Supporting Information

for

NIR absorbing ferrocenyl perylenediimide based donor-acceptor chromophores

Mohd Wazid and Rajneesh Misra*

Department of Chemistry, Indian Institute of Technology Indore (M.P.) 453552, India

E-mail: rajneeshmisra@iiti.ac.in

General Methods

All the moisture and oxygen-sensitive reactions were performed in an inert atmosphere using the standard inert atmosphere method. ^{1}H NMR spectra were measured on a Bruker Advance (III) 400 MHz/500 MHz, and $^{13}C\{^{1}H\}$ NMR spectra were measured at 100 MHz/125 MHz using $CDCl_3$ as the internal solvent. The ^{1}H NMR chemical shifts are recorded in parts per million (ppm) relative to the solvent residual peak ($CDCl_3$, 7.26 ppm). The $^{13}C\{^{1}H\}$ NMR shifts are reported relative to the solvent residual peak ($CDCl_3$, 77.16 ppm). The multiplicities are given as s (singlet), d (doublet), t (triplet), q (quartet), and m (multiple), and the coupling constant values (J) are reported in Hz. Thermogravimetric analysis was performed on a Mettler Toledo thermal analysis system. The UV-visible absorption spectra of all compounds were recorded in a PerkinElmer LAMBDA 35 UV-visible Spectrophotometer in DCM solvent at room temperature. Cyclic voltammograms (CVs) and differential pulse voltammetry (DPVs) were recorded on a PalmSens 4 electrochemical analyzer using glassy carbon as a working electrode, Pt wire as the counter electrode, and Ag/AgCl as the reference electrode. The scan rate was 50 mV s^{-1} for cyclic voltammetry. A solution of (TBA)ClO_4 in CH_2Cl_2 (0.1 M) was used as the supporting electrolyte.

Characterization

^{1}H-NMR, ^{13}C-NMR, MALDI of PDI derivatives 1–5.

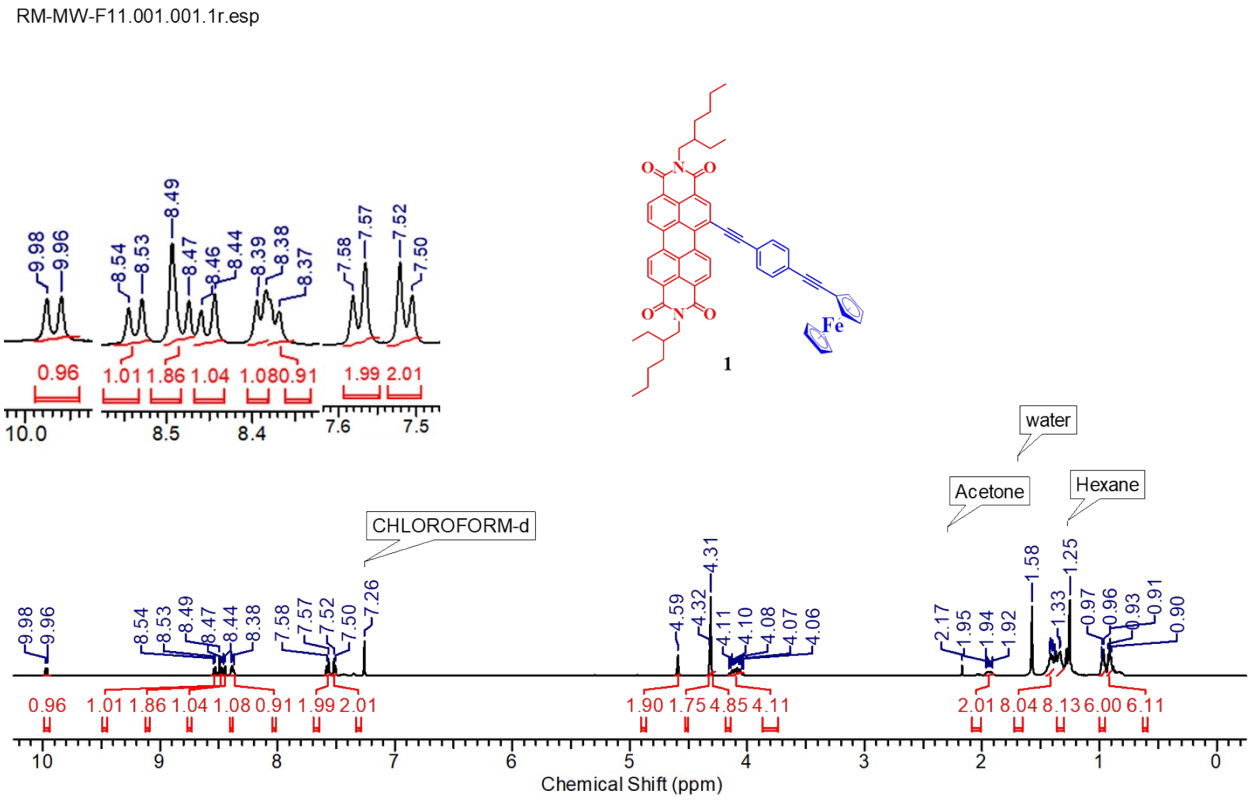

Figure S1. ^{1}H NMR of compound **1**.

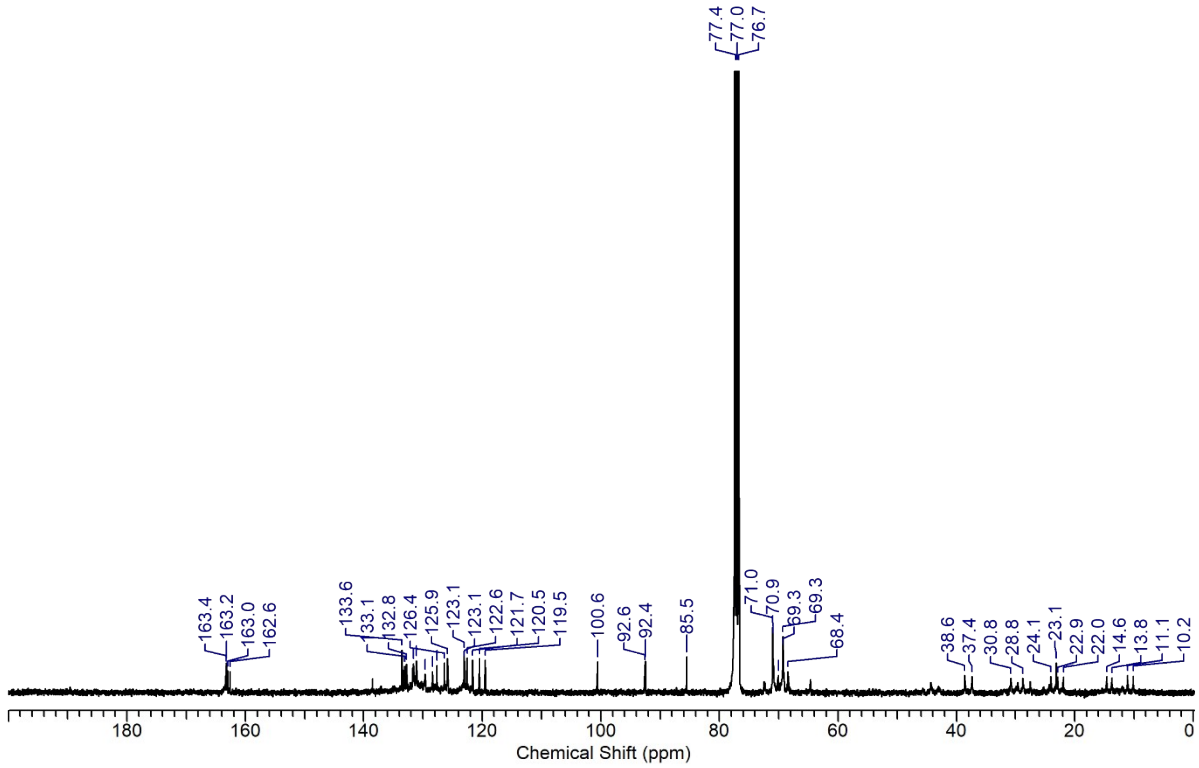

Figure S2. ^{13}C NMR of compound **1**.

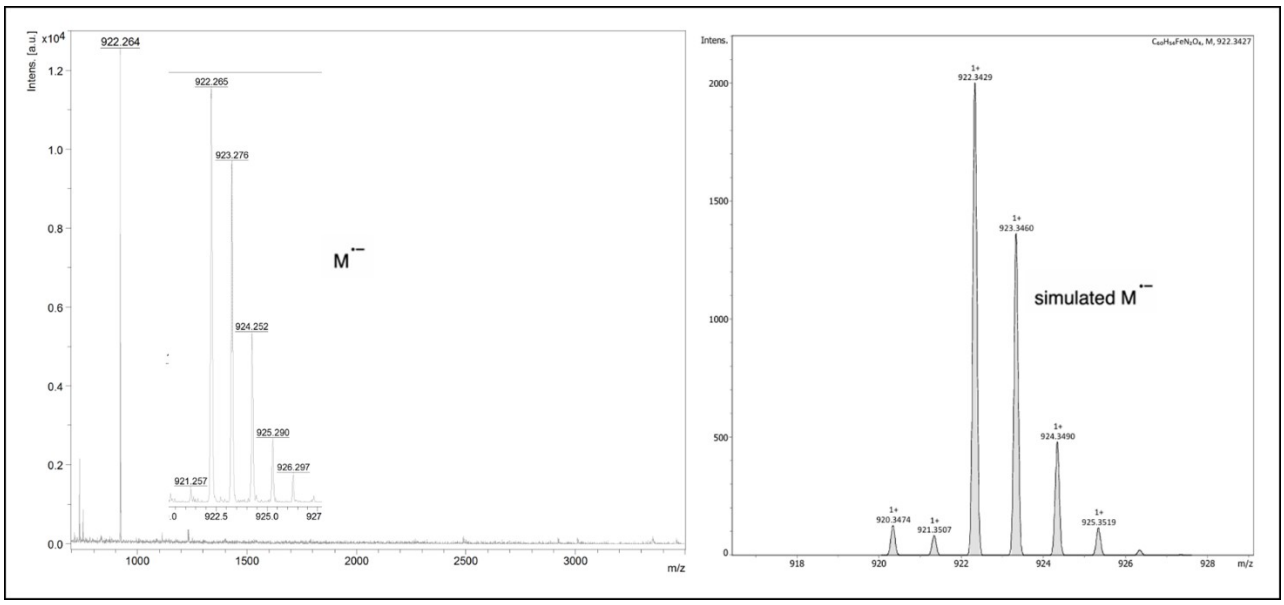

Figure S3. HRMS (MALDI-TOF) of compound **1**.

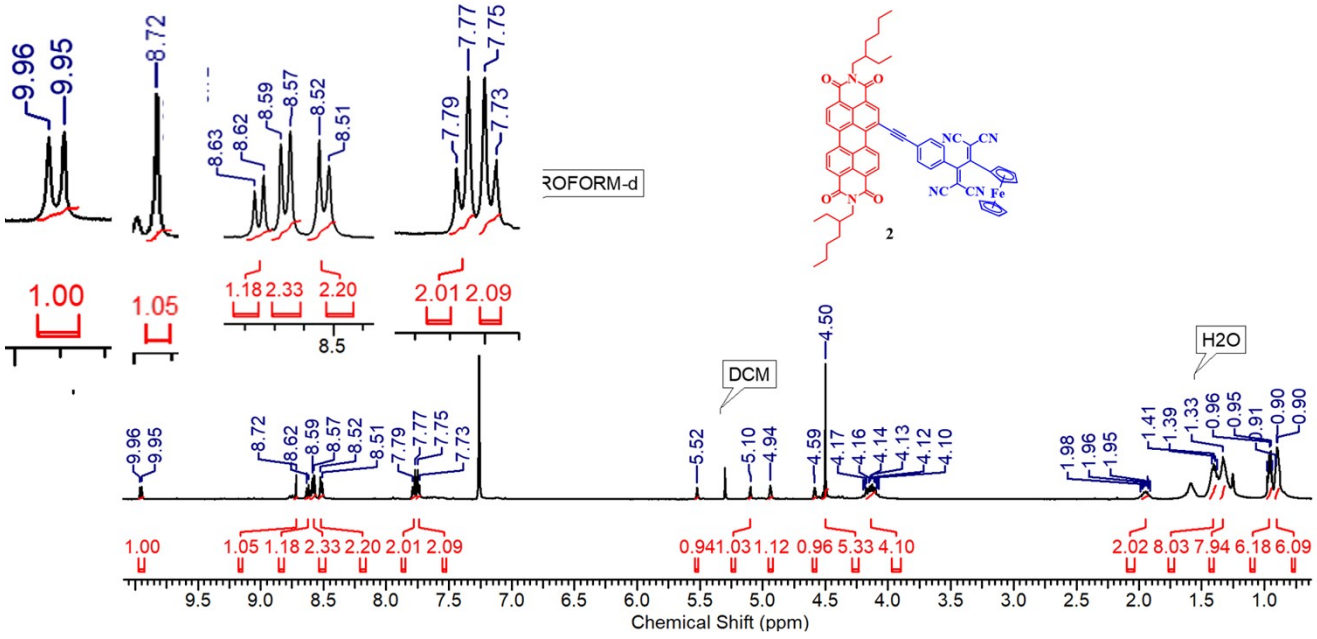

Figure S4. ^{1}H NMR of compound **2**.

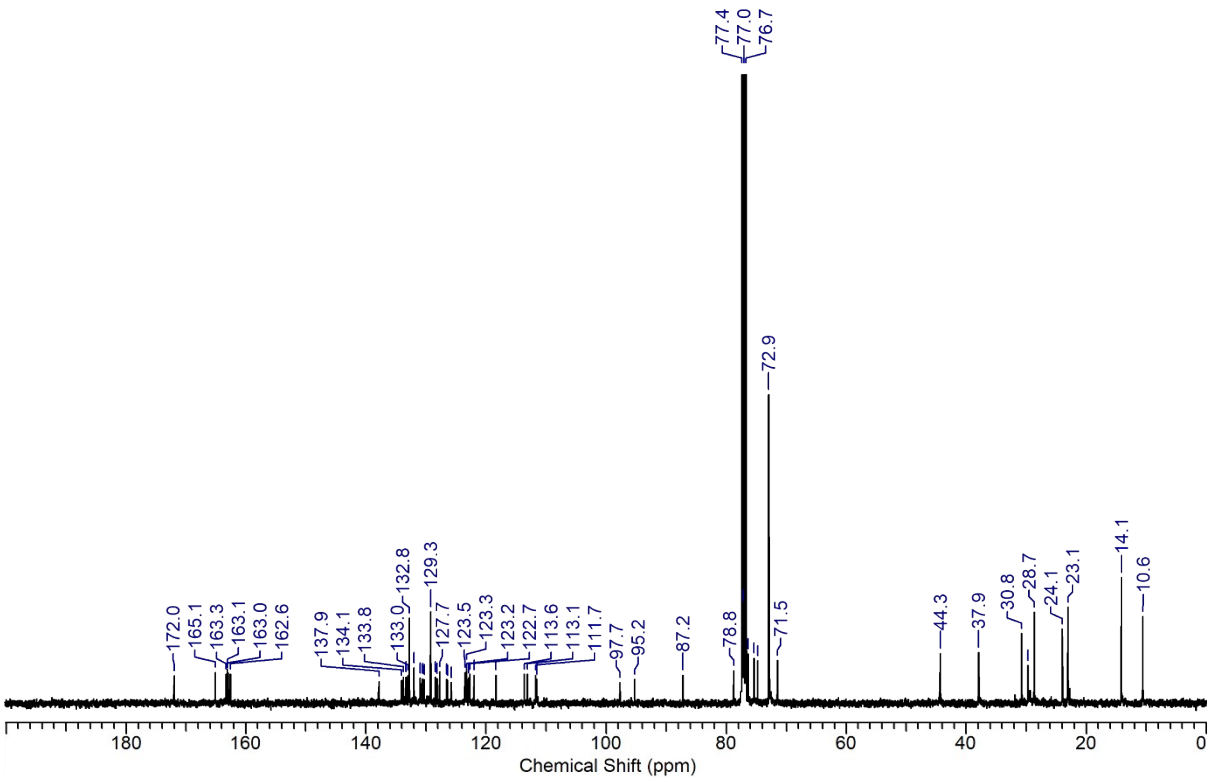

Figure S5. ^{13}C NMR of compound **2**.

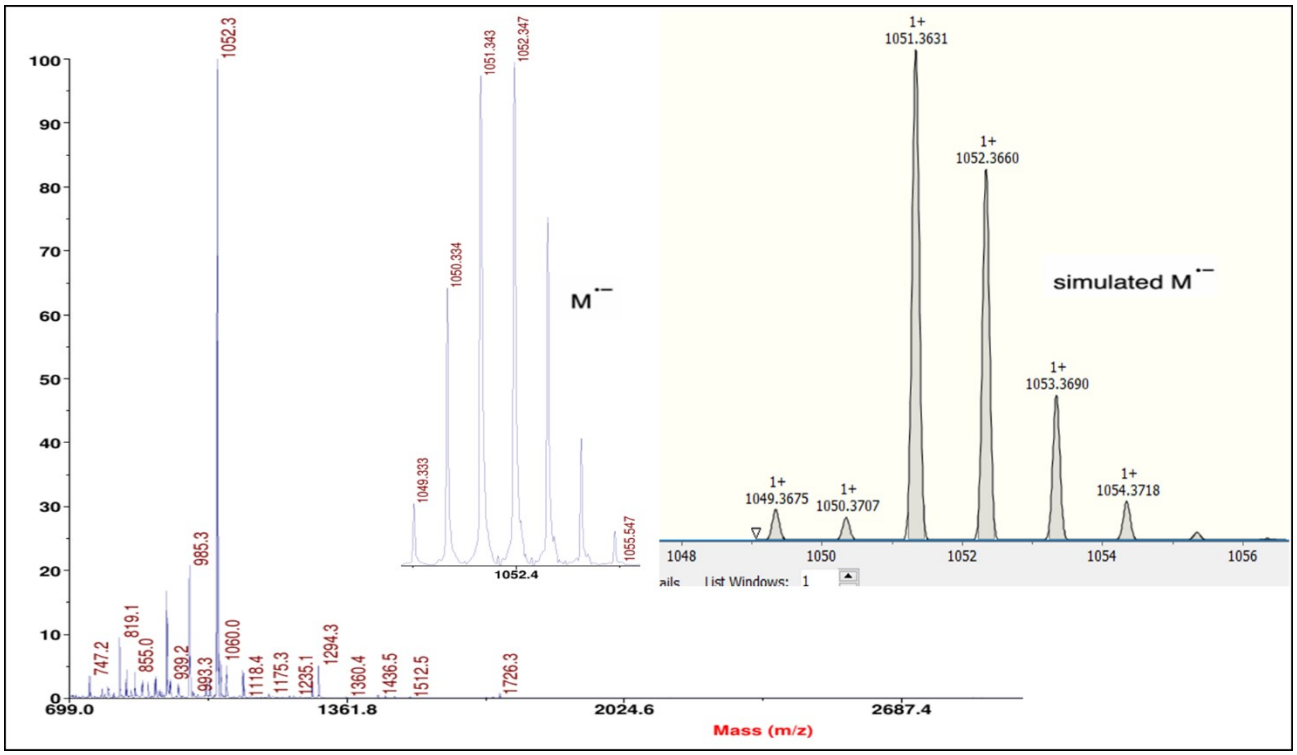

Figure S6. HRMS (MALDI-TOF) of compound **2**.

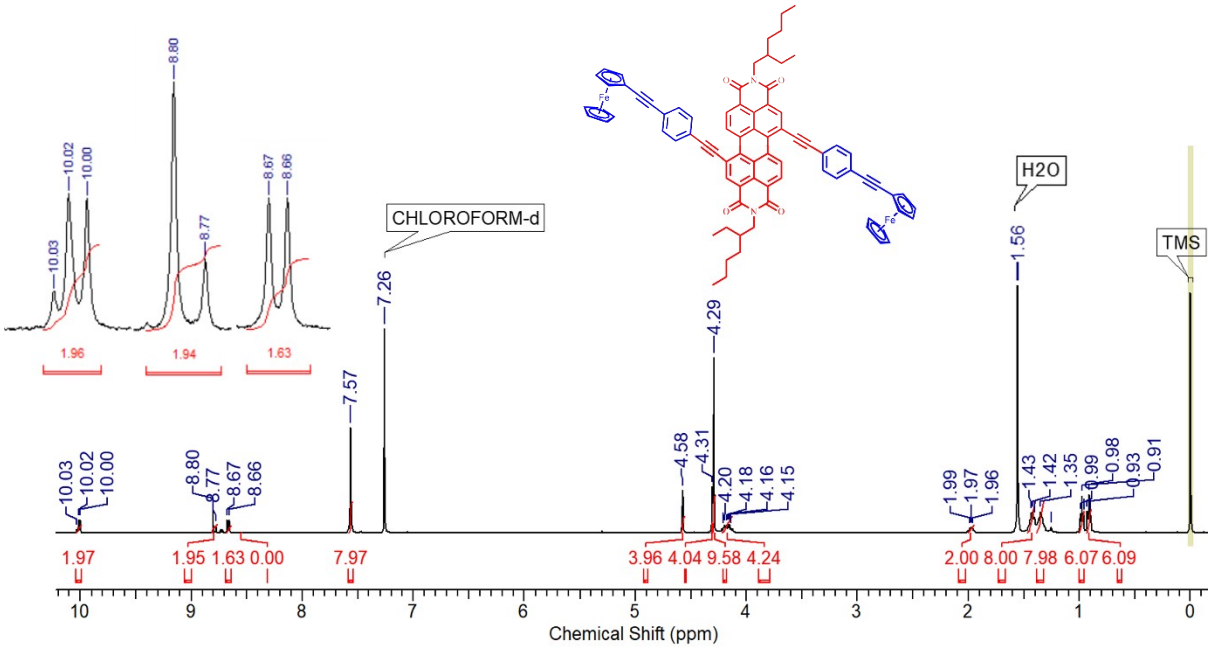

Figure S7. ^{1}H NMR of compound **3**.

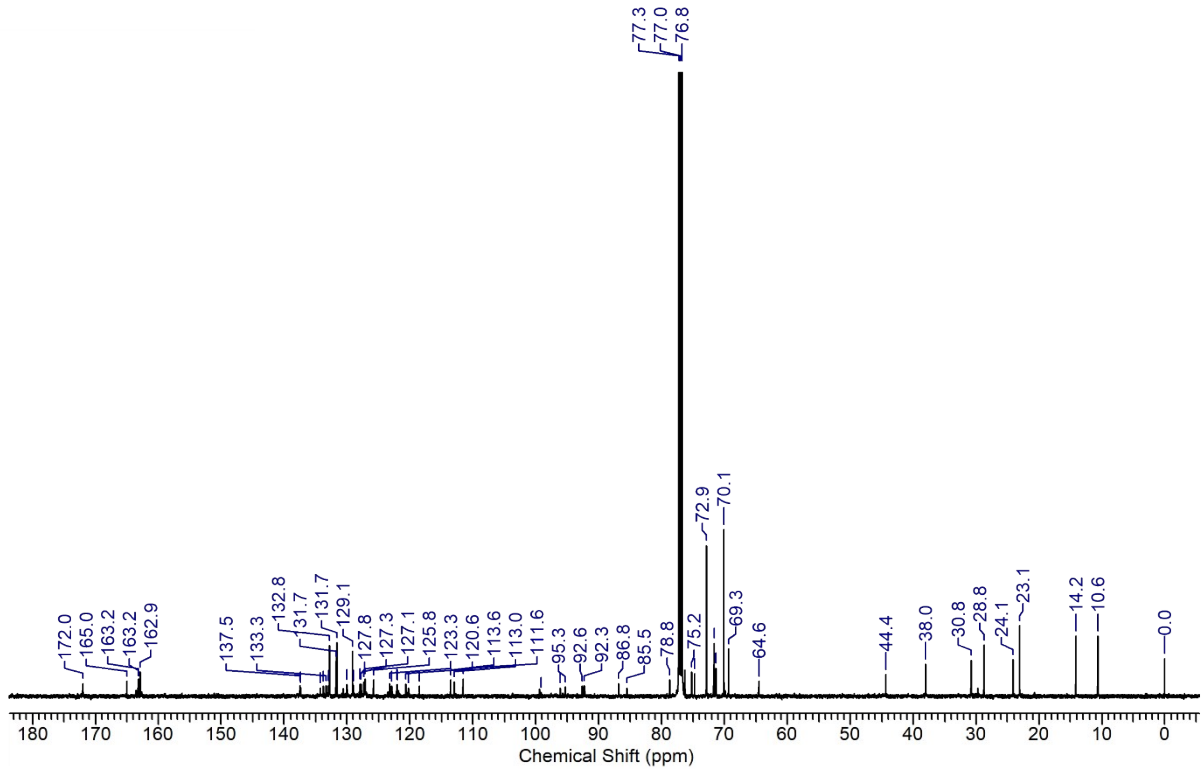

Figure S8. ^{13}C NMR of compound **3**.

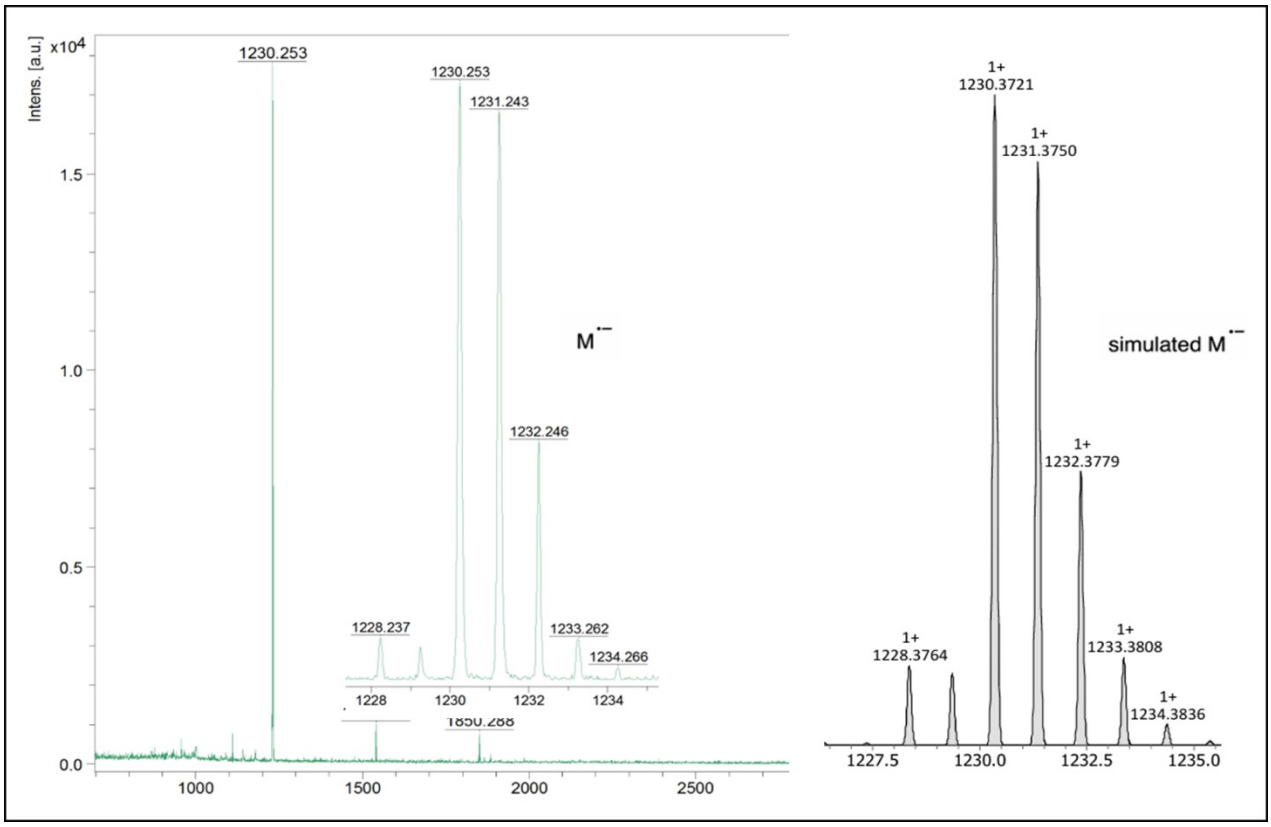

Figure S9. HRMS (MALDI-TOF) of compound **3**.

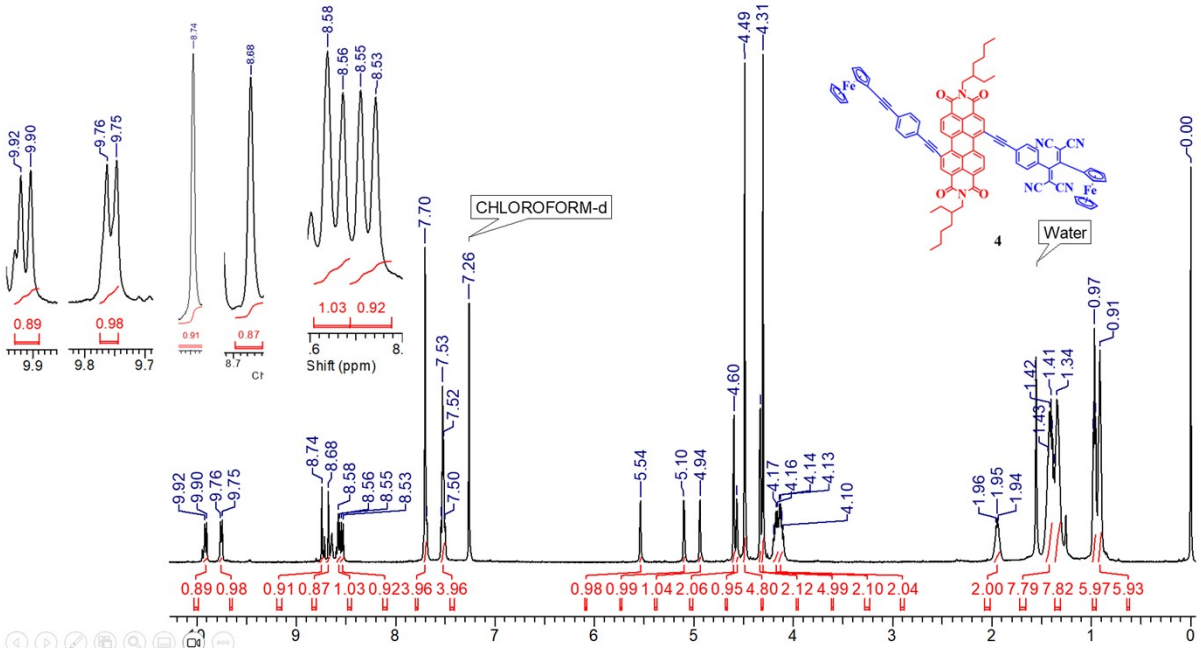

Figure S10. ^{1}H NMR of compound **4**.

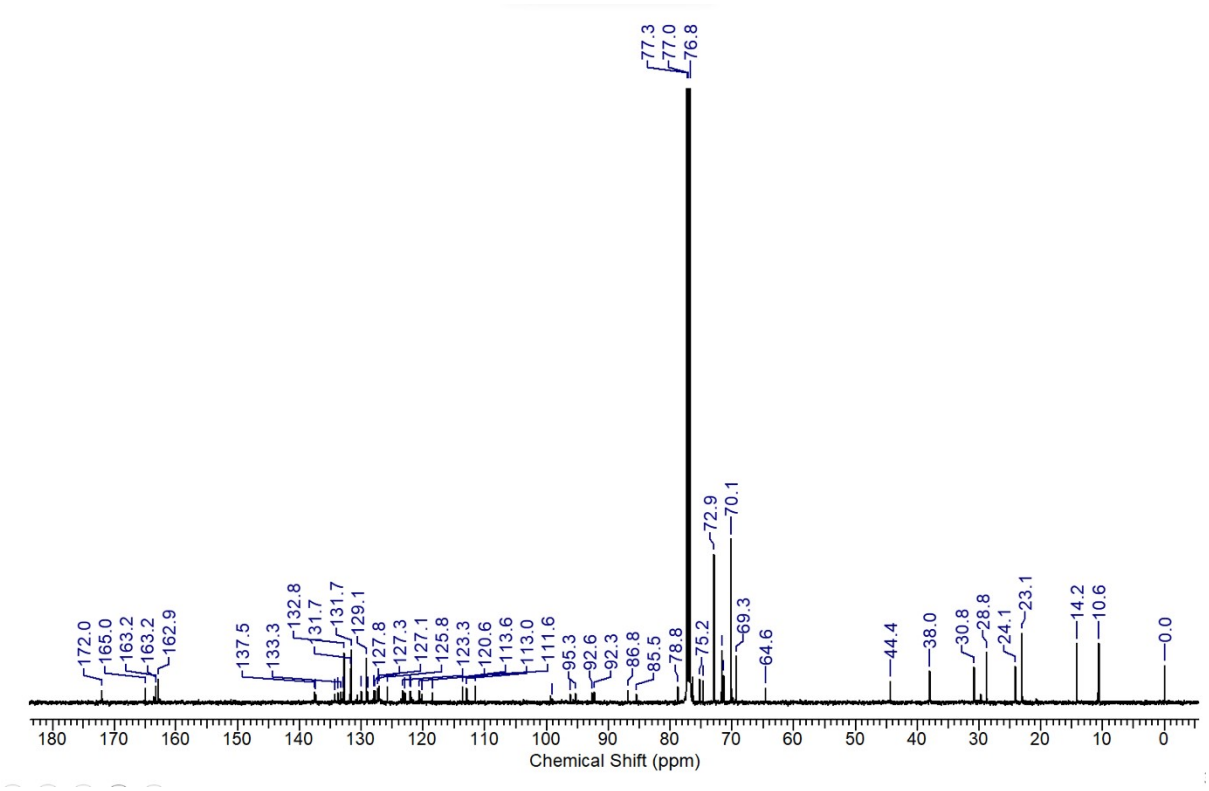

Figure S11. ^{13}C NMR of compound **4**.

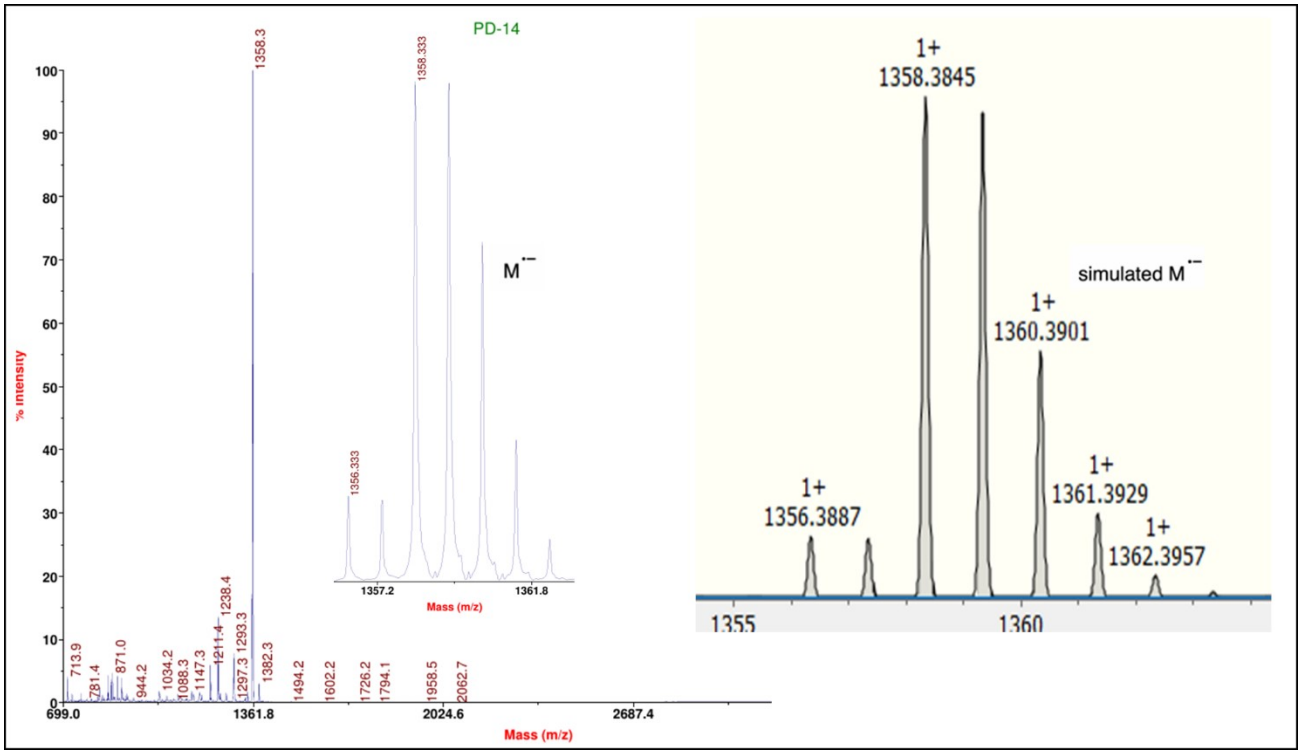

Figure S12. HRMS (MALDI-TOF) of compound **4**.

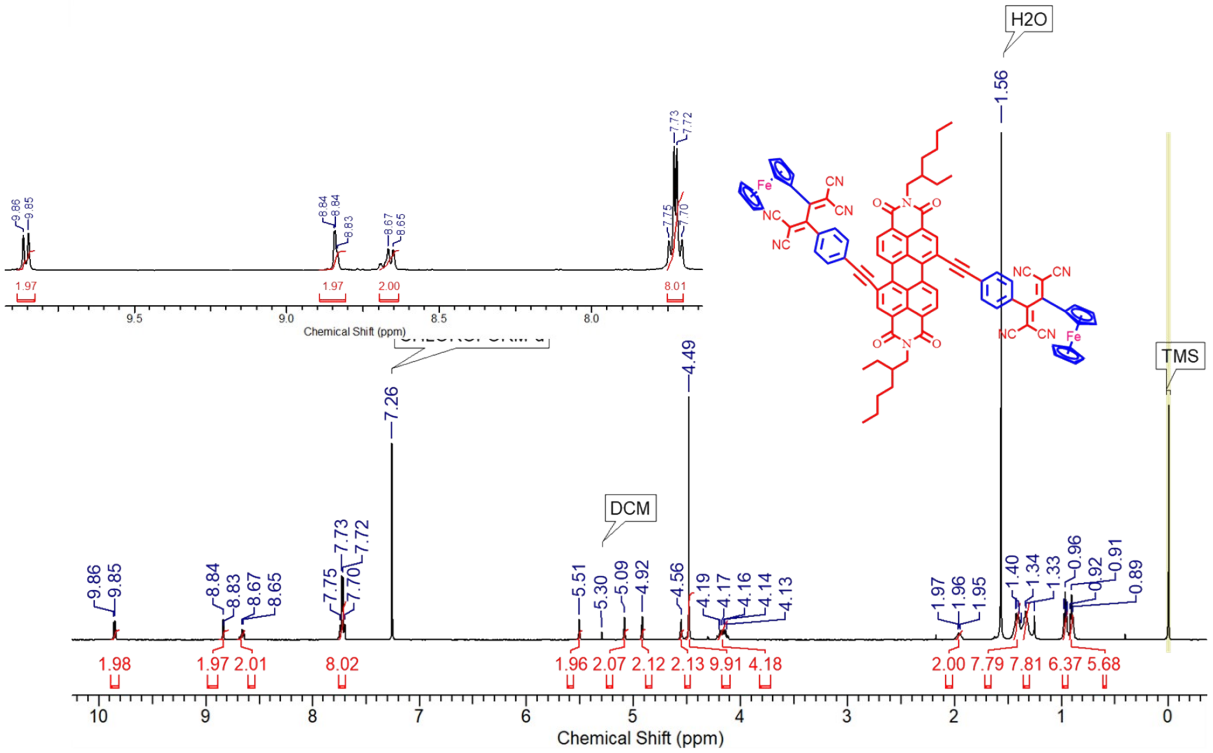

Figure S13. ^{1}H NMR of compound **5**.

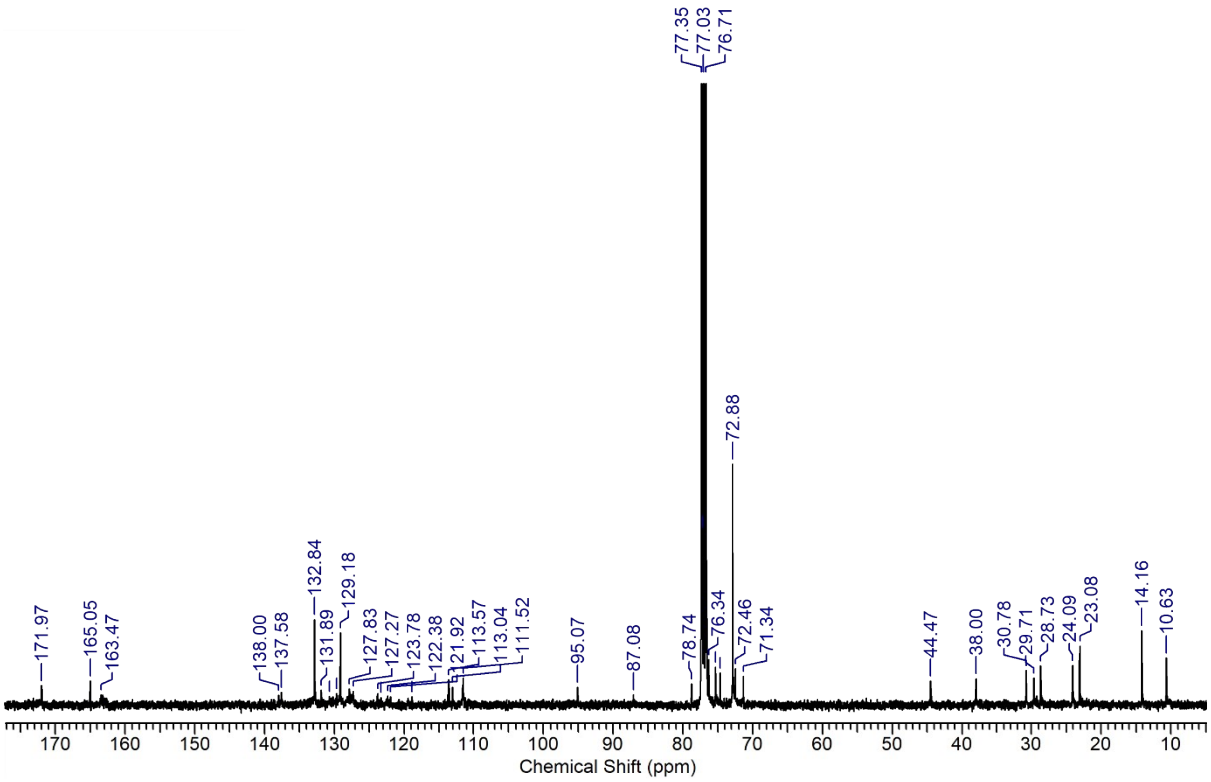

Figure S14. ^{13}C NMR of compound **5**.

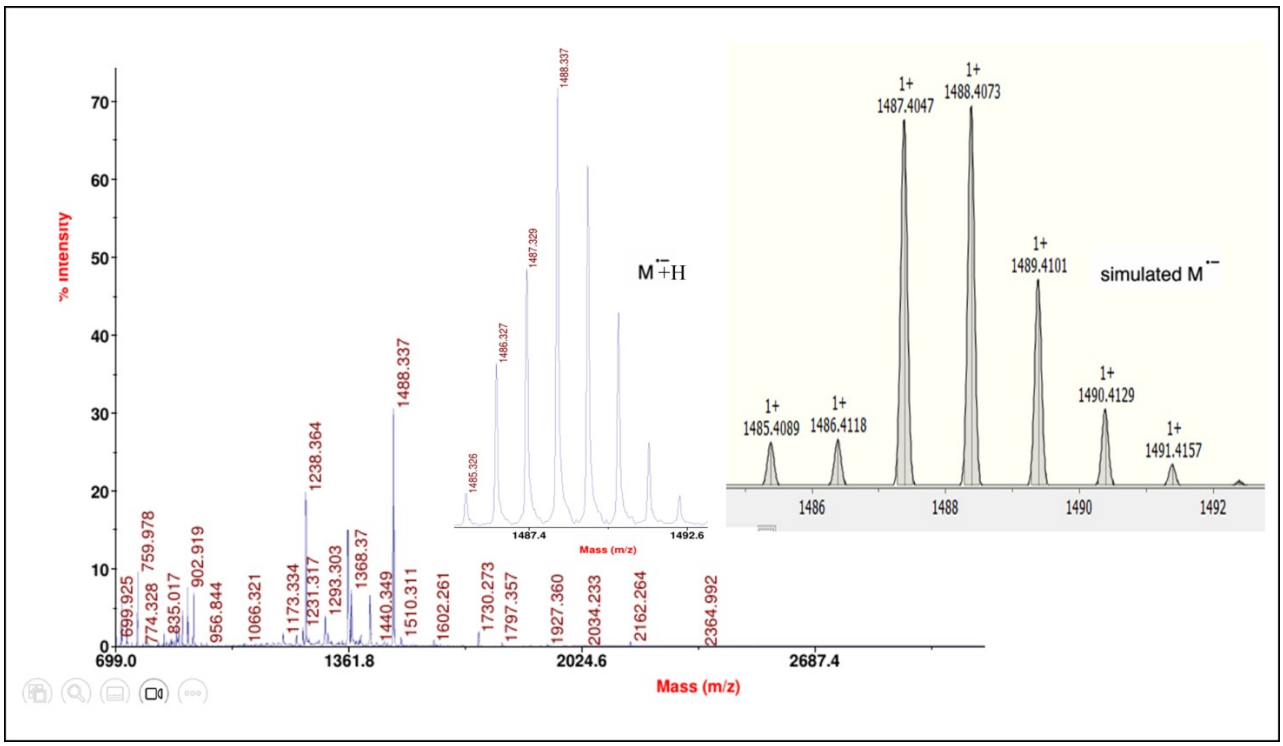

Figure S15. HRMS (MALDI-TOF) of compound **5**.

Photophysical Study

Solvatochromic study:

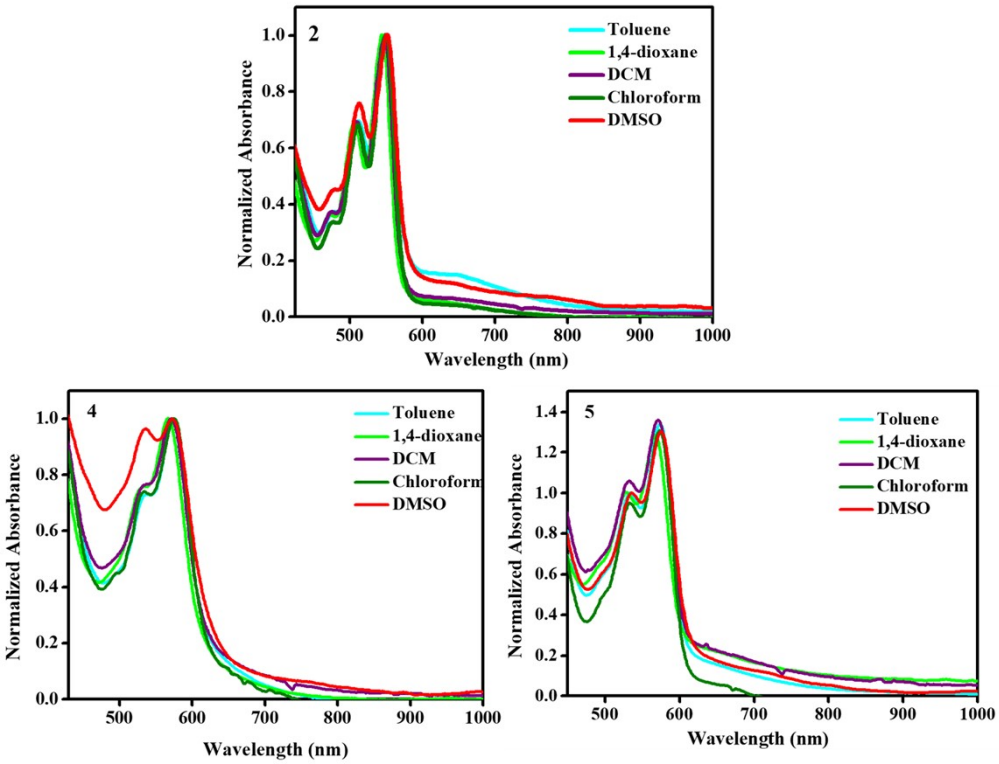

Figure S16. Absorption spectra of chromophores **1–5** in toluene to DMSO.

Electrochemistry Study

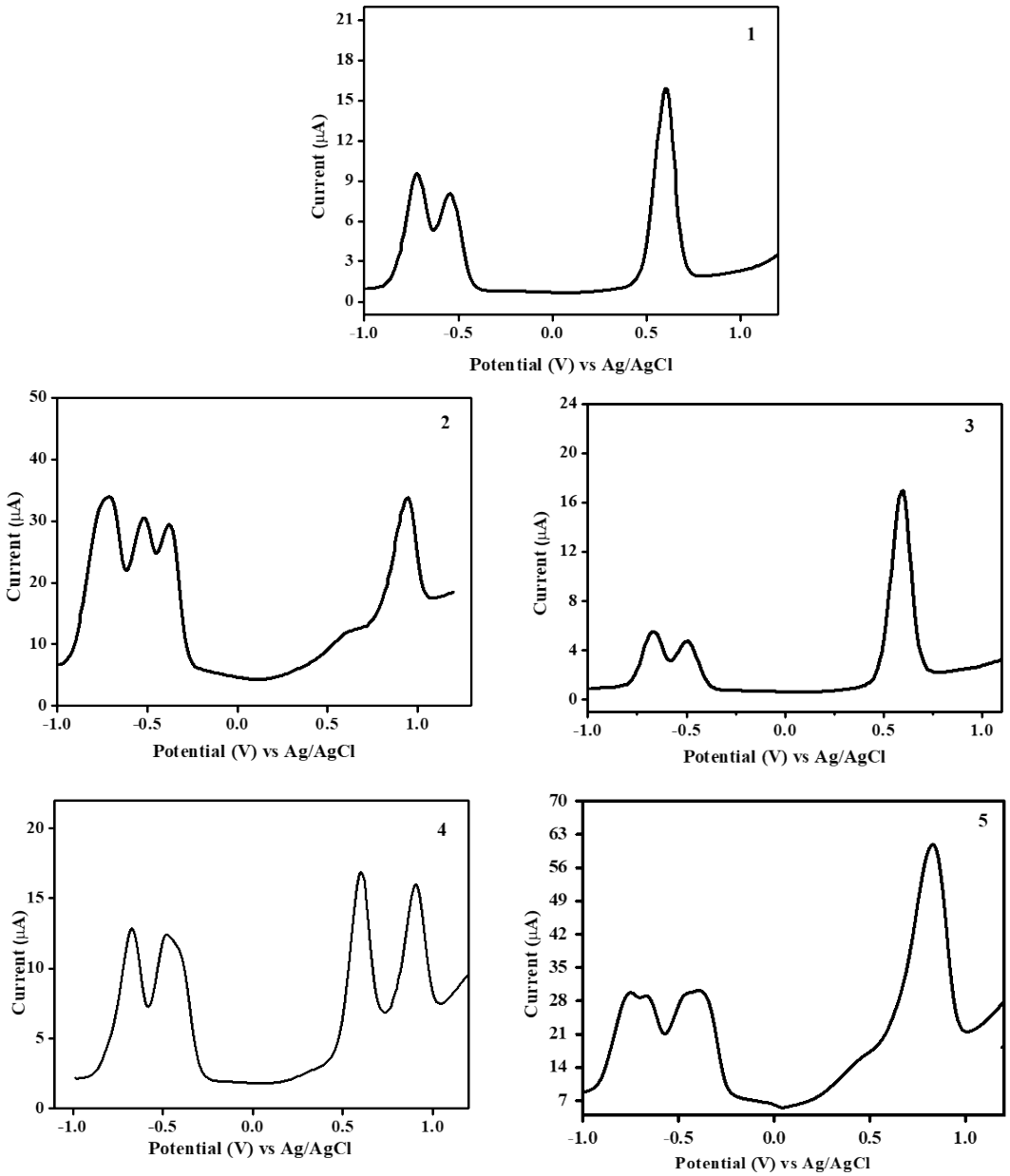

Figure S17. DPVs of donor-acceptor PDI derivatives **1–5**.

Table 1. Redox properties of derivatives **1–5**.

Compounds	wave	$E_{1/2}$ (V)	E_{pa} (mV)	E_{pc} (mV)	ΔE_p (mV)	E_{HOMO} (eV)[a]	E_{LUMO} (eV)[a]	E_g (eV)[a]
1	i	–0.50	–460	–539	79	–5.04	–3.90	1.14
	ii	–0.67	–640	–719	79			
	iii	0.64	679	599	80			
2	i	–0.29	–319	–389	70	–5.36	–4.11	1.25
	ii	–0.45	–459	–539	80			
	iii	–0.61	–649	–689	40			
	iv	–0.83	–739	–769	30			
	v	0.96	999	919	80			
3	i	–0.44	–400	–479	79	–5.04	–3.96	1.08
	ii	– 0.62	–579	–659	80			
	iii	0.64	609	679	70			
4	i	–0.47	–449	–489	40	–4.89	–3.93	0.96
	ii	–0.57	– 529	–609	80			
	iii	–0.75	–719	–779	60			
	iv	–0.85	–829	–869	40			
	v	0.49	529	459	70			
	vi	0.83	869	789	80			
5	i	–0.34	–309	–379	70	–5.05	–4.06	0.99
	ii	–0.46	–429	–489	70			
	iii	–0.64	–609	–669	60			
	iv	–0.76	–719	–799	80			

	v	0.96	999	919	80			

PDI derivatives **1–5** in 0.1 M solution of (TBA)ClO_4 as the supporting electrolyte in dichloromethane at 100 mV s^{-1} scan rate *versus* Ag/AgCl at 25 °C. E_g = – (HOMO-LUMO), $E_{1/2}$ calculated by $E_{pa}+E_{pc}$ /2 and $\Delta E_p = E_{pa}-E_{pc}$.

Spectroelectrochemistry Study

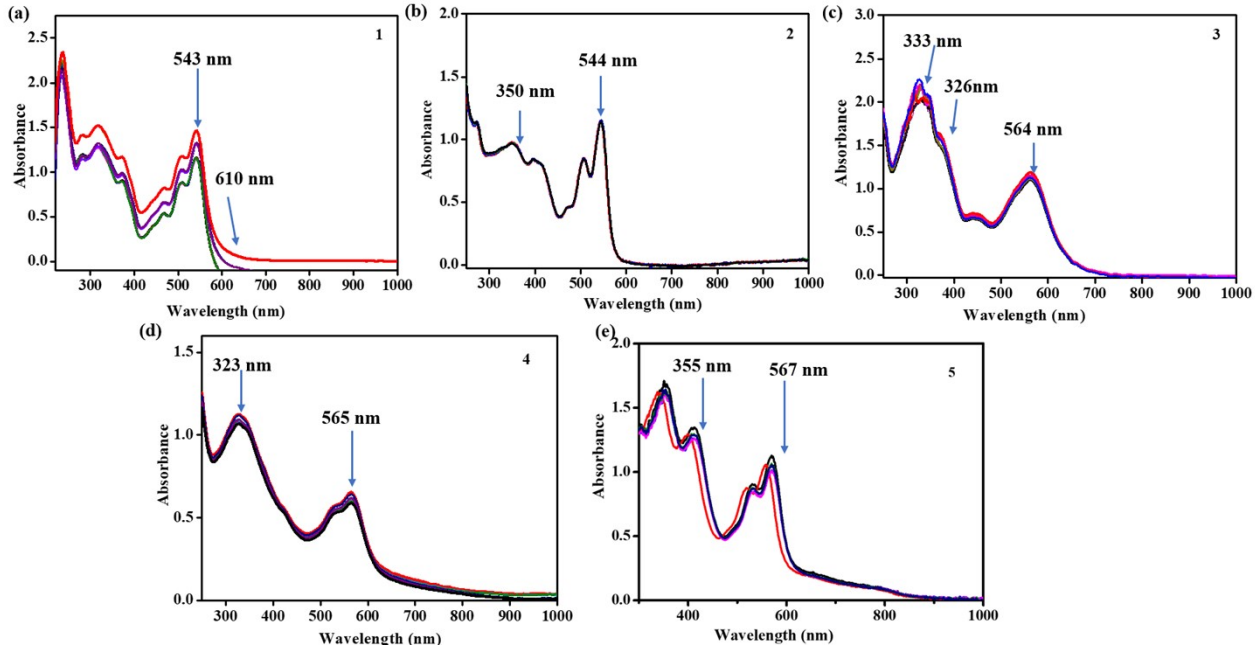

Figure S18. Oxidation of the PDI derivatives **1–5** under Spectroelectrochemical conditions in a DCM/0.50 M $TBAPF_6$ system. Spectroelectrochemical changes were observed (**a**) for **1**, (**b**) for **2**, **(c)** for **3**, **(d)**, for **4**, and (**e**) for **5** in oxidation cycles. initial spectrum: black.

Molecular electrostatic potential map.

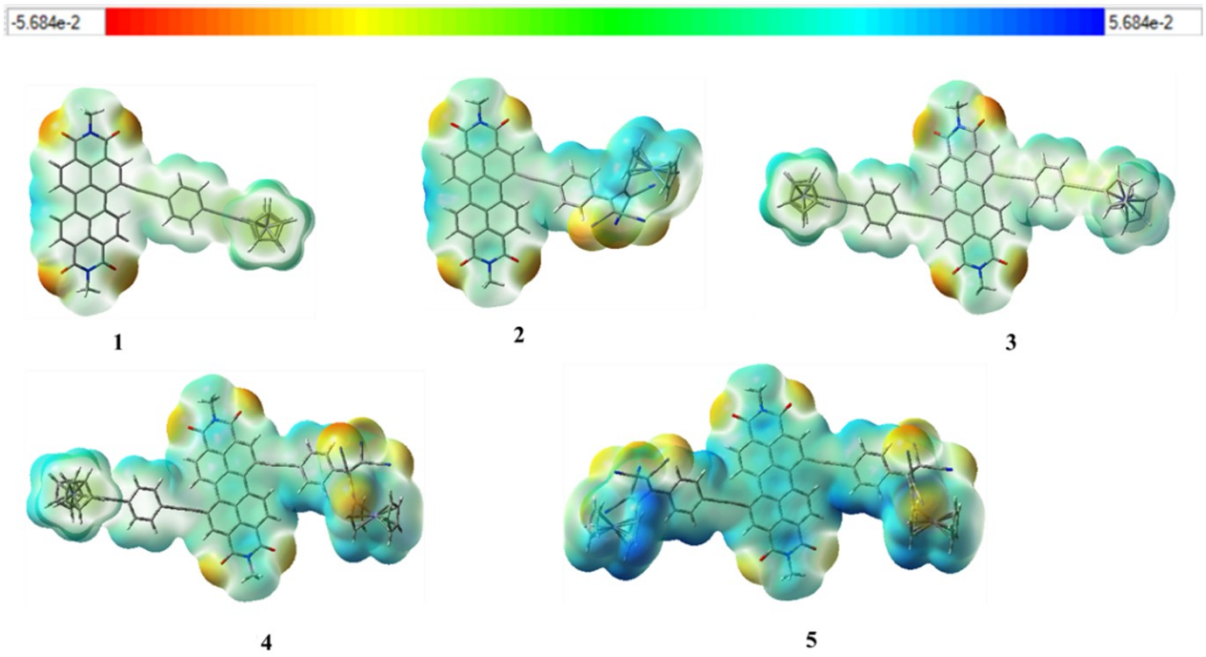

Fig. S19 Molecular electrostatic potential (MEP) map of PDI compounds **1–5**.

TDOS spectrum

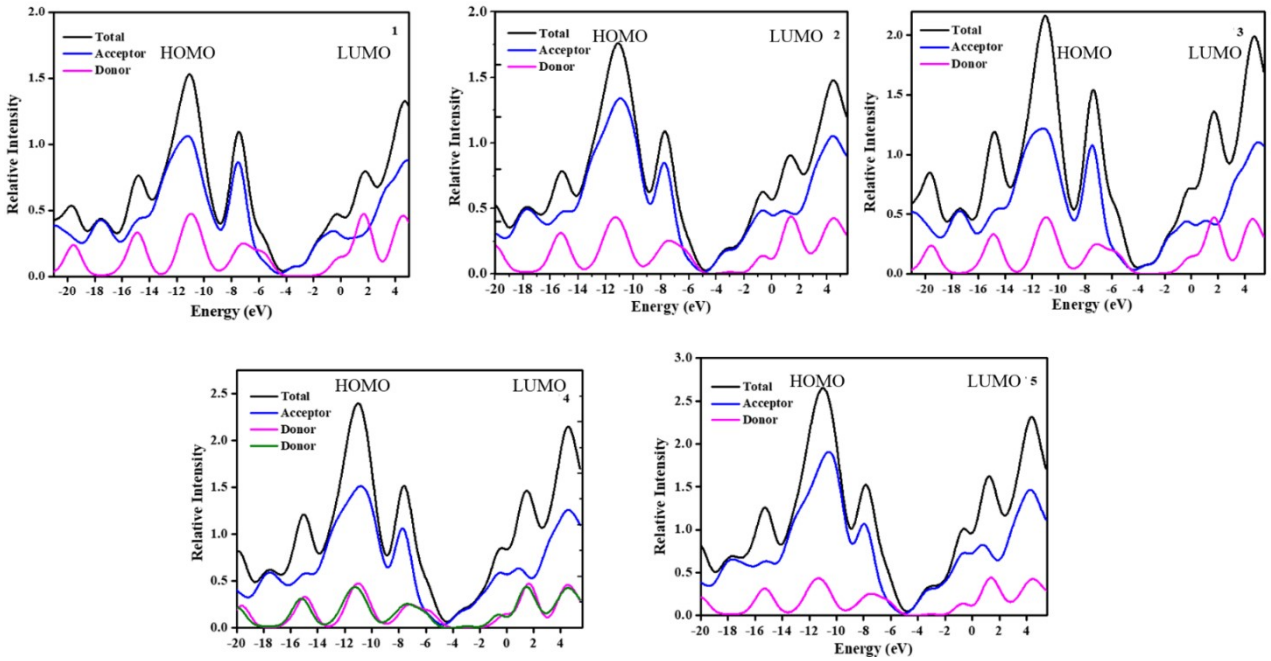

Fig. S20 Density of state (DOS) analysis of the PDI derivatives **1**−**5**.

DFT calculation:

The computational study was performed by using the Gaussian 09W program[1]

DFT of compound (1)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	7.661529	-2.279659	0.613213
2	6	0	7.455888	-0.900162	0.650832
3	6	0	6.202721	-0.329779	0.408282
4	6	0	5.101801	-1.184040	0.074012
5	6	0	5.320736	-2.596723	0.080586
6	6	0	6.602103	-3.130236	0.342807
7	6	0	3.804082	-0.654032	-0.242732
8	6	0	2.731727	-1.571810	-0.405303
9	6	0	2.983414	-2.970102	-0.382273
10	6	0	4.240904	-3.479188	-0.171800
11	6	0	5.988394	1.117591	0.495564
12	6	0	4.741640	1.652039	0.052022
13	6	0	3.667434	0.804400	-0.379560
14	6	0	6.966778	1.992710	0.976226
15	6	0	6.773900	3.376424	0.988696
16	6	0	5.597445	3.921320	0.502345
17	6	0	4.572229	3.071268	0.023055
18	6	0	3.383340	3.637512	-0.497694

19	6	0	2.398433	2.805366	-0.997546
20	6	0	2.538615	1.414295	-0.936424
21	6	0	4.430160	-4.952832	-0.181176
22	7	0	5.729410	-5.414793	0.071264
23	6	0	6.834297	-4.594109	0.331719
24	6	0	5.428941	5.393532	0.492086
25	7	0	4.230357	5.893696	-0.031659
26	6	0	3.184802	5.106586	-0.538828
27	8	0	3.507651	-5.727261	-0.396200
28	8	0	7.933707	-5.090342	0.538924
29	8	0	6.284051	6.160973	0.914973
30	8	0	2.165456	5.614618	-0.987827
31	6	0	1.358562	-1.233471	-0.545165
32	6	0	0.147906	-1.107569	-0.622247
33	6	0	-1.253806	-0.900112	-0.709499
34	6	0	5.976835	-6.860907	0.069420
35	6	0	4.082037	7.353049	-0.041016
36	6	0	-2.122241	-1.968710	-1.018830
37	6	0	-3.490642	-1.765890	-1.100993
38	6	0	-4.046372	-0.487941	-0.874190
39	6	0	-3.176266	0.580281	-0.565008
40	6	0	-1.807782	0.378728	-0.484250
41	6	0	-5.449869	-0.281409	-0.949527
42	1	0	8.639836	-2.707866	0.800788
43	1	0	8.304974	-0.264029	0.867771
44	1	0	2.160300	-3.658511	-0.532339
45	1	0	7.903315	1.605276	1.357813
46	1	0	7.540503	4.045298	1.363963
47	1	0	1.510444	3.253097	-1.430207
48	1	0	1.744766	0.804392	-1.338598

49	1	0	5.028879	-7.358328	-0.118067
50	1	0	6.702690	-7.111511	-0.707048
51	1	0	6.389180	-7.164777	1.033439
52	1	0	4.890319	7.802448	-0.621365
53	1	0	3.116727	7.584403	-0.483692
54	1	0	4.139868	7.737466	0.979435
55	1	0	-1.706454	-2.955481	-1.193448
56	1	0	-4.150040	-2.593341	-1.340176
57	1	0	-3.592449	1.566375	-0.388743
58	1	0	-1.149727	1.206021	-0.239471
59	6	0	-6.652452	-0.102603	-1.012088
60	6	0	-8.050722	0.112372	-1.093904
61	26	0	-9.439023	-0.087124	0.410605
62	6	0	-8.739027	1.357175	-0.860504
63	6	0	-9.049905	-0.866779	-1.441837
64	6	0	-8.446687	-0.750587	2.081324
65	6	0	-9.494040	-1.655569	1.735530
66	6	0	-9.030191	0.528429	2.326446
67	6	0	-10.726816	-0.935677	1.766710
68	6	0	-10.440120	0.413870	2.132269
69	6	0	-10.128004	1.144719	-1.083258
70	6	0	-10.319497	-0.224268	-1.441329
71	1	0	-8.264274	2.285976	-0.577490
72	1	0	-8.850279	-1.903466	-1.673320
73	1	0	-7.391002	-0.983282	2.115986
74	1	0	-9.373685	-2.700138	1.482800
75	1	0	-8.496732	1.428622	2.599450
76	1	0	-11.704866	-1.339664	1.543495
77	1	0	-11.163321	1.211483	2.234820
78	1	0	-10.905515	1.889680	-0.984212

79	1	0	-11.267426	-0.696119	-1.660494

Rotational constants (GHZ): 0.0630221 0.0167274 0.0136357

DFT of compound (2)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	8.174211	3.024703	-0.178107
2	6	0	8.182707	1.629598	-0.227138
3	6	0	7.006929	0.878410	-0.151440
4	6	0	5.757748	1.559475	0.019686
5	6	0	5.762434	2.988938	0.020058
6	6	0	6.974812	3.709373	-0.068710
7	6	0	4.522693	0.841455	0.167736
8	6	0	3.314825	1.588237	0.154698
9	6	0	3.353031	3.007656	0.139964
10	6	0	4.539167	3.698367	0.102610
11	6	0	7.019067	-0.583976	-0.250176
12	6	0	5.819110	-1.297608	0.044505
13	6	0	4.587298	-0.619679	0.325922
14	6	0	8.166123	-1.303642	-0.595016
15	6	0	8.180512	-2.701532	-0.610095
16	6	0	7.047003	-3.414325	-0.258316
17	6	0	5.858148	-2.725314	0.080760
18	6	0	4.712788	-3.460288	0.471683
19	6	0	3.564477	-2.784054	0.840172

20	6	0	3.504473	-1.387026	0.765973
21	6	0	4.512650	5.182382	0.112636
22	7	0	5.746623	5.836312	0.044800
23	6	0	6.991612	5.193383	-0.046694
24	6	0	7.096049	-4.896649	-0.241090
25	7	0	5.931173	-5.568297	0.148973
26	6	0	4.730679	-4.944277	0.520054
27	8	0	3.472937	5.824140	0.177678
28	8	0	8.033492	5.831722	-0.105450
29	8	0	8.099031	-5.527103	-0.547718
30	6	0	2.004592	1.038681	0.093556
31	6	0	0.833729	0.715527	-0.006730
32	6	0	-0.509846	0.272099	-0.119927
33	6	0	5.710579	7.303261	0.064139
34	6	0	5.998756	-7.034161	0.168495
35	6	0	-1.584324	1.152882	0.124823
36	6	0	-2.893892	0.710493	0.028965
37	6	0	-3.183626	-0.619140	-0.344955
38	6	0	-2.107106	-1.500827	-0.575503
39	6	0	-0.796447	-1.065313	-0.464589
40	1	0	9.095620	3.593409	-0.234138
41	1	0	9.138126	1.127880	-0.317719
42	1	0	2.424284	3.565734	0.156024
43	1	0	9.075804	-0.780881	-0.864255
44	1	0	9.076534	-3.249388	-0.880024
45	1	0	2.709477	-3.358117	1.180134
46	1	0	2.589706	-0.900404	1.067731
47	1	0	5.133913	7.669903	-0.787502
48	1	0	5.225839	7.647792	0.979686
49	1	0	6.736055	7.659656	0.014604

50	1	0	6.777092	-7.359013	0.861959
51	1	0	5.026972	-7.406152	0.482280
52	1	0	6.250991	-7.404660	-0.826988
53	1	0	-1.376931	2.182258	0.395712
54	1	0	-3.700973	1.407151	0.223114
55	1	0	-2.295085	-2.541836	-0.806039
56	1	0	0.019711	-1.758408	-0.635968
57	6	0	-4.577947	-1.084630	-0.431503
58	6	0	-5.025385	-2.021268	-1.327800
59	6	0	-5.665132	-1.116710	1.772590
60	6	0	-4.231269	-2.551565	-2.398338
61	6	0	-6.368920	-2.521273	-1.287828
62	6	0	-4.873298	-2.268405	2.086636
63	6	0	-6.575209	-0.696347	2.792939
64	7	0	-3.637547	-2.991646	-3.296836
65	7	0	-7.450759	-2.949531	-1.282724
66	7	0	-4.225170	-3.199225	2.347666
67	7	0	-7.319492	-0.374109	3.627912
68	8	0	3.752477	-5.594151	0.862302
69	6	0	-5.554691	-0.493479	0.551769
70	6	0	-6.215624	0.739368	0.149422
71	26	0	-8.192382	1.138571	-0.259385
72	6	0	-6.737277	1.790757	1.003112
73	6	0	-6.376257	1.194441	-1.215497
74	6	0	-9.342143	-0.530843	0.125083
75	6	0	-9.437892	-0.170201	-1.251101
76	6	0	-9.790473	0.570691	0.909240
77	6	0	-9.951614	1.159134	-1.319489
78	6	0	-10.168487	1.617638	0.014875
79	6	0	-7.155034	2.863234	0.172465

80	6	0	-6.944241	2.493593	-1.189796
81	1	0	-6.764445	1.778079	2.081521
82	1	0	-6.097703	0.641382	-2.100934
83	1	0	-8.962415	-1.471118	0.498682
84	1	0	-9.158582	-0.799018	-2.084257
85	1	0	-9.811398	0.610862	1.989523
86	1	0	-10.132964	1.726254	-2.222507
87	1	0	-10.539505	2.593156	0.298832
88	1	0	-7.583372	3.793387	0.519515
89	1	0	-7.192546	3.090423	-2.056363

Rotational constants (GHZ): 0.0539441 0.0147663 0.0121130

DFT of compound (3)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.899851	-2.140535	-1.963312
2	6	0	2.663444	-0.773084	-1.808204
3	6	0	1.374554	-0.255734	-1.632389
4	6	0	0.261146	-1.158546	-1.713483
5	6	0	0.525267	-2.560152	-1.801848
6	6	0	1.848025	-3.040854	-1.925298
7	6	0	-1.090547	-0.685626	-1.709482
8	6	0	-2.139217	-1.638496	-1.597753

9	6	0	-1.839344	-3.025328	-1.639461
10	6	0	-0.550228	-3.481894	-1.773096
11	6	0	1.126137	1.169091	-1.392323
12	6	0	-0.202970	1.653776	-1.613759
13	6	0	-1.301525	0.758866	-1.845633
14	6	0	1.823712	3.481177	-0.937241
15	6	0	0.581829	3.962456	-1.275594
16	6	0	-0.458077	3.059747	-1.608645
17	6	0	-1.735627	3.564277	-1.939456
18	6	0	-2.750944	2.683510	-2.273705
19	6	0	-2.536196	1.304896	-2.215865
20	6	0	-0.305787	-4.942849	-1.857074
21	7	0	1.024795	-5.354722	-1.990344
22	6	0	2.132149	-4.492411	-2.033607
23	6	0	0.344902	5.426955	-1.258577
24	7	0	-0.937246	5.864210	-1.608899
25	6	0	-2.006788	5.022291	-1.953883
26	8	0	-1.207183	-5.769692	-1.816336
27	8	0	3.270343	-4.926570	-2.153349
28	8	0	1.212973	6.235908	-0.958806
29	8	0	-3.103726	5.478141	-2.249151
30	6	0	-3.510731	-1.332072	-1.389146
31	6	0	-4.703082	-1.214864	-1.162117
32	6	0	-6.084910	-1.019639	-0.901883
33	6	0	1.253470	-6.800692	-2.084036
34	6	0	-1.156841	7.314620	-1.599920
35	6	0	-6.991255	-2.099202	-0.971670
36	6	0	-8.340133	-1.906715	-0.718821
37	6	0	-8.836821	-0.628553	-0.382768
38	6	0	-7.928859	0.450424	-0.312604

39	6	0	-6.580187	0.259327	-0.567199
40	6	0	-10.218688	-0.433130	-0.116487
41	1	0	3.906484	-2.519655	-2.100171
42	1	0	3.507653	-0.100694	-1.829673
43	1	0	-2.645479	-3.746494	-1.574264
44	1	0	2.594196	4.183383	-0.641493
45	1	0	-3.714915	3.085289	-2.565426
46	1	0	-3.353379	0.647103	-2.470475
47	1	0	0.894784	-7.292319	-1.177201
48	1	0	0.700917	-7.206523	-2.933641
49	1	0	2.321528	-6.958899	-2.208322
50	1	0	-0.451049	7.797952	-2.278188
51	1	0	-2.180685	7.495629	-1.916462
52	1	0	-0.989583	7.708911	-0.595279
53	1	0	-6.620403	-3.086017	-1.228084
54	1	0	-9.029306	-2.742451	-0.776502
55	1	0	-8.299661	1.436738	-0.054908
56	1	0	-5.890741	1.094922	-0.505976
57	6	0	-11.402862	-0.265880	0.110953
58	6	0	-12.782481	-0.064512	0.364674
59	26	0	-13.773455	-0.274037	2.155088
60	6	0	-13.408658	1.173881	0.754441
61	6	0	-13.825473	-1.054335	0.263531
62	6	0	-12.430580	-0.998709	3.528962
63	6	0	-13.578293	-1.843693	3.466882
64	6	0	-12.863810	0.309515	3.900007
65	6	0	-14.722955	-1.057694	3.799656
66	6	0	-14.281238	0.272810	4.067802
67	6	0	-14.808868	0.947068	0.866906
68	6	0	-15.065489	-0.424713	0.564515

69	1	0	-12.890073	2.107935	0.917920
70	1	0	-13.675581	-2.089711	-0.008058
71	1	0	-11.413915	-1.289049	3.301057
72	1	0	-13.581797	-2.891922	3.200858
73	1	0	-12.231007	1.178048	4.020399
74	1	0	-15.746036	-1.406789	3.832830
75	1	0	-14.911474	1.108443	4.340246
76	1	0	-15.548256	1.684130	1.148429
77	1	0	-16.033253	-0.906941	0.576232
78	6	0	2.122722	2.094314	-0.978734
79	6	0	3.429296	1.752061	-0.538174
80	6	0	4.556214	1.593319	-0.100288
81	6	0	5.865032	1.343199	0.389458
82	6	0	6.280274	0.027398	0.688423
83	6	0	6.778881	2.401242	0.581843
84	6	0	7.561190	-0.220428	1.155494
85	1	0	5.582549	-0.792119	0.550881
86	6	0	8.060428	2.152085	1.046720
87	1	0	6.468413	3.416385	0.357819
88	6	0	8.478885	0.836280	1.341505
89	1	0	7.870755	-1.235040	1.382421
90	1	0	8.756653	2.971652	1.189153
91	6	0	9.795323	0.581353	1.811482
92	6	0	10.924398	0.365744	2.212293
93	6	0	12.235886	0.118029	2.689000
94	26	0	13.878111	-0.461112	1.593930
95	6	0	13.299925	1.083053	2.807433
96	6	0	12.751272	-1.142617	3.161076
97	6	0	13.260603	-0.736456	-0.344471
98	6	0	13.873684	-1.924911	0.152910

99	6	0	14.219333	0.318293	-0.274641
100	6	0	15.212704	-1.604788	0.531765
101	6	0	15.426381	-0.218583	0.266923
102	6	0	14.434580	0.427049	3.361497
103	6	0	14.096732	-0.943178	3.579254
104	1	0	13.227383	2.124958	2.529205
105	1	0	12.193811	-2.067926	3.195936
106	1	0	12.237034	-0.641836	-0.680709
107	1	0	13.402647	-2.894498	0.239558
108	1	0	14.055689	1.346044	-0.568591
109	1	0	15.935549	-2.290187	0.953016
110	1	0	16.339263	0.330450	0.453640
111	1	0	15.391836	0.885515	3.568187
112	1	0	14.753684	-1.702644	3.980462

Rotational constants (GHZ): 0.0445943 0.0055853 0.0053348

DFT of compound (4)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.123540	-0.820274	-3.043691
2	6	0	1.787304	0.443714	-2.553445
3	6	0	0.475817	0.775732	-2.194168
4	6	0	-0.563976	-0.181550	-2.442103
5	6	0	-0.194127	-1.490685	-2.877147

6	6	0	1.152101	-1.798961	-3.171788
7	6	0	-1.945497	0.149272	-2.265394
8	6	0	-2.903795	-0.897567	-2.334530
9	6	0	-2.496515	-2.201806	-2.722677
10	6	0	-1.187059	-2.491363	-3.022991
11	6	0	0.128225	2.069210	-1.599250
12	6	0	-1.243698	2.471596	-1.650302
13	6	0	-2.279462	1.559793	-2.047042
14	6	0	0.667700	4.256721	-0.614595
15	6	0	-0.622992	4.694994	-0.793494
16	6	0	-1.605397	3.808530	-1.298995
17	6	0	-2.934827	4.260478	-1.455008
18	6	0	-3.895171	3.394417	-1.950805
19	6	0	-3.572245	2.063704	-2.228457
20	6	0	-0.837483	-3.864996	-3.469139
21	7	0	0.515144	-4.102068	-3.755748
22	6	0	1.537772	-3.153031	-3.636031
23	6	0	-0.972582	6.088396	-0.420099
24	7	0	-2.301689	6.480252	-0.612504
25	6	0	-3.319175	5.652064	-1.112712
26	8	0	-1.677514	-4.746523	-3.584134
27	8	0	2.692880	-3.453885	-3.907000
28	8	0	-0.154006	6.875938	0.034152
29	8	0	-4.462403	6.064319	-1.254901
30	6	0	-4.275091	-0.776009	-1.987677
31	6	0	-5.451022	-0.818934	-1.667062
32	6	0	-6.815750	-0.809116	-1.278246
33	6	0	0.915255	-5.438383	-4.210745
34	6	0	-2.632485	7.863077	-0.249175
35	6	0	-7.639736	-1.932187	-1.506109

36	6	0	-8.970754	-1.920977	-1.121178
37	6	0	-9.531057	-0.788423	-0.490682
38	6	0	-8.705633	0.334931	-0.264685
39	6	0	-7.375009	0.325202	-0.650343
40	6	0	-10.892588	-0.781267	-0.086548
41	1	0	3.144964	-1.059877	-3.317948
42	1	0	2.568951	1.182512	-2.457071
43	1	0	-3.236564	-2.989924	-2.794919
44	1	0	1.394080	4.932087	-0.177922
45	1	0	-4.902570	3.765814	-2.102865
46	1	0	-4.350312	1.412301	-2.597273
47	1	0	0.017138	-6.046087	-4.283728
48	1	0	1.411711	-5.362820	-5.179918
49	1	0	1.618015	-5.877553	-3.499409
50	1	0	-2.020344	8.554018	-0.832192
51	1	0	-3.688180	8.016160	-0.457071
52	1	0	-2.420060	8.027683	0.809111
53	1	0	-7.219371	-2.808591	-1.988066
54	1	0	-9.596479	-2.788706	-1.300449
55	1	0	-9.125786	1.210280	0.218883
56	1	0	-6.748443	1.191650	-0.465981
57	6	0	-12.059103	-0.775404	0.261995
58	6	0	-13.419569	-0.762983	0.657405
59	26	0	-14.214527	-1.421304	2.435973
60	6	0	-14.102442	0.305640	1.342815
61	6	0	-14.385150	-1.810020	0.434115
62	6	0	-12.675716	-2.199293	3.551582
63	6	0	-13.693800	-3.180506	3.361387
64	6	0	-13.257960	-1.081420	4.220751
65	6	0	-14.907248	-2.668935	3.913348

66	6	0	-14.637697	-1.372018	4.444792
67	6	0	-15.462809	-0.074761	1.513225
68	6	0	-15.637052	-1.376918	0.953492
69	1	0	-13.647245	1.235041	1.654551
70	1	0	-14.180126	-2.750219	-0.058031
71	1	0	-11.650182	-2.273792	3.216043
72	1	0	-13.570532	-4.137965	2.873917
73	1	0	-12.746169	-0.170335	4.499017
74	1	0	-15.864451	-3.172280	3.920124
75	1	0	-15.355280	-0.720152	4.924047
76	1	0	-16.228588	0.515767	1.996986
77	1	0	-16.557778	-1.943695	0.939922
78	6	0	1.066816	2.950307	-0.997732
79	6	0	2.407209	2.607389	-0.672862
80	6	0	3.550243	2.410028	-0.298895
81	6	0	4.875860	2.106681	0.105377
82	6	0	5.365570	0.786162	0.010809
83	6	0	5.725185	3.106678	0.622489
84	6	0	6.655971	0.482358	0.411110
85	1	0	4.717746	0.005711	-0.373260
86	6	0	7.020432	2.802241	1.009699
87	1	0	5.353261	4.119681	0.728001
88	6	0	7.519807	1.487427	0.898068
89	1	0	7.006217	-0.539422	0.325470
90	1	0	7.635254	3.584008	1.437128
91	6	0	8.884428	1.147896	1.331420
92	6	0	9.965014	1.987915	1.233417
93	6	0	9.085588	-0.219330	1.932744
94	6	0	9.943092	3.253269	0.558703
95	6	0	11.245057	1.630461	1.772275

96	6	0	8.881701	-0.344150	3.286665
97	6	0	9.382174	-1.299066	1.002650
98	7	0	9.983359	4.274344	0.002430
99	7	0	12.296099	1.369277	2.197779
100	6	0	8.483681	0.780245	4.080072
101	6	0	9.074288	-1.567829	4.002240
102	26	0	11.060223	-2.468188	0.776365
103	6	0	9.075852	-2.709924	1.151144
104	6	0	9.948431	-1.133486	-0.318908
105	7	0	8.153150	1.689600	4.726918
106	7	0	9.239000	-2.552435	4.600886
107	6	0	12.444807	-2.012248	2.237851
108	6	0	12.990193	-1.762680	0.944530
109	6	0	12.078409	-3.387029	2.312055
110	6	0	12.966283	-2.989372	0.216035
111	6	0	12.402362	-3.992870	1.060259
112	6	0	9.407725	-3.360999	-0.065698
113	6	0	9.954267	-2.396361	-0.964237
114	1	0	8.633707	-3.175028	2.018537
115	1	0	10.295524	-0.202538	-0.743516
116	1	0	12.308434	-1.269512	3.010936
117	1	0	13.347750	-0.806917	0.588893
118	1	0	11.611662	-3.872006	3.158218
119	1	0	13.302701	-3.132134	-0.801974
120	1	0	12.234340	-5.027179	0.792108
121	1	0	9.286354	-4.416975	-0.263900
122	1	0	10.326529	-2.594191	-1.959722

Rotational constants (GHZ): 0.0323739 0.0053513 0.0051167

DFT of compound (5)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.929500	-1.136113	-2.562545
2	6	0	2.741625	0.196521	-2.186849
3	6	0	1.499817	0.680061	-1.761151
4	6	0	0.368798	-0.201840	-1.819794
5	6	0	0.591792	-1.576742	-2.137703
6	6	0	1.877176	-2.034014	-2.504980
7	6	0	-0.961200	0.267041	-1.573553
8	6	0	-2.002143	-0.692813	-1.459405
9	6	0	-1.737962	-2.061104	-1.728230
10	6	0	-0.486008	-2.494389	-2.093113
11	6	0	1.311860	2.052116	-1.279887
12	6	0	-0.023840	2.564994	-1.253850
13	6	0	-1.160178	1.716873	-1.477197
14	6	0	2.107514	4.268365	-0.571285
15	6	0	0.842507	4.794987	-0.672593
16	6	0	-0.247147	3.953897	-1.005399
17	6	0	-1.545160	4.504494	-1.095554
18	6	0	-2.610144	3.687969	-1.434704
19	6	0	-2.417601	2.314804	-1.612099
20	6	0	-0.280535	-3.930175	-2.409329
21	7	0	1.012703	-4.318690	-2.775134
22	6	0	2.118502	-3.457560	-2.849348

23	6	0	0.637326	6.241513	-0.402833
24	7	0	-0.669455	6.726787	-0.512605
25	6	0	-1.787478	5.950023	-0.853197
26	8	0	-1.184274	-4.753164	-2.361049
27	8	0	3.223371	-3.866846	-3.179076
28	8	0	1.554606	6.990806	-0.098585
29	6	0	-3.330515	-0.414035	-1.037094
30	6	0	-4.484278	-0.321195	-0.655787
31	6	0	-5.824960	-0.148760	-0.222989
32	6	0	1.200999	-5.738276	-3.096272
33	6	0	-0.858669	8.158480	-0.248823
34	6	0	-6.763419	-1.194231	-0.351387
35	6	0	-8.078866	-1.012382	0.043602
36	6	0	-8.503243	0.208886	0.609468
37	6	0	-7.564533	1.254679	0.729140
38	6	0	-6.251721	1.080472	0.321420
39	1	0	3.900397	-1.491314	-2.889664
40	1	0	3.586520	0.866979	-2.234230
41	1	0	-2.541399	-2.784670	-1.656415
42	1	0	2.921981	4.917221	-0.271482
43	1	0	-3.593412	4.131852	-1.544452
44	1	0	-3.272432	1.706427	-1.866374
45	1	0	0.939828	-6.350523	-2.230743
46	1	0	0.546680	-6.018652	-3.924008
47	1	0	2.244018	-5.880917	-3.366244
48	1	0	-0.285811	8.746504	-0.968940
49	1	0	-1.920054	8.374320	-0.338254
50	1	0	-0.497750	8.397163	0.753180
51	1	0	-6.448306	-2.143098	-0.771333
52	1	0	-8.780505	-1.830694	-0.068533

53	1	0	-7.871192	2.222188	1.106018
54	1	0	-5.545603	1.898703	0.409526
55	6	0	-9.909888	0.400318	1.001528
56	6	0	-10.321325	1.171173	2.058307
57	6	0	-11.388182	0.377346	-0.961897
58	6	0	-9.430540	1.765788	3.012657
59	6	0	-11.711118	1.409601	2.320036
60	6	0	-10.870993	1.669942	-1.299221
61	6	0	-12.393259	-0.134694	-1.841522
62	7	0	-8.751071	2.246813	3.825284
63	7	0	-12.830027	1.621223	2.558757
64	7	0	-10.445997	2.716394	-1.580197
65	7	0	-13.218489	-0.531916	-2.559947
66	8	0	-2.902992	6.442636	-0.941978
67	6	0	2.368754	2.903843	-0.861878
68	6	0	3.712444	2.493866	-0.645090
69	6	0	4.880319	2.268076	-0.380089
70	6	0	6.235454	1.953324	-0.099051
71	6	0	6.668049	0.610741	-0.057861
72	6	0	7.174238	2.974705	0.153422
73	6	0	7.991543	0.304675	0.214706
74	1	0	5.952450	-0.184384	-0.236643
75	6	0	8.500627	2.666251	0.410415
76	1	0	6.849504	4.009188	0.154240
77	6	0	8.940914	1.326569	0.429290
78	1	0	8.298155	-0.734447	0.237532
79	1	0	9.191333	3.469550	0.634009
80	6	0	10.345771	0.993177	0.720651
81	6	0	11.416686	1.746736	0.313957
82	6	0	11.316872	2.870278	-0.572483

83	6	0	12.756596	1.431689	0.716902
84	6	0	10.603503	-0.115732	2.899212
85	7	0	11.291460	3.771055	-1.308252
86	7	0	13.855386	1.204322	1.024497
87	6	0	10.367011	1.156050	3.514553
88	6	0	10.867978	-1.197101	3.797389
89	7	0	10.167219	2.186568	4.017318
90	7	0	11.094045	-2.064333	4.540198
91	6	0	10.597707	-0.251889	1.530780
92	6	0	10.715280	-1.497154	0.786806
93	26	0	12.314638	-2.764296	0.519756
94	6	0	10.415922	-2.841298	1.245104
95	6	0	11.058568	-1.603223	-0.615608
96	6	0	13.928677	-2.116902	1.632200
97	6	0	14.256833	-2.130015	0.244927
98	6	0	13.557384	-3.437237	2.017436
99	6	0	14.093041	-3.465460	-0.230216
100	6	0	13.660479	-4.273251	0.864406
101	6	0	10.531995	-3.718887	0.135570
102	6	0	10.937414	-2.961729	-1.004171
103	1	0	10.116461	-3.119491	2.243558
104	1	0	11.344299	-0.782997	-1.258345
105	1	0	13.933868	-1.241610	2.266136
106	1	0	14.567232	-1.272285	-0.334446
107	1	0	13.230093	-3.740127	3.002472
108	1	0	14.254329	-3.804972	-1.244425
109	1	0	13.434332	-5.330154	0.823030
110	1	0	10.363969	-4.786668	0.162059
111	1	0	11.137363	-3.355551	-1.990904
112	6	0	-10.947182	-0.291824	0.155462

113	6	0	-11.306760	-1.646720	0.547386
114	26	0	-13.083328	-2.426157	1.233241
115	6	0	-11.783581	-2.722607	-0.302152
116	6	0	-11.143826	-2.204933	1.872962
117	6	0	-14.541048	-0.964645	1.249547
118	6	0	-14.345371	-1.482988	2.562941
119	6	0	-14.923535	-2.039335	0.395693
120	6	0	-14.612723	-2.884322	2.524120
121	6	0	-14.970024	-3.228138	1.185302
122	6	0	-11.859195	-3.901631	0.484691
123	6	0	-11.478454	-3.582070	1.822518
124	1	0	-12.001161	-2.650174	-1.356397
125	1	0	-10.811005	-1.664958	2.747508
126	1	0	-14.391479	0.064888	0.956724
127	1	0	-14.041219	-0.907191	3.425388
128	1	0	-15.114806	-1.965837	-0.665868
129	1	0	-14.543744	-3.569001	3.358567
130	1	0	-15.215078	-4.219271	0.828234
131	1	0	-12.177770	-4.871819	0.129197
132	1	0	-11.465457	-4.264895	2.660541

Rotational constants (GHZ): 0.0328778 0.0044724 0.0041821

TD-DFT Calculation

Compound (1)

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.2080 eV 561.52 nm f=0.0001 <S**2>=0.000

184 ->197	0.17657
184 ->198	0.20724
185 ->189	0.13733
185 ->192	-0.12440
185 ->193	-0.11829
185 ->195	-0.13442
185 ->197	0.35361
185 ->198	-0.29424
185 ->199	0.11457
186 ->197	-0.18882
186 ->198	-0.22610
187 ->198	-0.10861

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-KS) = -3441.48004991

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 2.2088 eV 561.32 nm f=0.0179 <S**2>=0.000

184 ->197	-0.22936
184 ->198	0.19226
185 ->197	0.27356
185 ->198	0.32539
186 ->197	0.24009
186 ->198	-0.19966
187 ->197	0.11208

Excited State 3: Singlet-A 2.4112 eV 514.21 nm f=0.7668 <S**2>=0.000

186 ->188 -0.28555

187 ->188 0.62702

Excited State 4: Singlet-A 2.5813 eV 480.31 nm f=0.0074 <S**2>=0.000

182 ->189 -0.10880

182 ->192 0.10425

182 ->193 0.10084

182 ->195 0.11736

182 ->197 -0.32922

182 ->198 0.24670

182 ->199 -0.10640

184 ->197 -0.10409

185 ->197 -0.23819

185 ->198 -0.32134

186 ->197 0.13999

186 ->198 -0.10366

Excited State 5: Singlet-A 2.6296 eV 471.49 nm f=0.0000 <S**2>=0.000

182 ->197 0.26120

182 ->198 0.35128

184 ->197 -0.18212

184 ->198 -0.24618

185 ->197 0.20649

185 ->198 -0.15006

186 ->197 0.16896

186 ->198 0.22660

Excited State 6: Singlet-A 3.1218 eV 397.16 nm f=0.8973 <S**2>=0.000

183 ->188 0.28840

184 ->188 0.36782

186 ->188 0.44603

187 ->188 0.20180

Excited State 7: Singlet-A 3.4466 eV 359.73 nm f=0.0013 <S**2>=0.000

182 ->189 0.12315

182 ->192 -0.10950

182 ->193 -0.10351

182 ->195 -0.11643

182 ->197 0.31616

182 ->198 -0.23753

184 ->197 -0.16013

184 ->198 0.11575

185 ->197 -0.22193

185 ->198 -0.30080

186 ->197 0.13488

Excited State 8: Singlet-A 3.5288 eV 351.35 nm f=0.0001 <S**2>=0.000

182 ->197 -0.30640

182 ->198 -0.40921

184 ->197 -0.10918

184 ->198 -0.14876

185 ->189 0.12310

185 ->197 0.19297

185 ->198 -0.14005

186 ->197 0.15217

186 ->198 0.20438

187 ->198 0.11246

Excited State 9: Singlet-A 3.6785 eV 337.05 nm f=0.5683 <S**2>=0.000

175 ->188 -0.13613

177 ->188 0.26987

179 ->188 0.13220

180 ->188 0.24470

183 ->188 -0.20421

186 ->188 0.11093

186 ->192 -0.11942

187 ->189 0.43229

Excited State 10: Singlet-A 3.7815 eV 327.87 nm f=0.1384 <S**2>=0.000

177 ->188 0.11399

180 ->188 0.54984

180 ->190 0.10849

183 ->188 0.10209

186 ->193 0.11391

187 ->189 -0.28372

187 ->193 -0.11267

Excited State 11: Singlet-A 3.8987 eV 318.01 nm f=0.0064 <S**2>=0.000

175 ->188 0.11856

177 ->188 -0.30870

180 ->188 0.11770

183 ->188 -0.24274

184 ->188 -0.20890

186 ->188 0.32024

186 ->189 0.10262

186 ->191 -0.14753

187 ->188 0.16067

187 ->189 -0.11906

187 ->191 0.19903

Excited State 12: Singlet-A 3.9229 eV 316.05 nm f=0.7205 <S**2>=0.000

175	->188	-0.19332
177	->188	0.32767
179	->188	0.11203
180	->188	-0.17663
183	->188	-0.14343
184	->188	-0.13467
184	->189	-0.12838
186	->188	0.24132
187	->188	0.14530
187	->189	-0.30849
187	->191	-0.16534

Excited State 13: Singlet-A 4.0198 eV 308.44 nm f=0.0002 <S**2>=0.000

185	->188	0.67498
185	->189	0.10965

Excited State 14: Singlet-A 4.1327 eV 300.01 nm f=0.0160 <S**2>=0.000

172	->188	-0.16858
172	->190	-0.10917
174	->188	-0.16508
175	->188	0.14945
177	->188	0.10862
184	->188	0.21414
186	->188	-0.10045
186	->190	-0.25114
186	->191	-0.11139
187	->189	-0.11437
187	->190	0.41116

187 ->191 0.12474

Excited State 15: Singlet-A 4.1512 eV 298.67 nm f=0.0017 <S**2>=0.000

172 ->188 0.46444

172 ->190 0.23423

172 ->195 -0.10288

173 ->188 -0.14833

174 ->188 0.17936

186 ->190 -0.15899

187 ->190 0.25277

SavETr: write IOETrn= 770 NScale= 10 NData= 16 NLR=1 NState= 15 LETran= 280.

Compound (2)

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 1.9811 eV 625.84 nm f=0.0003 <S**2>=0.000

217 -> 221 0.10351

217 -> 222 0.42433

217 -> 229 0.10207

217 -> 234 -0.44617

218 -> 231 0.11374

218 -> 232 0.13551

218 -> 233 0.17829

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-KS) = -3888.86959312

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 2.0327 eV 609.94 nm f=0.0130 <S**2>=0.000

217 -> 231 -0.12728

217 -> 232 -0.15126

217 -> 233 -0.19878

218 -> 222 0.39322

218 -> 234 -0.44428

Excited State 3: Singlet-A 2.4412 eV 507.88 nm f=0.0170 <S**2>=0.000

213 -> 222 0.21108

213 -> 234 -0.29769

214 -> 222 0.18636

214 -> 234 -0.25797

215 -> 234 -0.12602

217 -> 231 0.18541

217 -> 232 0.22130

217 -> 233 0.29259

Excited State 4: Singlet-A 2.4514 eV 505.76 nm f=0.7395 <S**2>=0.000

219 -> 220 0.68528

Excited State 5: Singlet-A 2.5924 eV 478.25 nm f=0.0001 <S**2>=0.000

213 -> 231 0.11902

213 -> 232 0.14203

213 -> 233 0.18769

214 -> 232 0.11826

214 -> 233 0.15609

215 -> 232 0.11221

215 -> 233 0.14834

217 -> 222 0.15534

218 -> 231 -0.23169

218 -> 232 -0.27627

218 -> 233 -0.36502

Excited State 6: Singlet-A 3.0729 eV 403.48 nm f=0.0132 <S**2>=0.000

213 -> 222 -0.20549

213 -> 234 0.19535

214 -> 222 -0.17499

214 -> 234 0.17279

215 -> 222 -0.14551

215 -> 234 0.10241

217 -> 231 0.18801

217 -> 232 0.22500

217 -> 233 0.29790

218 -> 222 0.32695

Excited State 7: Singlet-A 3.2465 eV 381.90 nm f=1.5450 <S**2>=0.000

216 -> 220 0.48237

216 -> 221 -0.19189

218 -> 220 0.10567

218 -> 221 -0.11210

219 -> 221 0.39205

Excited State 8: Singlet-A 3.2953 eV 376.24 nm f=0.0034 <S**2>=0.000

213 -> 231 -0.14751

213 -> 232 -0.17577

213 -> 233 -0.23208

214 -> 231 -0.13008

214 -> 232 -0.15534

214 -> 233 -0.20533

217 -> 222 0.40088

217 -> 234 0.19036

218 -> 231 -0.10409

218 -> 232 -0.12414

218 -> 233 -0.16379

Excited State 9: Singlet-A 3.4309 eV 361.38 nm f=0.0026 <S**2>=0.000

211 -> 220 0.16245

216 -> 220 0.42214

216 -> 221 0.17961

218 -> 221 0.17598

219 -> 221 -0.37235

219 -> 224 -0.11936

219 -> 225 0.12866

Excited State 10: Singlet-A 3.4717 eV 357.12 nm f=0.0815 <S**2>=0.000

215 -> 221 0.11904

216 -> 221 -0.10287

218 -> 220 -0.33845

218 -> 221 0.51159

218 -> 222 -0.15764

219 -> 221 0.20258

Excited State 11: Singlet-A 3.6565 eV 339.08 nm f=0.0202 <S**2>=0.000

217 -> 220 -0.34572

217 -> 221 0.50867

217 -> 222 -0.18690

218 -> 222 0.12380

218 -> 234 0.15404

Excited State 12: Singlet-A 3.7308 eV 332.33 nm f=0.0352 <S**2>=0.000

209 -> 220 -0.16922

211 -> 220 -0.23847

212 -> 220 0.55154

212 -> 221 0.14142

212 -> 223 0.10789

219 -> 226 0.13985

Excited State 13: Singlet-A 3.7644 eV 329.36 nm f=0.1894 <S**2>=0.000

215 -> 221 0.10842

215 -> 222 0.23916

217 -> 220 0.14462

217 -> 221 -0.21071

217 -> 233 -0.10265

218 -> 222 0.36781

218 -> 234 0.39247

Excited State 14: Singlet-A 3.8006 eV 326.22 nm f=0.0007 <S**2>=0.000

213 -> 231 -0.10662

213 -> 232 -0.12727

213 -> 233 -0.16813

214 -> 232 -0.11348

214 -> 233 -0.14978

217 -> 221 -0.12604

217 -> 222 -0.24942

217 -> 229 0.10112

217 -> 234 -0.45434

218 -> 231 -0.10987

218 -> 232 -0.13062

218 -> 233 -0.17253

218 -> 234 -0.10129

Excited State 15: Singlet-A 3.8786 eV 319.66 nm f=0.0404 <S**2>=0.000

203 -> 220 -0.10664

209 -> 220 0.25932

210 -> 220 -0.14068

211 -> 220 0.38556

211 -> 221 0.12322

212 -> 220 0.27850

216 -> 221 -0.15024

219 -> 224 -0.20369

219 -> 225 -0.15446

SavETr: write IOETrn= 770 NScale= 10 NData= 16 NLR=1 NState= 15 LETran= 280.

Compound (3)

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.1995 eV 563.69 nm f=0.2907 <S**2>=0.000

260 -> 281 -0.14623

261 -> 278 0.21750

261 -> 282 -0.10554

262 -> 279 -0.18839

263 -> 279 -0.11957

263 -> 280 0.25662

264 -> 281 -0.20987

265 -> 278 -0.16418

266 -> 267 0.32604

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-KS) = -5473.96302368

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 2.2072 eV 561.72 nm f=0.0001 <S**2>=0.000

260 -> 280 0.14000

261 -> 280 -0.21029

263 -> 269 -0.10492

263 -> 272 -0.11276

263 -> 273 -0.12844

263 -> 278 0.30719

263 -> 279 0.14155

263 -> 281 0.30799

263 -> 282 -0.15286

264 -> 279 -0.10162

264 -> 280 0.21496

265 -> 280 0.16661

Excited State 3: Singlet-A 2.2095 eV 561.15 nm f=0.0000 <S**2>=0.000

260 -> 279 -0.13093

261 -> 279 -0.20326

261 -> 280 -0.10414

262 -> 269 -0.10496

262 -> 272 0.11207

262 -> 273 -0.12653

262 -> 278 -0.31993

262 -> 281 0.31487

262 -> 282 0.15093

264 -> 279 -0.19657

264 -> 280 -0.10657

265 -> 279 0.15993

Excited State 4: Singlet-A 2.2099 eV 561.04 nm f=0.0056 <S**2>=0.000

260 -> 278 -0.16699

261 -> 281 0.24965

262 -> 279 0.27452

262 -> 280 0.14514

263 -> 279 -0.11877

263 -> 280 0.24410

264 -> 278 -0.24677

264 -> 282 0.12021

265 -> 281 -0.18860

Excited State 5: Singlet-A 2.2434 eV 552.65 nm f=0.6568 <S**2>=0.000

261 -> 278 -0.11768

262 -> 279 0.13408

263 -> 280 -0.13645

264 -> 267 0.20218

264 -> 281 0.11953

266 -> 267 0.56636

Excited State 6: Singlet-A 2.5805 eV 480.46 nm f=0.0032 <S**2>=0.000

256 -> 278 -0.25256

256 -> 281 -0.16735

256 -> 282 0.12777

257 -> 278 -0.10363

257 -> 281 -0.21661

263 -> 279 -0.16125

263 -> 280 0.34629

264 -> 278 0.11510

Excited State 7: Singlet-A 2.5822 eV 480.16 nm f=0.0068 <S**2>=0.000

256 -> 278 0.11374

256 -> 281 -0.21293

257 -> 278 -0.26580

257 -> 281 0.16690

257 -> 282 0.12873

261 -> 278 -0.10174

262 -> 279 -0.31618

262 -> 280 -0.17282

262 -> 281 0.14158

264 -> 281 0.11166

265 -> 278 0.10045

Excited State 8: Singlet-A 2.6289 eV 471.62 nm f=0.0000 <S**2>=0.000

256 -> 279 0.14109

256 -> 280 -0.30676

257 -> 279 0.10998

257 -> 280 -0.23846

260 -> 280 -0.16476

261 -> 279 -0.10516

261 -> 280 0.22883

263 -> 278 0.17210

263 -> 281 0.16885

264 -> 280 -0.20888

265 -> 280 -0.15077

Excited State 9: Singlet-A 2.6304 eV 471.34 nm f=0.0000 <S**2>=0.000

256 -> 279 0.21571

256 -> 280 0.11806

257 -> 279 -0.28607

257 -> 280 -0.15707

257 -> 281 0.12439

260 -> 279 0.15181

261 -> 279 0.20599

261 -> 280 0.11426

262 -> 278 -0.18250

262 -> 281 0.16203

264 -> 279 0.19153

264 -> 280 0.10503

265 -> 279 -0.13676

Excited State 10: Singlet-A 2.9288 eV 423.33 nm f=0.0827 <S**2>=0.000

259 -> 267 0.26128

261 -> 267 0.26762

265 -> 267 0.56297

Excited State 11: Singlet-A 3.1692 eV 391.22 nm f=1.3333 <S**2>=0.000

258 -> 267 0.32886

260 -> 267 0.40491

264 -> 267 -0.40146

266 -> 267 0.14981

Excited State 12: Singlet-A 3.4456 eV 359.83 nm f=0.0012 <S**2>=0.000

256 -> 278 0.22426

256 -> 281 0.18969

256 -> 282 -0.10995

257 -> 278 0.13837

257 -> 281 0.18094

261 -> 281 -0.11519

263 -> 279 -0.15243

263 -> 280 0.33129

264 -> 278 0.10472

Excited State 13: Singlet-A 3.4476 eV 359.63 nm f=0.0011 <S**2>=0.000

256 -> 278 -0.14655

256 -> 281 0.17665

257 -> 278 0.23853

257 -> 281 -0.19068

257 -> 282 -0.11050

261 -> 278 -0.12760

262 -> 279 -0.30150

262 -> 280 -0.16614

262 -> 281 0.13693

Excited State 14: Singlet-A 3.5282 eV 351.41 nm f=0.0001 <S**2>=0.000

256 -> 279 -0.16681

256 -> 280 0.35834

257 -> 279 -0.12853

257 -> 280 0.27880

261 -> 280 0.15136

263 -> 278 0.16407

263 -> 281 0.15508

264 -> 280 -0.18195

265 -> 280 -0.15614

Excited State 15: Singlet-A 3.5292 eV 351.31 nm f=0.0004 <S**2>=0.000

256 -> 279 -0.25143

256 -> 280 -0.13825

256 -> 281 0.10777

257 -> 279 0.33354

257 -> 280 0.18201

257 -> 281 -0.14337

261 -> 279 0.13699

262 -> 278 -0.17418

262 -> 281 0.15002

264 -> 279 0.16716

265 -> 279 -0.14177

SavETr: write IOETrn= 770 NScale= 10 NData= 16 NLR=1 NState= 15 LETran= 280.

Compound (4)

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 1.9835 eV 625.08 nm f=0.0003 <S**2>=0.000
293 -> 301 0.42268
293 -> 309 -0.10126
293 -> 315 0.44673
294 -> 314 0.25327
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -5921.35221861
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 2.0332 eV 609.80 nm f=0.0119 <S**2>=0.000
293 -> 314 -0.28124
294 -> 301 0.39183
294 -> 315 0.44458

Excited State 3: Singlet-A 2.2046 eV 562.39 nm f=0.1538 <S**2>=0.000
295 -> 316 0.27255
296 -> 316 0.10594
296 -> 317 -0.38033
297 -> 302 0.10059
297 -> 306 -0.10586
297 -> 316 0.26780
298 -> 299 -0.23377
298 -> 316 -0.12446

Excited State 4: Singlet-A 2.2082 eV 561.46 nm f=0.0001 <S**2>=0.000
295 -> 317 0.27026
296 -> 302 0.12995
296 -> 306 -0.16146
296 -> 312 0.13460
296 -> 316 0.43224
296 -> 317 0.11985
296 -> 318 -0.15336
297 -> 317 0.27722
298 -> 317 -0.13035

Excited State 5: Singlet-A 2.2487 eV 551.36 nm f=0.7705 <S**2>=0.000
296 -> 317 -0.15699
297 -> 299 0.27305
297 -> 316 0.10387
298 -> 299 0.57898

Excited State 6: Singlet-A 2.4422 eV 507.67 nm f=0.0027 <S**2>=0.000
286 -> 301 0.21648
286 -> 315 0.30594

287 -> 301 0.18050
287 -> 315 0.24963
289 -> 301 0.10009
289 -> 315 0.13335
293 -> 314 -0.40834
294 -> 314 0.12432

Excited State 7: Singlet-A 2.5808 eV 480.42 nm f=0.0057 <S**2>=0.000
290 -> 302 -0.10173
290 -> 306 0.13440
290 -> 312 -0.11628
290 -> 316 -0.38603
290 -> 318 0.13912
295 -> 316 0.12761
296 -> 317 0.39083
297 -> 316 0.16164

Excited State 8: Singlet-A 2.5917 eV 478.38 nm f=0.0001 <S**2>=0.000
286 -> 314 0.26742
287 -> 314 0.21010
289 -> 314 0.21266
293 -> 301 -0.15548
293 -> 314 0.14875
294 -> 314 0.50649

Excited State 9: Singlet-A 2.6301 eV 471.40 nm f=0.0000 <S**2>=0.000
290 -> 316 0.10035
290 -> 317 -0.42108
291 -> 317 -0.11224
295 -> 317 -0.30687
296 -> 316 0.24264
297 -> 317 -0.26711
298 -> 317 0.11399

Excited State 10: Singlet-A 2.9701 eV 417.44 nm f=0.2093 <S**2>=0.000
291 -> 299 0.21835
292 -> 299 -0.18416
295 -> 299 -0.34913
297 -> 299 0.43790
298 -> 299 -0.19428
298 -> 300 0.12524

Excited State 11: Singlet-A 3.0743 eV 403.29 nm f=0.0172 <S**2>=0.000
286 -> 301 -0.20908
286 -> 315 -0.19994
287 -> 301 -0.16805
287 -> 315 -0.16766
289 -> 301 -0.14995
289 -> 315 -0.10684
293 -> 314 -0.41317

294 -> 301 -0.32683
294 -> 314 0.10571

Excited State 12: Singlet-A 3.2154 eV 385.59 nm f=1.8019 <S**2>=0.000
291 -> 299 0.19219
292 -> 299 0.41356
292 -> 300 0.18249
295 -> 300 0.14283
297 -> 299 0.12884
297 -> 300 -0.25184
298 -> 300 -0.29144

Excited State 13: Singlet-A 3.2951 eV 376.27 nm f=0.0013 <S**2>=0.000
286 -> 314 0.33131
287 -> 314 0.27728
289 -> 314 0.12919
293 -> 301 0.40218
293 -> 315 -0.19067
294 -> 301 -0.10414
294 -> 314 -0.22828

Excited State 14: Singlet-A 3.3603 eV 368.96 nm f=0.0126 <S**2>=0.000
281 -> 299 0.10619
283 -> 299 0.15563
291 -> 299 0.13237
292 -> 299 0.40950
292 -> 300 -0.15577
297 -> 300 0.20479
298 -> 300 0.34662

Excited State 15: Singlet-A 3.4492 eV 359.46 nm f=0.0412 <S**2>=0.000
289 -> 300 -0.12159
294 -> 299 0.34343
294 -> 300 0.54333
294 -> 301 -0.15898
298 -> 300 -0.10477
SavETr: write IOETrn= 770 NScale= 10 NData= 16 NLR=1 NState= 15 LETran= 280.

Compound (5)

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 1.9828 eV 625.30 nm f=0.0003 <S**2>=0.000

326 -> 334 0.32003

326 -> 335 0.28032

326 -> 345 -0.10090

326 -> 352 0.44300

328 -> 350 -0.19413

328 -> 351 -0.10921

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-KS) = -6368.73337332

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 1.9829 eV 625.27 nm f=0.0003 <S**2>=0.000

327 -> 334 -0.27756

327 -> 335 0.31093

327 -> 353 -0.44402

329 -> 350 0.13428

329 -> 351 -0.18421

Excited State 3: Singlet-A 2.0324 eV 610.04 nm f=0.0146 <S**2>=0.000

327 -> 350 -0.15734

327 -> 351 0.21134

328 -> 335 -0.10250

328 -> 353 0.13380

329 -> 334 -0.25240

329 -> 335 0.27044

329 -> 353 -0.42233

Excited State 4: Singlet-A 2.0334 eV 609.74 nm f=0.0115 <S**2>=0.000

326 -> 349 0.10188

326 -> 350 0.22591

326 -> 351 0.12401

328 -> 334 0.28969

328 -> 335 0.24290

328 -> 352 0.42291

329 -> 352 0.12876

Excited State 5: Singlet-A 2.2949 eV 540.26 nm f=0.9202 <S**2>=0.000

330 -> 331 0.68569

Excited State 6: Singlet-A 2.4421 eV 507.69 nm f=0.0028 <S**2>=0.000

318 -> 334 0.16570

318 -> 335 0.14470

318 -> 352 0.30725

320 -> 334 0.13587

320 -> 335 0.11871

320 -> 352 0.24740

322 -> 352 0.10859

326 -> 349 0.14859

326 -> 350 0.33367

326 -> 351 0.18575

Excited State 7: Singlet-A 2.4424 eV 507.64 nm f=0.0021 <S**2>=0.000

319 -> 334 0.14337

319 -> 335 -0.16010

319 -> 353 0.30781

321 -> 334 0.11739

321 -> 335 -0.13113

321 -> 353 0.24753

323 -> 353 0.11019

327 -> 349 -0.11552

327 -> 350 0.23247

327 -> 351 -0.31610

Excited State 8: Singlet-A 2.5930 eV 478.15 nm f=0.0000 <S**2>=0.000

318 -> 350 -0.21931

318 -> 351 -0.12344

320 -> 350 -0.16882

322 -> 350 -0.14299

323 -> 350 -0.10119

326 -> 334 -0.11740

326 -> 335 -0.10279

326 -> 350 -0.10849

328 -> 349 -0.17816

328 -> 350 -0.39662

328 -> 351 -0.22306

329 -> 350 -0.12162

Excited State 9: Singlet-A 2.5934 eV 478.08 nm f=0.0001 <S**2>=0.000

319 -> 350 -0.15229

319 -> 351 0.20906

321 -> 350 -0.11670

321 -> 351 0.15996

323 -> 351 0.13636

327 -> 334 -0.10215

327 -> 335 0.11422

327 -> 351 0.10753

328 -> 351 -0.11858

329 -> 349 0.13865

329 -> 350 -0.27491

329 -> 351 0.37713

Excited State 10: Singlet-A 3.0719 eV 403.60 nm f=0.0155 <S**2>=0.000

319 -> 334 0.13783

319 -> 335 -0.15405

319 -> 353 0.20094

321 -> 334 0.10851

321 -> 335 -0.12121

321 -> 353 0.16432

327 -> 349 0.11752

327 -> 350 -0.23317

327 -> 351 0.32142

329 -> 334 0.20395

329 -> 335 -0.22950

Excited State 11: Singlet-A 3.0749 eV 403.22 nm f=0.0127 <S**2>=0.000

318 -> 334 -0.15933

318 -> 335 -0.13929

318 -> 352 -0.20047

320 -> 334 -0.12589

320 -> 335 -0.10995

320 -> 352 -0.16451

326 -> 349 0.15122

326 -> 350 0.33730

326 -> 351 0.19075

328 -> 334 -0.23620

328 -> 335 -0.20860

Excited State 12: Singlet-A 3.1239 eV 396.89 nm f=0.1321 <S**2>=0.000

324 -> 332 0.15654

325 -> 331 0.55923

330 -> 332 0.28081

Excited State 13: Singlet-A 3.2686 eV 379.32 nm f=2.4497 <S**2>=0.000

316 -> 333 -0.10344

324 -> 331 0.51300

325 -> 332 0.24241

329 -> 332 -0.11252

330 -> 333 -0.28990

Excited State 14: Singlet-A 3.2928 eV 376.54 nm f=0.0153 <S**2>=0.000

319 -> 350 -0.18815

319 -> 351 0.25836

321 -> 350 -0.15439

321 -> 351 0.21207

327 -> 334 0.26062

327 -> 335 -0.29317

327 -> 353 -0.19078

329 -> 350 0.12110

329 -> 351 -0.16791

Excited State 15: Singlet-A 3.2974 eV 376.01 nm f=0.0031 <S**2>=0.000

318 -> 349 0.12256

318 -> 350 0.27226

318 -> 351 0.15331

320 -> 349 0.10047

320 -> 350 0.22375

320 -> 351 0.12596

326 -> 334 -0.30249

326 -> 335 -0.26678

326 -> 352 0.18787

328 -> 350 -0.17777

328 -> 351 -0.10110

SavETr: write IOETrn= 770 NScale= 10 NData= 16 NLR=1 NState= 15 LETran= 280.

References

[1] Frisch, M. J.; Trucks, G. W.; Schlegel, G. W.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Li, Nakatsuji, X.; Caricato, M.; Marenich, A.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Ortiz, J. V.; Izmaylov, A. F.; Sonnenberg, J. L.; Williams-Young, D.; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery, J. A.; Peralta, J. E., Jr.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Keith, T.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J. B.; Fox, D. J. Gaussian 09, rev. A.02; Gaussian, Inc.: Wallingford, CT, **2016**.