Supporting Information

Near-infrared absorbing tetracyanobutadiene bridged diketopyrrolopyrroles

Yuvraj Patil[a], Charu Popli[a] and Rajneesh Misra*[a]

[a] Yuvraj Patil, Charu Popli and Rajneesh Misra
Department of Chemistry
Indian Institute of Technology Indore
Indore 453552 (India)
E-mail: rajneeshmisra@iiti.ac.in

Table of Contents……..……Page No.

Scheme S1 Synthesis ethyne bridged **DPP**s **I**–**IV**……..……..….**S2**

Fig. S1 Cyclic voltammetry plots of **DPP-VIII**…….……..…….……**S2**

Fig. S2 ^{1}H NMR spectrum of **DPP-V**……..……..**S3**

Fig. S3 ^{13}C NMR spectrum of **DPP-V** ……**S4**

Fig. S4 HRMS of **DPP-V** ……..…….…….....**S5**

Fig. S5 ^{1}H NMR spectrum of **DPP-VI** ……**S5**

Fig. S6 ^{13}C NMR spectrum of **DPP-VI** …….……..**S6**

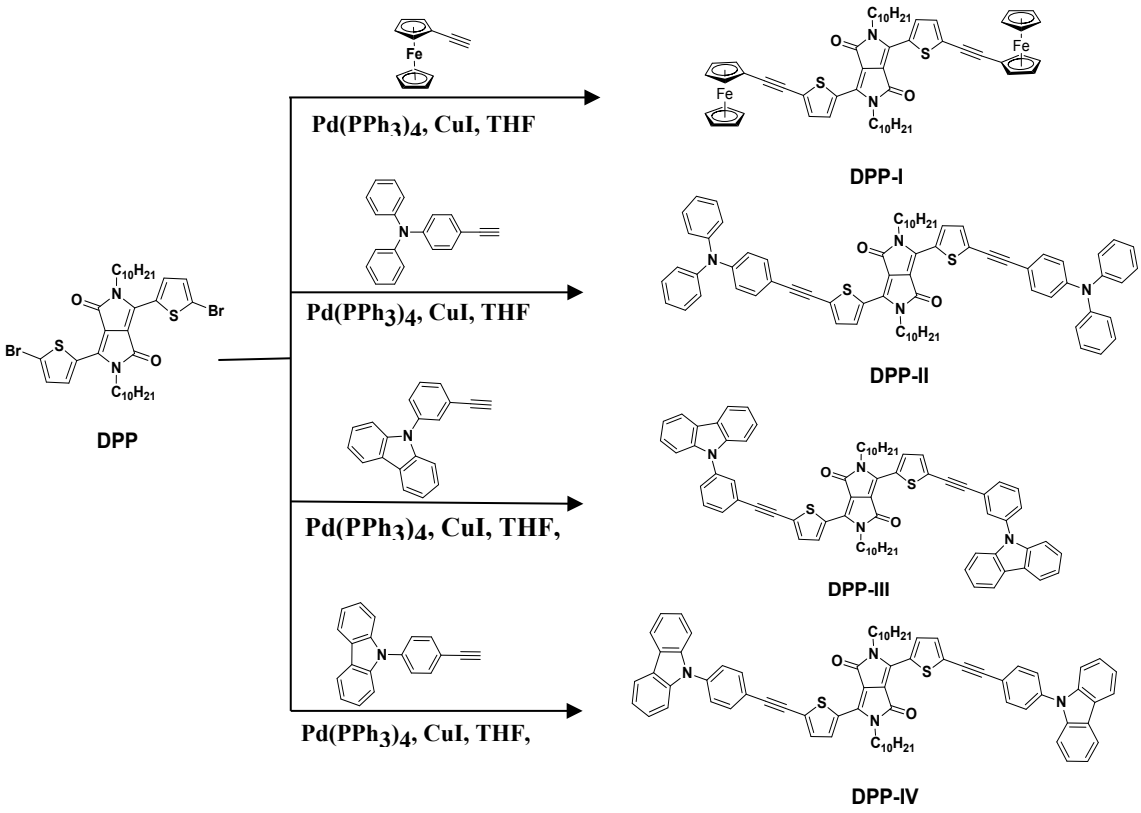
Fig. S7 HRMS of **DPP-VI** ……..…….**S6**

Fig. S8 ^{1}H NMR spectrum of **DPP-VII** ……**S7**

Fig. S9 ^{13}C NMR spectrum of **DPP-VII** ……..**S7**

Fig. S10 HRMS of **DPP-VII** ……..…….**S8**

DFT and TD-DFT Calculation data ……..……..……....….....**S8–S18**



Scheme S1 Synthesis of donor functionalized **DPP**s **I**–**IV.**

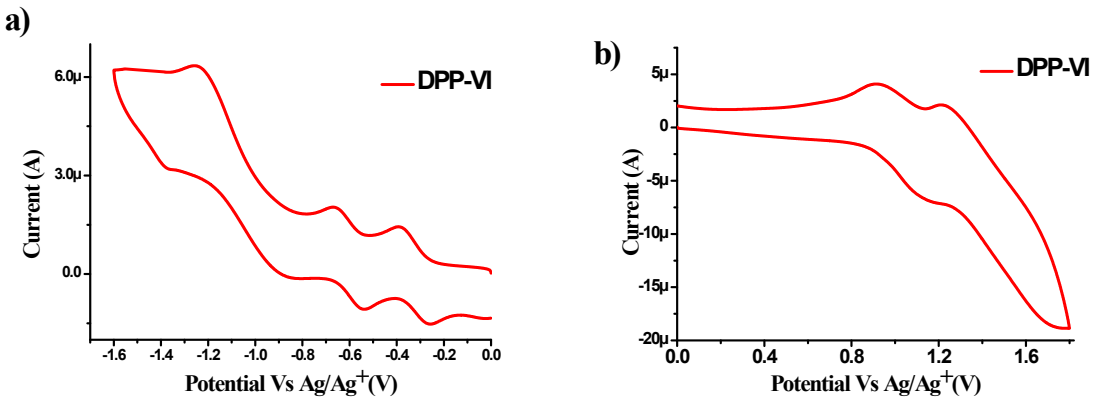


Fig. S1 Cyclic voltammetry plots of **DPP-VI**.

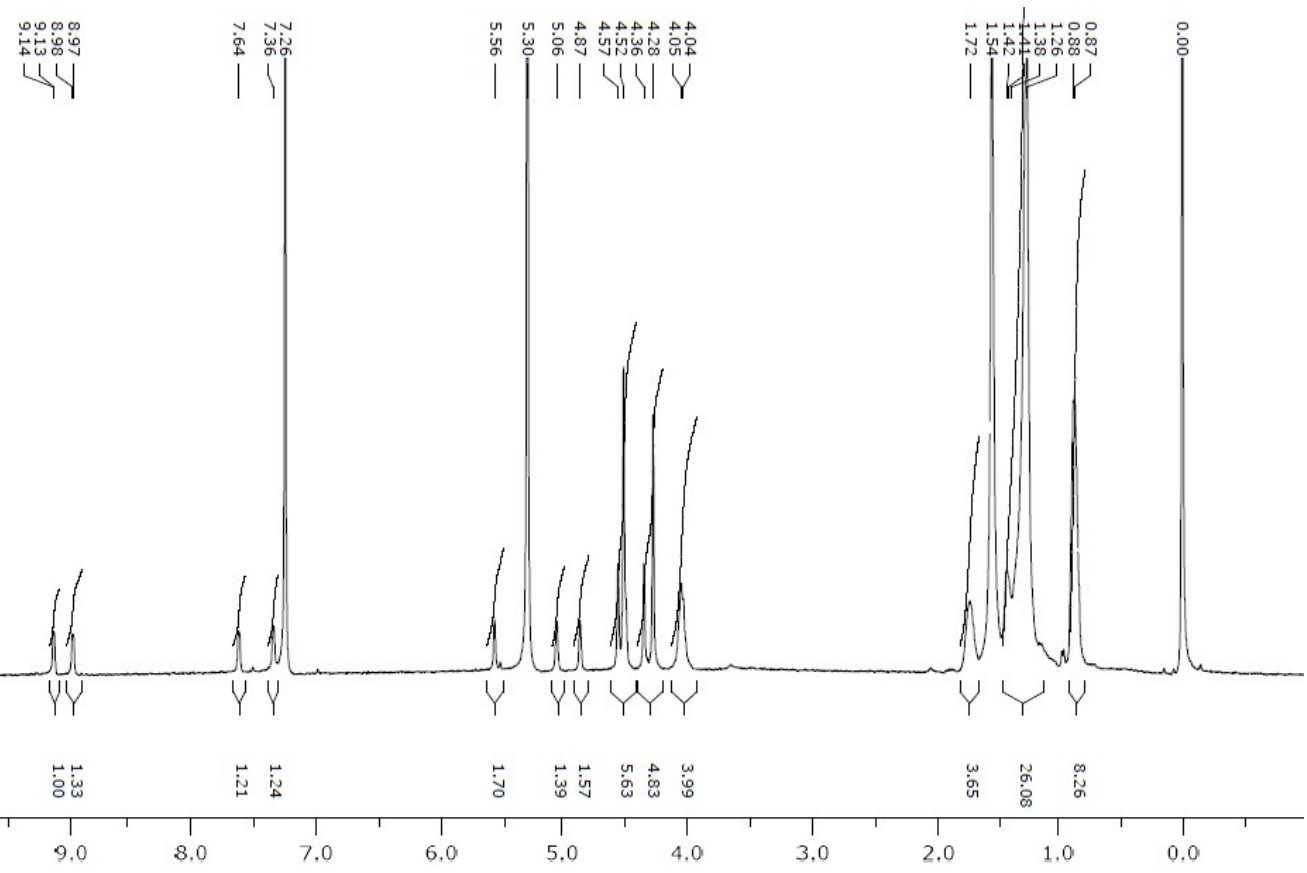


Fig. S2 ^{1}H NMR spectrum of **DPP-V.**

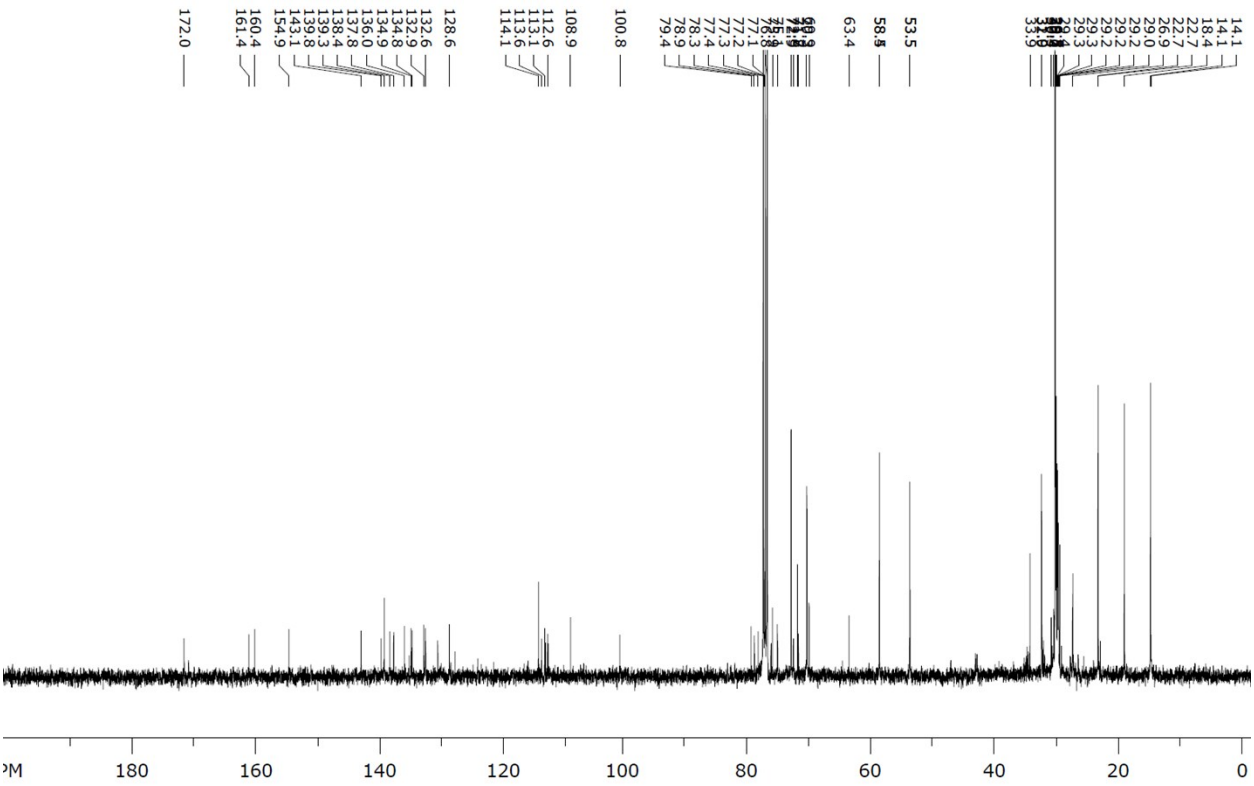


Fig. S3 ^{13}C NMR of **DPP-V.**

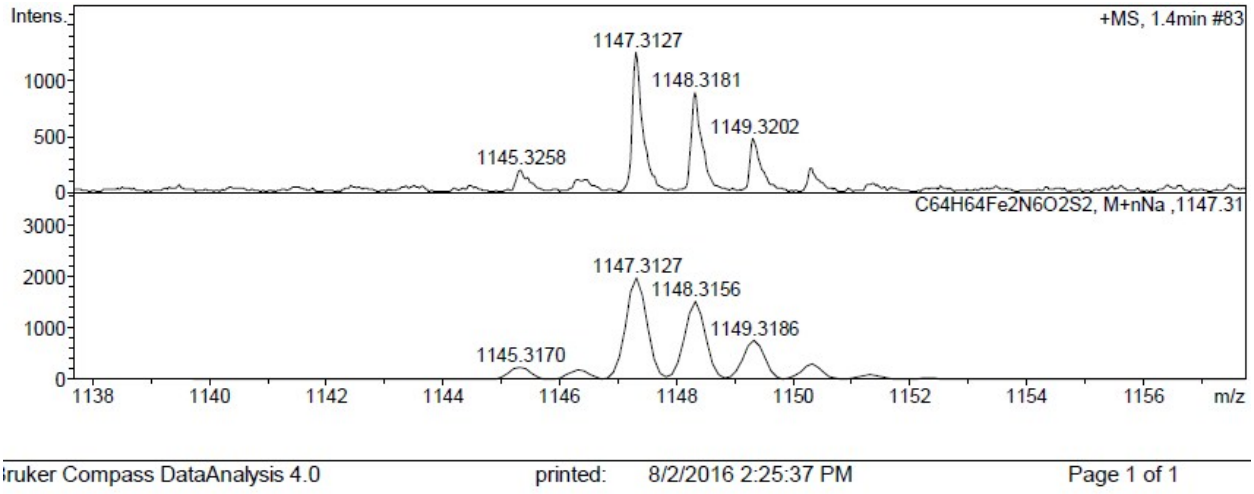


Fig. S4 HRMS of **DPP-V.**

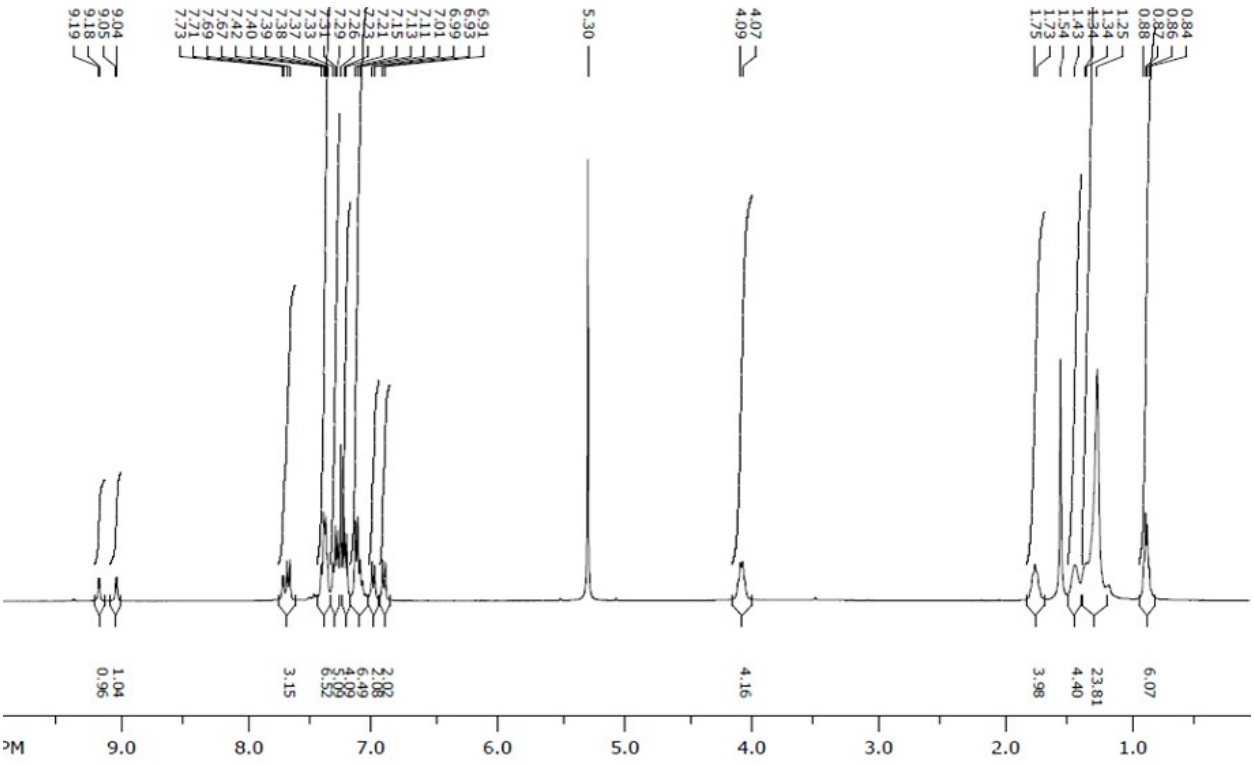


Fig. S5 [1] H NMR spectrum of **DPP-VI.**

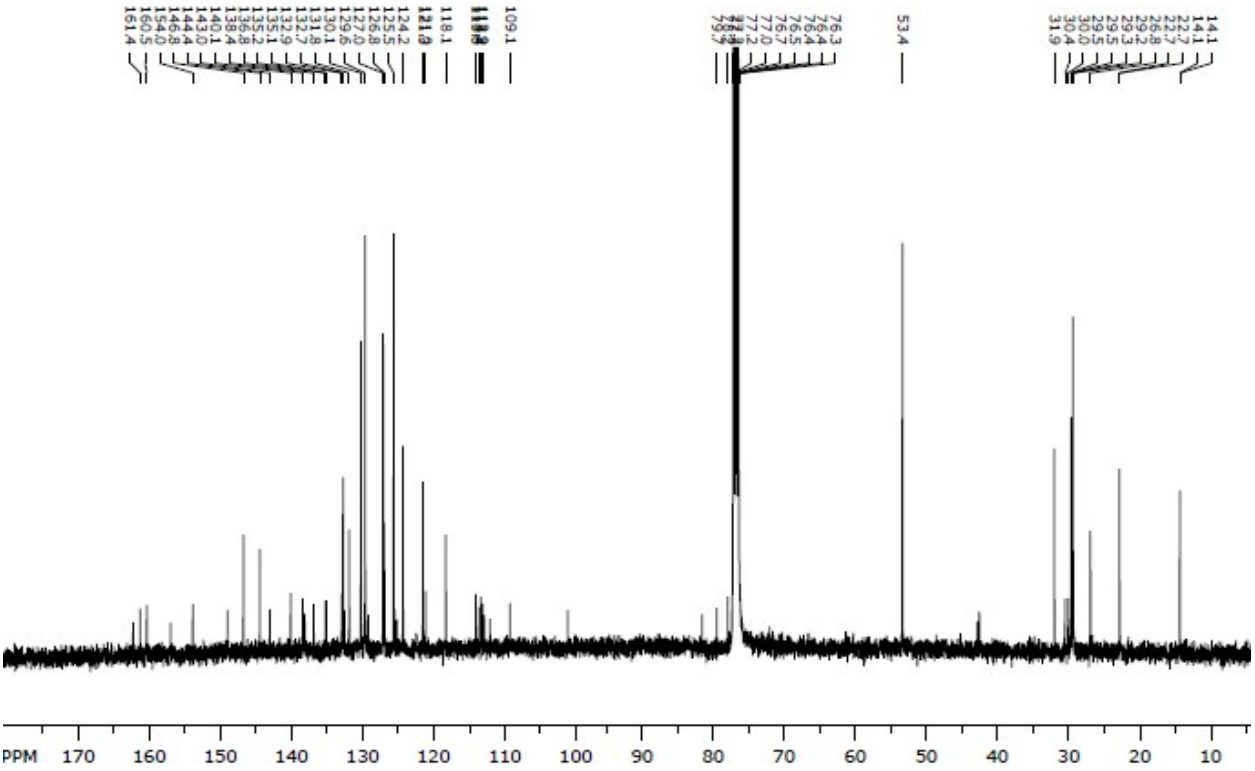


Fig. S6 ^{13}C NMR of **DPP-VI.**

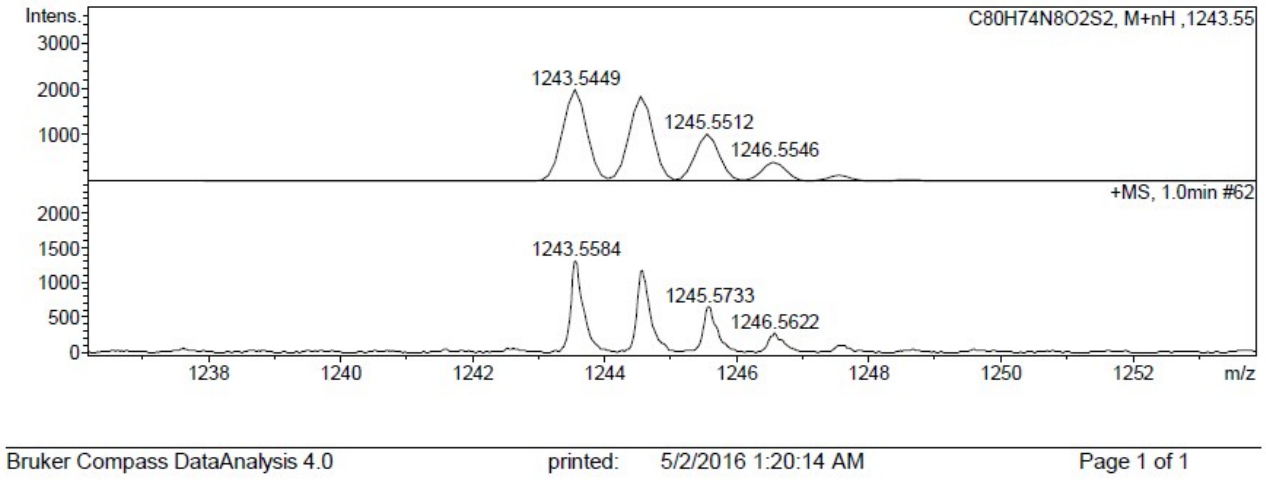


Fig. S7 HRMS of **DPP-VI.**

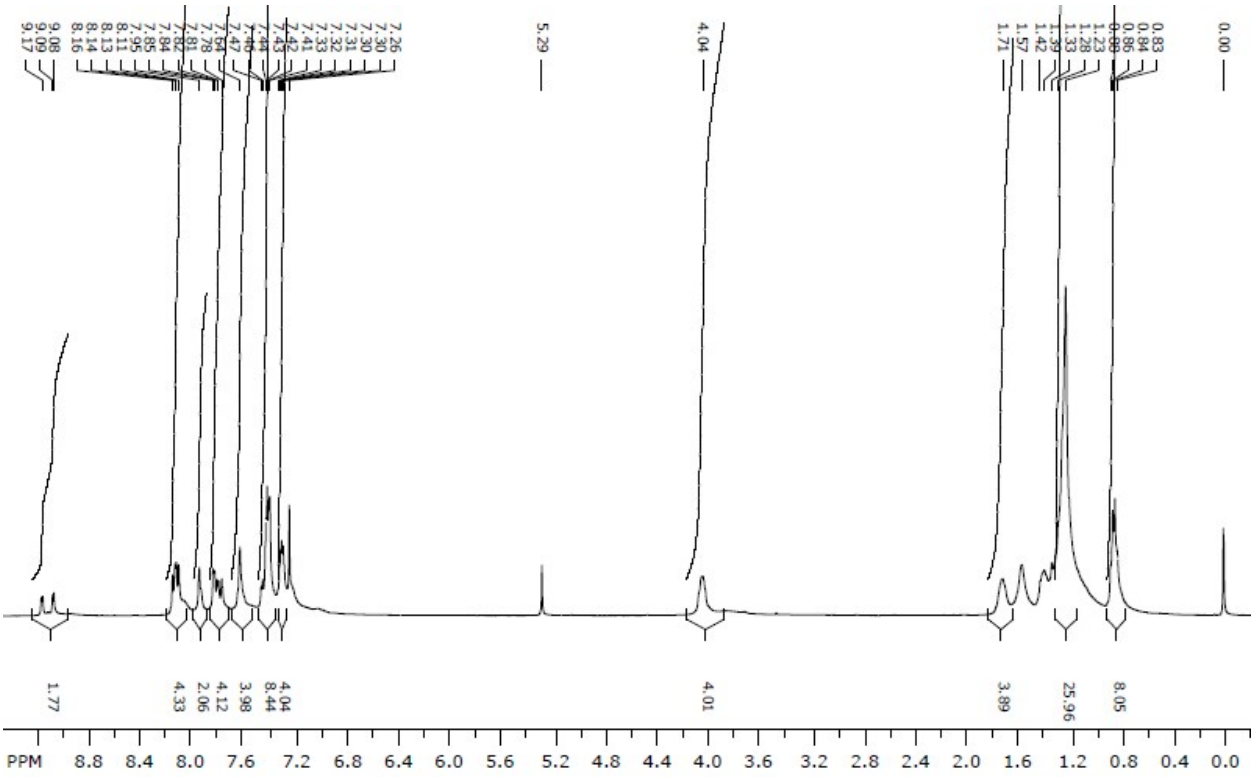


Fig. S8 [1] H NMR spectrum of **DPP-VII**.

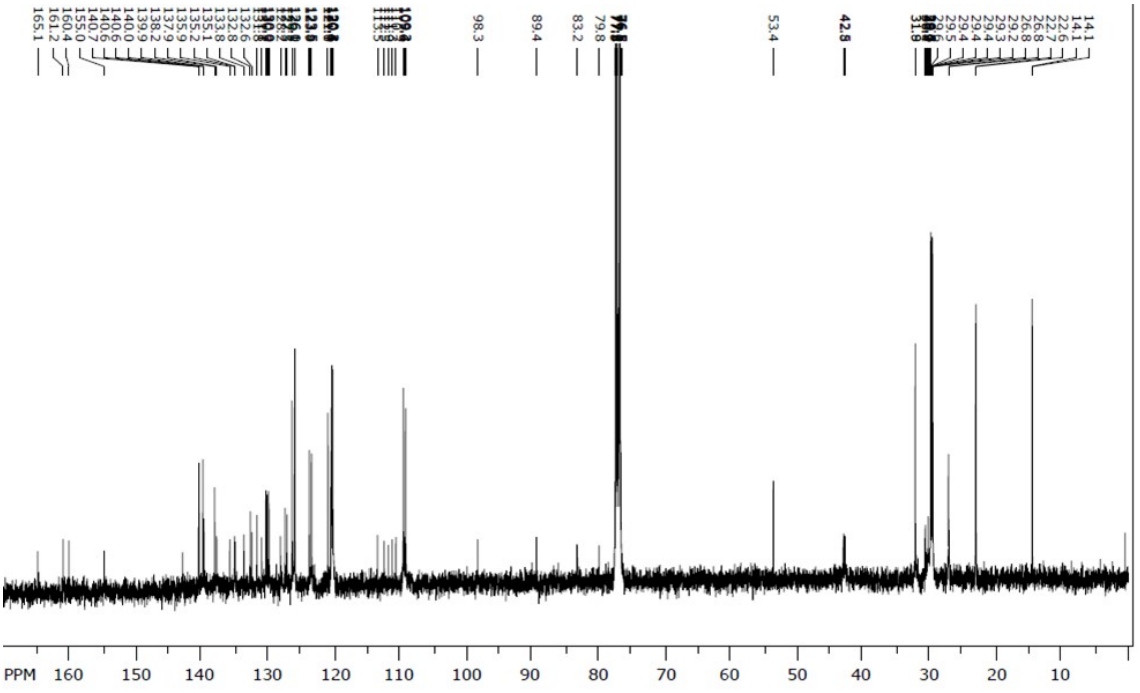


Fig. S9 [13]C NMR of **DPP-VII**.

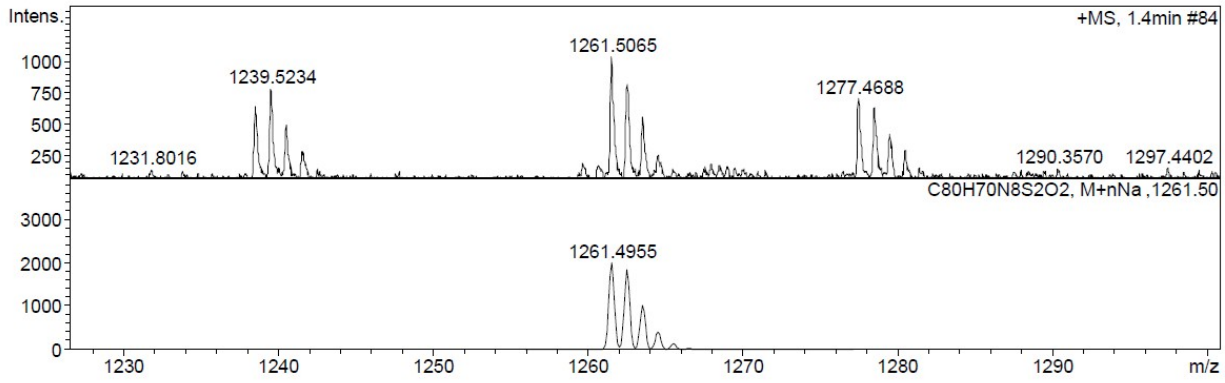


Fig. S10 HRMS of **DPP-VII.**

DFT and TD-DFT Calculation Data

DPP-V

DFT Calculation Data

Calculation method: B3LYP/6-31G(d, p) level B3LYP/6-31+G** for C, H, N, B, and Lanl2DZ for Fe.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.201013	-0.967962	-0.197267
2	6	0	-2.226513	0.079986	0.295328
3	6	0	-1.205586	1.043352	0.371389
4	6	0	0.036229	0.438821	0.074698
5	6	0	-0.973853	2.446282	0.644333
6	6	0	1.052272	1.400415	0.144965
7	8	0	0.535463	-1.903842	-0.495564
8	8	0	-1.712890	3.379968	0.952275
9	6	0	-3.621426	0.304447	0.532492
10	6	0	-4.160582	1.536567	0.909523
11	16	0	-4.905910	-0.894510	0.393506
12	6	0	-5.551619	1.518379	1.083402
13	1	0	-3.536945	2.415611	1.044788
14	6	0	-6.128576	0.276008	0.843484
15	1	0	-6.138942	2.380427	1.374590
16	6	0	2.449970	1.171445	-0.095524
17	6	0	2.996844	-0.064407	-0.459182
18	16	0	3.704540	2.386428	0.029688
19	6	0	4.380444	-0.023618	-0.630968

20	1	0	2.384733	-0.950684	-0.590072
21	6	0	4.955551	1.232274	-0.407911
22	1	0	4.970542	-0.885955	-0.911618
23	7	0	-1.614408	-1.125915	-0.040360
24	7	0	0.438054	2.607040	0.480457
25	6	0	1.020937	3.930767	0.714557
26	1	0	1.827193	4.101869	-0.001640
27	1	0	0.222321	4.638121	0.480067
28	6	0	1.485413	4.142992	2.157855
29	1	0	0.640094	4.040321	2.843612
30	1	0	2.260201	3.427551	2.447081
31	1	0	1.899703	5.149768	2.267831
32	6	0	-2.202714	-2.443701	-0.283995
33	1	0	-1.412874	-3.159410	-0.044638
34	1	0	-3.017033	-2.607480	0.425078
35	6	0	-2.656281	-2.645797	-1.732495
36	1	0	-3.426138	-1.925502	-2.022510
37	1	0	-1.805671	-2.540203	-2.411084
38	1	0	-3.068655	-3.652391	-1.854951
39	6	0	6.352296	1.536329	-0.514470
40	6	0	6.969093	2.753161	-0.271494
41	6	0	7.263642	0.397845	-0.909723
42	6	0	8.383586	2.898909	-0.423335
43	6	0	6.283080	3.933532	0.142837
44	7	0	9.534928	3.031195	-0.538478
45	7	0	5.752379	4.911809	0.488152
46	6	0	-10.010560	-0.779120	1.115974
47	26	0	-11.509784	-0.450723	-0.290481
48	6	0	-10.599511	-2.029987	0.703646
49	6	0	-11.066974	0.025283	1.680718
50	6	0	-11.982849	-1.994168	1.030100
51	6	0	-12.270065	-0.730542	1.631514
52	6	0	-10.683760	0.474573	-1.959299
53	6	0	-11.677804	1.314805	-1.373134
54	6	0	-12.918953	0.608315	-1.392988
55	6	0	-12.690492	-0.668483	-1.988833
56	6	0	-11.307963	-0.751641	-2.338042
57	1	0	-10.068871	-2.839999	0.223996
58	1	0	-10.947718	1.028452	2.064177
59	1	0	-12.700207	-2.776785	0.825763
60	1	0	-13.242303	-0.391550	1.961227
61	1	0	-9.631423	0.705968	-2.052228
62	1	0	-11.513599	2.300839	-0.961038
63	1	0	-13.859185	0.964292	-0.994645
64	1	0	-13.427861	-1.448363	-2.121053
65	1	0	-10.814997	-1.604338	-2.784291
66	6	0	7.988087	-0.247462	0.175586
67	26	0	7.818202	-2.198583	0.899265
68	6	0	9.260831	-0.933946	0.121794
69	6	0	7.575941	-0.232678	1.560019
70	6	0	9.619260	-1.293042	1.445953
71	6	0	8.578839	-0.872661	2.329966
72	6	0	6.559485	-3.366384	-0.287246
73	6	0	6.022748	-3.252528	1.031407

74	6	0	6.983141	-3.791049	1.939999
75	6	0	8.109398	-4.233396	1.182056
76	6	0	7.848500	-3.968644	-0.196899
77	1	0	9.846862	-1.118851	-0.764818
78	1	0	6.651795	0.182382	1.935920
79	1	0	10.514150	-1.829980	1.728054
80	1	0	8.543123	-1.045157	3.396464
81	1	0	6.087129	-3.035386	-1.202109
82	1	0	5.068001	-2.819963	1.296868
83	1	0	6.889605	-3.824297	3.016782
84	1	0	9.019356	-4.655480	1.585994
85	1	0	8.519990	-4.146809	-1.024874
86	6	0	7.380819	0.107904	-2.247430
87	6	0	6.687393	0.870892	-3.242830
88	6	0	8.160970	-0.982564	-2.748974
89	7	0	8.767458	-1.879674	-3.175557
90	7	0	6.129215	1.472412	-4.067874
91	6	0	-7.477575	-0.088759	0.925541
92	6	0	-8.650649	-0.412883	1.003855

Total Energy (HF) = -3370.4401355 Hartree

TDDFT Calculation Data

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 1.6832 eV 736.61 nm f=1.2451
<S**2>=0.000

221 -> 222	0.69378
221 <- 222	-0.11504

Excited State 2: Singlet-A 1.8167 eV 682.46 nm f=0.0002
<S**2>=0.000

217 -> 222	-0.15668
217 -> 223	0.49009
217 -> 224	0.14284
217 -> 227	-0.16377
217 -> 228	0.32011
218 -> 226	-0.24815

Excited State 3: Singlet-A 1.8737 eV 661.70 nm f=0.0115
<S**2>=0.000

217 -> 226	0.26895
218 -> 222	-0.20121
218 -> 223	0.44316
218 -> 224	0.12119
218 -> 227	-0.17079
218 -> 228	0.33353

Excited State 4: Singlet-A 1.9230 eV 644.75 nm f=0.0001
<S**2>=0.000

219 -> 222	0.48226
219 -> 224	-0.17352
219 -> 225	0.18225

```
     219 -> 227        0.25657
     219 -> 228        0.13574
     219 -> 231        0.18430
     220 -> 229       -0.24052

 Excited State   5:      Singlet-A      1.9711 eV  629.01 nm  f=0.0242
<S**2>=0.000
     219 -> 229        0.26400
     220 -> 222        0.46315
     220 -> 224       -0.13375
     220 -> 225        0.15175
     220 -> 227        0.23056
     220 -> 228        0.12357
     220 -> 231        0.17775
     221 -> 222       -0.13970

 Excited State   6:      Singlet-A      2.0935 eV  592.23 nm  f=0.0005
<S**2>=0.000
     217 -> 226        0.10291
     218 -> 222        0.67070
     218 -> 224        0.11505
```

DPP-VI

DFT Calculation Data

Calculation method: B3LYP/6-31G(d, p) level B3LYP/6-31+G** for C, H, N, B.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.074107	-0.257476	1.107344
2	6	0	-1.915631	-0.945394	0.100848
3	6	0	-0.867707	-1.720429	-0.425690
4	6	0	0.353032	-1.328186	0.166749
5	6	0	-0.593221	-2.783007	-1.369916
6	6	0	1.397302	-2.097348	-0.361849
7	8	0	0.779718	0.406886	1.860355
8	8	0	-1.302943	-3.446521	-2.123953
9	6	0	-3.300859	-1.044521	-0.246659
10	6	0	-3.809230	-1.942077	-1.188931
11	16	0	-4.613951	-0.085002	0.435362
12	6	0	-5.197520	-1.862767	-1.358893
13	1	0	-3.163729	-2.630990	-1.725958
14	6	0	-5.806466	-0.904658	-0.554442
15	1	0	-5.761779	-2.481956	-2.044936
16	6	0	2.785196	-1.997359	-0.005548
17	6	0	3.287882	-1.138296	0.977524

18	16	0	4.082656	-2.917570	-0.739582
19	6	0	4.669650	-1.233823	1.137751
20	1	0	2.647119	-0.471883	1.544842
21	6	0	5.289755	-2.154769	0.285868
22	1	0	5.223050	-0.645690	1.858755
23	7	0	-1.340101	-0.063568	1.014134
24	7	0	0.821059	-2.974408	-1.281106
25	6	0	1.442065	-3.992651	-2.131923
26	1	0	2.248088	-4.479390	-1.579140
27	1	0	0.662220	-4.739615	-2.296130
28	6	0	1.921858	-3.448605	-3.479492
29	1	0	1.078486	-3.036776	-4.040057
30	1	0	2.677885	-2.667949	-3.359539
31	1	0	2.365819	-4.257790	-4.067051
32	6	0	-1.966543	0.935648	1.880461
33	1	0	-1.191192	1.683595	2.061023
34	1	0	-2.772776	1.427916	1.332402
35	6	0	-2.448673	0.363827	3.215952
36	1	0	-3.203256	-0.414928	3.076905
37	1	0	-1.606687	-0.060056	3.769397
38	1	0	-2.890209	1.160783	3.822630
39	6	0	6.695628	-2.436200	0.251117
40	6	0	7.365508	-3.251663	-0.646404
41	6	0	7.543993	-1.758971	1.303814
42	6	0	7.524743	-2.327460	2.560671
43	6	0	6.801321	-3.538129	2.815762
44	6	0	8.166747	-1.771901	3.712628
45	6	0	8.778496	-3.449123	-0.545937
46	6	0	6.739530	-3.951035	-1.721323
47	7	0	6.219468	-4.519550	3.047022
48	7	0	8.655452	-1.343844	4.678927
49	7	0	9.928919	-3.620485	-0.487308
50	7	0	6.260711	-4.529001	-2.612785
51	6	0	8.306144	-0.585537	0.896041
52	6	0	7.879574	0.184539	-0.211445
53	6	0	9.497469	-0.178194	1.539992
54	6	0	8.570682	1.305767	-0.629627
55	1	0	6.982706	-0.099993	-0.750874
56	6	0	10.203925	0.931600	1.117730
57	1	0	9.892455	-0.748651	2.370115
58	6	0	9.755557	1.708784	0.025955
59	1	0	8.210295	1.869472	-1.481429
60	1	0	11.115838	1.206459	1.633244
61	7	0	10.467773	2.830689	-0.399965
62	6	0	9.816107	3.899073	-1.093598
63	6	0	10.357684	4.392377	-2.287981
64	6	0	8.651069	4.478187	-0.570991
65	6	0	9.738695	5.451869	-2.949003
66	1	0	11.260340	3.943757	-2.689256
67	6	0	8.030120	5.527003	-1.246973
68	1	0	8.240520	4.105983	0.362001
69	6	0	8.571405	6.020466	-2.435717
70	1	0	10.166263	5.826335	-3.874263
71	1	0	7.128502	5.968944	-0.833453

72	1	0	8.089311	6.842323	-2.955797
73	6	0	11.875962	2.944864	-0.165942
74	6	0	12.741211	1.898578	-0.514811
75	6	0	12.397800	4.119584	0.391071
76	6	0	14.111248	2.024948	-0.291369
77	1	0	12.337759	0.993444	-0.956923
78	6	0	13.770881	4.243307	0.595775
79	1	0	11.724962	4.927289	0.659451
80	6	0	14.632202	3.196832	0.260767
81	1	0	14.773227	1.208250	-0.562889
82	1	0	14.165994	5.157186	1.029177
83	1	0	15.700470	3.293913	0.427237
84	6	0	-7.159827	-0.567343	-0.467397
85	6	0	-8.339117	-0.264139	-0.377041
86	6	0	-9.708521	0.078911	-0.275569
87	6	0	-10.139571	1.091654	0.608615
88	6	0	-10.685368	-0.581515	-1.052038
89	6	0	-11.479829	1.424005	0.715956
90	1	0	-9.407438	1.604890	1.223408
91	6	0	-12.025192	-0.244403	-0.952486
92	1	0	-10.375548	-1.355152	-1.746904
93	6	0	-12.451908	0.764079	-0.063919
94	1	0	-11.787388	2.195222	1.412649
95	1	0	-12.754774	-0.756216	-1.569303
96	7	0	-13.812541	1.104201	0.041894
97	6	0	-14.205323	2.440596	0.353550
98	6	0	-15.182708	2.677781	1.330847
99	6	0	-13.632317	3.527542	-0.323536
100	6	0	-15.580220	3.981684	1.620643
101	1	0	-15.625420	1.838059	1.856103
102	6	0	-14.023538	4.828901	-0.014671
103	1	0	-12.884356	3.345651	-1.088169
104	6	0	-15.000769	5.063421	0.954749
105	1	0	-16.338102	4.151756	2.379696
106	1	0	-13.572296	5.661560	-0.546254
107	1	0	-15.308560	6.078085	1.187337
108	6	0	-14.828061	0.121907	-0.159815
109	6	0	-15.939073	0.413572	-0.964426
110	6	0	-14.736641	-1.135583	0.455728
111	6	0	-16.941447	-0.537611	-1.144677
112	1	0	-16.010597	1.385090	-1.441918
113	6	0	-15.735378	-2.086629	0.255418
114	1	0	-13.884247	-1.359981	1.088455
115	6	0	-16.843754	-1.792896	-0.541367
116	1	0	-17.796555	-0.298846	-1.770187
117	1	0	-15.652468	-3.056122	0.737815
118	1	0	-17.623391	-2.533625	-0.689148

Total Energy (HF) = =-3848.8688579 Hartree

TDDFT Calculation Data

Excitation energies and oscillator strengths:

```
 Excited State   1:      Singlet-A      1.5608 eV  794.38 nm  f=1.5810
<S**2>=0.000
     265 -> 266        0.70234

 Excited State   2:      Singlet-A      1.7896 eV  692.81 nm  f=0.0051
<S**2>=0.000
     263 -> 266        0.67206
     264 -> 266        0.20166

 Excited State   3:      Singlet-A      1.9539 eV  634.53 nm  f=0.1108
<S**2>=0.000
     263 -> 266       -0.19701
     264 -> 266        0.66266

 Excited State   4:      Singlet-A      2.0694 eV  599.12 nm  f=0.1231
<S**2>=0.000
     264 -> 267       -0.13142
     265 -> 267        0.68069

 Excited State   5:      Singlet-A      2.4554 eV  504.94 nm  f=0.2670
<S**2>=0.000
     261 -> 266        0.17669
     262 -> 266       -0.13892
     265 -> 268        0.64970

 Excited State   6:      Singlet-A      2.5824 eV  480.11 nm  f=0.0181
<S**2>=0.000
     264 -> 267        0.68235
     265 -> 267        0.13301

 Excited State   7:      Singlet-A      2.6558 eV  466.84 nm  f=0.4448
<S**2>=0.000
     263 -> 267        0.69807

 Excited State   8:      Singlet-A      2.8011 eV  442.63 nm  f=0.1811
<S**2>=0.000
     262 -> 266        0.47130
     264 -> 268        0.47339
     265 -> 268        0.13704
```

DPP-VII

DFT Calculation Data

Calculation method: B3LYP/6-31G(d, p) level B3LYP/6-31+G** for C, H, N, B.

```
                         Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
```

1	6	0	0.285174	-1.324303	0.670472
2	6	0	2.410310	-0.393680	0.434079
3	6	0	1.469014	0.647673	0.375283
4	6	0	0.168753	0.115561	0.516593
5	6	0	1.357094	2.083610	0.217541
6	6	0	-0.769421	1.153677	0.455592
7	8	0	-0.535694	-2.222768	0.824834
8	8	0	2.181625	2.981072	0.060187
9	6	0	3.833475	-0.256199	0.325441
10	6	0	4.488635	0.961336	0.130969
11	16	0	5.009692	-1.563914	0.418989
12	6	0	5.884446	0.848792	0.057578
13	1	0	3.943832	1.897259	0.049214
14	6	0	6.346194	-0.454557	0.194527
15	1	0	6.554531	1.686511	-0.089576
16	6	0	-2.194754	1.009318	0.562101
17	6	0	-2.850910	-0.208178	0.771987
18	16	0	-3.351420	2.318690	0.439003
19	6	0	-4.237783	-0.081647	0.837363
20	1	0	-2.313880	-1.145572	0.870888
21	6	0	-4.708935	1.227205	0.677939
22	1	0	-4.897783	-0.924642	0.997746
23	7	0	1.692369	-1.574784	0.604322
24	7	0	-0.049318	2.335148	0.283401
25	6	0	-0.518875	3.715692	0.135094
26	1	0	-1.370430	3.879476	0.798588
27	1	0	0.302117	4.335477	0.502078
28	6	0	-0.840856	4.095764	-1.311957
29	1	0	0.051313	3.992672	-1.935169
30	1	0	-1.635351	3.472790	-1.731666
31	1	0	-1.173275	5.137241	-1.353910
32	6	0	2.165944	-2.950118	0.771723
33	1	0	1.346476	-3.579304	0.417414
34	1	0	3.015698	-3.118554	0.106831
35	6	0	2.495315	-3.304949	2.223783
36	1	0	3.291486	-2.673815	2.627607
37	1	0	1.606847	-3.190075	2.850105
38	1	0	2.823828	-4.347182	2.284637
39	6	0	-6.086131	1.628303	0.701226
40	6	0	-6.596493	2.898644	0.488304
41	6	0	-7.098173	0.540794	0.966955
42	6	0	-7.269537	0.123073	2.258866
43	6	0	-6.574079	0.746449	3.349230
44	6	0	-8.098343	-0.986379	2.632342
45	6	0	-8.002232	3.143067	0.578046
46	6	0	-5.802893	4.044248	0.183338
47	7	0	-6.021543	1.235709	4.248155
48	7	0	-8.723577	-1.902902	2.981946
49	7	0	-9.145868	3.350921	0.650309
50	7	0	-5.182105	4.996468	-0.072848
51	6	0	7.665987	-0.922120	0.170968
52	6	0	8.809018	-1.345066	0.152593
53	6	0	10.144821	-1.830205	0.130191

54	6	0	11.214077	-0.948074	-0.118457
55	6	0	10.410503	-3.199085	0.338168
56	6	0	12.527498	-1.422091	-0.136161
57	1	0	11.016072	0.100520	-0.307589
58	6	0	11.721651	-3.662399	0.307477
59	1	0	9.586515	-3.879565	0.522433
60	6	0	12.781612	-2.783840	0.082843
61	1	0	11.924689	-4.715481	0.475211
62	6	0	13.867232	0.648936	0.336889
63	6	0	14.577086	-0.672321	-1.372803
64	6	0	13.196973	1.193965	1.435186
65	6	0	15.025645	1.260935	-0.204808
66	6	0	14.708852	-1.660681	-2.351685
67	6	0	15.476364	0.420726	-1.295133
68	6	0	13.693692	2.378884	1.974384
69	1	0	12.323810	0.711776	1.860524
70	6	0	15.503066	2.451041	0.355854
71	6	0	15.772949	-1.550657	-3.244411
72	1	0	14.005533	-2.482988	-2.422315
73	6	0	16.537295	0.506473	-2.203835
74	6	0	14.831895	3.006385	1.440991
75	1	0	13.188896	2.822711	2.827298
76	1	0	16.389027	2.931803	-0.048758
77	6	0	16.682576	-0.482432	-3.172070
78	1	0	15.897041	-2.307301	-4.013435
79	1	0	17.234862	1.337656	-2.156138
80	1	0	15.191612	3.929882	1.883808
81	1	0	17.502089	-0.427416	-3.881796
82	7	0	13.600635	-0.527769	-0.377280
83	6	0	-7.838916	0.004195	-0.192005
84	6	0	-7.169517	-0.165560	-1.419085
85	6	0	-9.213056	-0.283838	-0.110119
86	6	0	-7.854561	-0.665258	-2.521600
87	1	0	-6.114558	0.070311	-1.499937
88	6	0	-9.901724	-0.767450	-1.228130
89	1	0	-9.765363	-0.075720	0.797826
90	6	0	-9.209610	-0.975440	-2.430937
91	1	0	-7.328134	-0.821652	-3.457671
92	6	0	-12.249052	-0.539017	-2.067358
93	6	0	-11.945432	-1.817910	-0.205484
94	6	0	-12.092885	0.325046	-3.154037
95	6	0	-13.522891	-1.030443	-1.689043
96	6	0	-11.415581	-2.534482	0.869341
97	6	0	-13.329198	-1.845051	-0.507162
98	6	0	-13.232305	0.669560	-3.878783
99	1	0	-11.123614	0.729614	-3.422965
100	6	0	-14.651138	-0.669680	-2.433934
101	6	0	-12.302106	-3.264470	1.658750
102	1	0	-10.357233	-2.530537	1.099695
103	6	0	-14.197406	-2.589075	0.299631
104	6	0	-14.499276	0.174966	-3.529475
105	1	0	-13.134707	1.339969	-4.727400
106	1	0	-15.633377	-1.039689	-2.154705
107	6	0	-13.678763	-3.292591	1.382433

108	1	0	-11.911600	-3.819168	2.506244
109	1	0	-15.260824	-2.617614	0.080272
110	1	0	-15.367051	0.461823	-4.115205
111	1	0	-14.341895	-3.870064	2.019058
112	7	0	-11.289509	-1.022706	-1.162083
113	1	0	-9.742355	-1.375036	-3.286631
114	1	0	13.805922	-3.139995	0.086282

Total Energy (HF) = =-3848.8688579 Hartree

TDDFT Calculation Data

Excitation energies and oscillator strengths:

```
 Excited State   1:      Singlet-A      1.4244 eV  870.44 nm  f=0.0027
<S**2>=0.000
     262 -> 264        0.41172
     263 -> 264        0.56735
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -3846.44629108
 Copying the excited state density for this state as the 1-particle RhoCI
density.

 Excited State   2:      Singlet-A      1.6477 eV  752.48 nm  f=0.4277
<S**2>=0.000
     261 -> 264        0.51498
     262 -> 264        0.39231
     263 -> 264       -0.27685

 Excited State   3:      Singlet-A      1.6939 eV  731.95 nm  f=0.8490
<S**2>=0.000
     261 -> 264        0.48006
     262 -> 264       -0.41045
     263 -> 264        0.30290

 Excited State   4:      Singlet-A      1.7482 eV  709.20 nm  f=0.0002
<S**2>=0.000
     260 -> 264        0.70312

 Excited State   5:      Singlet-A      1.8918 eV  655.37 nm  f=0.0104
<S**2>=0.000
     262 -> 265        0.37568
     263 -> 265        0.58461

 Excited State   6:      Singlet-A      2.0080 eV  617.46 nm  f=0.0064
<S**2>=0.000
     259 -> 264        0.69187
     262 -> 265       -0.11229

 Excited State   7:      Singlet-A      2.0109 eV  616.56 nm  f=0.1749
<S**2>=0.000
     259 -> 264        0.13683
```

```
     262 -> 264        0.10174
     262 -> 265        0.56498
     263 -> 265       -0.35873

 Excited State   8:      Singlet-A      2.2317 eV  555.57 nm  f=0.0000
<S**2>=0.000
     260 -> 265        0.69868
```