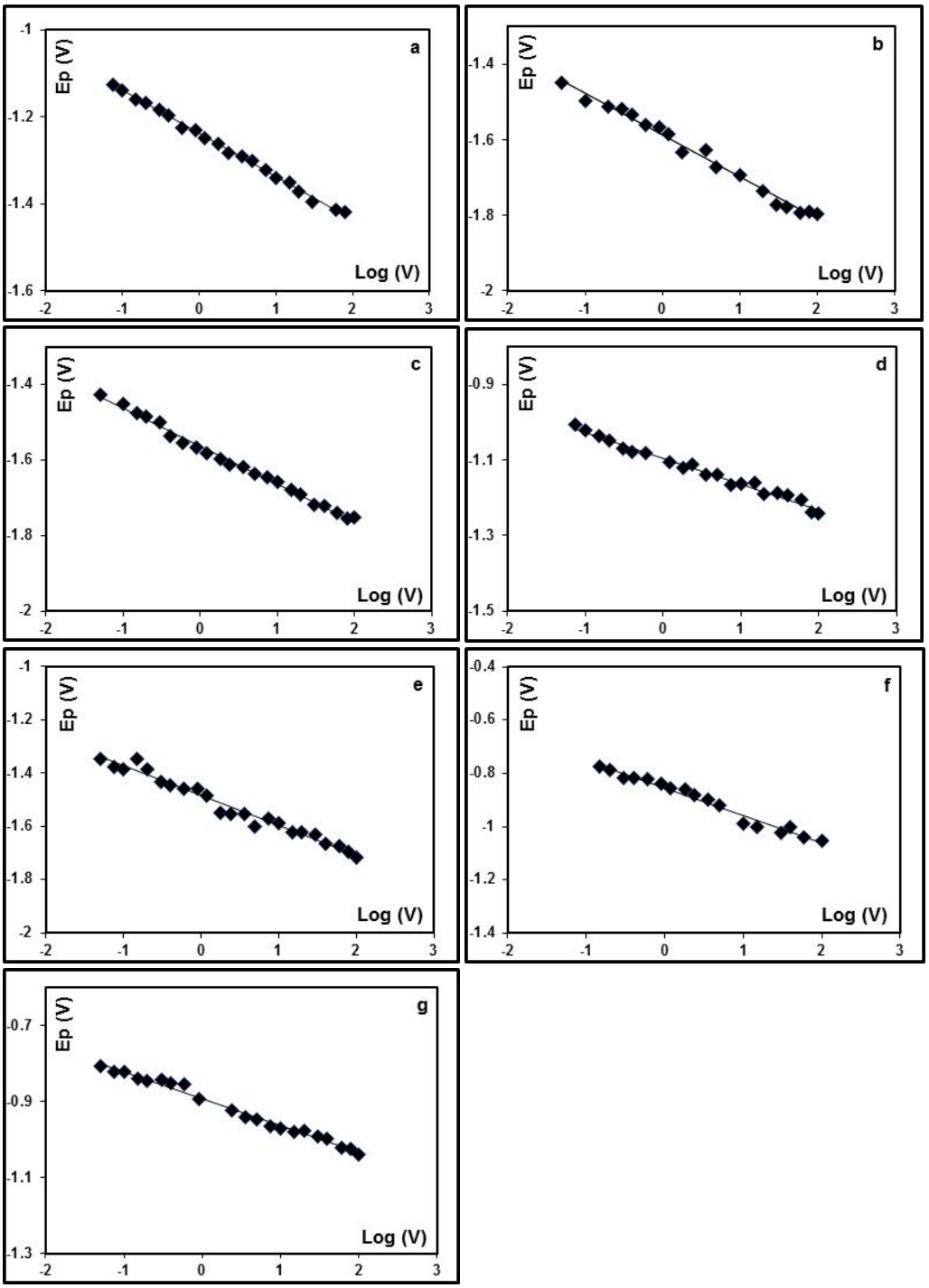

Figure S5: Variation of the reduction peak potential with the log of the scan rate (log (ν)) for (a) **1a** (2.06 mM); (b) **1b** (1.52 mM); (c): **1c** (1.53 mM); (d): **1d** (1.90 mM); (e): **1e** (1.20 mM); (f) **1f** (2.03 mM); and (g) **1g** (1.70 mM);

II-6. Cyclic voltammetry as a function of the concentration and the scan rate

II-6.1. 4-methylphenyl sulfonyl chloride (**1b**):

Similar to what is reported for the phenyl sulfonyl chloride in the manuscript, all the investigated compounds show a similar dependence on the concentration and scan rate. Two additional examples are presented here. The variation of the cyclic voltammograms of the sulfonyl chloride **1b** in CH_3CN/Bu_4NPF_6 (0.1 M) with the scan rate at two different concentrations (1.4 mM and 5.7 mM) are shown as a typical example on Figure S6. For the low concentration (1.4 mM), the crossing observed at 0.2 V/s (Figure S6a) decreases very quickly as the scan rate is increased to 0.3V/s (Figure S6b) and is eliminated at 0.6 V/s (Figure S6c). For the higher concentration (5.7 mM), the crossing that is more pronounced at 0.2 V/s (Figure S6d) still persists when increasing the scan rate to 0.6 V/s (Figure S6e) and disappears only at much higher scan rates (5 V/s or higher) as shown on Figure S6f. These results confirm the occurrence of an autocatalytic process that is more pronounced for high concentrations and low scan rates. Similar observations can be made for the 4-nitrophenyl sulfonyl chloride as shown in Figure S7.

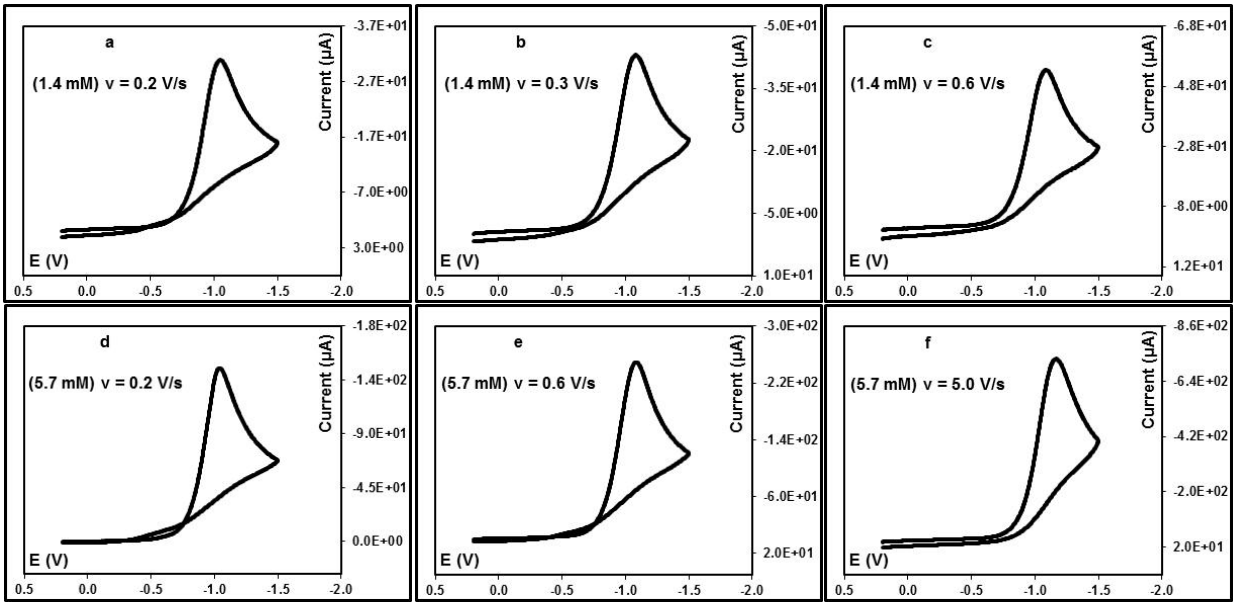

Figure S6. Cyclic voltammetry in CH_3CN/Bu_4NPF_6 (0.1 M) at a glassy carbon electrode of **1b** at (a) 1.4 mM, v = 0.2 V/s; (b) 1.4 mM, v = 0.3 V/s (c): 1.4 mM, v = 0.6 V/s; (d): 5.7 mM, v = 0.2 V/s; (e): 5.7 mM, v = 0.6 V/s; and (f) 5.7 mM, v = 5 V/s.

II-6.2. 4-nitrophenyl sulfonyl chloride (**1g**):

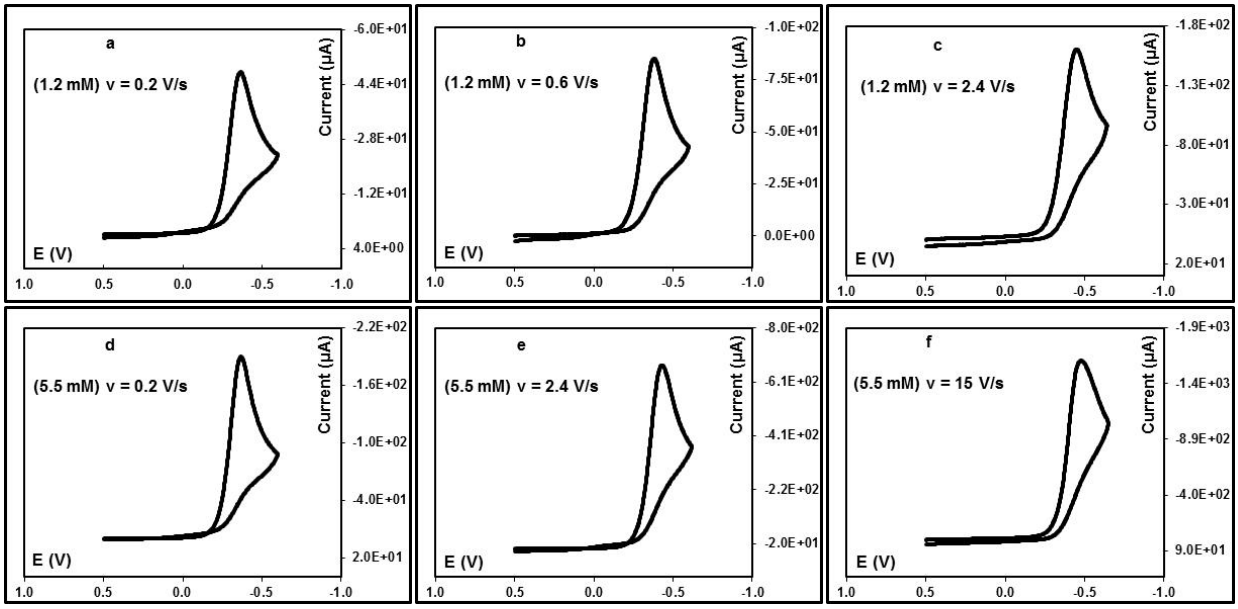

Figure S7. Cyclic voltammetry in CH_3CN/ Bu_4NPF_6 (0.1 M) at a glassy carbon electrode of **1g** at (a) 1.2 mM, v = 0.2 V/s; (b) 1.2 mM, v = 0.6 V/s (c): 1.2 mM, v = 2.4 V/s; (d): 5.5 mM, v = 0.2 V/s; (e): 5.5 mM, v = 2.4 V/s; and (f) 5.5 mM, v = 15 V/s.

II-7 Cyclic voltammetry of phenyl sulfonyl chloride (**1c**) in the presence of a proton donor (pentachlorophenol)

Figure S8 shows cyclic voltammograms of phenyl sulfonyl chloride (**1c**) in the absence (Figure S8a) and in the presence of a proton donor, pentachlorophenol, (Figure S8a). Upon addition of pentachlorophenol to the initial solution of phenyl sulfonyl chloride (**1c**) (1:1), the trace crossing is totally eliminated. This provides further support for the autocatalytic process described in the mechanism (Scheme 1) in the manuscript.

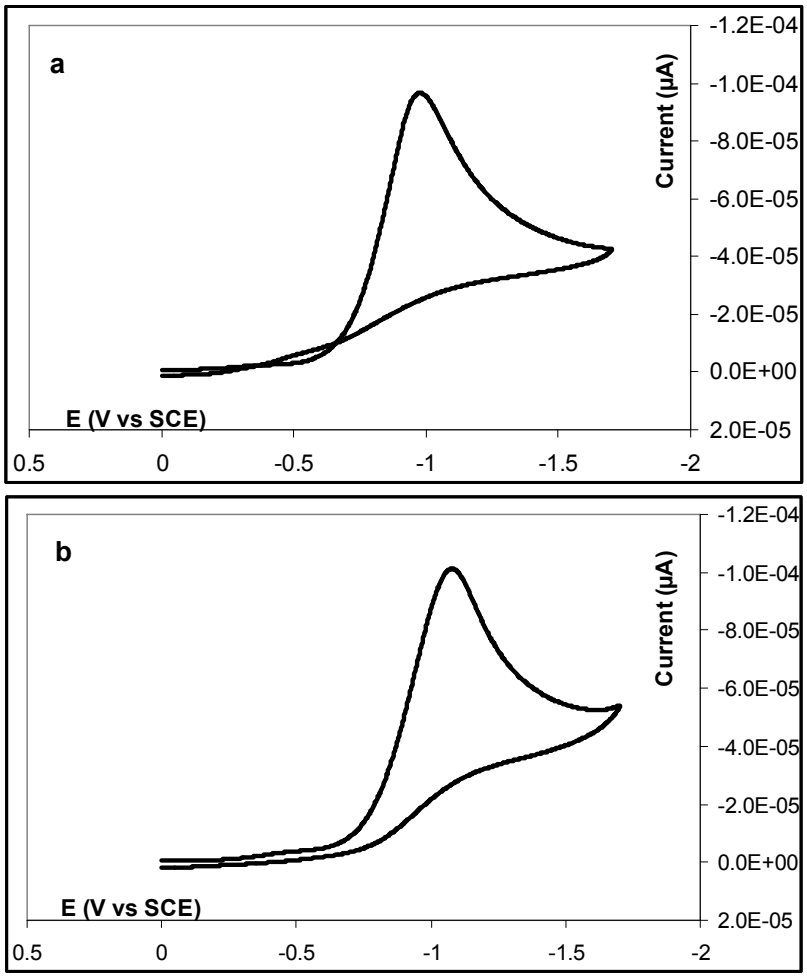

Figure S8. Cyclic voltammetry in CH_3CN/Bu_4NPF_6 (0.1 M) at a glassy carbon electrode at a scan rate v = 0.2 V/s of (a) 1c (2.5 mM) and (b) 1c (2.5 mM) + pentachlorophenol (2.5 mM).

II-8. Electrolysis of phenylthiophenylsulfonate (**2c**)

The electrolysis of phenylthiophenylsulfonate (**2c**) has been performed in acetonitrile, in the presence of tetramethyl ammounium hexafluorophsphate (Me_4NPF_6, 0.10 M). The consumption of the initial compound and the formation of the electrolytic products were monitored by cyclic voltammetry (Figure S9) and HPLC. This compound consumed one electron per molecule with the formation of diphenyl disulfide (**4c**) and phenyl sulfinate anion as final products in quantitative yields.

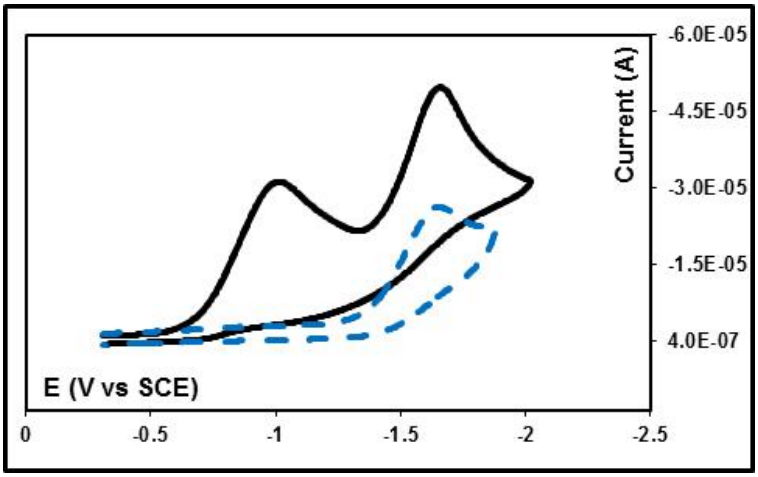

Figure S9. Cyclic voltammetry in CH_3CN/Bu_4NPF_6 (0.1 M) at a glassy carbon electrode of **2c** at a scan rate v = 0.2 V/s before (solid line) and after (dashed line) electrolysis.

III- Computational calculations

All of the calculations were performed using the Gaussian 03 package.[1] The LUMOs and SOMOs were calculated after a full optimization without imposed symmetry of the conformations using the B3LYP method with the 6-31G+(d,p) basis set starting from preliminary optimizations performed with semi-empirical methods. The obtained conformations were verified by running frequency calculations for the B3LYP calculations.

1. Gaussian 03, Revision B.03, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, Jr. J. A. Montgomery, T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li,; J. E. Knox, H. P. Hratchian, J. B. Cross, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O.Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala,; K. Morokuma, G. A.Voth, P. Salvador,; J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. D. Farkas, K. Malick,; A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui,; A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez and J. A. Pople, Gaussian, Inc., Pittsburgh PA, 2003.

Total Energies and Coordinates

p-Methoxylphenyl sulfonyl chloride (1a).

Total Energy: -1354.97340788 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.268220	0.365447	-0.006717
2	6	0	0.192908	0.139100	1.367139
3	6	0	1.358677	0.173293	2.131461
4	6	0	2.610198	0.417080	1.549280
5	6	0	2.683313	0.641342	0.183733
6	6	0	1.515691	0.614613	-0.602628
7	1	0	-0.640863	0.347359	-0.594608
8	1	0	-0.764477	-0.050617	1.839820
9	1	0	3.503596	0.440418	2.163268
10	1	0	3.632550	0.841786	-0.300991
11	16	0	1.256225	-0.122687	3.879624
12	8	0	2.426766	0.443543	4.542467
13	8	0	-0.103292	0.137567	4.343046
14	17	0	1.503814	-2.246717	3.991129
15	8	0	1.698471	0.842623	-1.925408
16	6	0	0.568658	0.818991	-2.798273
17	1	0	0.964321	1.016750	-3.794269
18	1	0	0.081008	-0.162499	-2.785906
19	1	0	-0.154254	1.598043	-2.530261

p-Methoxylphenyl sulfonyl chloride reduced form (1a+e).

Total Energy: -1354.76338159 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.231269	0.747609	0.318739
2	6	0	-0.086707	0.407274	1.663765
3	6	0	1.146259	-0.058388	2.116845
4	6	0	2.231752	-0.199990	1.264371
5	6	0	2.093999	0.141564	-0.088055
6	6	0	0.860822	0.618487	-0.552278
7	1	0	-1.172168	1.112810	-0.076956
8	1	0	-0.911655	0.479966	2.362797
9	1	0	3.165452	-0.587833	1.654751
10	1	0	2.942166	0.032391	-0.753123
11	16	0	1.353060	-0.489240	3.933058
12	8	0	-0.206534	-0.922274	4.359389

13	8	0	2.482919	-1.721946	3.865377
14	8	0	0.615560	0.988773	-1.881931
15	6	0	1.708733	0.916740	-2.825590
16	1	0	2.077630	-0.110790	-2.938497
17	1	0	1.295608	1.262688	-3.773798
18	1	0	2.540956	1.566552	-2.526860
19	17	0	2.343176	2.200739	4.530155

p-Methylphenyl sulfonyl chloride (1b).

Total Energy: -1279.76397460 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.098585	-0.395769	0.026490
2	6	0	0.116861	-0.364759	1.419010
3	6	0	1.268292	0.097904	2.059685
4	6	0	2.391702	0.517976	1.346651
5	6	0	2.348385	0.477380	-0.046446
6	6	0	1.209768	0.018571	-0.726922
7	1	0	-0.795447	-0.743682	-0.483635
8	1	0	-0.744692	-0.677829	1.998270
9	1	0	3.269853	0.879948	1.869738
10	1	0	3.213018	0.811822	-0.612702
11	6	0	1.183191	-0.050052	-2.234324
12	1	0	1.935778	0.606770	-2.678739
13	1	0	1.389630	-1.071063	-2.578464
14	1	0	0.203218	0.234702	-2.629304
15	16	0	1.304092	0.154017	3.843340
16	8	0	2.328302	1.096297	4.282287
17	8	0	-0.060615	0.191006	4.358915
18	17	0	2.055209	-1.788516	4.325355

p-Methylbenzene sulfonyl chloride reduced form (1b+e)

Total Energy: -1279.84882231 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.116214	-0.450330	0.023759
2	6	0	0.105737	-0.383256	1.420714
3	6	0	1.202249	0.157251	2.086566
4	6	0	2.313132	0.612106	1.374952
5	6	0	2.311421	0.538864	-0.017974
6	6	0	1.214999	0.006552	-0.715806

7	1	0	-0.742273	-0.869495	-0.497597
8	1	0	-0.744257	-0.736070	1.995452
9	1	0	3.160332	1.021536	1.914997
10	1	0	3.177590	0.895242	-0.572892
11	16	0	1.228609	0.191915	3.920156
12	8	0	2.045303	1.411015	4.257818
13	8	0	-0.225988	0.194761	4.311700
14	17	0	2.642518	-2.295591	4.143904
15	6	0	1.224311	-0.062684	-2.227050
16	1	0	1.207581	0.939433	-2.675090
17	1	0	2.123678	-0.567775	-2.599516
18	1	0	0.353977	-0.608765	-2.604892

Phenyl sulfonyl chloride (1c).

Total Energy: -1240.44160636 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.080744	0.452166	0.033414
2	6	0	0.107370	0.392696	1.427632
3	6	0	1.260366	-0.093277	2.046937
4	6	0	2.381623	-0.510552	1.327250
5	6	0	2.335818	-0.442910	-0.065920
6	6	0	1.190965	0.038176	-0.709201
7	1	0	-0.807479	0.820166	-0.470272
8	1	0	-0.744276	0.703274	2.022449
9	1	0	3.256947	-0.885824	1.845524
10	1	0	3.193331	-0.767543	-0.646732
11	16	0	1.304796	-0.179464	3.834553
12	8	0	-0.057915	-0.176863	4.355666
13	8	0	2.296174	-1.165827	4.250217
14	17	0	2.128410	1.724646	4.333289
15	1	0	1.163305	0.088902	-1.793457

Phenyl sulfonyl chloride reduced form (1c+e).

Total Energy: -1240.52857159 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.160581	0.577183	0.020606
2	6	0	0.149122	0.499647	1.416393
3	6	0	1.202781	-0.136072	2.072230
4	6	0	2.274812	-0.676100	1.361954
5	6	0	2.280092	-0.594408	-0.033047

6	6	0	1.224700	0.031778	-0.705140
7	1	0	-0.659921	1.065565	-0.499581
8	1	0	-0.666627	0.912558	2.000563
9	1	0	3.081591	-1.158542	1.903529
10	1	0	3.109346	-1.016964	-0.595211
11	16	0	1.217500	-0.200861	3.908282
12	8	0	-0.236743	-0.117676	4.291922
13	8	0	1.952107	-1.476043	4.227351
14	17	0	2.767395	2.190694	4.211956
15	1	0	1.233445	0.097006	-1.790460

p-Chlorophenyl sulfonyl chloride (1d).

Total Energy: -1700.03383484 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.079840	0.456765	0.033032
2	6	0	0.113427	0.391620	1.424775
3	6	0	1.263097	-0.096299	2.048701
4	6	0	2.381361	-0.513260	1.324363
5	6	0	2.344099	-0.446819	-0.067281
6	6	0	1.195247	0.038660	-0.698564
7	1	0	-0.801680	0.824850	-0.479467
8	1	0	-0.741398	0.703499	2.014467
9	1	0	3.258288	-0.892318	1.837222
10	1	0	3.194730	-0.770016	-0.656511
11	17	0	1.151150	0.122060	-2.444906
12	16	0	1.306279	-0.185825	3.833602
13	8	0	-0.058198	-0.214302	4.348207
14	8	0	2.318239	-1.152869	4.243723
15	17	0	2.085815	1.731985	4.339985

p-Chlorophenyl sulfonyl chloride reduced form (1d+e).

Total Energy: -1700.12688874 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.010952	-0.029888	0.043725
2	6	0	-0.004508	0.085452	1.436136
3	6	0	1.208294	0.154145	2.119695
4	6	0	2.420499	0.091715	1.434486
5	6	0	2.425641	-0.023603	0.042064
6	6	0	1.207032	-0.083409	-0.633603
7	1	0	-0.945056	-0.079328	-0.506012

8	1	0	-0.933862	0.133358	1.993789
9	1	0	3.350350	0.144432	1.990877
10	1	0	3.359237	-0.068228	-0.508945
11	17	0	1.206203	-0.228767	-2.399280
12	16	0	1.209273	0.252123	3.953673
13	17	0	1.216478	-2.577412	4.263269
14	8	0	2.496802	0.961901	4.278959
15	8	0	-0.081634	0.954889	4.280744

p-Fluorophenyl sulfonyl chloride (1e).

Total Energy: -1339.68070010 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.015831	-0.009868	0.028086
2	6	0	-0.016014	0.041863	1.420765
3	6	0	1.207965	0.074235	2.094160
4	6	0	2.432075	0.046377	1.420772
5	6	0	2.432055	-0.005414	0.028132
6	6	0	1.208146	-0.034560	-0.634602
7	1	0	-0.939057	-0.028497	-0.539859
8	1	0	-0.947186	0.068935	1.975346
9	1	0	3.363242	0.076969	1.975196
10	1	0	3.355304	-0.020757	-0.539874
11	9	0	1.208296	-0.085952	-1.984743
12	16	0	1.207637	0.144212	3.878974
13	8	0	2.483836	0.677658	4.342115
14	8	0	-0.073024	0.667135	4.341818
15	17	0	1.216284	-1.924890	4.393290

p-Fluorophenyl sulfonyl chloride (1e+e).

Total Energy: -1339.77232599 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.012401	-0.035946	0.043027
2	6	0	-0.006274	0.084004	1.435648
3	6	0	1.207570	0.156325	2.118680
4	6	0	2.421701	0.092223	1.435344
5	6	0	2.428296	-0.027686	0.042724
6	6	0	1.208068	-0.090451	-0.618314
7	1	0	-0.937496	-0.090207	-0.521680
8	1	0	-0.934548	0.132428	1.994740
9	1	0	3.349763	0.146935	1.994207

10	1	0	3.353600	-0.075672	-0.522208
11	9	0	1.208301	-0.208571	-1.983855
12	16	0	1.207455	0.256852	3.951133
13	8	0	2.493461	0.969189	4.277918
14	8	0	-0.084703	0.957783	4.278314
15	17	0	1.220936	-2.579757	4.273899

p-Cyanophenyl sulfonyl chloride (1f).

Total Energy: -1332.68031235 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.076051	-0.522420	-0.009478
2	6	0	0.020270	-0.090655	1.316626
3	6	0	1.139340	0.391036	1.997622
4	6	0	2.358470	0.438321	1.326618
5	6	0	2.438840	0.008849	-0.009893
6	6	0	1.297777	-0.472954	-0.675550
7	1	0	-0.813440	-0.897504	-0.502950
8	1	0	1.058625	0.710621	3.030461
9	1	0	3.246524	0.802872	1.830944
10	1	0	1.373545	-0.806321	-1.704625
11	16	0	-1.551039	-0.162743	2.182039
12	8	0	-2.414885	-1.133576	1.521391
13	8	0	-1.303372	-0.180284	3.618581
14	6	0	3.697220	0.059899	-0.699938
15	7	0	4.716471	0.100788	-1.258761
16	17	0	-2.354396	1.753127	1.736903

p-Cyanophenyl sulfonyl chloride (1f+e).

Total Energy: -1332.78224517 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.146955	0.549435	0.017240
2	6	0	0.139020	0.470807	1.407987
3	6	0	1.201204	-0.147538	2.068075
4	6	0	2.282658	-0.676151	1.361760
5	6	0	2.297483	-0.600470	-0.028333
6	6	0	1.228249	0.014130	-0.707388
7	1	0	-0.674578	1.020324	-0.513500
8	1	0	-0.684963	0.871590	1.988523
9	1	0	3.093866	-1.147978	1.905376
10	1	0	3.127722	-1.011058	-0.594337

11	6	0	1.237952	0.089090	-2.139609
12	7	0	1.246225	0.151582	-3.303423
13	16	0	1.216096	-0.196363	3.906918
14	8	0	-0.240216	-0.124086	4.281235
15	8	0	1.964146	-1.461581	4.228432
16	17	0	2.716862	2.194960	4.045011

p-Nitrophenyl sulfonyl chloride (1g).

Total Energy: -1444.94370886 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.128447	0.529034	0.023024
2	6	0	0.154490	0.485047	1.415837
3	6	0	1.260214	-0.088959	2.045631
4	6	0	2.341004	-0.618390	1.338372
5	6	0	2.312965	-0.573801	-0.054450
6	6	0	1.208847	0.000881	-0.682393
7	1	0	-0.707795	0.959856	-0.513243
8	1	0	-0.669535	0.877930	2.000445
9	1	0	3.177895	-1.063583	1.864229
10	1	0	3.124175	-0.974824	-0.649097
11	16	0	1.290713	-0.154934	3.842202
12	8	0	-0.074869	-0.065186	4.343731
13	8	0	2.216497	-1.199072	4.263042
14	17	0	2.222371	1.696055	4.300213
15	7	0	1.180831	0.049266	-2.162859
16	8	0	2.143417	-0.424046	-2.763852
17	8	0	0.197211	0.560395	-2.694861

p-Nitrophenyl sulfonyl chloride (1g+e).

Energy = -1445.04837875 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.002490	0.020679	-0.001537
2	6	0	-0.004469	0.018988	1.391009
3	6	0	1.208596	-0.002992	2.082798
4	6	0	2.429129	-0.045186	1.404908
5	6	0	2.443415	-0.044323	0.012963
6	6	0	1.224417	-0.011101	-0.671638
7	1	0	-0.923947	0.048018	-0.569840
8	1	0	-0.933761	0.048270	1.949236
9	1	0	3.352376	-0.065147	1.973397

10	1	0	3.371568	-0.067346	-0.544484
11	16	0	1.196793	-0.064688	3.919643
12	8	0	2.476054	0.621405	4.314457
13	8	0	-0.102450	0.592011	4.297148
14	17	0	1.216700	-2.879263	3.913586
15	7	0	1.233459	-0.001381	-2.135665
16	8	0	2.325856	-0.028488	-2.714725
17	8	0	0.148382	0.035230	-2.728029

P-Methoxylphenyl sulfonyl radical.

Total Energy: - 894.75438521 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.198939	-0.271539	0.076918
2	6	0	-0.082806	-0.507719	1.438616
3	6	0	1.077602	-0.092386	2.106311
4	6	0	2.130606	0.513080	1.421291
5	6	0	2.012740	0.751693	0.051131
6	6	0	0.846599	0.357515	-0.624875
7	1	0	-1.091040	-0.560864	-0.468169
8	1	0	-0.887764	-0.982970	1.988592
9	1	0	3.023023	0.819539	1.956276
10	1	0	2.824914	1.242358	-0.470869
11	16	0	1.265938	-0.462072	3.862587
12	8	0	2.283586	0.477840	4.417119
13	8	0	-0.100607	-0.577179	4.450455
14	8	0	0.632576	0.539427	-1.952415
15	6	0	1.644868	1.166841	-2.738183
16	1	0	2.572866	0.583274	-2.726942
17	1	0	1.249042	1.201672	-3.753102
18	1	0	1.843050	2.186426	-2.387542

P-Methylphenyl sulfonyl radical.

Total Energy: -819.54523656 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.000571	-0.292767	-0.037386
2	6	0	-0.048895	-0.353555	1.353926
3	6	0	1.119372	-0.095817	2.075527
4	6	0	2.328792	0.183381	1.438518
5	6	0	2.351931	0.239048	0.044135
6	6	0	1.195833	-0.000088	-0.714112

7	1	0	-0.908719	-0.471634	-0.607113
8	1	0	-0.976255	-0.569172	1.873389
9	1	0	3.222456	0.378395	2.021311
10	1	0	3.284381	0.476274	-0.460699
11	16	0	1.086108	-0.232052	3.882938
12	8	0	2.225202	0.569566	4.416558
13	8	0	-0.318139	0.004705	4.326812
14	6	0	1.232840	0.036956	-2.222823
15	1	0	2.155160	0.494847	-2.589970
16	1	0	1.175142	-0.976044	-2.639441
17	1	0	0.386993	0.602473	-2.627327

Phenyl sulfonyl radical.

Total Energy: -780.22316376 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.005875	-0.003775	0.012185
2	6	0	-0.016895	0.043891	1.407799
3	6	0	1.206177	0.085319	2.080251
4	6	0	2.430253	0.046259	1.409444
5	6	0	2.421234	-0.001460	0.013831
6	6	0	1.208167	-0.028652	-0.681675
7	1	0	-0.945812	-0.019711	-0.530890
8	1	0	-0.947732	0.072787	1.963503
9	1	0	3.360307	0.077052	1.966360
10	1	0	3.361928	-0.015652	-0.527977
11	16	0	1.205099	0.082394	3.898441
12	8	0	2.507163	0.653295	4.348107
13	8	0	-0.099452	0.648843	4.346514
14	1	0	1.208939	-0.069020	-1.766767

p-Chlorophenyl sulfonyl radical.

Total Energy: -1239.81570375 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.011932	0.001051	0.011281
2	6	0	-0.014310	0.045543	1.405135
3	6	0	1.206174	0.085855	2.082250
4	6	0	2.427637	0.047766	1.406708
5	6	0	2.427196	0.003171	0.012881
6	6	0	1.208084	-0.021499	-0.670398
7	1	0	-0.945096	-0.013815	-0.540625

8	1	0	-0.948154	0.072838	1.955928
9	1	0	3.360768	0.076926	1.958623
10	1	0	3.361094	-0.010143	-0.537817
11	16	0	1.205262	0.077494	3.897229
12	8	0	2.508136	0.647135	4.344618
13	8	0	-0.100538	0.641542	4.343175
14	17	0	1.209294	-0.082405	-2.419860

p-Fluorophenyl sulfonyl radical.

Total Energy: -879.46239993 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.004477	0.262496	-0.054123
2	6	0	-0.050697	0.329010	1.338178
3	6	0	1.118173	0.091424	2.066316
4	6	0	2.340313	-0.175052	1.442458
5	6	0	2.387310	-0.241963	0.050452
6	6	0	1.214049	-0.019154	-0.665018
7	1	0	-0.889465	0.421935	-0.660058
8	1	0	-0.982504	0.537142	1.852529
9	1	0	3.230289	-0.351361	2.036533
10	1	0	3.308437	-0.463342	-0.477096
11	9	0	1.260058	-0.081463	-2.015260
12	16	0	1.071837	0.241340	3.873172
13	8	0	-0.333124	-0.007430	4.304190
14	8	0	2.216526	-0.546147	4.414117

p-Cyanophenyl sulfonyl radical.

Total Energy: -872.46288826 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.013319	0.013618	-0.000141
2	6	0	-0.016867	0.049048	1.392292
3	6	0	1.206148	0.082585	2.064779
4	6	0	2.430050	0.051431	1.393755
5	6	0	2.428264	0.015963	0.001332
6	6	0	1.207903	-0.005086	-0.697407
7	1	0	-0.948387	0.002413	-0.549493
8	1	0	-0.948428	0.073631	1.946685
9	1	0	3.360918	0.077915	1.949226
10	1	0	3.364005	0.006506	-0.546902
11	16	0	1.205196	0.065381	3.886223

12	8	0	2.508760	0.633271	4.330462
13	8	0	-0.100640	0.629146	4.329031
14	6	0	1.208815	-0.045897	-2.132641
15	7	0	1.209584	-0.079559	-3.295457

p-Nitrophenyl sulfonyl radical.

Total Energy: -984.72647834 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.016126	0.410182	-0.042183
2	6	0	-0.013549	0.464177	1.350572
3	6	0	1.131130	0.095093	2.060067
4	6	0	2.312949	-0.297737	1.428467
5	6	0	2.341273	-0.351354	0.035673
6	6	0	1.193460	0.006181	-0.671215
7	1	0	-0.850280	0.672567	-0.636514
8	1	0	-0.913016	0.764144	1.876310
9	1	0	3.182020	-0.576897	2.013452
10	1	0	3.229164	-0.663657	-0.499913
11	7	0	1.225472	-0.047280	-2.149670
12	8	0	2.273988	-0.407174	-2.682748
13	8	0	0.201879	0.272500	-2.752217
14	16	0	1.112587	0.224741	3.879172
15	8	0	-0.309331	0.120316	4.309386
16	8	0	2.169498	-0.690528	4.392374