Supporting Information

Cartesian coordinates of all non-planar oligomers:

2-thiophene

Atom#	atomic #		x	y	z
1	6	0	0.093103	0.718207	0.074374
2	6	0	-0.093103	-0.718207	0.074374
3	16	0	-1.238659	1.788533	-0.248795
4	16	0	1.238659	-1.788533	-0.248795
5	6	0	1.238659	1.438025	0.298991
6	6	0	-1.238659	-1.438025	0.298991
7	6	0	1.044626	2.841743	0.222419
8	6	0	-1.044626	-2.841743	0.222419
9	6	0	-0.244703	3.180453	-0.057250
10	6	0	0.244703	-3.180453	-0.057250
11	1	0	2.185614	0.973100	0.534299
12	1	0	-2.185614	-0.973100	0.534299
13	1	0	1.830164	3.566766	0.378849
14	1	0	-1.830164	-3.566766	0.378849
15	1	0	-0.669230	4.165364	-0.163638
16	1	0	0.669230	-4.165364	-0.163638

6-thiophene

Atom#	atomic #		x	y	z
1	6	0	-0.021265	8.474277	0.181850
2	6	0	0.333428	7.084240	0.011509
3	16	0	1.178987	9.653872	0.623190
4	16	0	-0.878525	5.840593	0.109401
5	6	0	-1.249694	9.072286	0.047790
6	6	0	1.566971	6.530419	-0.227242
7	6	0	-1.223333	10.469783	0.287991
8	6	0	1.539290	5.125013	-0.354404
9	6	0	0.021265	10.926878	0.601097
10	6	0	0.283018	4.586089	-0.215528
11	1	0	-2.139131	8.527845	-0.236311
12	1	0	2.463890	7.123162	-0.338190
13	1	0	-2.092548	11.107803	0.221357
14	1	0	2.413305	4.527781	-0.572658
15	1	0	0.326525	11.936454	0.822644
16	6	0	-0.125335	3.206474	-0.296760
17	16	0	1.039579	1.922950	-0.141553
18	6	0	-1.384256	2.687569	-0.482886
19	6	0	-0.176027	0.698446	-0.370267
20	6	0	-1.412803	1.278014	-0.524192
21	1	0	-2.259976	3.306906	-0.615757
22	6	0	0.176027	-0.698446	-0.370267
23	1	0	-2.313073	0.703812	-0.691442
24	16	0	-1.039579	-1.922950	-0.141553

25	6	0	1.412803	-1.278014	-0.524192
26	6	0	0.125335	-3.206474	-0.296760
27	6	0	1.384256	-2.687569	-0.482886
28	1	0	2.313073	-0.703812	-0.691442
29	1	0	2.259976	-3.306906	-0.615757
30	6	0	-0.283018	-4.586089	-0.215528
31	16	0	0.878525	-5.840593	0.109401
32	6	0	-1.539290	-5.125013	-0.354404
33	6	0	-0.333428	-7.084240	0.011509
34	6	0	-1.566971	-6.530419	-0.227242
35	1	0	-2.413305	-4.527781	-0.572658
36	6	0	0.021265	-8.474277	0.181850
37	1	0	-2.463890	-7.123162	-0.338190
38	16	0	-1.178987	-9.653872	0.623190
39	6	0	1.249694	-9.072286	0.047790
40	6	0	-0.021265	-10.926878	0.601097
41	6	0	1.223333	-10.469783	0.287991
42	1	0	2.139131	-8.527845	-0.236311
43	1	0	-0.326525	-11.936454	0.822644
44	1	0	2.092548	-11.107803	0.221357

12-thiophene

Atom#	atomic #		x	y	z
1	6	0	-0.208421	19.967938	1.404402
2	6	0	0.178748	18.619018	1.061064
3	16	0	0.948843	21.089621	2.059221
4	16	0	-1.011761	17.356394	0.947984
5	6	0	-1.440528	20.563579	1.296416
6	6	0	1.430005	18.120914	0.793316
7	6	0	-1.450873	21.914600	1.727543
8	6	0	1.433312	16.745423	0.477029
9	6	0	-0.230021	22.339222	2.158217
10	6	0	0.183794	16.174401	0.497791
11	1	0	-2.305812	20.052887	0.898041
12	1	0	2.318318	18.736511	0.794334
13	1	0	-2.327797	22.545205	1.708471
14	1	0	2.324951	16.195989	0.209936
15	1	0	0.046256	23.312264	2.530212
16	6	0	-0.195352	14.813568	0.214015
17	16	0	0.992994	13.542029	0.208936
18	6	0	-1.439402	14.304267	-0.072347
19	6	0	-0.192147	12.341797	-0.220363
20	6	0	-1.437715	12.915325	-0.316462
21	1	0	-2.324957	14.920743	-0.134562
22	6	0	0.188989	10.966936	-0.417344
23	1	0	-2.322394	12.355459	-0.584944
24	16	0	-1.005900	9.701545	-0.409888
25	6	0	1.441600	10.438508	-0.621360
26	6	0	0.190153	8.475604	-0.721505
27	6	0	1.442181	9.038966	-0.792055
28	1	0	2.333093	11.047148	-0.675166
29	1	0	2.334720	8.462364	-0.989754
30	6	0	-0.190183	7.093984	-0.861618

31	16	0	1.001873	5.828723	-0.770481
32	6	0	-1.439149	6.557524	-1.067584
33	6	0	-0.189712	4.590955	-1.049091
34	6	0	-1.438965	5.151690	-1.172884
35	1	0	-2.328572	7.163379	-1.167767
36	6	0	0.190182	3.203620	-1.114834
37	1	0	-2.328342	4.567395	-1.362023
38	16	0	-1.004465	1.945249	-0.978297
39	6	0	1.441788	2.657151	-1.273486
40	6	0	0.190294	0.694264	-1.173567
41	6	0	1.441788	1.247835	-1.306319
42	1	0	2.333271	3.256946	-1.390228
43	1	0	2.333655	0.654447	-1.449989
44	6	0	-0.190294	-0.694264	-1.173567
45	16	0	1.004465	-1.945249	-0.978297
46	6	0	-1.441788	-1.247835	-1.306319
47	6	0	-0.190182	-3.203620	-1.114834
48	6	0	-1.441788	-2.657151	-1.273486
49	1	0	-2.333655	-0.654447	-1.449989
50	6	0	0.189712	-4.590955	-1.049091
51	1	0	-2.333271	-3.256946	-1.390228
52	16	0	-1.001873	-5.828723	-0.770481
53	6	0	1.438965	-5.151690	-1.172884
54	6	0	0.190183	-7.093984	-0.861618
55	6	0	1.439149	-6.557524	-1.067584
56	1	0	2.328342	-4.567395	-1.362023
57	6	0	-0.190153	-8.475604	-0.721505
58	1	0	2.328572	-7.163379	-1.167767
59	16	0	1.005900	-9.701545	-0.409888
60	6	0	-1.442181	-9.038966	-0.792055
61	6	0	-0.188989	-10.966936	-0.417344
62	6	0	-1.441600	-10.438508	-0.621360
63	1	0	-2.334720	-8.462364	-0.989754
64	6	0	0.192147	-12.341797	-0.220363
65	1	0	-2.333093	-11.047148	-0.675166
66	16	0	-0.992994	-13.542029	0.208936
67	6	0	1.437715	-12.915325	-0.316462
68	6	0	0.195352	-14.813568	0.214015
69	6	0	1.439402	-14.304267	-0.072347
70	1	0	2.322394	-12.355459	-0.584944
71	6	0	-0.183794	-16.174401	0.497791
72	1	0	2.324957	-14.920743	-0.134562
73	16	0	1.011761	-17.356394	0.947984
74	6	0	-1.433312	-16.745423	0.477029
75	6	0	-0.178748	-18.619018	1.061064
76	6	0	-1.430005	-18.120914	0.793316
77	1	0	-2.324951	-16.195989	0.209936
78	6	0	0.208421	-19.967938	1.404402
79	1	0	-2.318318	-18.736511	0.794334
80	16	0	-0.948843	-21.089621	2.059221
81	6	0	1.440528	-20.563579	1.296416
82	6	0	0.230021	-22.339222	2.158217
83	6	0	1.450873	-21.914600	1.727543
84	1	0	2.305812	-20.052887	0.898041
85	1	0	-0.046256	-23.312264	2.530212

86	1	0	2.327797	-22.545205	1.708471

18-thiophene

Atom#	atomic #		x	y	z
1	6	0	0.691403	-30.827446	4.145860
2	6	0	0.302349	-29.580701	3.528668
3	16	0	-0.495072	-31.872164	4.872533
4	16	0	1.467908	-28.315548	3.271601
5	6	0	1.945228	-31.372791	4.269771
6	6	0	-0.934143	-29.188840	3.078105
7	6	0	1.950033	-32.624876	4.935755
8	6	0	-0.944446	-27.896404	2.511195
9	6	0	0.703704	-33.025584	5.312629
10	6	0	0.285265	-27.283451	2.520277
11	1	0	2.832882	-30.898657	3.875353
12	1	0	-1.805318	-29.826591	3.127736
13	1	0	2.842633	-33.205315	5.118427
14	1	0	-1.824560	-27.440012	2.080699
15	1	0	0.418561	-33.929914	5.824884
16	6	0	0.653863	-25.983601	2.018857
17	16	0	-0.557660	-24.776422	1.698026
18	6	0	1.904894	-25.491558	1.732431
19	6	0	0.630579	-23.632647	1.141592
20	6	0	1.891743	-24.170325	1.239328
21	1	0	2.805885	-26.077380	1.846889
22	6	0	0.235857	-22.328693	0.673679
23	1	0	2.781799	-23.637452	0.935906
24	16	0	1.396169	-21.036859	0.556513
25	6	0	-1.006116	-21.891193	0.278749
26	6	0	0.204841	-19.930600	-0.064067
27	6	0	-1.023507	-20.543512	-0.135921
28	1	0	-1.875472	-22.533045	0.260151
29	1	0	-1.907423	-20.043921	-0.506340
30	6	0	0.564628	-18.580687	-0.415110
31	16	0	-0.653863	-17.348625	-0.577286
32	6	0	1.810842	-18.053813	-0.658316
33	6	0	0.524377	-16.143864	-1.012870
34	6	0	1.788127	-16.684482	-0.994269
35	1	0	2.714623	-18.645561	-0.625125
36	6	0	0.120660	-14.796812	-1.324166
37	1	0	2.672904	-16.116846	-1.245477
38	16	0	1.278739	-13.497551	-1.321569
39	6	0	-1.128769	-14.320974	-1.644290
40	6	0	0.075437	-12.332096	-1.793107
41	6	0	-1.154251	-12.935996	-1.907626
42	1	0	-1.998457	-14.958587	-1.716474
43	1	0	-2.045582	-12.400823	-2.202940
44	6	0	0.428702	-10.951522	-2.002241
45	16	0	-0.793309	-9.712464	-2.018850
46	6	0	1.671157	-10.398637	-2.203340
47	6	0	0.378074	-8.465021	-2.337685
48	6	0	1.642651	-9.001523	-2.391765
49	1	0	2.576031	-10.988256	-2.243778

50	6	0	-0.031326	-7.093657	-2.498076
51	1	0	2.523982	-8.408302	-2.590498
52	16	0	1.128179	-5.799848	-2.394004
53	6	0	-1.288383	-6.589151	-2.733482
54	6	0	-0.086362	-4.593579	-2.707865
55	6	0	-1.319399	-5.184458	-2.851148
56	1	0	-2.160805	-7.216982	-2.846819
57	6	0	0.262451	-3.198026	-2.779156
58	1	0	-2.218009	-4.623013	-3.064155
59	16	0	-0.957848	-1.966328	-2.628999
60	6	0	1.499795	-2.624637	-2.952893
61	6	0	0.205809	-0.690040	-2.844544
62	6	0	1.467908	-1.215495	-2.989650
63	1	0	2.402671	-3.204854	-3.080409
64	6	0	-0.205809	0.690040	-2.844544
65	1	0	2.344182	-0.602771	-3.147326
66	16	0	0.957848	1.966328	-2.628999
67	6	0	-1.467908	1.215495	-2.989650
68	6	0	-0.262451	3.198026	-2.779156
69	6	0	-1.499795	2.624637	-2.952893
70	1	0	-2.344182	0.602771	-3.147326
71	6	0	0.086362	4.593579	-2.707865
72	1	0	-2.402671	3.204854	-3.080409
73	16	0	-1.128179	5.799848	-2.394004
74	6	0	1.319399	5.184458	-2.851148
75	6	0	0.031326	7.093657	-2.498076
76	6	0	1.288383	6.589151	-2.733482
77	1	0	2.218009	4.623013	-3.064155
78	6	0	-0.378074	8.465021	-2.337685
79	1	0	2.160805	7.216982	-2.846819
80	16	0	0.793309	9.712464	-2.018850
81	6	0	-1.642651	9.001523	-2.391765
82	6	0	-0.428702	10.951522	-2.002241
83	6	0	-1.671157	10.398637	-2.203340
84	1	0	-2.523982	8.408302	-2.590498
85	1	0	-2.576031	10.988256	-2.243778
86	6	0	-0.075437	12.332096	-1.793107
87	16	0	-1.278739	13.497551	-1.321569
88	6	0	1.154251	12.935996	-1.907626
89	6	0	-0.120660	14.796812	-1.324166
90	6	0	1.128769	14.320974	-1.644290
91	1	0	2.045582	12.400823	-2.202940
92	6	0	-0.524377	16.143864	-1.012870
93	1	0	1.998457	14.958587	-1.716474
94	16	0	0.653863	17.348625	-0.577286
95	6	0	-1.788127	16.684482	-0.994269
96	6	0	-0.564628	18.580687	-0.415110
97	6	0	-1.810842	18.053813	-0.658316
98	1	0	-2.672904	16.116846	-1.245477
99	6	0	-0.204841	19.930600	-0.064067
100	1	0	-2.714623	18.645561	-0.625125
101	16	0	-1.396169	21.036859	0.556513
102	6	0	1.023507	20.543512	-0.135921
103	6	0	-0.235857	22.328693	0.673679
104	6	0	1.006116	21.891193	0.278749

105	1	0	1.907423	20.043921	-0.506340
106	6	0	-0.630579	23.632647	1.141592
107	1	0	1.875472	22.533045	0.260151
108	16	0	0.557660	24.776422	1.698026
109	6	0	-1.891743	24.170325	1.239328
110	6	0	-0.653863	25.983601	2.018857
111	6	0	-1.904894	25.491558	1.732431
112	1	0	-2.781799	23.637452	0.935906
113	6	0	-0.285265	27.283451	2.520277
114	1	0	-2.805885	26.077380	1.846889
115	16	0	-1.467908	28.315548	3.271601
116	6	0	0.944446	27.896404	2.511195
117	6	0	-0.302349	29.580701	3.528668
118	6	0	0.934143	29.188840	3.078105
119	1	0	1.824560	27.440012	2.080699
120	6	0	-0.691403	30.827446	4.145860
121	1	0	1.805318	29.826591	3.127736
122	16	0	0.495072	31.872164	4.872533
123	6	0	-1.945228	31.372791	4.269771
124	6	0	-0.703704	33.025584	5.312629
125	6	0	-1.950033	32.624876	4.935755
126	1	0	-2.832882	30.898657	3.875353
127	1	0	-0.418561	33.929914	5.824884
128	1	0	-2.842633	33.205315	5.118427

2-pyrrole

Atom#	atomic #		x	y	z
1	6	0	-0.721116	0.052953	0.039904
2	6	0	0.721116	-0.052937	0.039907
3	7	0	-1.518131	-1.023776	-0.252214
4	7	0	1.518143	1.023781	-0.252210
5	6	0	-1.562735	1.117303	0.300086
6	6	0	1.562722	-1.117297	0.300096
7	6	0	-2.895182	0.659364	0.152098
8	6	0	2.895174	-0.659377	0.152096
9	6	0	-2.836181	-0.667988	-0.190851
10	6	0	2.836189	0.667975	-0.190855
11	1	0	-1.251971	2.101812	0.611067
12	1	0	1.251945	-2.101798	0.611088
13	1	0	-3.794638	1.235079	0.295466
14	1	0	3.794622	-1.235106	0.295451
15	1	0	-3.615458	-1.382247	-0.393330
16	1	0	3.615474	1.382229	-0.393321
17	1	0	-1.166847	-1.913809	-0.555183
18	1	0	1.166872	1.913828	-0.555156

6-pyrrole

Atom#	atomic #		x	y	z
1	6	0	7.740086	-0.173890	-0.225126
2	6	0	6.449741	0.456401	-0.077158

3	7	0	8.718597	0.371059	-1.016776
4	7	0	5.327170	-0.271576	0.222212
5	6	0	8.261491	-1.332364	0.319306
6	6	0	6.056627	1.777552	-0.183013
7	6	0	9.582902	-1.480156	-0.167923
8	6	0	4.664544	1.833093	0.051166
9	6	0	9.837107	-0.413262	-0.993080
10	6	0	4.227343	0.544770	0.298168
11	1	0	7.761461	-1.972773	1.027940
12	1	0	6.712217	2.617256	-0.348745
13	1	0	10.273370	-2.271992	0.071176
14	1	0	4.057284	2.722640	0.097679
15	1	0	10.713428	-0.149772	-1.559667
16	1	0	8.584857	1.178506	-1.597652
17	1	0	5.287191	-1.274938	0.210378
18	6	0	2.916790	0.021722	0.591589
19	7	0	1.777801	0.675039	0.195115
20	6	0	2.514346	-1.119725	1.260467
21	6	0	0.661338	-0.023042	0.579972
22	1	0	1.766255	1.451369	-0.441672
23	6	0	1.102453	-1.147488	1.253411
24	1	0	3.166653	-1.822307	1.753364
25	6	0	-0.665841	0.450292	0.276303
26	1	0	0.475188	-1.876609	1.740624
27	7	0	-1.736654	-0.402327	0.202919
28	6	0	-1.148140	1.722424	0.024943
29	6	0	-2.886416	0.285234	-0.087016
30	1	0	-1.686063	-1.394745	0.345903
31	6	0	-2.536844	1.618737	-0.204541
32	1	0	-0.566285	2.629754	0.039616
33	1	0	-3.205094	2.425330	-0.459796
34	6	0	-4.155087	-0.385180	-0.229871
35	7	0	-5.342736	0.275401	-0.049476
36	6	0	-4.469949	-1.691385	-0.559075
37	6	0	-6.403741	-0.567891	-0.249798
38	1	0	-5.426137	1.244587	0.199106
39	6	0	-5.877159	-1.806229	-0.568596
40	1	0	-3.762906	-2.469715	-0.797208
41	6	0	-7.767830	-0.114928	-0.109796
42	1	0	-6.445994	-2.703180	-0.753288
43	7	0	-8.796511	-0.715432	-0.789963
44	6	0	-8.324125	0.898895	0.647080
45	6	0	-9.981417	-0.104369	-0.491060
46	1	0	-8.669153	-1.434083	-1.478858
47	6	0	-9.719065	0.903125	0.403070
48	1	0	-7.791276	1.534206	1.336325
49	1	0	-10.904937	-0.434455	-0.934399
50	1	0	-10.448644	1.561754	0.844424

12-pyrrole

Atom#	atomic #		x	y	z
1	6	0	-18.245777	0.766255	0.647233
2	6	0	-16.953466	1.135583	0.120751

3	7	0	-19.123275	1.706846	1.123119
4	7	0	-15.896617	0.262512	0.140324
5	6	0	-18.858861	-0.464448	0.789185
6	6	0	-16.499460	2.304318	-0.461752
7	6	0	-20.131664	-0.246808	1.370285
8	6	0	-15.137055	2.122403	-0.787910
9	6	0	-20.266516	1.104729	1.567299
10	6	0	-14.778403	0.844326	-0.401062
11	1	0	-18.452934	-1.409118	0.464820
12	1	0	-17.100519	3.171343	-0.683948
13	1	0	-20.870048	-0.995756	1.604282
14	1	0	-14.502770	2.824066	-1.305202
15	1	0	-21.074173	1.682280	1.982636
16	1	0	-18.905886	2.682550	1.212395
17	1	0	-15.895188	-0.608622	0.639886
18	6	0	-13.526331	0.136157	-0.488928
19	7	0	-12.327838	0.800364	-0.547638
20	6	0	-13.240104	-1.216094	-0.532164
21	6	0	-11.285188	-0.088854	-0.613115
22	1	0	-12.220209	1.784433	-0.379260
23	6	0	-11.837164	-1.356827	-0.610186
24	1	0	-13.966742	-2.011686	-0.566073
25	6	0	-9.916222	0.357899	-0.674716
26	1	0	-11.292579	-2.281440	-0.715097
27	7	0	-8.879048	-0.437305	-0.262037
28	6	0	-9.360060	1.544783	-1.117882
29	6	0	-7.679042	0.204363	-0.427337
30	1	0	-8.984457	-1.364278	0.108812
31	6	0	-7.960859	1.449530	-0.960918
32	1	0	-9.903243	2.374931	-1.539578
33	1	0	-7.238786	2.218644	-1.183191
34	6	0	-6.431634	-0.415238	-0.055148
35	7	0	-5.240008	-0.027038	-0.610121
36	6	0	-6.142818	-1.419693	0.851539
37	6	0	-4.200955	-0.752358	-0.087454
38	1	0	-5.141569	0.690643	-1.305142
39	6	0	-4.747978	-1.632408	0.829342
40	1	0	-6.856285	-1.922774	1.484087
41	6	0	-2.840051	-0.542836	-0.514496
42	1	0	-4.204473	-2.370324	1.397071
43	7	0	-1.775985	-0.888493	0.277439
44	6	0	-2.316121	-0.022352	-1.684465
45	6	0	-0.590595	-0.603631	-0.348942
46	1	0	-1.854996	-1.292596	1.192993
47	6	0	-0.909366	-0.057857	-1.579880
48	1	0	-2.885516	0.316181	-2.535029
49	1	0	-0.205064	0.304544	-2.311288
50	6	0	0.680616	-0.860968	0.280063
51	7	0	1.830587	-1.002488	-0.452459
52	6	0	1.034518	-0.996689	1.610932
53	6	0	2.905392	-1.225692	0.368289
54	1	0	1.879077	-0.952067	-1.453904
55	6	0	2.425464	-1.227280	1.666025
56	1	0	0.368001	-0.907845	2.453639
57	6	0	4.234360	-1.414012	-0.156428

58	1	0	3.010572	-1.407677	2.553227
59	7	0	5.347991	-1.168985	0.606205
60	6	0	4.680396	-1.835517	-1.395863
61	6	0	6.489746	-1.407723	-0.115420
62	1	0	5.331259	-0.704740	1.496449
63	6	0	6.092151	-1.831046	-1.370488
64	1	0	4.057552	-2.168440	-2.210498
65	6	0	7.798191	-1.212244	0.455620
66	1	0	6.748240	-2.160113	-2.160013
67	7	0	8.892579	-0.949688	-0.328629
68	6	0	8.237917	-1.235385	1.766533
69	6	0	10.014145	-0.790681	0.444936
70	1	0	8.843932	-0.720815	-1.305155
71	6	0	9.625151	-0.972073	1.759734
72	1	0	7.635814	-1.477586	2.627327
73	6	0	11.297547	-0.493675	-0.139763
74	1	0	10.280005	-0.975325	2.616213
75	7	0	12.291307	0.121559	0.576449
76	6	0	11.802608	-0.727843	-1.406438
77	6	0	13.413366	0.288033	-0.192850
78	1	0	12.209814	0.408279	1.535064
79	6	0	13.125031	-0.236522	-1.440325
80	1	0	11.284192	-1.228423	-2.208129
81	6	0	14.599195	0.923189	0.326183
82	1	0	13.785498	-0.237186	-2.292411
83	7	0	15.835286	0.701604	-0.223720
84	6	0	14.778868	1.816318	1.367204
85	6	0	16.796909	1.421687	0.434959
86	1	0	16.014673	0.093776	-1.002481
87	6	0	16.154636	2.125482	1.437308
88	1	0	13.999177	2.224927	1.989775
89	6	0	18.187689	1.354505	0.052219
90	1	0	16.631518	2.765020	2.162412
91	7	0	19.049267	2.394248	0.292689
92	6	0	18.920688	0.359816	-0.566980
93	6	0	20.299673	2.087489	-0.164647
94	1	0	18.765909	3.283355	0.662115
95	6	0	20.250849	0.826079	-0.703157
96	1	0	18.549856	-0.613448	-0.845967
97	1	0	21.113537	2.785305	-0.069390
98	1	0	21.080606	0.290879	-1.134344

18-pyrrole

Atom#	atomic #		x	y	z
1	6	0	28.573284	2.061438	-0.874668
2	6	0	27.224778	2.466153	-0.556241
3	7	0	29.369298	2.806618	-1.706668
4	7	0	26.267650	1.551230	-0.200679
5	6	0	29.319154	0.967721	-0.477157
6	6	0	26.622575	3.710310	-0.528366
7	6	0	30.589391	1.065198	-1.095411
8	6	0	25.272466	3.527507	-0.155044
9	6	0	30.590480	2.211013	-1.850895

10	6	0	25.069533	2.173959	0.041436
11	1	0	28.999647	0.209843	0.219901
12	1	0	27.117908	4.652818	-0.697759
13	1	0	31.413477	0.379634	-0.986913
14	1	0	24.543423	4.303474	0.014152
15	1	0	31.352340	2.647769	-2.473144
16	1	0	29.054565	3.618822	-2.205170
17	1	0	26.382381	0.556723	-0.279544
18	6	0	23.895938	1.430731	0.425207
19	7	0	22.632871	1.912694	0.193929
20	6	0	23.751488	0.203490	1.046099
21	6	0	21.687396	1.022664	0.636856
22	1	0	22.430916	2.710883	-0.380887
23	6	0	22.368960	-0.051584	1.178889
24	1	0	24.555031	-0.411142	1.418399
25	6	0	20.277842	1.291749	0.502102
26	1	0	21.920414	-0.898839	1.672172
27	7	0	19.349452	0.283725	0.477667
28	6	0	19.581044	2.481702	0.388414
29	6	0	18.082765	0.792612	0.352245
30	1	0	19.567736	-0.693815	0.545860
31	6	0	18.208393	2.169267	0.292222
32	1	0	20.014229	3.468603	0.406836
33	1	0	17.400674	2.871213	0.161014
34	6	0	16.924226	-0.063177	0.290013
35	7	0	15.674692	0.392339	0.621431
36	6	0	16.780949	-1.386718	-0.086808
37	6	0	14.739493	-0.598054	0.468745
38	1	0	15.472018	1.324984	0.932788
39	6	0	15.414902	-1.722013	0.027471
40	1	0	17.570457	-2.032046	-0.436795
41	6	0	13.345784	-0.375539	0.763316
42	1	0	14.975890	-2.688564	-0.160536
43	7	0	12.359055	-1.140340	0.197509
44	6	0	12.719219	0.535904	1.594533
45	6	0	11.123479	-0.744959	0.639909
46	1	0	12.519771	-1.887780	-0.453124
47	6	0	11.329088	0.306557	1.515317
48	1	0	13.212483	1.265920	2.215832
49	1	0	10.558550	0.868593	2.017935
50	6	0	9.914484	-1.384013	0.183467
51	7	0	8.756676	-1.340725	0.915830
52	6	0	9.633804	-2.098906	-0.967593
53	6	0	7.747855	-2.006689	0.269803
54	1	0	8.660527	-0.884961	1.805202
55	6	0	8.279144	-2.490303	-0.912628
56	1	0	10.322235	-2.290471	-1.774874
57	6	0	6.427759	-2.117225	0.837709
58	1	0	7.754640	-3.089329	-1.639291
59	7	0	5.323588	-2.331648	0.052528
60	6	0	5.984773	-2.052913	2.146305
61	6	0	4.188984	-2.392006	0.820962
62	1	0	5.323080	-2.268009	-0.949626
63	6	0	4.583390	-2.224538	2.135910
64	1	0	6.609986	-1.954940	3.019203

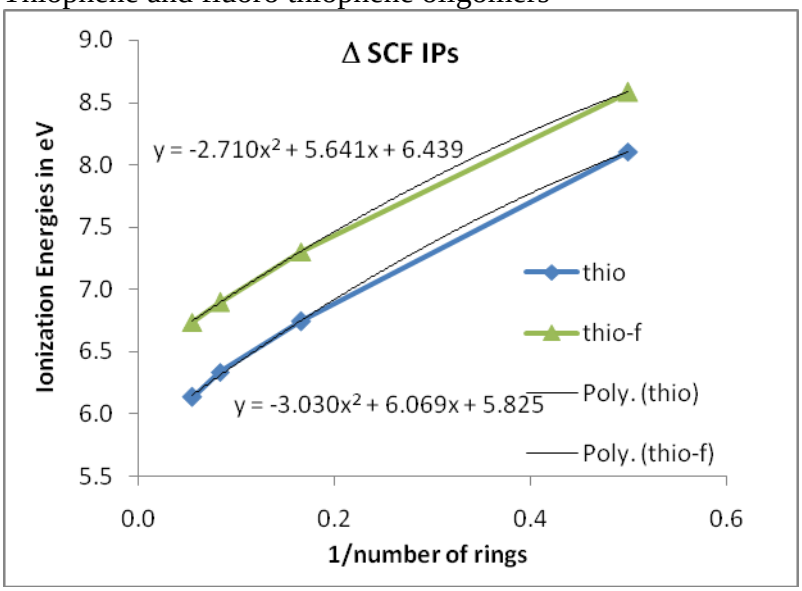
65	6	0	2.888935	-2.598513	0.234808
66	1	0	3.938813	-2.282731	2.998004
67	7	0	1.743593	-2.181352	0.863802
68	6	0	2.502796	-3.193126	-0.952588
69	6	0	0.639951	-2.480480	0.106036
70	1	0	1.729196	-1.580502	1.668255
71	6	0	1.094977	-3.119351	-1.032986
72	1	0	3.159640	-3.682175	-1.653617
73	6	0	-0.690067	-2.140196	0.545312
74	1	0	0.476193	-3.542034	-1.808113
75	7	0	-1.722251	-1.971447	-0.340540
76	6	0	-1.209899	-1.935050	1.811014
77	6	0	-2.883868	-1.665504	0.319784
78	1	0	-1.639680	-2.063128	-1.336920
79	6	0	-2.581747	-1.636133	1.669699
80	1	0	-0.664970	-2.025297	2.736704
81	6	0	-4.117398	-1.426922	-0.387724
82	1	0	-3.268695	-1.392809	2.464147
83	7	0	-5.337032	-1.599600	0.213548
84	6	0	-4.364835	-1.001627	-1.680734
85	6	0	-6.354099	-1.299855	-0.654975
86	1	0	-5.467209	-1.907283	1.160264
87	6	0	-5.763850	-0.924430	-1.848694
88	1	0	-3.617403	-0.743075	-2.413323
89	6	0	-7.738475	-1.415765	-0.269388
90	1	0	-6.285227	-0.654870	-2.752999
91	7	0	-8.726645	-0.716504	-0.912199
92	6	0	-8.356433	-2.175343	0.708144
93	6	0	-9.954430	-1.005174	-0.375688
94	1	0	-8.573228	-0.081984	-1.674888
95	6	0	-9.742177	-1.916576	0.643351
96	1	0	-7.865669	-2.865727	1.375089
97	1	0	-10.500327	-2.325638	1.291497
98	6	0	-11.160539	-0.388849	-0.869893
99	7	0	-12.388199	-0.976790	-0.708274
100	6	0	-11.372857	0.805902	-1.534716
101	6	0	-13.375755	-0.196548	-1.251067
102	1	0	-12.542600	-1.860704	-0.257923
103	6	0	-12.758223	0.925239	-1.775186
104	1	0	-10.614960	1.528995	-1.789794
105	6	0	-14.759959	-0.597304	-1.223459
106	1	0	-13.250748	1.725607	-2.303193
107	7	0	-15.775160	0.321300	-1.308222
108	6	0	-15.352052	-1.843335	-1.125532
109	6	0	-16.995996	-0.301443	-1.253566
110	1	0	-15.645458	1.314377	-1.235203
111	6	0	-16.751733	-1.658272	-1.143874
112	1	0	-14.832671	-2.787939	-1.105139
113	6	0	-18.227130	0.444950	-1.312611
114	1	0	-17.500702	-2.433594	-1.140400
115	7	0	-19.392088	-0.046751	-0.780959
116	6	0	-18.521066	1.684923	-1.849754
117	6	0	-20.416644	0.849311	-0.951200
118	1	0	-19.444359	-0.856962	-0.190036
119	6	0	-19.891811	1.937798	-1.623870

120	1	0	-17.836236	2.310201	-2.399458
121	6	0	-21.747452	0.573578	-0.470958
122	1	0	-20.449351	2.793549	-1.969213
123	7	0	-22.631170	1.579779	-0.178463
124	6	0	-22.401836	-0.619744	-0.222564
125	6	0	-23.827970	1.066565	0.249175
126	1	0	-22.428759	2.559237	-0.265526
127	6	0	-23.702513	-0.311309	0.229969
128	1	0	-21.995519	-1.605141	-0.383668
129	6	0	-24.923865	1.921532	0.632648
130	1	0	-24.456391	-1.017732	0.538088
131	7	0	-26.221732	1.480368	0.619561
132	6	0	-24.951605	3.233075	1.071701
133	6	0	-27.075618	2.468849	1.032890
134	1	0	-26.510202	0.559102	0.343738
135	6	0	-26.298516	3.576406	1.319159
136	1	0	-24.091795	3.864967	1.226339
137	6	0	-28.502714	2.258201	1.099152
138	1	0	-26.666776	4.538156	1.637920
139	7	0	-29.292945	2.968545	1.966490
140	6	0	-29.337743	1.408647	0.398337
141	6	0	-30.598134	2.585282	1.838995
142	1	0	-28.936932	3.602713	2.658106
143	6	0	-30.657269	1.616894	0.868317
144	1	0	-29.037038	0.747001	-0.398151
145	1	0	-31.369997	3.029710	2.443224
146	1	0	-31.550077	1.122393	0.523010

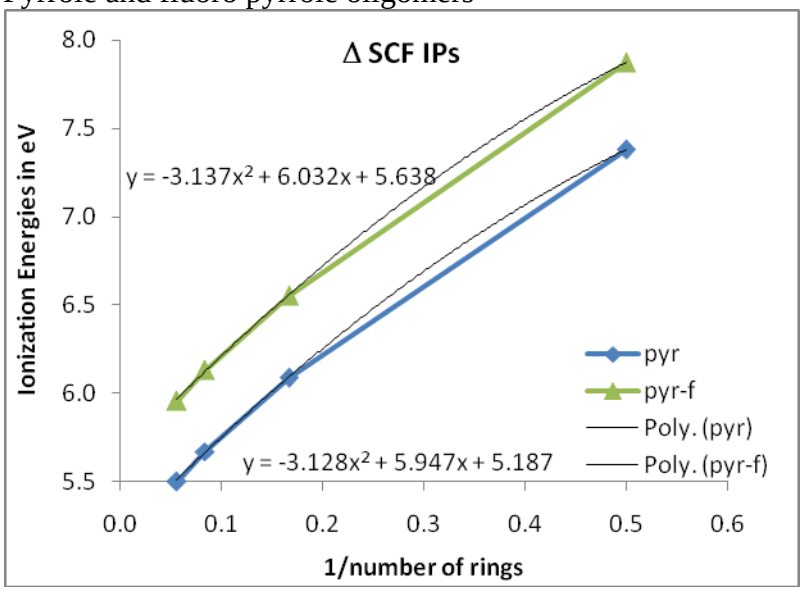
Plots for extrapolating oligomer data to infinite chain length

ΔSCF IPs

Thiophene and fluoro thiophene oligomers

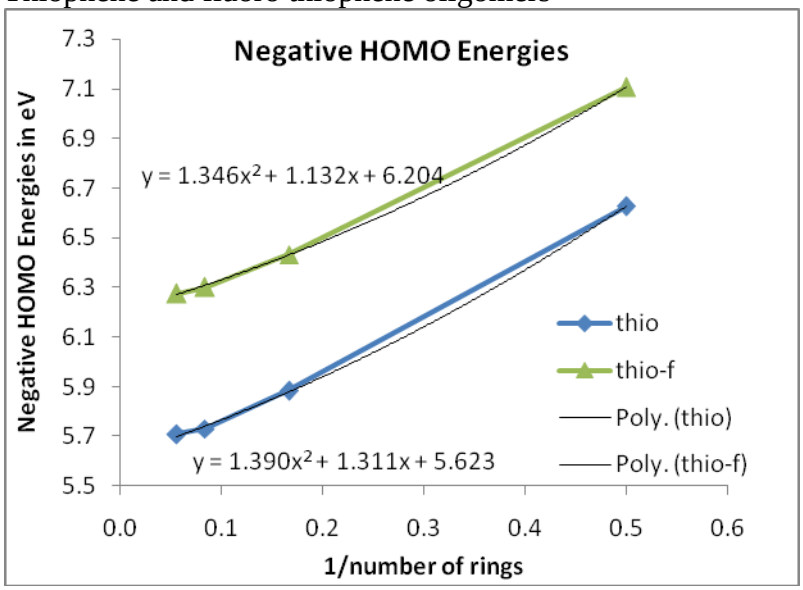


Pyrrole and fluoro pyrrole oligomers

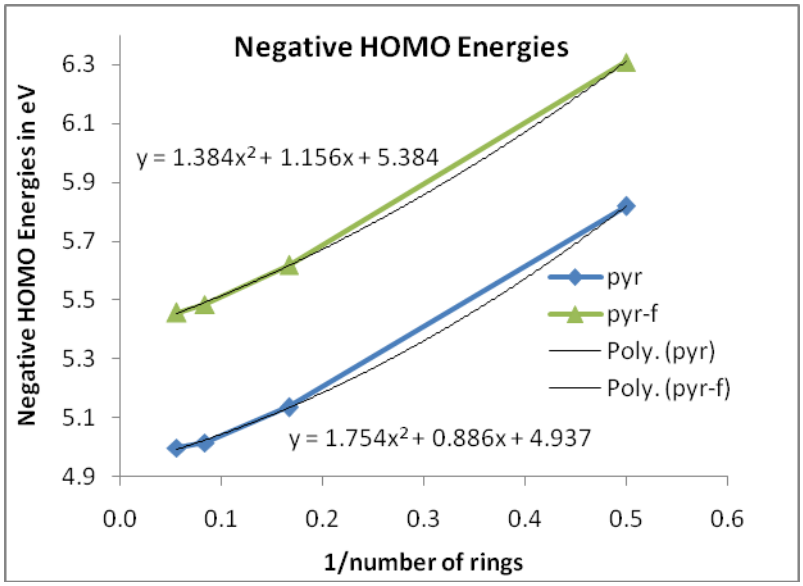


Negative HOMO energies

Thiophene and fluoro thiophene oligomers

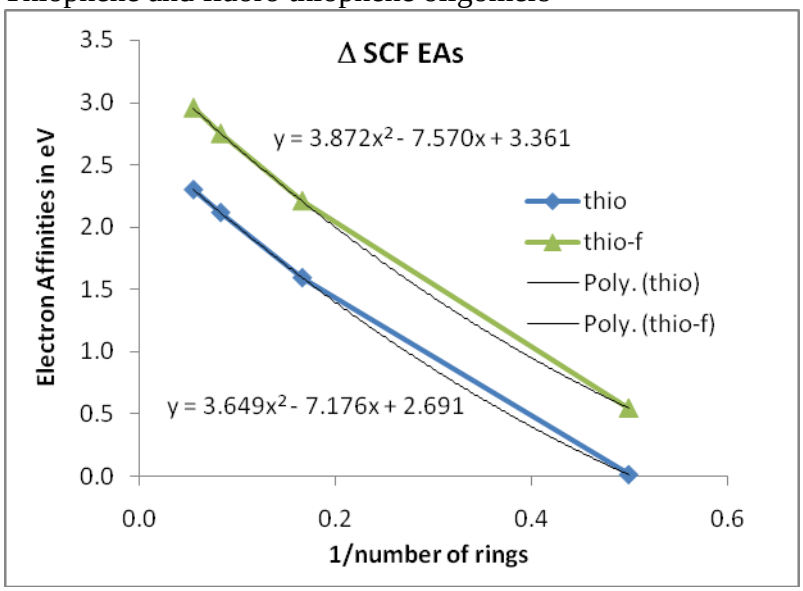


Pyrrole and fluoro pyrrole oligomers

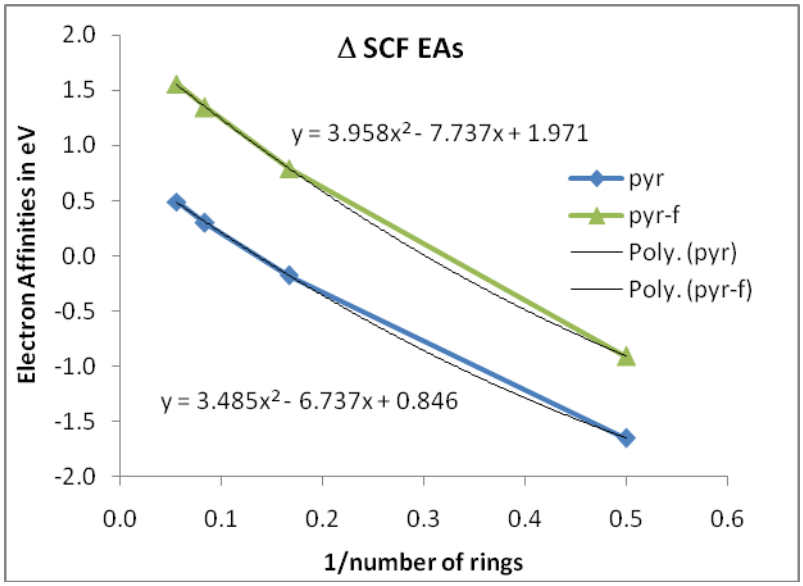


ΔSCF EAs

Thiophene and fluoro thiophene oligomers

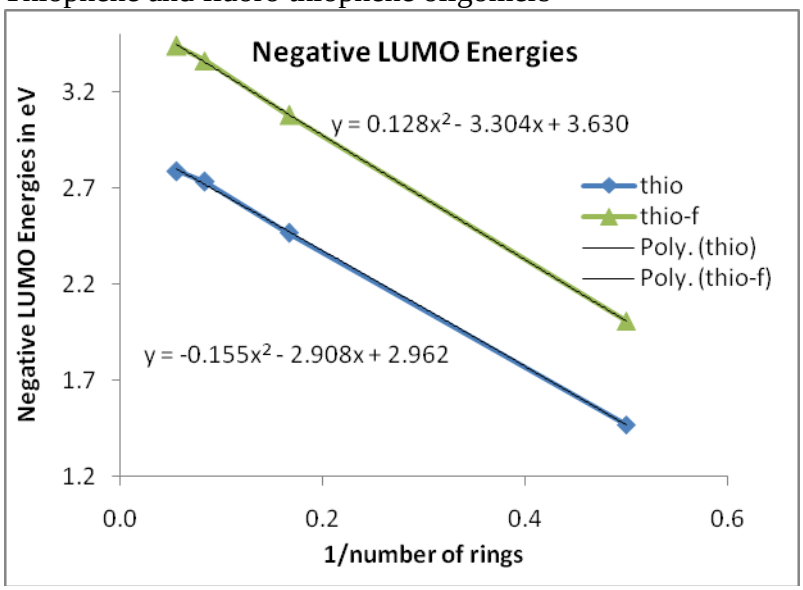


Pyrrole and fluoro pyrrole oligomers

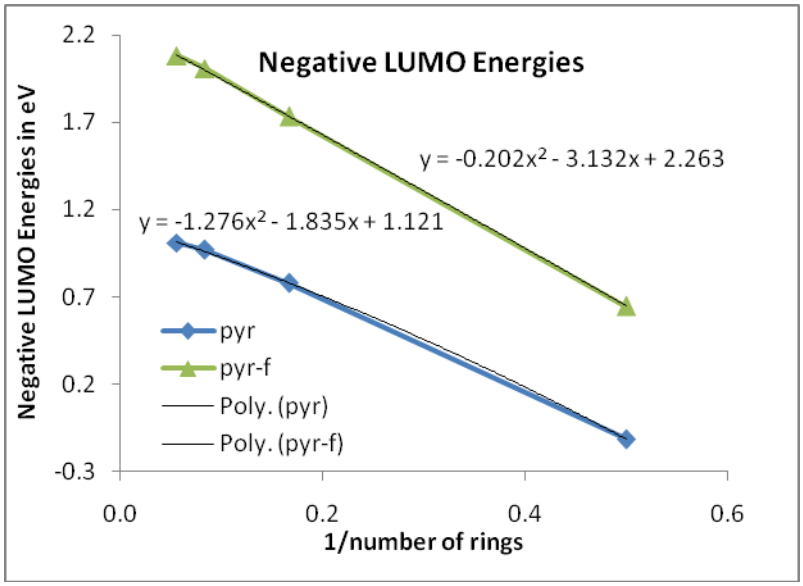


Negative LUMO energies

Thiophene and fluoro thiophene oligomers



Pyrrole and fluoro pyrrole oligomers


Negative LUMO Energies
Negative LUMO Energies in eV
1/number of rings
y = -0.202x² - 3.132x + 2.263
y = -1.276x² - 1.835x + 1.121
pyr
pyr-f
Poly. (pyr)
Poly. (pyr-f)
2.2
1.7
1.2
0.7
0.2
-0.3
0.0
0.2
0.4
0.6