Electrochemical Reduction of N-(Arylthio)succinimides: The effect of Aryl Substituents

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Supplementary Information

I- Experimental Section

Cyclic Voltammetry. Electrochemical measurements were conducted in three electrode glass cells, thermostatted at 25 ^{0}C, and under dry nitrogen. The working electrode is a 2 mm diameter glassy carbon electrode (Ekochemie). The electrode was carefully polished and ultrasonically rinsed with ethanol before each run. The reference electrode is a saturated calomel electrode (SCE). The counter electrode was a platinum wire. The electrochemical instrument used is an Autolab PGSTAT30 especially configured to carry high scan rate CV experiments. A feedback correction was applied to minimize the Ohmic drop between the working and reference electrodes.

Electrolyses. The electrolyses were carried out in 20 cm^3 cells with a glassy carbon (Electrosynthesis) rectangular plate working electrode of 8 cm^2. The counter electrode was a platinum grid, separated from the cathodic compartment by means of a glass frit. The reference electrode was the same as for CV. The cell was thermostatted at 25 ^{0}C, and the solution was kept under a nitrogen stream during the whole electrolysis. The disappearance of the starting material and the formation of the products were followed by in situ cyclic voltammetry. The supporting electrolyte, tetramethylammonium hexafluorophosphate, was extracted and chromatographic analyses (HPLC and GCMS) were performed by comparison with authentic samples of the product.

Chemicals. Acetonitrile (Aldrich), the supporting electrolytes, tetramethylammonium and tetrabutylammonium hexafluorophosphate (Fluka, *puriss*) were used as received. All investigated N-(Arylthio)succinimides (**1a-e**) were synthesised and characterized (see Syhthetic Procedure in Part II below) .

Theoretical calculation. Computational investigations were conducted with Gaussian 16[32] using DFT at the B3LYP level and a 6-311G ++ (2d,p) basis set in the solvent phase (acetonitrile) via the PCM. The neutral structures for all compounds **1a-e** were optimized and their energies and molecular orbitals were determined. All potential fragments including substituted phenyl thiyl radicals, their corresponding thiolate anions, the succinimidyl radical and its anion were optimized and their energies were calculated. Frequency determinations for the calculations were performed to check that the obtained conformations were real minima.

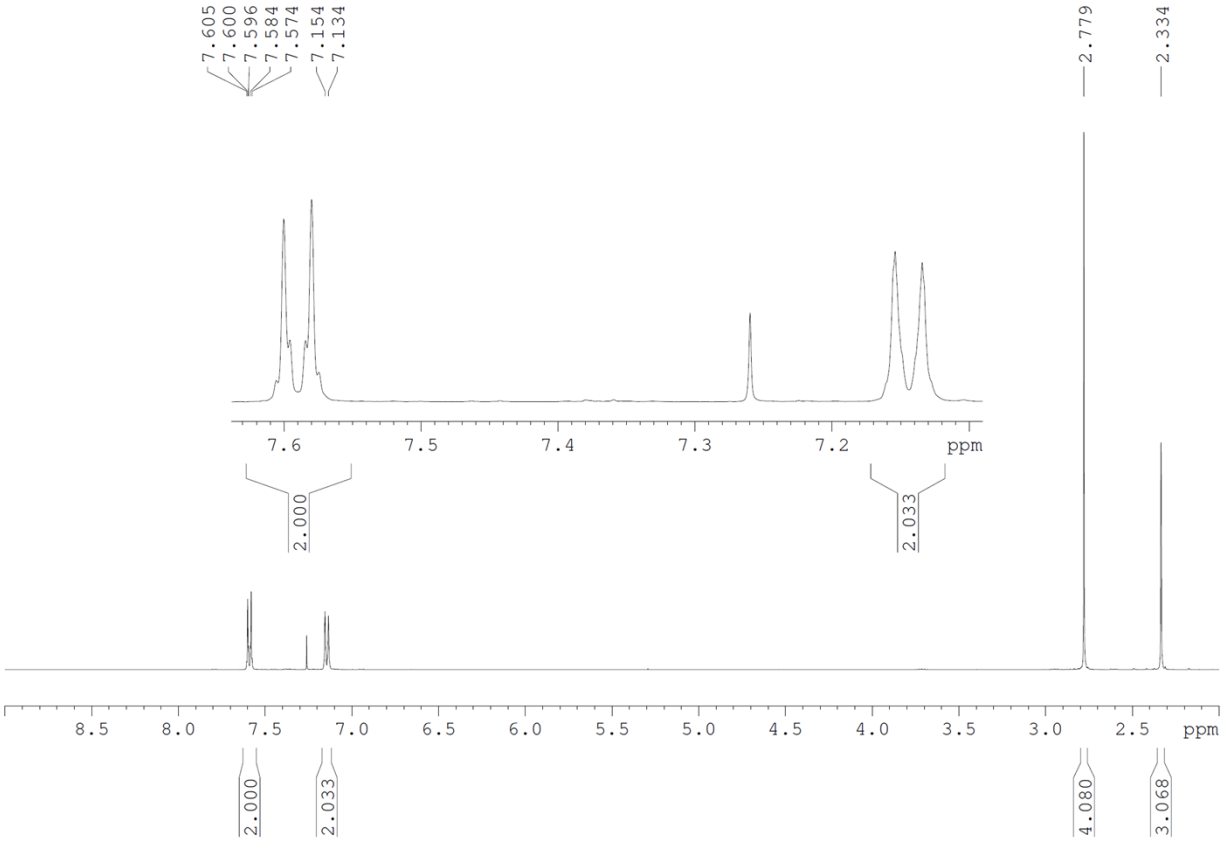
II- Synthetic Procedure

All glassware was dried overnight in an oven at 110 ^{o}C, and cooled under and argon atmosphere. To a 100 mL round-bottom flask 0.5 equivalents of disulfide was dissolved in anhydrous dichloromethane, and the solution was cooled to -20 ^{o}C under argon. To the round-bottom flask 3 drops of triethylamine was added. A second solution of 1.1 equivalents of sulfuryl chloride dissolved in ~ 5 mL of dichloromethane was prepared and added to the round-bottom flask dropwise, via an addition funnel. An immediate colour change to an orange-red colour occurred upon addition of the sulfuryl chloride solution. The solution was left to mix for 1 hour, where it was then concentrated under vacuum and vacuum distilled to yield the corresponding sulfenyl chloride.

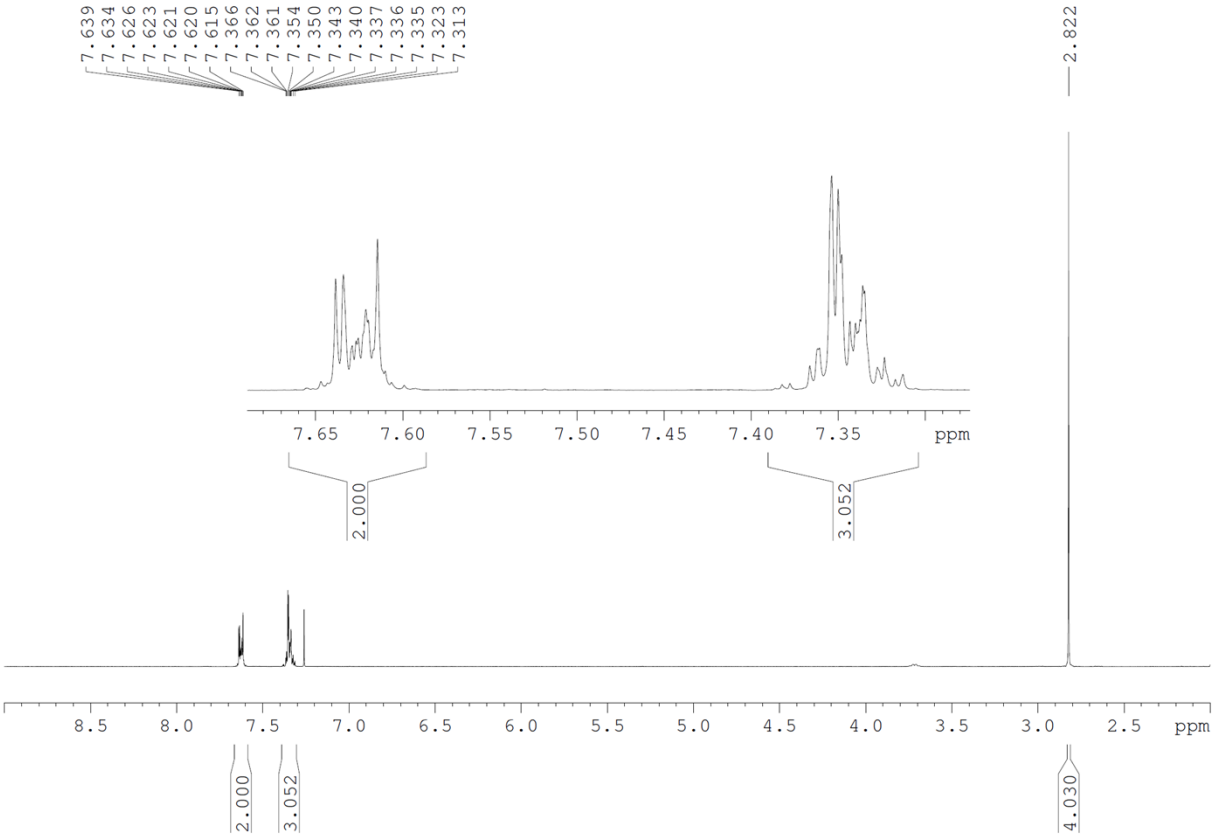
To a second 50 mL round-bottom flask 1.0 equivalent of succinimide and 1.0 equivalent of triethylamine was dissolved in anhydrous acetonitrile. A second solution was prepared from the corresponding sulfenyl chloride, synthesized in the previous step, dissolved in minimal acetonitrile. The second solution was added to the round-bottom flask dropwise, and a pale-yellow precipitate quickly began to form. The solutions were mixed for 1 hour and then the mixture was filtered. The precipitate was washed with cold acetonitrile several times and then recrystallized from acetonitrile prior to electrochemical analysis.

III- NMR Spectra

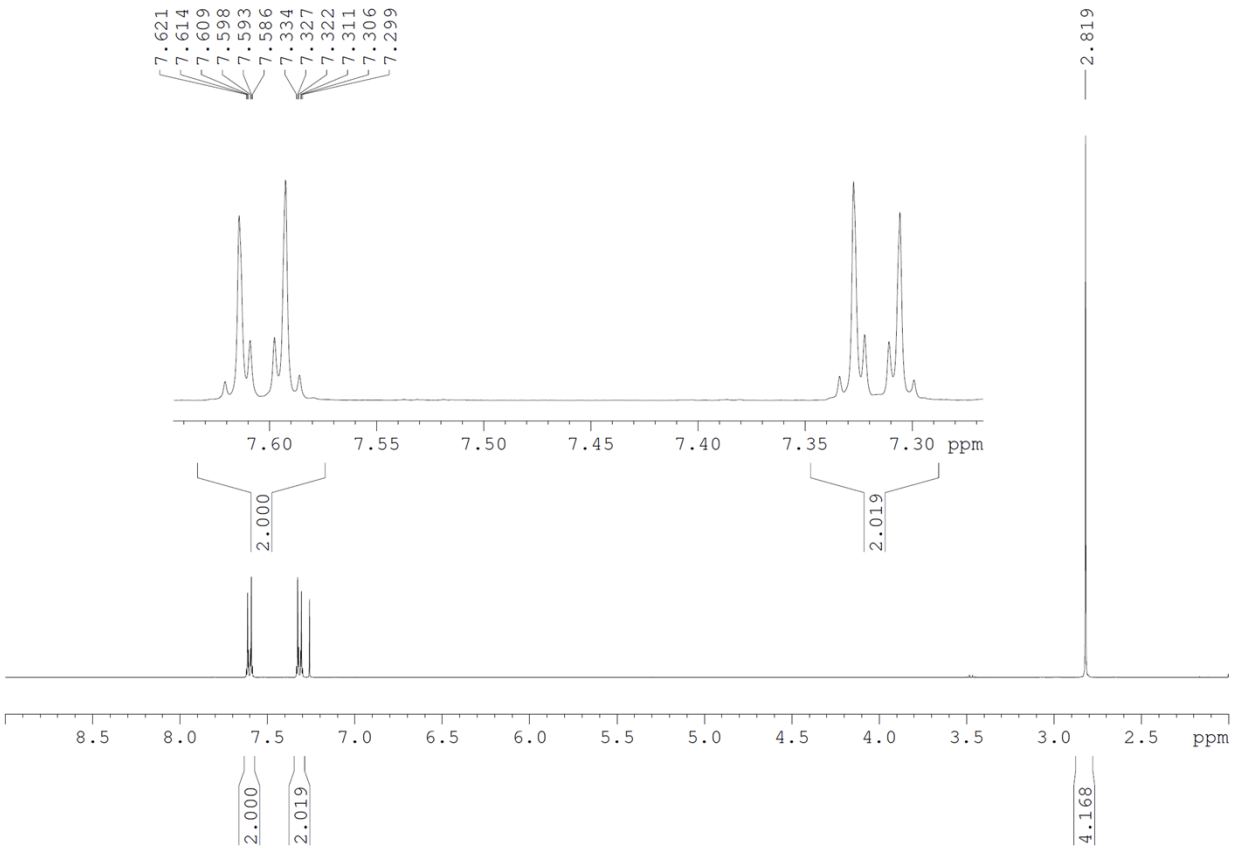
a) N-(4-methylphenylthio)succinimide (**1a**)



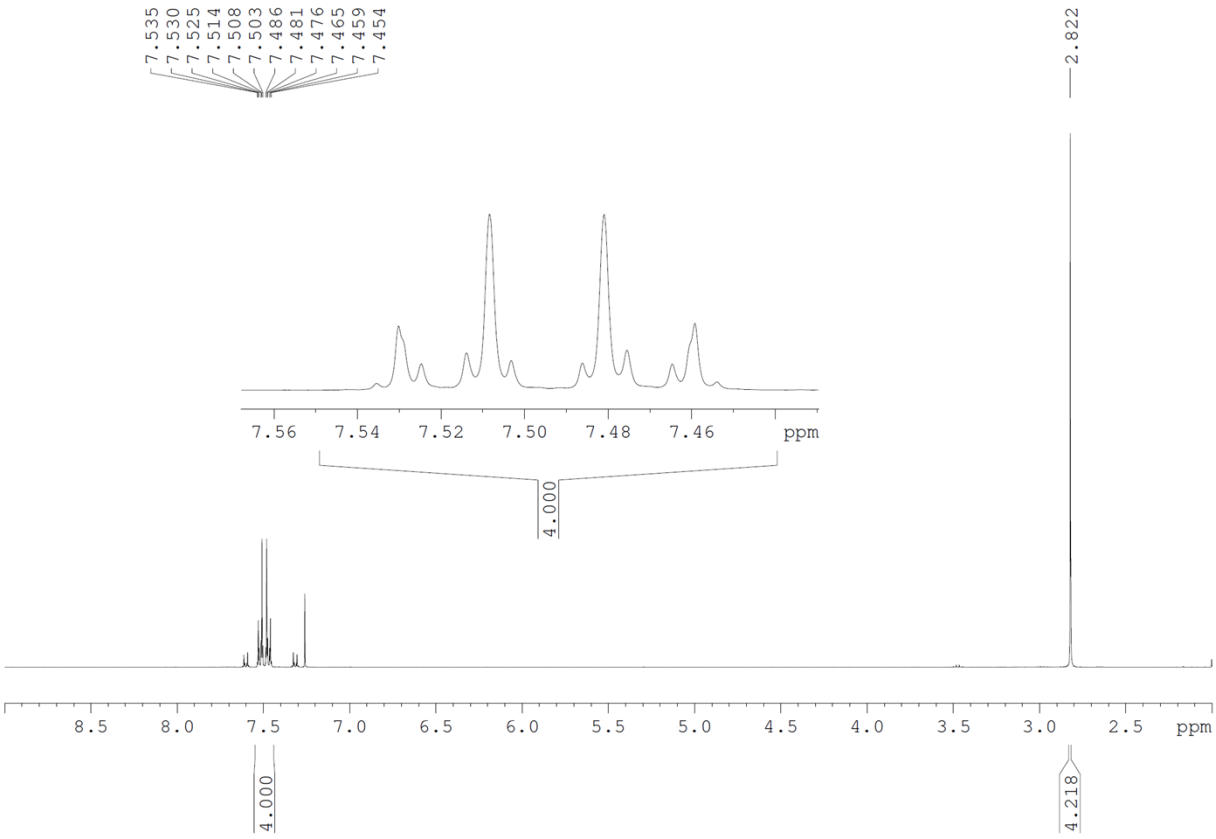
b) N-(phenylthio)succinimide (**1b**)



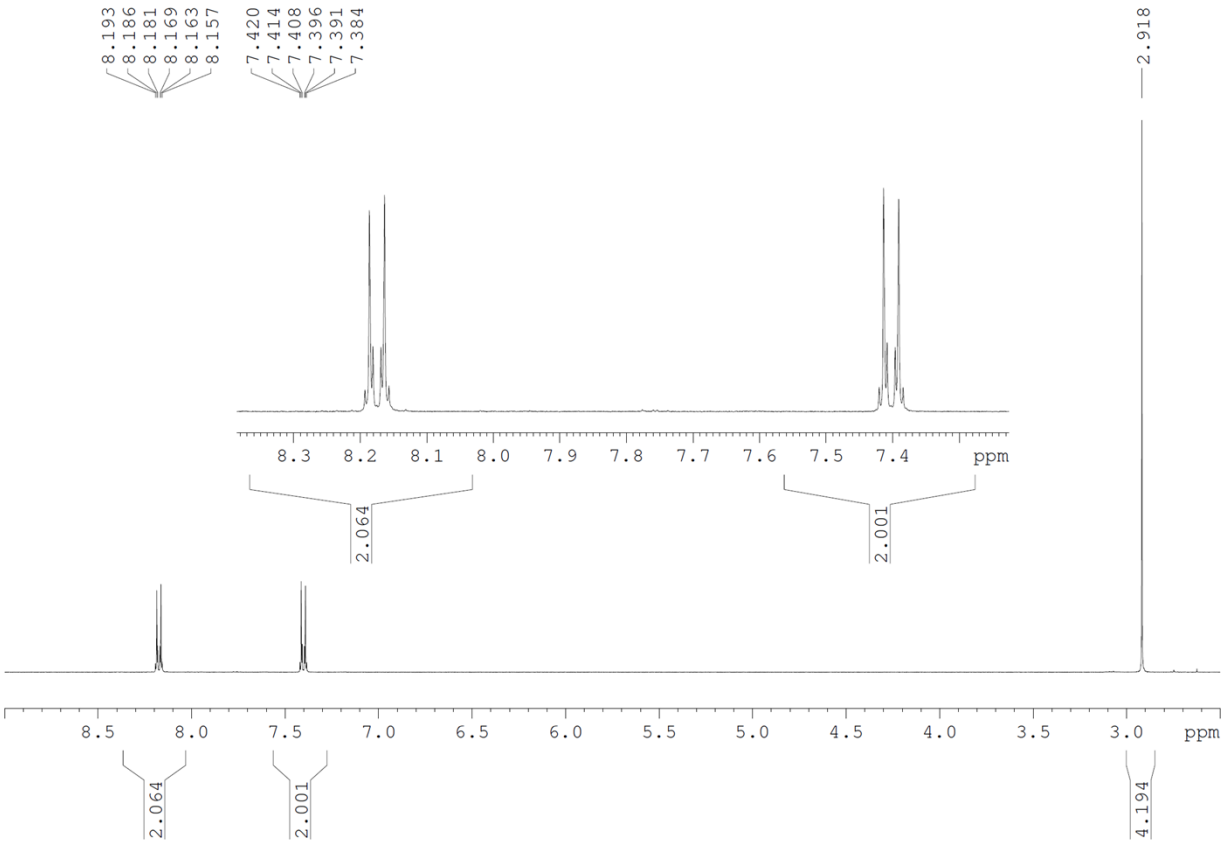
c) N-(4-chlorophenylthio)succinimide (**1c**)



d) N-(4-bromophenylthio)succinimide (**1d**)



e) N-(4-nitrophenylthio)succinimide (**1e**)



IV- Supplementary Electrochemical Data

Cyclic voltammetry of compounds **1b**, **1c** and **1d** and their corresponding disulfides. The data for compound **1a** is provided in the manuscript.

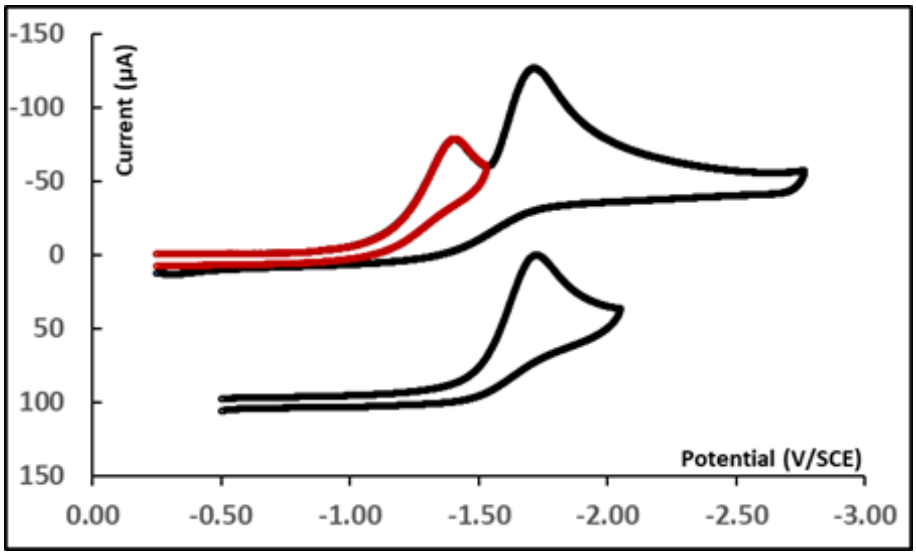


Figure S1. Cyclic voltammograms, in acetonitrile in the presence of 0.1 M $^{n}Bu_4NPF_6$ at a scan rate of v = 0.2 Vs^{-1} using a glassy carbon electrode, of (Top): N-(phenylthio)succinimide (**1b**, 2.68 mM) and (Bottom): bis(phenyl)disulfide (1.11 mM).

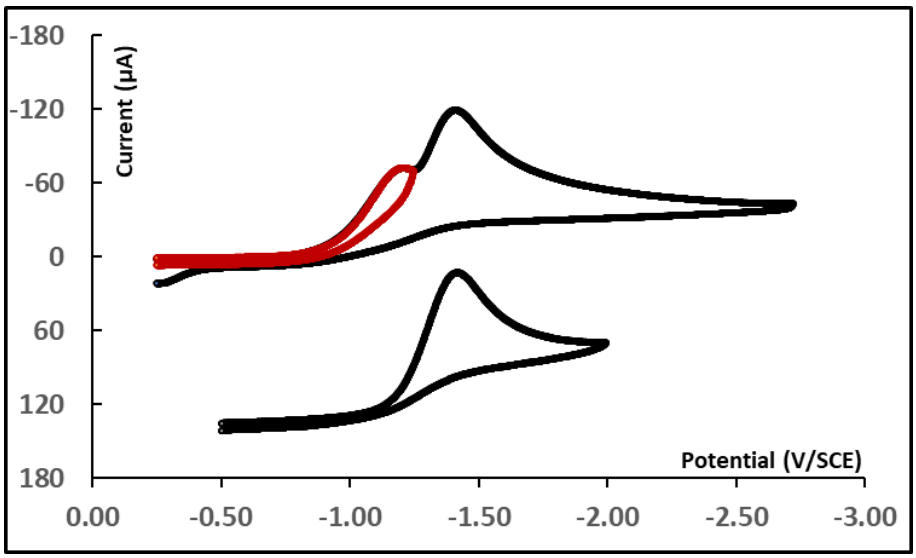


Figure S2. Cyclic voltammograms, in acetonitrile in the presence of 0.1 M $^{n}Bu_4NPF_6$ at a scan rate of v = 0.2 Vs^{-1} using a glassy carbon electrode, of (Top): N-(4-chlorophenylthio)succinimide (**1c**, 2.66 mM) and (Bottom): bis(4-chlorophenyl)disulfide (1.20 mM).

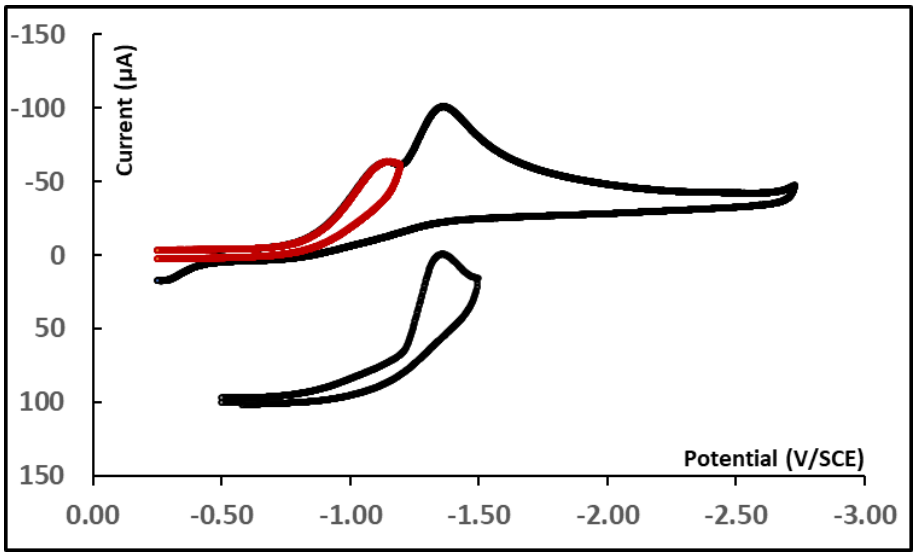


Figure S3. Cyclic voltammograms, in acetonitrile in the presence of 0.1 M $^{n}Bu_4NPF_6$ at a scan rate of v = 0.2 Vs^{-1} using a glassy carbon electrode, of (Top): N-(4-bromorophenylthio)succinimide (**1d**, 2.20 mM) and (Bottom): bis(4-bromophenyl)disulfide (1.18 mM).

Ep vs log v plots for **1a**, **1b**, and **1e**. For **1c** and **1d**, the first and second peak merge when the scan rate is increased.

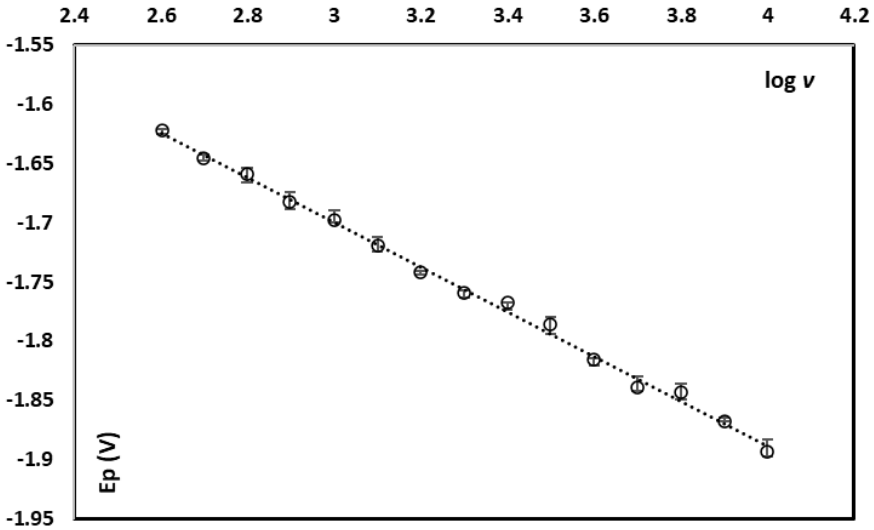


Figure S4: Variation of the first reduction peak potential (E_{p1}) with log ν for N-(4-methylphenylthio)succinimide (**1a**). Cyclic voltammetry in in acetonitrile in the presence of 0.1 M $^{n}Bu_4NPF_6$.

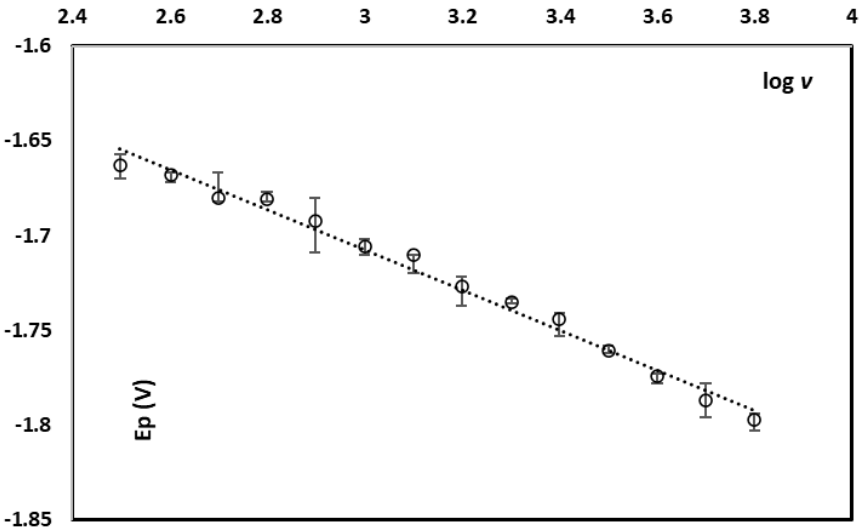


Figure S5: Variation of the first reduction peak potential (E_{p1}) with log ν for N-(phenylthio)succinimide (**1b**). Cyclic voltammetry in in acetonitrile in the presence of 0.1 M $^{n}Bu_4NPF_6$.

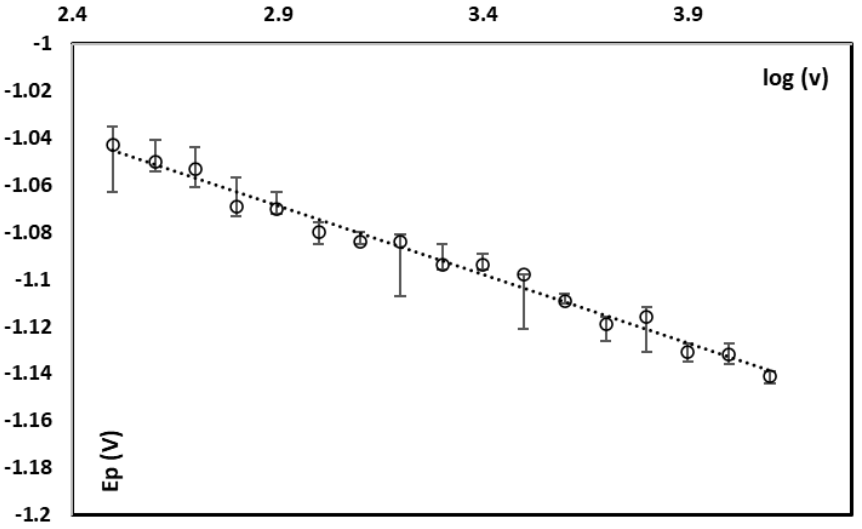


Figure S6: Variation of the first reduction peak potential (E_{p1}) with log ν for N-(4-nitrophenylthio)succinimide (**1e**). Cyclic voltammetry in in acetonitrile in the presence of 0.1 M $^{n}Bu_4NPF_6$.

V- Computational Results

N-(4-methylphenylthio)succinimide (1a)

Total Energy: -1029.437612 Hartrees

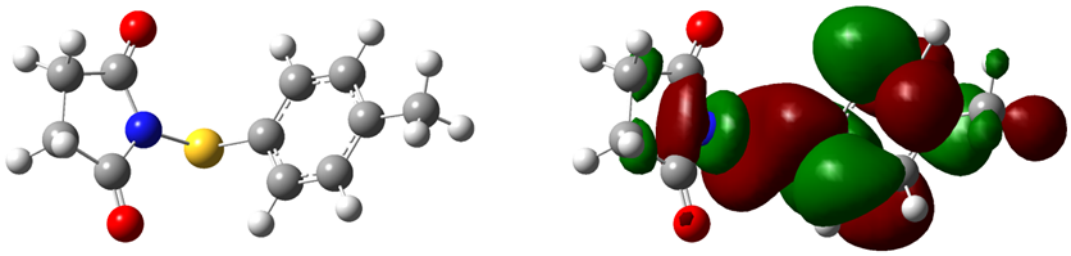


Figure S7: Structure and LUMO of **1a**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.264663	1.164282	-0.304164
2	6	0	2.277244	-1.175239	-0.159965
3	7	0	1.731133	0.025923	0.325292
4	8	0	1.949889	2.301891	-0.050998
5	8	0	1.969602	-2.276667	0.226977
6	6	0	-0.981275	0.042483	0.765132
7	6	0	-1.558333	-1.184201	0.430689
8	6	0	-1.661642	1.226605	0.480005
9	6	0	-2.796948	-1.217813	-0.196209
10	1	0	-1.035701	-2.104502	0.656690
11	6	0	-2.903672	1.179308	-0.141937
12	1	0	-1.218931	2.179132	0.740704
13	6	0	-3.491624	-0.039802	-0.490200
14	1	0	-3.233217	-2.175288	-0.457967
15	1	0	-3.422141	2.105736	-0.361772
16	6	0	3.276452	0.699633	-1.330985
17	1	0	4.238836	1.158912	-1.103120
18	1	0	2.964993	1.062288	-2.311295

19	6	0	3.293114	-0.828766	-1.228629
20	1	0	3.007334	-1.327767	-2.155087
21	1	0	4.261672	-1.229166	-0.926762
22	16	0	0.586163	0.098637	1.626876
23	6	0	-4.849786	-0.087428	-1.139526
24	1	0	-5.632978	-0.209749	-0.384952
25	1	0	-5.061639	0.832576	-1.685893
26	1	0	-4.929861	-0.927991	-1.830699

N-(phenylthio)succinimide (1b)

Total Energy: -990.108037 Hartrees

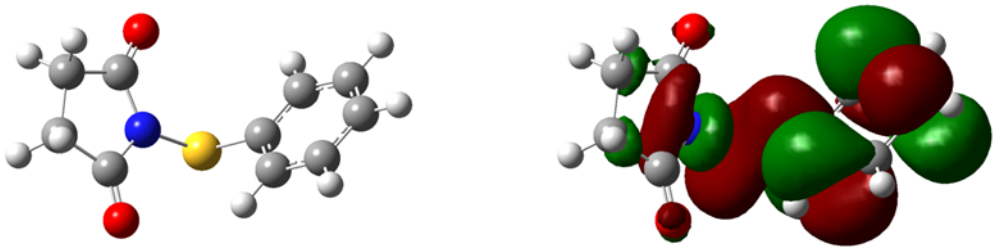


Figure S8: Structure and LUMO of **1b**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.834044	1.208541	-0.294785
2	6	0	2.010445	-1.108611	0.061079
3	7	0	1.320918	0.079401	0.375032
4	8	0	1.404793	2.331186	-0.176592
5	8	0	1.743164	-2.198390	0.508635
6	6	0	-1.423006	0.006791	0.513877
7	6	0	-1.766754	-1.223890	-0.057274
8	6	0	-2.252065	1.119889	0.347893
9	6	0	-2.931689	-1.328780	-0.813593
10	1	0	-1.128286	-2.086031	0.090444
11	6	0	-3.427384	1.000244	-0.393754

12	1	0	-1.978414	2.068672	0.792741
13	6	0	-3.763761	-0.219743	-0.978701
14	1	0	-3.196120	-2.279088	-1.262811
15	1	0	-4.072260	1.862087	-0.520200
16	6	0	2.986604	0.748318	-1.164917
17	1	0	3.879241	1.310048	-0.884400
18	1	0	2.756746	0.996445	-2.202794
19	6	0	3.113740	-0.759958	-0.917938
20	1	0	2.980569	-1.359823	-1.819723
21	1	0	4.069978	-1.043867	-0.474495
22	1	0	-4.674157	-0.308575	-1.560213
23	16	0	0.040724	0.160321	1.546785

N-(4-chlorophenylthio)succinimide (1c)

Total Energy: -1449.732453 Hartrees

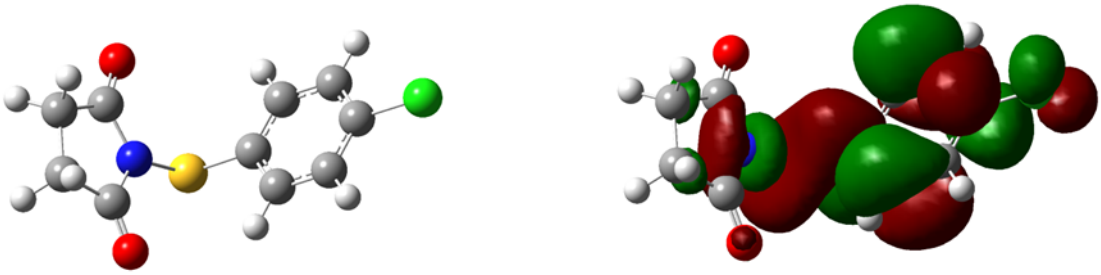


Figure S9: Structure and LUMO of **1c**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.371436	-1.219184	-0.043681
2	6	0	-1.100288	-1.106584	0.503561
3	6	0	-0.602306	0.146016	0.867270
4	6	0	-1.389954	1.284592	0.701266
5	6	0	-2.671062	1.177900	0.171338
6	6	0	-3.142987	-0.073506	-0.199962

7	1	0	-2.760968	-2.185793	-0.332933
8	1	0	-0.496367	-1.992800	0.646416
9	1	0	-1.005548	2.255965	0.982813
10	1	0	-3.286901	2.057577	0.042908
11	16	0	1.010507	0.301871	1.631153
12	6	0	3.491145	0.549612	-1.545152
13	6	0	3.588296	-0.943689	-1.215411
14	1	0	3.106817	0.744228	-2.547084
15	1	0	4.441448	1.076105	-1.451477
16	1	0	3.283187	-1.590002	-2.038798
17	1	0	4.589368	-1.252105	-0.911306
18	7	0	2.074182	0.074773	0.285117
19	6	0	2.645398	-1.166030	-0.051769
20	6	0	2.518646	1.126187	-0.537957
21	8	0	2.402891	-2.207900	0.507006
22	8	0	2.163082	2.274529	-0.434676
23	17	0	-4.757583	-0.214790	-0.880027

N-(4-bromophenylthio)succinimide (1d)

Total Energy: -3563.646218 Hartrees

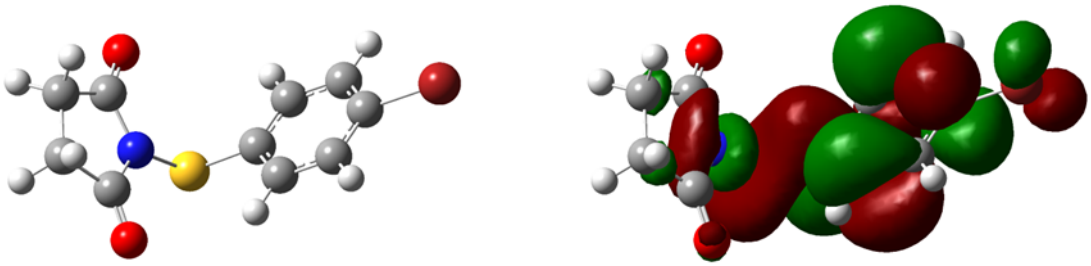


Figure S10: Structure and LUMO of **1d**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	1.711058	-1.129686	-0.231373
2	6	0	0.406052	-0.980754	-0.683185
3	6	0	-0.099937	0.291482	-0.955255
4	6	0	0.712053	1.413293	-0.796667
5	6	0	2.027648	1.270111	-0.366882
6	6	0	2.507385	-0.000308	-0.083326
7	1	0	2.102067	-2.113996	-0.013192
8	1	0	-0.215893	-1.855110	-0.822950
9	1	0	0.321089	2.400751	-1.004113
10	1	0	2.658204	2.140279	-0.246828
11	16	0	-1.758258	0.505146	-1.598116
12	6	0	-4.040602	0.320879	1.726318
13	6	0	-4.163068	-1.116276	1.208759
14	1	0	-3.598657	0.383240	2.721400
15	1	0	-4.992430	0.851987	1.757366
16	1	0	-3.810466	-1.863963	1.919756
17	1	0	-5.181879	-1.386665	0.928640
18	7	0	-2.735195	0.096207	-0.230702
19	6	0	-3.293207	-1.179605	-0.028923
20	6	0	-3.125763	1.028384	0.749077
21	8	0	-3.090804	-2.137149	-0.735036
22	8	0	-2.771586	2.181316	0.777005
23	35	0	4.315596	-0.204879	0.525076

N-(4-nitrophenylthio)succinimide (1e)

Total Energy: -1194.682041 Hartrees

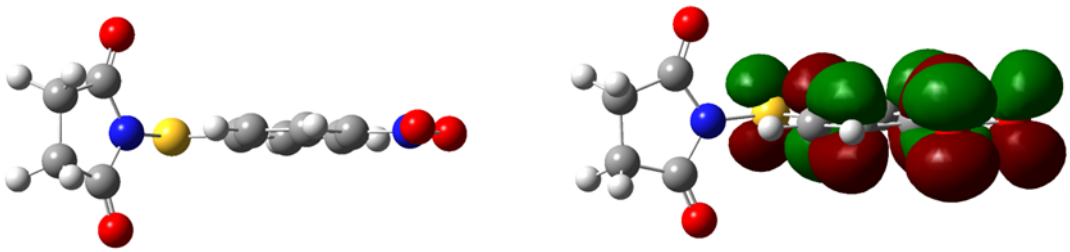


Figure S11: Structure and LUMO of **1e**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.861881	-0.277881	1.175371
2	6	0	-2.878983	-0.210085	-1.182268
3	7	0	-2.307149	0.295797	0.008027
4	8	0	-2.538079	0.019421	2.296328
5	8	0	-2.567598	0.147378	-2.289076
6	6	0	0.377034	0.845629	0.016628
7	6	0	0.590082	-0.532605	-0.008517
8	6	0	1.464573	1.728594	0.029462
9	6	0	1.883248	-1.029015	-0.019584
10	1	0	-0.239939	-1.223993	-0.019344
11	6	0	2.755575	1.236570	0.018413
12	1	0	1.302749	2.799342	0.048130
13	6	0	2.953316	-0.141782	-0.005655
14	1	0	2.063243	-2.093780	-0.038233
15	1	0	3.602573	1.906435	0.028265
16	6	0	-3.890811	-1.298154	0.740655
17	1	0	-4.847929	-1.037152	1.193149
18	1	0	-3.598682	-2.272455	1.134040
19	6	0	-3.910355	-1.245670	-0.791559
20	1	0	-3.645237	-2.194028	-1.259751
21	1	0	-4.874839	-0.939213	-1.198093
22	16	0	-1.223373	1.616942	0.037369
23	7	0	4.313731	-0.666257	-0.016171
24	8	0	5.247045	0.135387	-0.003323
25	8	0	4.468028	-1.886764	-0.037270

N-(4-nitrophenylthio)succinimide radical anion (1e$^{\bullet-}$)

Total Energy: -1194.813212 Hartrees

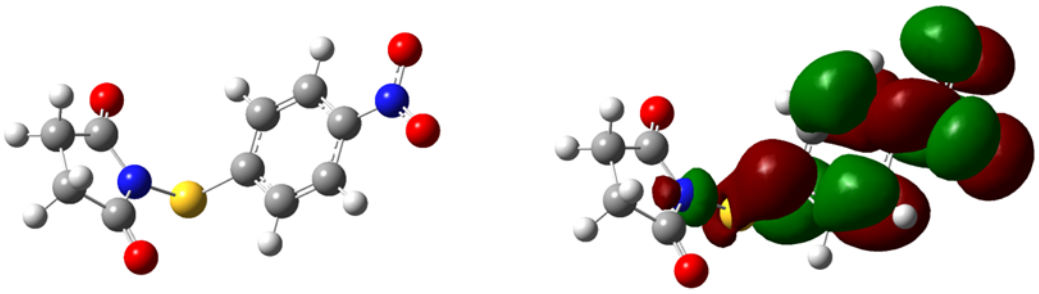


Figure S12: Structure and SOMO of **1e**$^{\bullet-}$.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.874045	-1.159021	0.280512
2	6	0	2.791122	1.175709	0.381676
3	7	0	2.340749	0.016875	-0.268298
4	8	0	2.631812	-2.276818	-0.109750
5	8	0	2.473171	2.302881	0.083874
6	6	0	-0.340586	0.015624	-0.949868
7	6	0	-0.975231	-1.203199	-0.651175
8	6	0	-1.035325	1.217428	-0.728165
9	6	0	-2.256425	-1.226799	-0.140135
10	1	0	-0.449681	-2.133774	-0.824495
11	6	0	-2.319604	1.209740	-0.223441
12	1	0	-0.554744	2.160002	-0.957803
13	6	0	-2.951748	-0.016587	0.081232
14	1	0	-2.745215	-2.161711	0.090053
15	1	0	-2.855666	2.131864	-0.055382
16	6	0	3.788455	-0.771741	1.425709
17	1	0	4.789007	-1.149995	1.212555
18	1	0	3.438436	-1.265735	2.332655
19	6	0	3.722977	0.756455	1.501082
20	1	0	3.317351	1.124119	2.444450
21	1	0	4.688841	1.239547	1.350075
22	16	0	1.280158	0.038238	-1.663678

23	7	0	-4.245904	-0.032698	0.588993
24	8	0	-4.803458	-1.160249	0.872435
25	8	0	-4.871629	1.080307	0.768107

Succinimidyl radical

Total Energy: -360.095887 Hartrees

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.145668	-0.239989	0.024739
2	6	0	1.145900	-0.242135	0.024872
3	7	0	-0.000905	-0.995147	0.349837
4	8	0	-2.229185	-0.736394	-0.181860
5	8	0	2.228297	-0.736676	-0.188803
6	6	0	-0.768443	1.234540	0.006341
7	1	0	-1.209315	1.727065	0.873963
8	1	0	-1.195849	1.691505	-0.886532
9	6	0	0.769758	1.233777	0.022429
10	1	0	1.218643	1.706533	-0.851201
11	1	0	1.190685	1.708327	0.909932

Succinimide anion

Total Energy: -360.324630 Hartrees

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.109363	-0.268989	0.000100
2	6	0	1.109487	-0.268963	-0.000085
3	7	0	-0.000014	-1.052420	0.000684
4	8	0	-2.276231	-0.683095	-0.000914
5	8	0	2.276167	-0.683128	0.000127
6	6	0	-0.762551	1.226510	0.001075
7	1	0	-1.201222	1.699537	0.882297

8	1	0	-1.205418	1.703408	-0.875750
9	6	0	0.762540	1.226564	-0.001197
10	1	0	1.202061	1.700726	-0.881240
11	1	0	1.204515	1.702321	0.876844

4-Methylphenylthiyl radical

Total Energy: -669.239749 Hartrees

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.762502	0.000753	-0.010776
2	6	0	-1.042897	-1.206190	-0.010501
3	6	0	0.336303	-1.214194	-0.004102
4	6	0	1.067962	0.000016	0.000142
5	6	0	0.336986	1.214370	-0.004092
6	6	0	-1.042554	1.207050	-0.010485
7	1	0	-1.583307	-2.145818	-0.017443
8	1	0	0.878502	-2.150899	-0.005197
9	1	0	0.879553	2.150859	-0.005194
10	1	0	-1.582445	2.146937	-0.017393
11	16	0	2.786887	-0.000363	0.006669
12	6	0	-3.263045	-0.000171	0.012936
13	1	0	-3.668874	-0.871414	-0.503082
14	1	0	-3.625093	-0.036555	1.046173
15	1	0	-3.670044	0.902899	-0.443318

4-Methylphenylthiolate

Total Energy: -669.402790 Hartrees

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.795082	-0.000309	-0.010795

2	6	0	1.063375	1.190640	-0.010927
3	6	0	-0.327714	1.194034	-0.004610
4	6	0	-1.072225	-0.000298	0.000384
5	6	0	-0.327932	-1.194380	-0.004577
6	6	0	1.063447	-1.190930	-0.010941
7	1	0	1.591223	2.140033	-0.018305
8	1	0	-0.854971	2.141513	-0.007734
9	1	0	-0.855126	-2.141902	-0.007600
10	1	0	1.591383	-2.140241	-0.018460
11	16	0	-2.848248	0.000266	0.007295
12	6	0	3.303849	0.000295	0.016692
13	1	0	3.712600	0.866081	-0.509384
14	1	0	3.688258	0.035877	1.042061
15	1	0	3.711307	-0.899930	-0.448657

Phenylthiyl radical

Total Energy: -629.892823 Hartrees

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.242895	-0.000008	-0.000102
2	6	0	-1.540182	-1.201571	-0.000073
3	6	0	-0.149339	-1.210679	-0.000007
4	6	0	0.552191	0.000009	0.000023
5	6	0	-0.149351	1.210688	-0.000009
6	6	0	-1.540196	1.201562	-0.000068
7	1	0	-3.325696	-0.000012	-0.000151
8	1	0	-2.073608	-2.144808	-0.000097
9	1	0	0.384316	-2.153065	0.000018
10	1	0	0.384293	2.153079	0.000014
11	1	0	-2.073634	2.144793	-0.000089
12	16	0	2.320185	0.000000	0.000107

Phenylthiolate

Total Energy: -630.075504 Hartrees

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.267717	0.000139	0.000110
2	6	0	-1.555318	1.198630	-0.000031
3	6	0	-0.164351	1.198943	-0.000060
4	6	0	0.576082	-0.000152	-0.000092
5	6	0	-0.164595	-1.199097	-0.000141
6	6	0	-1.555495	-1.198499	0.000051
7	1	0	-3.351222	0.000195	0.000161
8	1	0	-2.086905	2.144613	-0.000087
9	1	0	0.368599	2.143048	-0.000087
10	1	0	0.368204	-2.143300	-0.000369
11	1	0	-2.087270	-2.144380	0.000191
12	16	0	2.348560	0.000002	0.000073

4-Chlorophenylthiyl radical

Total Energy: -1089.533490 Hartrees

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.335847	0.000000	0.000062
2	6	0	-0.655590	1.218690	0.000031
3	6	0	0.724739	1.215786	-0.000033
4	6	0	1.451998	0.000000	-0.000068
5	6	0	0.724739	-1.215786	-0.000033
6	6	0	-0.655590	-1.218690	0.000030
7	1	0	-1.206529	2.149299	0.000057
8	1	0	1.266376	2.152268	-0.000057

9	1	0	1.266376	-2.152268	-0.000059
10	1	0	-1.206529	-2.149299	0.000056
11	16	0	3.171784	0.000000	-0.000147
12	17	0	-3.082056	0.000000	0.000142

4-Chlorophenylthiolate

Total Energy: -1089.702897 Hartrees

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.355240	0.000001	-0.000071
2	6	0	-0.667029	-1.205645	-0.000042
3	6	0	0.722971	-1.197563	0.000018
4	6	0	1.466050	-0.000006	0.000056
5	6	0	0.722976	1.197555	0.000019
6	6	0	-0.667026	1.205644	-0.000045
7	1	0	-1.207100	-2.144198	-0.000072
8	1	0	1.249924	-2.144274	0.000041
9	1	0	1.249933	2.144263	0.000027
10	1	0	-1.207095	2.144198	-0.000054
11	16	0	3.233283	0.000003	0.000173
12	17	0	-3.126729	0.000003	-0.000137

4-Bromophenylthiyl radical

Total Energy: -3203.447119 Hartrees

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.664952	0.000000	-0.000032
2	6	0	-0.015311	1.218120	0.000000
3	6	0	-1.396394	1.215423	0.000065
4	6	0	-2.123540	0.000000	0.000095
5	6	0	-1.396394	-1.215423	0.000066

6	6	0	-0.015311	-1.218120	0.000001
7	1	0	0.530719	2.151445	-0.000024
8	1	0	-1.937397	2.152297	0.000092
9	1	0	-1.937397	-2.152297	0.000093
10	1	0	0.530719	-2.151445	-0.000024
11	16	0	-3.843624	0.000000	0.000180
12	35	0	2.571524	0.000000	-0.000120

4-Bromophenylthiolate

Total Energy: -3203.617049 Hartrees

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.675280	-0.000004	-0.000022
2	6	0	0.012740	-1.205627	0.000006
3	6	0	1.402989	-1.197354	0.000066
4	6	0	2.146446	-0.000008	0.000122
5	6	0	1.402992	1.197341	0.000072
6	6	0	0.012741	1.205619	0.000002
7	1	0	-0.522902	-2.146500	-0.000025
8	1	0	1.929387	-2.144392	0.000085
9	1	0	1.929394	2.144376	0.000081
10	1	0	-0.522904	2.146490	-0.000018
11	16	0	3.912801	0.000007	0.000179
12	35	0	-2.606673	0.000003	-0.000127

4-Nitrophenylthiyl radical

Total Energy: -834.468658 Hartrees

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.523727	0.000000	-0.000009
2	8	0	-3.108647	-1.083929	-0.000004

3	8	0	-3.108647	1.083929	-0.000014
4	6	0	-1.069718	0.000000	-0.000001
5	6	0	-0.387702	1.213973	0.000001
6	6	0	-0.387702	-1.213973	-0.000001
7	6	0	0.994566	1.215291	0.000005
8	1	0	-0.937578	2.143736	0.000002
9	6	0	0.994566	-1.215291	0.000000
10	1	0	-0.937578	-2.143736	-0.000003
11	6	0	1.697927	0.000000	0.000002
12	1	0	1.527085	2.157135	0.000009
13	1	0	1.527085	-2.157135	0.000001
14	16	0	3.448363	0.000000	0.000010

4-Nitrophenylthiolate

Total Energy: -834.663506 Hartrees

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.515979	-0.000001	0.000007
2	8	0	-3.120762	1.087701	0.000001
3	8	0	-3.120783	-1.087692	0.000038
4	6	0	-1.092037	-0.000005	-0.000013
5	6	0	-0.390684	-1.214998	-0.000016
6	6	0	-0.390693	1.214987	-0.000018
7	6	0	0.984629	-1.209063	-0.000040
8	1	0	-0.939004	-2.146374	0.000016
9	6	0	0.984623	1.209061	0.000004
10	1	0	-0.939013	2.146364	-0.000023
11	6	0	1.732107	0.000005	-0.000059
12	1	0	1.520467	-2.149881	-0.000017
13	1	0	1.520444	2.149889	0.000030
14	16	0	3.463353	0.000001	0.000031