Supporting Information

Synthesis and Characterization of Heteroatom Substituted Carbazole Derivatives: Potential Host Materials for Phosphorescent Organic Light-emitting Diodes

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Ye Tao, and Run-feng Chen

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Figure 14. ^{13}C NMR shift spectra of C-SO in $CDCl_3$

Table S1-S6. The details of quantum chemical calculations

NMR Spectra

(1) 9-Ethyl-carbazole (E-C)

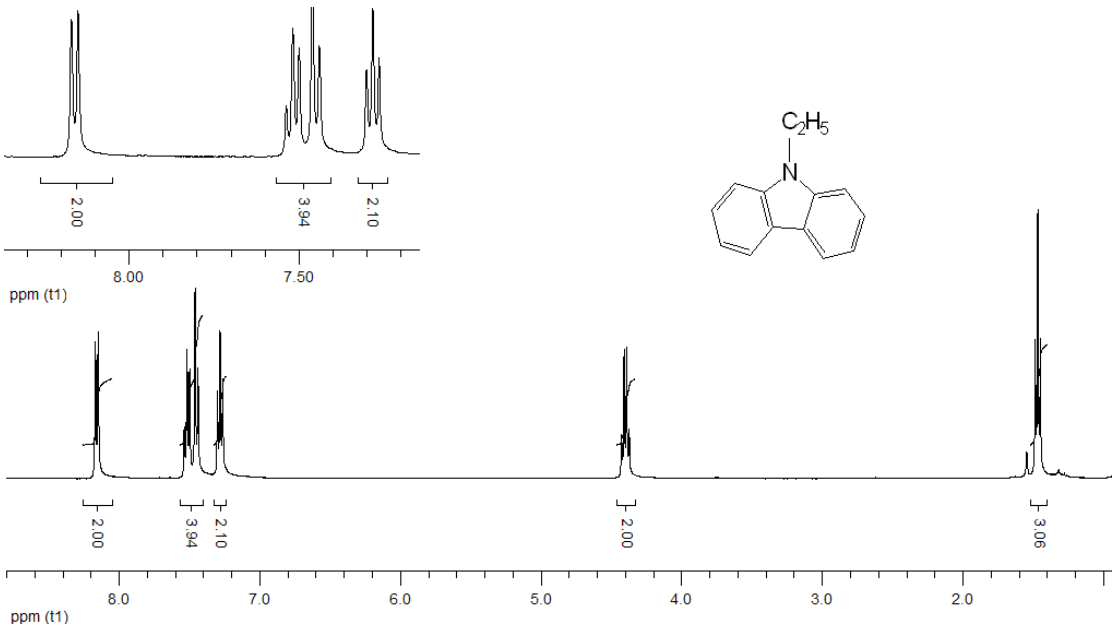


Figure 1. ^{1}H NMR shift spectra of E-C in $CDCl_3$

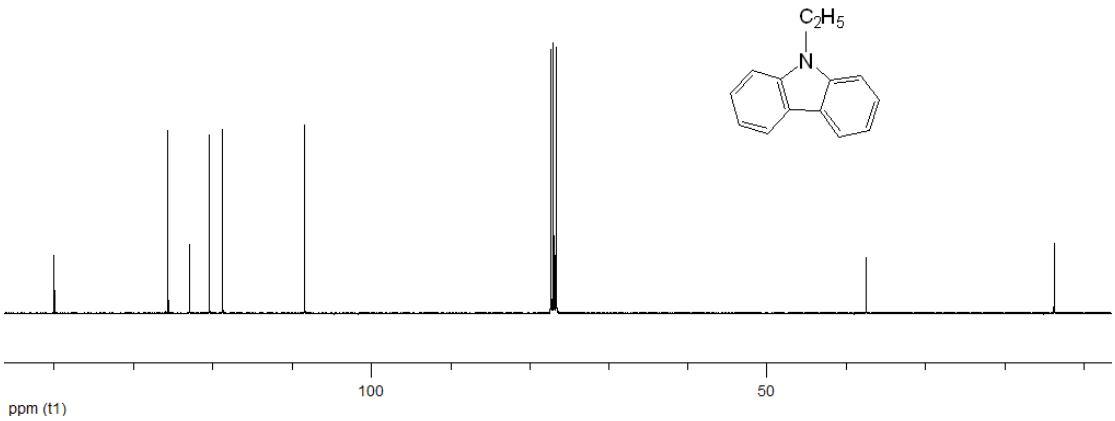


Figure 2. ^{13}C NMR shift spectra of E-C in $CDCl_3$

(2) 3-Iodo-9ethyl-carbazole(C-I)

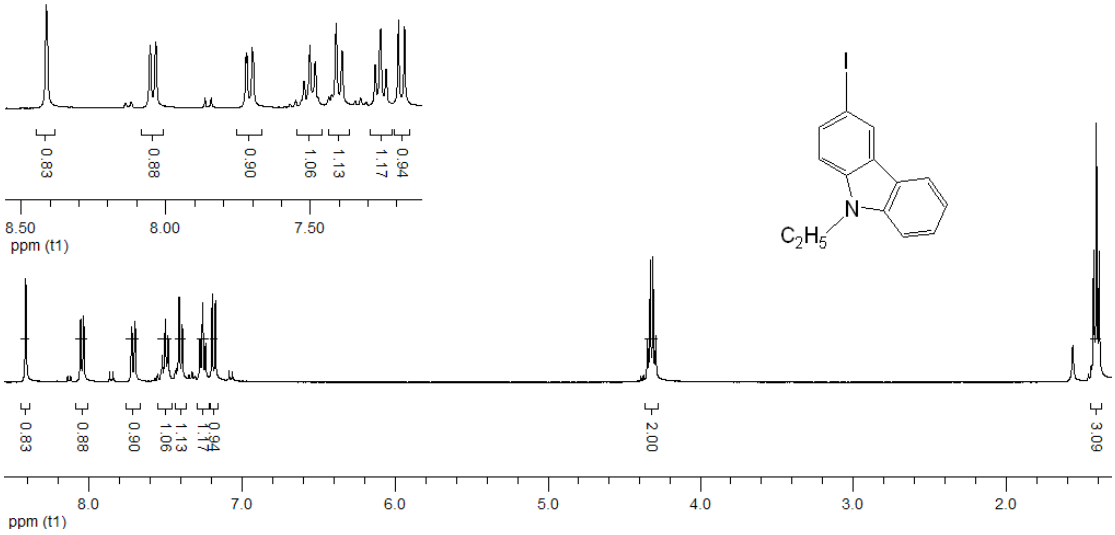


Figure 3. ^{1}H NMR shift spectra of C-I in $CDCl_3$

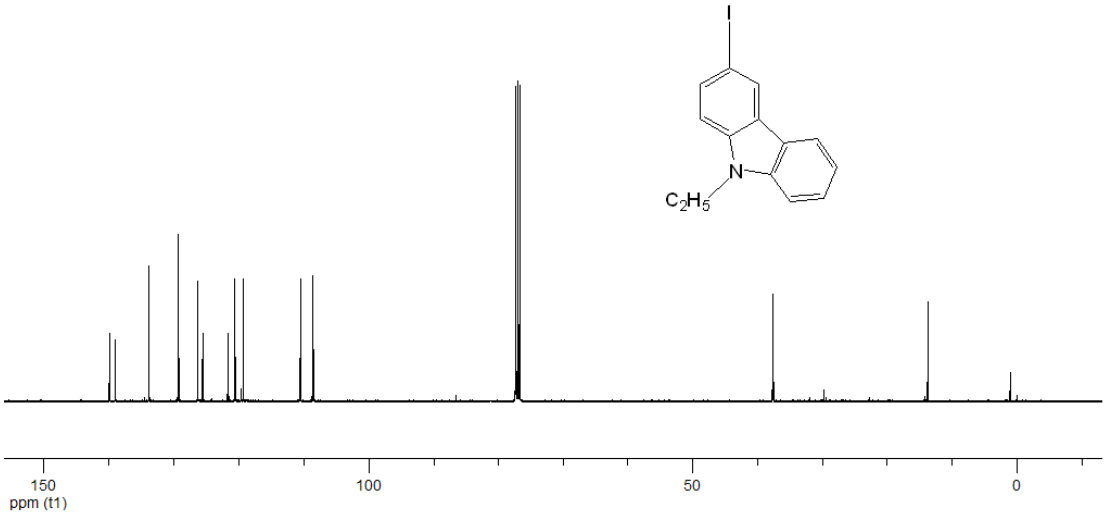


Figure 4. ^{13}C NMR shift spectra of C-I in $CDCl_3$

(3) 9-Ethyl-9H-3,9'-bicarbazole (C-C)

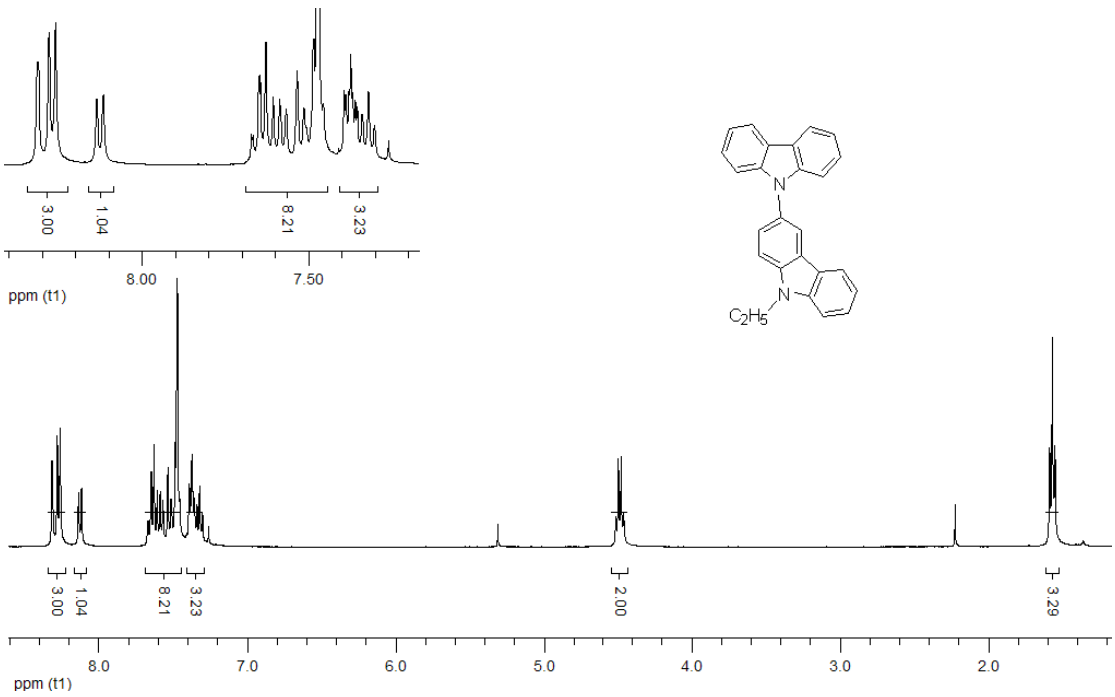


Figure 5. ^{1}H NMR shift spectra of (C-C) in $CDCl_3$

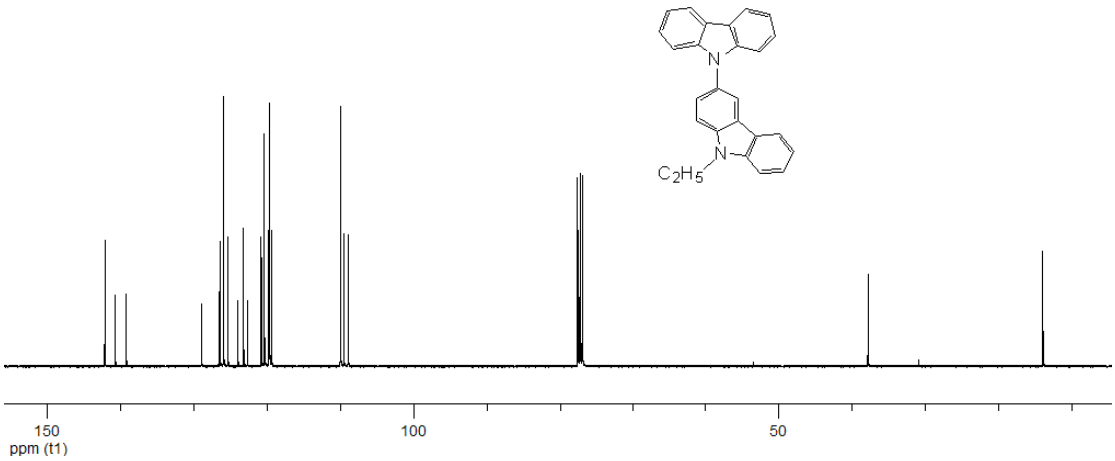


Figure 6. ^{13}C NMR shift spectra of C-C in $CDCl_3$

(4) 9-Ethyl-N,N-diphenyl-9H-carbazol-3-amine (C-N)

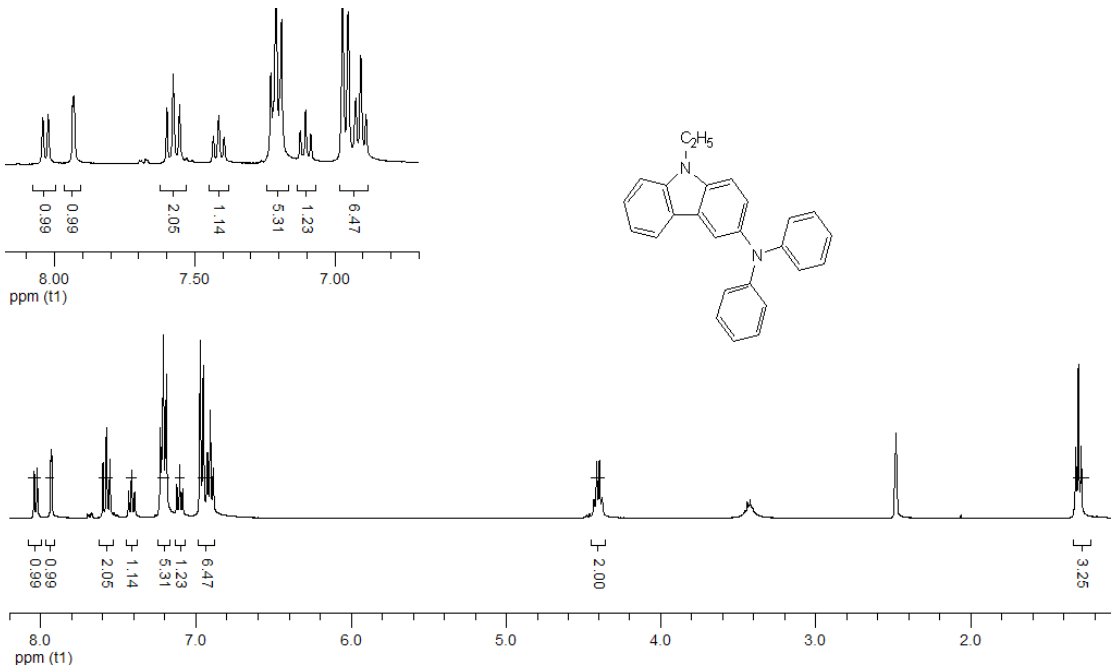


Figure 7. ^{1}H NMR shift spectra of C-N in $CDCl_3$

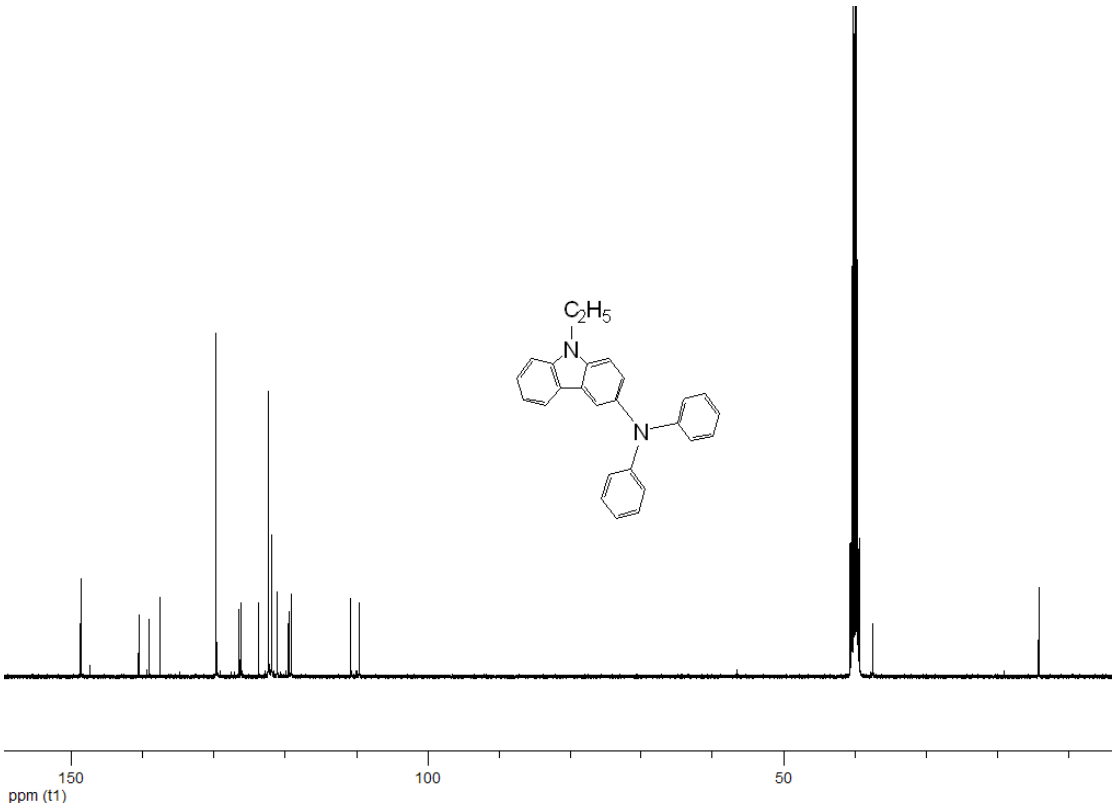


Figure 8. ^{13}C NMR shift spectra of C-N in $CDCl_3$

(5) 10-(9-Ethyl-9H-carbazol-3-yl)-10H-phenoxazine (C-O)

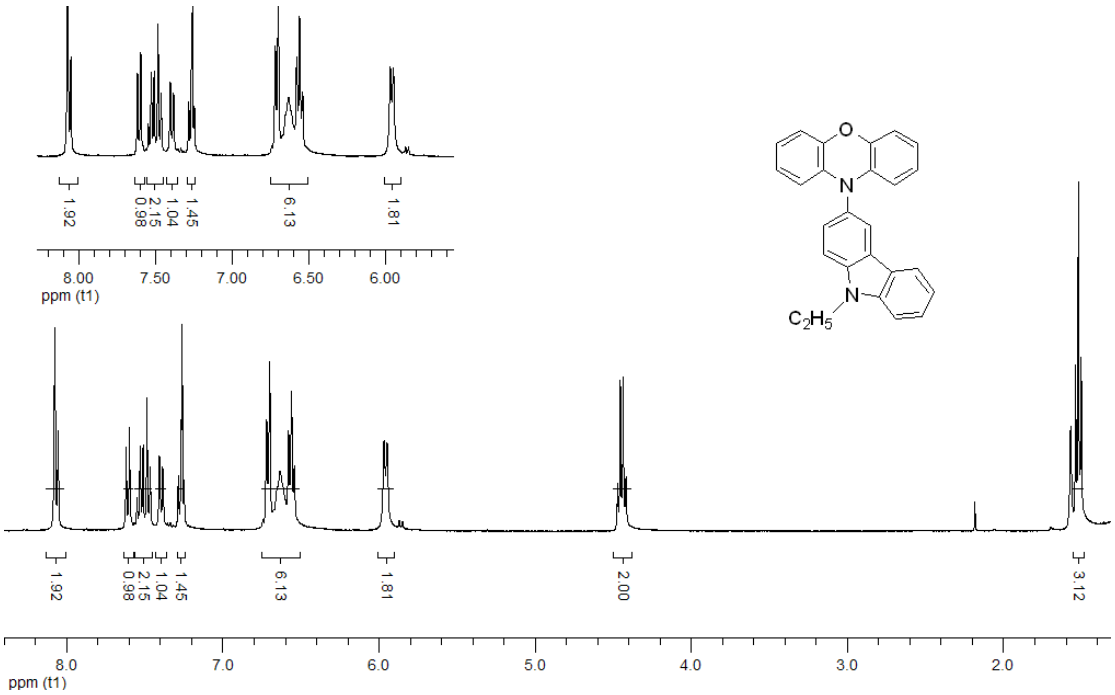


Figure 9. ^{1}H NMR shift spectra of C-O in $CDCl_3$

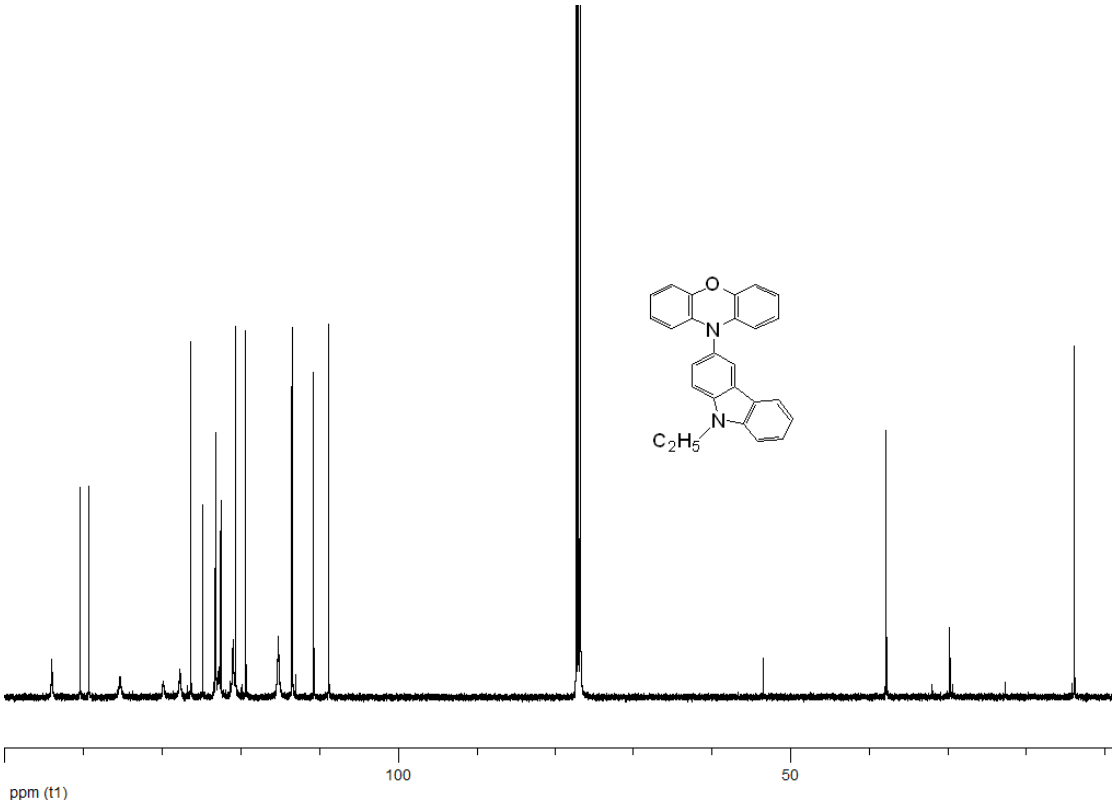


Figure 10. ^{13}C NMR shift spectra of C-O in $CDCl_3$

(6) 10-(9-Ethyl-9H-carbazol-3-yl)-10H-phenothiazine (C-S)

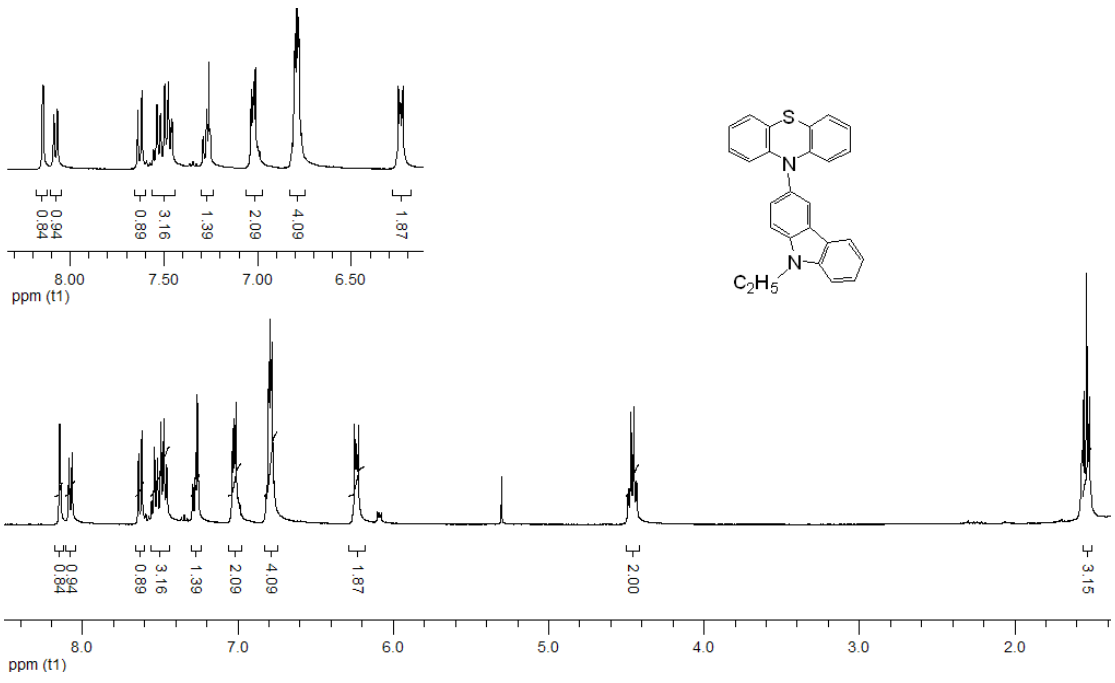


Figure 11. ^{1}H NMR shift spectra of C-S in $CDCl_3$

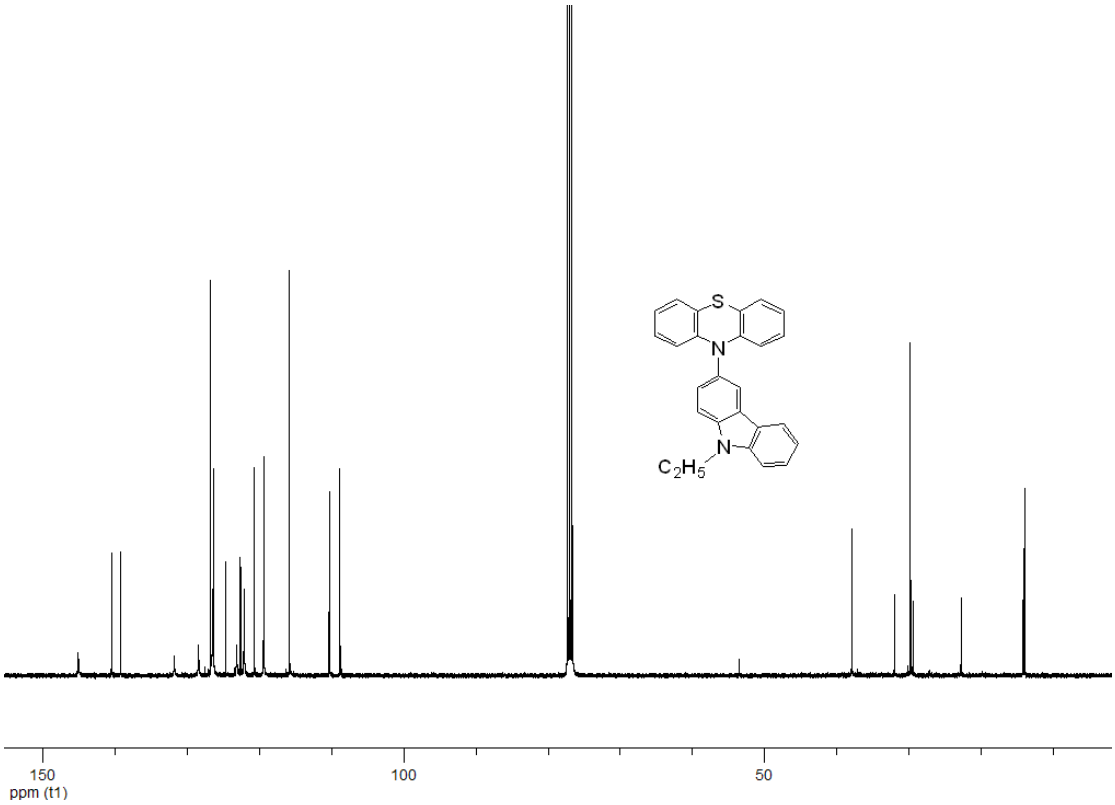


Figure 12. ^{13}C NMR shift spectra of C-S in $CDCl_3$

(7) 10-(9-Ethyl-9H-carbazol-3-yl)-10H-phenothiazine-S,S-dioxide(C-SO)

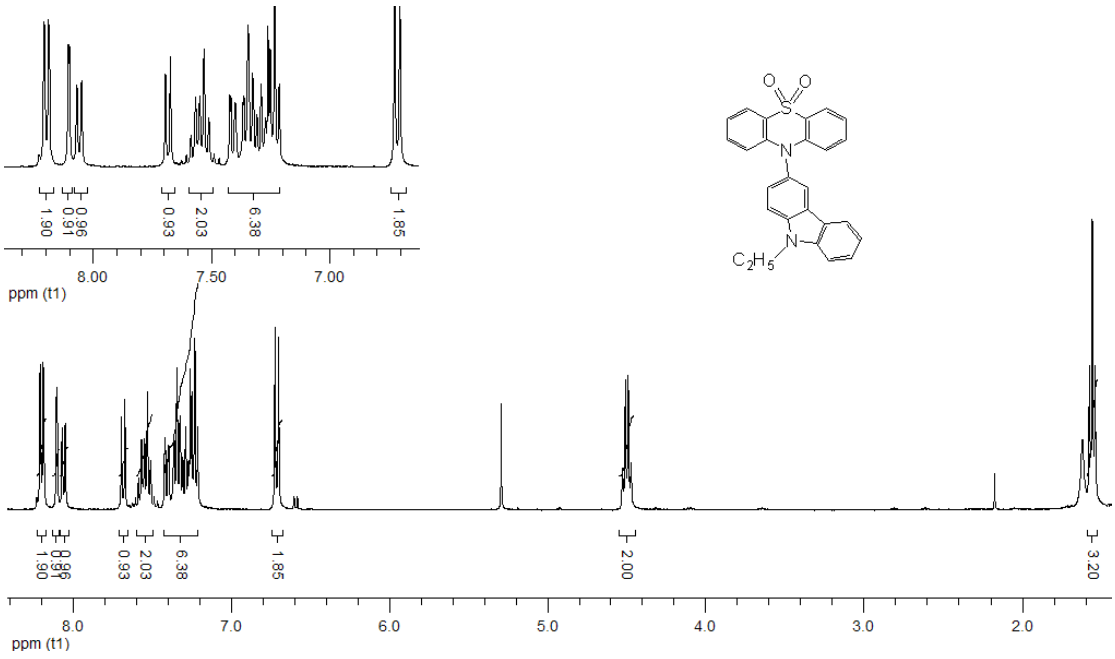


Figure 13. ^{1}H NMR shift spectra of C-SO in $CDCl_3$

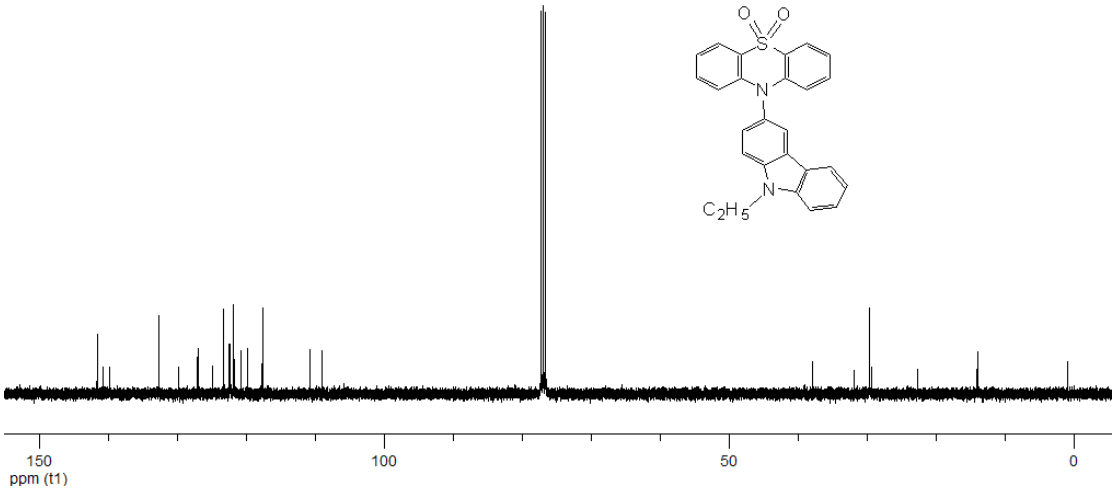
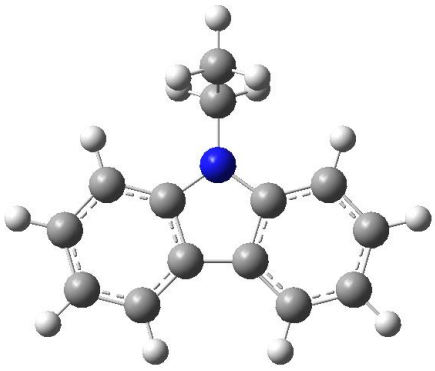


Figure 14. ^{13}C NMR shift spectra of C-SO in $CDCl_3$

The details of quantum chemical calculations

All the optimized geometries with Q-chem 3.2 suite of program are as follows

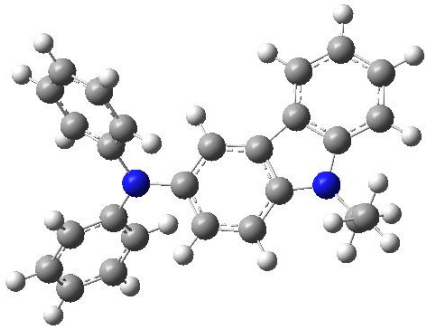
Compound E-C DFT/6-31G(d) B3LYP/6-31G(d) C1 symmetry	
Nuclear Repulsion Energy = 921.568656Hartree DFT SCF Energy = -596.082261 Hatree	

	Atoms	Coordinates (Angstroms)		
		X	Y	Z
1	C	3.041708	-1.702558	0.121568
2	C	3.426417	-0.364367	-0.069687
3	C	2.481277	0.648877	-0.218158

4	C	1.129668	0.292147	-0.174695
5	C	0.724188	-1.055263	0.023440
6	C	1.694903	-2.052610	0.169118
7	N	-0.000079	1.092907	-0.308509
8	C	-1.129617	0.291796	-0.174745
9	C	-0.723724	-1.055473	0.023477
10	C	-2.481318	0.648119	-0.218213
11	C	-3.426151	-0.365425	-0.069772
12	C	-3.041041	-1.703500	0.121454
13	C	-1.694124	-2.053135	0.169081
14	C	-0.001217	3.303787	0.856741
15	C	-0.000399	2.537462	-0.470831
16	H	3.803605	-2.468490	0.235046
17	H	4.482791	-0.110959	-0.100076
18	H	2.793633	1.679540	-0.358430
19	H	1.400456	-3.088179	0.319468
20	H	-2.794016	1.678697	-0.358366
21	H	-4.482599	-0.112325	-0.100169
22	H	-3.802712	-2.469671	0.234833
23	H	-1.399350	-3.088609	0.319435
24	H	-0.001038	4.384299	0.672603
25	H	-0.887581	3.055956	1.449769
26	H	0.884333	3.055831	1.450933
27	H	0.876808	2.807403	-1.068684
28	H	-0.877196	2.807014	-1.069473

Table S1. E-C

Compound C-N
DFT/6-31G(d)
B3LYP/6-31G(d)
C1 symmetry



Nuclear Repulsion Energy = 2368.446603 Hartree
DFT SCF Energy = -1113.546145 Hatree

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4	C	-2.489782	1.300592	0.385884
5	C	-1.903610	2.025857	1.437405
6	C	-2.315664	3.328092	1.711951
7	N	-2.055939	-0.018550	0.094618
8	C	-2.974260	-1.020137	-0.310904
9	C	-4.253519	-1.101773	0.266782
10	C	-2.612949	-1.964158	-1.287288
11	C	-3.507271	-2.962530	-1.668706
12	C	-4.780736	-3.033651	-1.100691
13	C	-5.145855	-2.093535	-0.134337
14	C	-0.666808	-0.339307	0.192453
15	C	-0.259676	-1.465862	0.939975
16	C	1.081229	-1.816177	1.058701
17	C	2.033026	-1.007007	0.430184
18	C	1.644405	0.140733	-0.310278
19	C	0.290034	0.460282	-0.439115
20	N	3.417480	-1.133346	0.386125
21	C	3.934208	-0.072599	-0.351101
22	C	2.863329	0.739911	-0.812116
23	C	5.264802	0.233790	-0.654479
24	C	5.510524	1.361818	-1.434696
25	C	4.461764	2.172999	-1.901687
26	C	3.138931	1.867316	-1.593925
27	C	4.571401	-1.741136	2.517582
28	C	4.197935	-2.140893	1.085633
29	H	-3.649328	4.942851	1.180352
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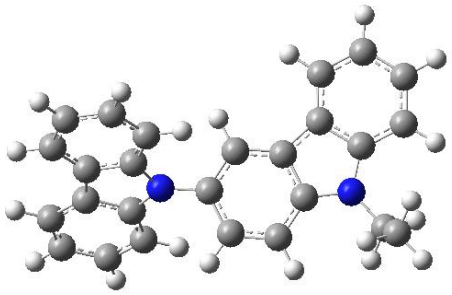
31	H	-3.950982	1.368792	-1.199532
32	H	-1.124259	1.562336	2.033461
33	H	-1.849012	3.870904	2.530113
34	H	-4.540746	-0.385374	1.029621
35	H	-1.629811	-1.907878	-1.743203
36	H	-3.207457	-3.681929	-2.426604
37	H	-5.477428	-3.809558	-1.404960
38	H	-6.129890	-2.138893	0.325554
39	H	-1.018338	-2.068139	1.429663
40	H	1.367684	-2.685941	1.642354
41	H	-0.026903	1.324868	-1.014471
42	H	6.086145	-0.379484	-0.295611
43	H	6.536605	1.619238	-1.683483
44	H	4.687982	3.046577	-2.506300
45	H	2.329732	2.497400	-1.954140

46	H	5.158234	-2.534990	2.993719
47	H	3.674273	-1.567761	3.120797
48	H	5.166633	-0.822246	2.523156
49	H	5.099109	-2.335938	0.494640
50	H	3.620841	-3.072055	1.085312

Table S2. C-N

Compound C-C
DFT/6-31G(d)
B3LYP/6-31G(d)
C1 symmetry



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DFT SCF Energy = -1112.371241 Hatree

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4	C	-2.847639	-1.009975	-0.404280
5	C	-4.127653	-0.400100	-0.343056
6	C	-5.244450	-1.095933	-0.821255
7	N	-1.897246	-0.129206	0.117998
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9	C	-3.938086	0.910016	0.243768
10	C	-2.024641	2.190723	1.108787
11	C	-2.908363	3.222062	1.418684
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13	C	-4.803479	1.962663	0.565074
14	C	-0.499457	-0.382930	0.230832
15	C	-0.049260	-1.437266	1.050500
16	C	1.306510	-1.720813	1.183620
17	C	2.218704	-0.916425	0.492751
18	C	1.779913	0.160128	-0.325250
19	C	0.412670	0.413987	-0.462911
20	N	3.604945	-0.987052	0.448298
21	C	4.074553	0.039904	-0.366139

22	C	2.969940	0.772340	-0.876680
23	C	5.390316	0.378228	-0.698211
24	C	5.585835	1.457000	-1.557967
25	C	4.502630	2.188571	-2.075426
26	C	3.194807	1.851589	-1.738885
27	C	4.808739	-1.389150	2.600466
28	C	4.432037	-1.910679	1.209350
29	H	-5.933649	-2.921111	-1.724251
30	H	-3.683776	-3.950949	-1.835559
31	H	-1.683485	-2.739628	-0.997787
32	H	-6.232009	-0.643256	-0.781581
33	H	-0.964370	2.275790	1.324011
34	H	-2.523440	4.127355	1.880684
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36	H	-5.868446	1.879304	0.363396
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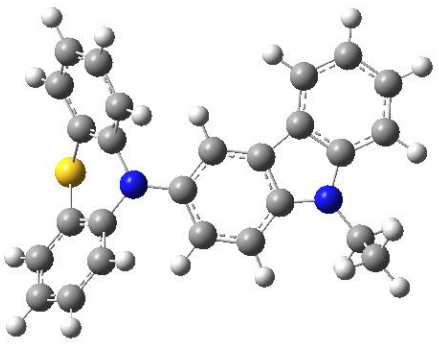
38	H	1.632997	-2.536570	1.821260
39	H	0.050855	1.215172	-1.100396
40	H	6.237548	-0.173413	-0.301844
41	H	6.599306	1.738456	-1.830845
42	H	4.690510	3.024860	-2.742489
43	H	2.358947	2.419630	-2.138985
44	H	5.432113	-2.122068	3.125114
45	H	3.914020	-1.204050	3.203704
46	H	5.368308	-0.451035	2.527034
47	H	5.331512	-2.117038	0.619752
48	H	3.890018	-2.859142	1.287889

Table S3. C-C

Compound C-S DFT/6-31G(d) B3LYP/6-31G(d) C1 symmetry	
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	Atoms	Coordinates (Angstroms)		
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1	C	-3.074198	1.665678	-0.500412
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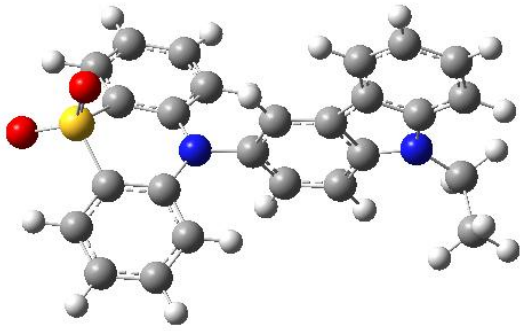
3	N	-1.711001	-0.113955	0.475011
4	C	-2.741710	-1.091291	0.349351
5	C	-3.721531	-0.937575	-0.645652
6	S	-3.634838	0.486917	-1.720561
7	C	-3.543786	2.982330	-0.506673
8	C	-3.097029	3.884655	0.457638
9	C	-2.217525	3.458825	1.456025
10	C	-1.771899	2.138056	1.480330
11	C	-2.838459	-2.172430	1.235309
12	C	-3.847896	-3.121895	1.083678
13	C	-4.800734	-2.977921	0.072103
14	C	-4.751144	-1.873914	-0.777739
15	C	-0.336033	-0.438389	0.258924
16	C	0.057962	-1.782224	0.051162
17	C	1.386524	-2.139167	-0.161163
18	C	2.355803	-1.136906	-0.177637
19	C	1.983741	0.215726	0.010624
20	C	0.645563	0.561372	0.221675
21	N	3.733184	-1.215292	-0.381006
22	C	4.259152	0.068086	-0.304204
23	C	3.203314	0.992837	-0.073260
24	C	5.586272	0.493822	-0.426170
25	C	5.844232	1.859271	-0.324442
26	C	4.810910	2.786214	-0.102273
27	C	3.491988	2.358646	0.024166
28	C	4.956183	-3.049704	0.793937
29	C	4.497121	-2.440839	-0.536184
30	H	-4.259160	3.291792	-1.263192
31	H	-3.454324	4.910401	0.443101
32	H	-1.890551	4.150378	2.227378
33	H	-1.106064	1.792967	2.265176
34	H	-2.106584	-2.264886	2.031839
35	H	-3.899691	-3.964800	1.767067
36	H	-5.595319	-3.710050	-0.040474
37	H	-5.509735	-1.730933	-1.541952
38	H	-0.688838	-2.565206	0.037289
39	H	1.639886	-3.183884	-0.316479
40	H	0.379015	1.604211	0.338440
41	H	6.396280	-0.210473	-0.592269

42	H	6.867981	2.212278	-0.416914
43	H	5.046169	3.844125	-0.027803
44	H	2.694661	3.077206	0.196989
45	H	5.523450	-3.970821	0.616857
46	H	4.097093	-3.290811	1.428422
47	H	5.596611	-2.350603	1.341543
48	H	5.359751	-2.220744	-1.174460
49	H	3.877682	3.154723	1.090282

Table S4. C-S

Compound C-SO
DFT/6-31G(d)
B3LYP/6-31G(d)
C1 symmetry



Nuclear Repulsion Energy = 3081.156329 Hartree
DFT SCF Energy = -1660.916761 Hatree

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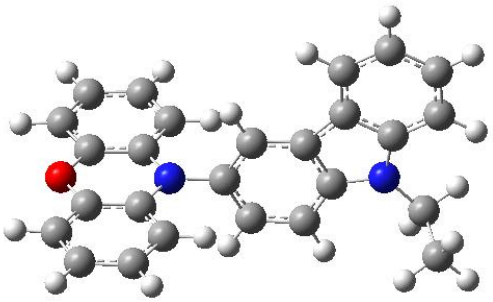
3	N	1.346993	0.045347	-0.383691
4	C	1.981463	1.283085	-0.160629
5	C	3.311173	1.366477	0.300640
6	S	4.100204	-0.088866	0.929663
7	C	4.150310	-2.439121	-0.452797
8	C	3.565006	-3.495390	-1.138376
9	C	2.222156	-3.392000	-1.517049
10	C	1.482052	-2.245034	-1.254341
11	C	1.320331	2.498774	-0.430120
12	C	1.979837	3.713465	-0.282278
13	C	3.316950	3.772115	0.125071
14	C	3.978638	2.587802	0.421467
15	C	-0.083136	0.031126	-0.580061
16	C	-0.626560	0.235132	-1.863025

17	C	-2.003230	0.228389	-2.070964
18	C	-2.833591	0.008325	-0.966010
19	C	-2.295107	-0.194103	0.335535
20	C	-0.910245	-0.183092	0.520821
21	N	-4.216703	-0.061476	-0.901435
22	C	-4.588347	-0.281758	0.423527
23	C	-3.420997	-0.379737	1.225285
24	C	-5.866620	-0.408447	0.976009
25	C	-5.959310	-0.643080	2.346119
26	C	-4.812375	-0.746812	3.152738
27	C	-3.542211	-0.616334	2.599642
28	O	5.556208	-0.003228	0.722874
29	O	3.590832	-0.343039	2.290106
30	C	-5.542872	1.616809	-2.193641
31	C	-5.132555	0.151423	-2.012471
32	H	5.182814	-2.479586	-0.120164
33	H	4.137388	-4.389613	-1.363963
34	H	1.742417	-4.213852	-2.041755
35	H	0.451368	-2.186682	-1.580335
36	H	0.292173	2.486027	-0.769010
37	H	1.440793	4.630358	-0.505153
38	H	3.826104	4.725912	0.220772
39	H	5.009787	2.582107	0.760676
40	H	0.047334	0.402493	-2.698022
41	H	-2.407217	0.393320	-3.064997
42	H	-0.467800	-0.335525	1.500945
43	H	-6.761813	-0.325095	0.367127
44	H	-6.941458	-0.745400	2.799489
45	H	-4.921295	-0.929127	4.217765
46	H	-2.657034	-0.695436	3.225110
47	H	-6.230089	1.716368	-3.041342
48	H	-6.044968	1.995446	-1.297558
49	H	-4.668224	2.247195	-2.384334
50	H	-4.652339	-0.229321	-2.920014

Table S5. C-SO

Compound C-O
DFT/6-31G(d)
B3LYP/6-31G(d)
C1 symmetry



Nuclear Repulsion Energy = 2518.889575 Hartree
DFT SCF Energy = -1187.563576 Hatree

	Atoms	Coordinates (Angstroms)		
		X	Y	Z
1	C	3.987700	-1.142961	0.048414
2	C	2.601531	-1.180636	-0.196822
3	N	1.860558	0.016847	-0.145473
4	C	2.527371	1.225843	0.135210
5	C	3.915169	1.206902	0.373416
6	O	4.647169	0.035548	0.340747
7	C	4.756204	-2.297111	0.009049
8	C	4.161142	-3.530181	-0.276904
9	C	2.792785	-3.584945	-0.520888
10	C	2.018883	-2.420601	-0.481671
11	C	1.868683	2.459144	0.191057
12	C	2.570363	3.635221	0.475282
13	C	3.941249	3.599060	0.708158
14	C	4.611967	2.372788	0.655134
15	C	0.453369	0.009692	-0.417409
1	C	0.000199	0.177070	-1.74088

6				4
1	C	-1.35733	0.173542	-2.04788
7		2		7
1	C	-2.26670	-0.00691	-0.99975
8		2	8	9
1	C	-1.82543	-0.17202	0.342106
9		6	6	
2	C	-0.45674	-0.16378	0.625626
0		1	3	
2	N	-3.65295	-0.06715	-1.03333
1		9	7	9
2	C	-4.12085	-0.24471	0.266495
2		5	6	
2	C	-3.01452	-0.32435	1.153169
3		6	8	
2	C	-5.43625	-0.34884	0.729575
4		8	3	
2	C	-5.62962	-0.54281	2.095687
5		3	9	
2	C	-4.54463	-0.62821	2.985433
6		0	4	
2	C	-3.23704	-0.51971	2.520979
7		9	1	
2	C	-4.86483	1.581040	-2.46877
8		6		8
2	C	-4.48252	0.118928	-2.21419
9		5		8
3	H	5.820251	-2.20957	0.205945
0			5	
3	H	4.768337	-4.42987	-0.30557
1			4	7
3	H	2.310904	-4.53258	-0.74407
2			1	6
3	H	0.953147	-2.47175	-0.67231
3			1	5
3	H	0.800229	2.495324	0.012076
4				
3	H	2.030316	4.577053	0.512203
5				
3	H	4.492676	4.507825	0.929543
6				
3	H	5.680879	2.299641	0.830394
7				
3	H	0.735121	0.312392	-2.52860

8				0
3	H	-1.68785	0.309869	-3.07299
9		3		5
4	H	-0.09027	-0.28949	1.640356
0		5	1	
4	H	-6.28469	-0.27909	0.055491
1		0	5	
4	H	-6.64275	-0.62692	2.479421
2		8	8	
4	H	-4.73088	-0.77870	4.044809
3		8	1	
4	H	-2.39975	-0.58466	3.210924
4		9	3	
4	H	-5.48891	1.659447	-3.36619
5		3		9
4	H	-5.42585	1.991019	-1.62277
6		8		2
4	H	-3.97265	2.198475	-2.61557
7		2		1
4	H	-3.93979	-0.29155	-3.07218
8		3	9	9
4	H	-5.37958	-0.49747	-2.09269
9		9	0	5

Table S6. C-O