Electronic Supplementary Information

Aggregation Induced Emission of Diketopyrrolopyrrole(DPP) Derivatives for Highly Fluorescent Red Film

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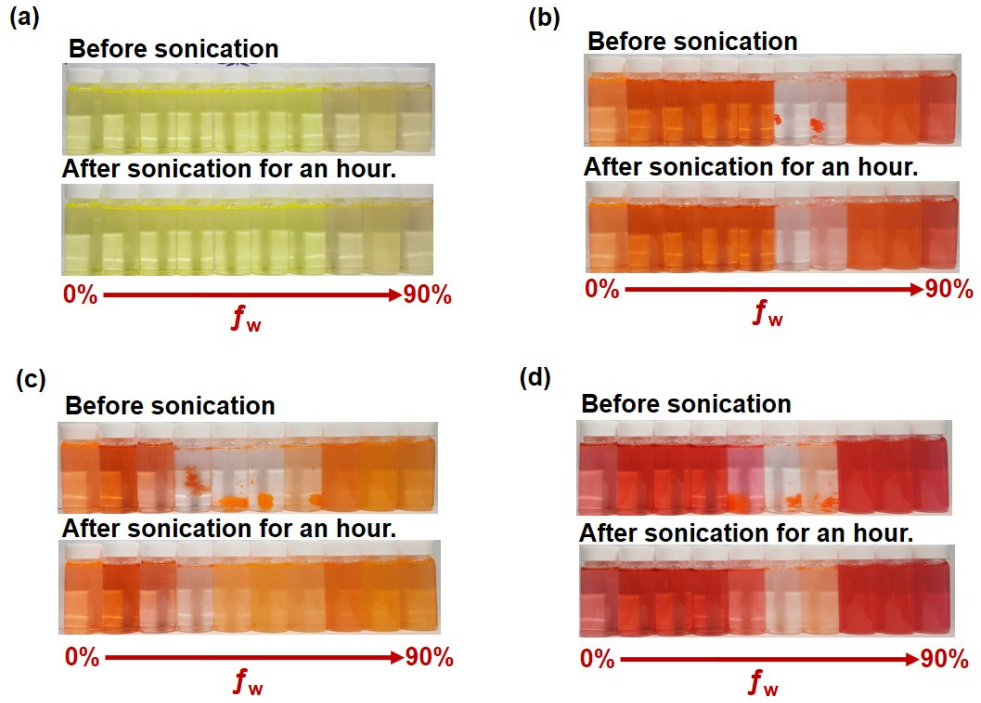

Figure S1. Optical images of (a)D6C, (b)T2, (c)D2, and (d)M2 in the THF/water mixtures before/after sonication for an hour.

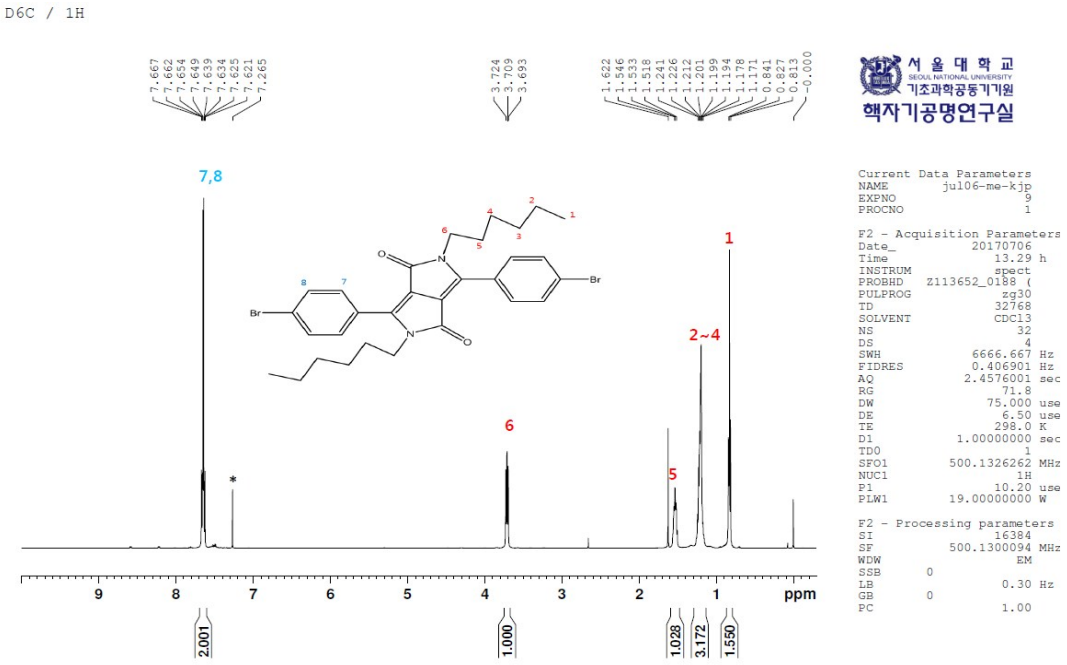

Figure S2. ^{1}H NMR spectrum of D6C in $CDCl_3$. The solvent peak is marked with asterisk.

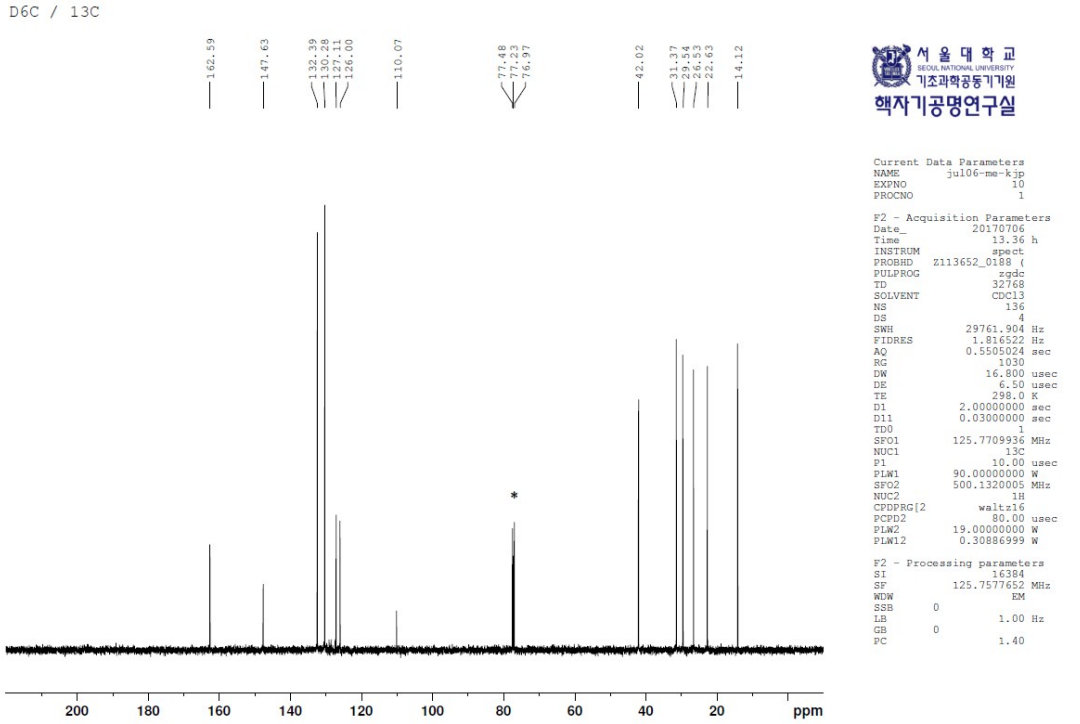

Figure S3. ^{13}C NMR spectrum of D6C in $CDCl_3$. The solvent peak is marked with asterisk.

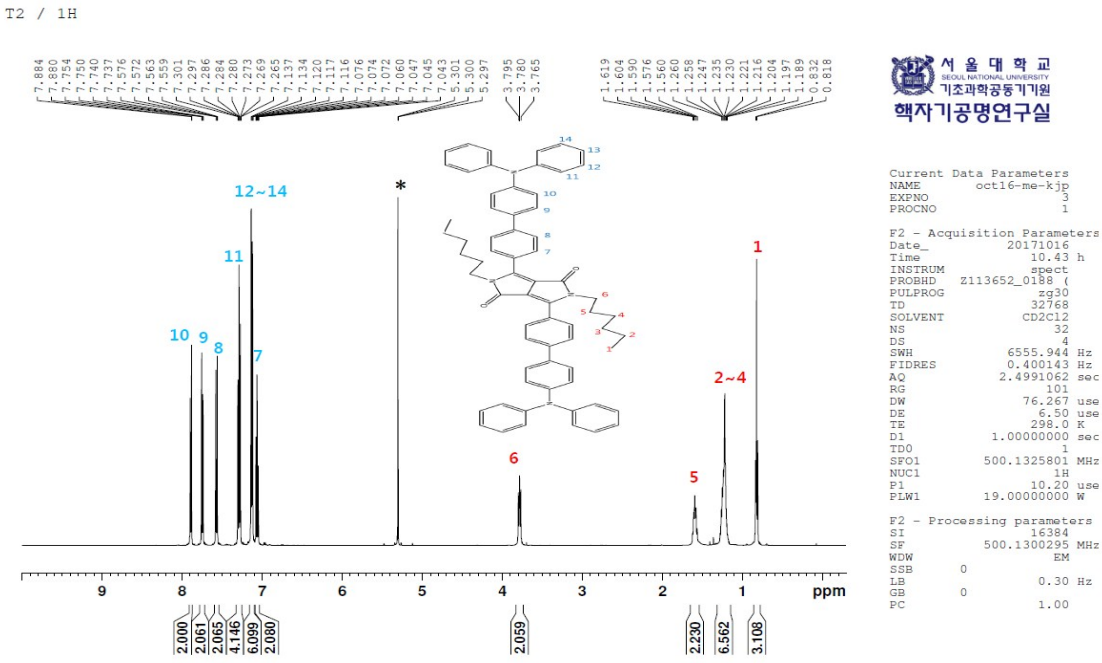

Figure S4. ^{1}H NMR spectrum of T2 in $CDCl_3$. The solvent peak is marked with asterisk.

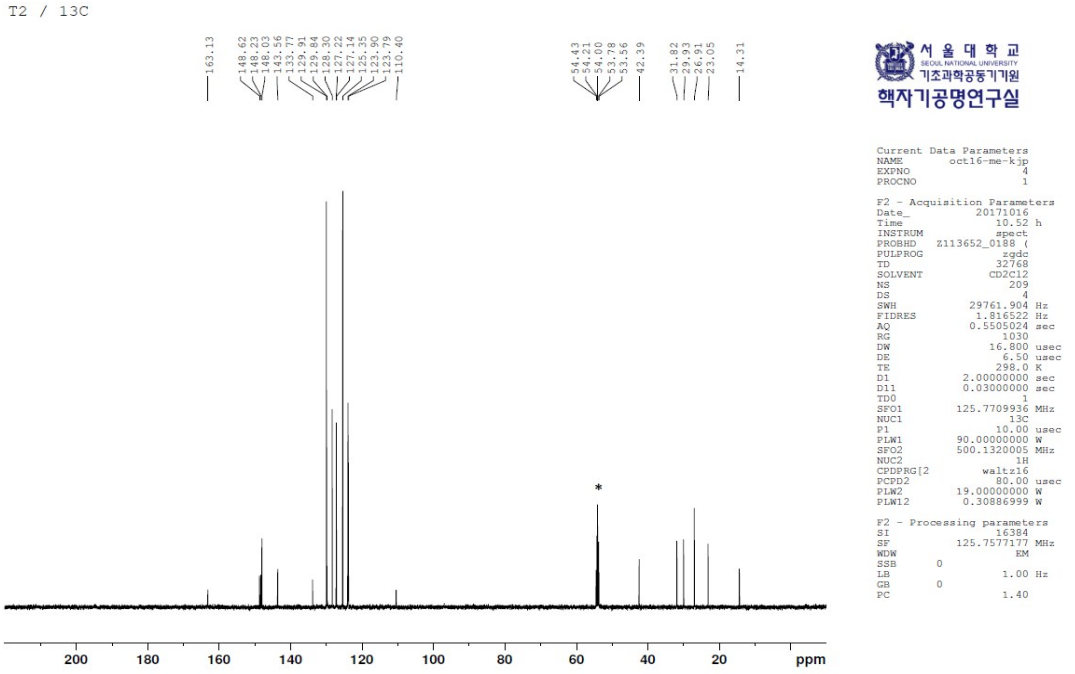

Figure S5. ^{13}C NMR spectrum of T2 in $CDCl_3$. The solvent peak is marked with asterisk.

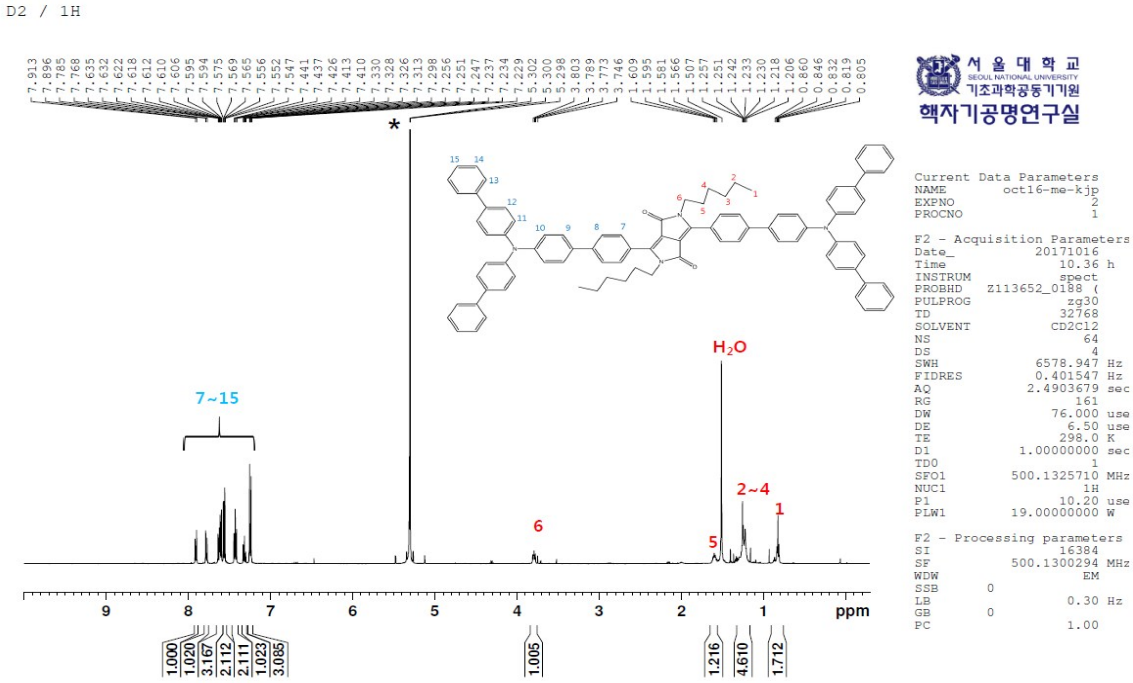

Figure S6. ^{1}H NMR spectrum of D2 in $CDCl_3$. The solvent peak is marked with asterisk.

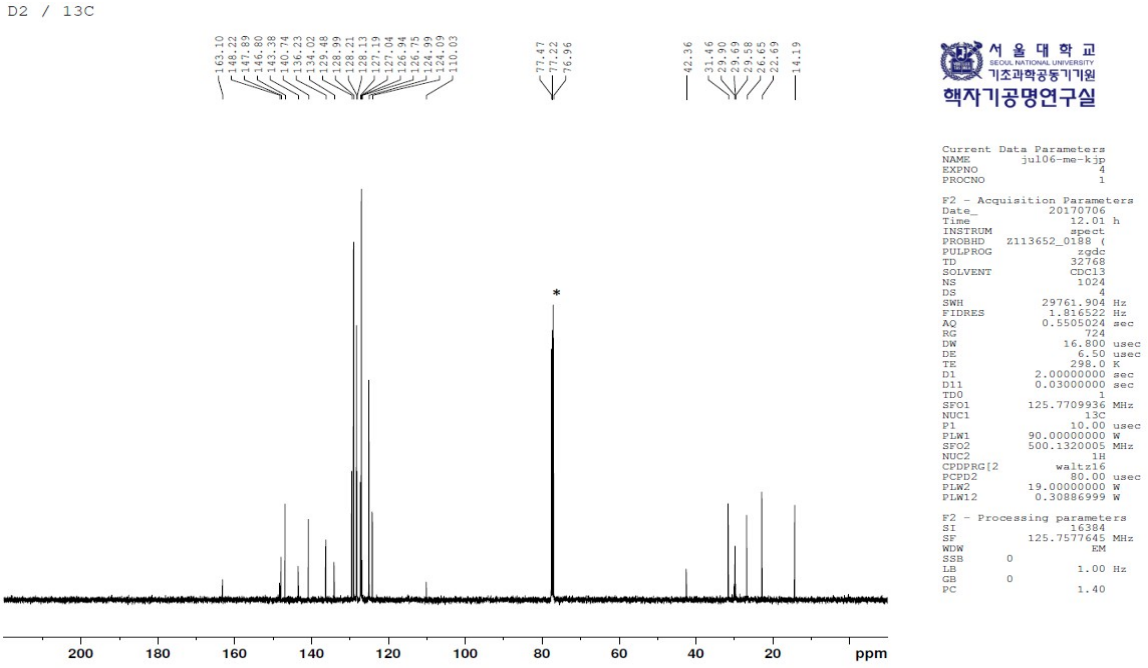

Figure S7. ^{13}C NMR spectrum of D2 in $CDCl_3$. The solvent peak is marked with asterisk.

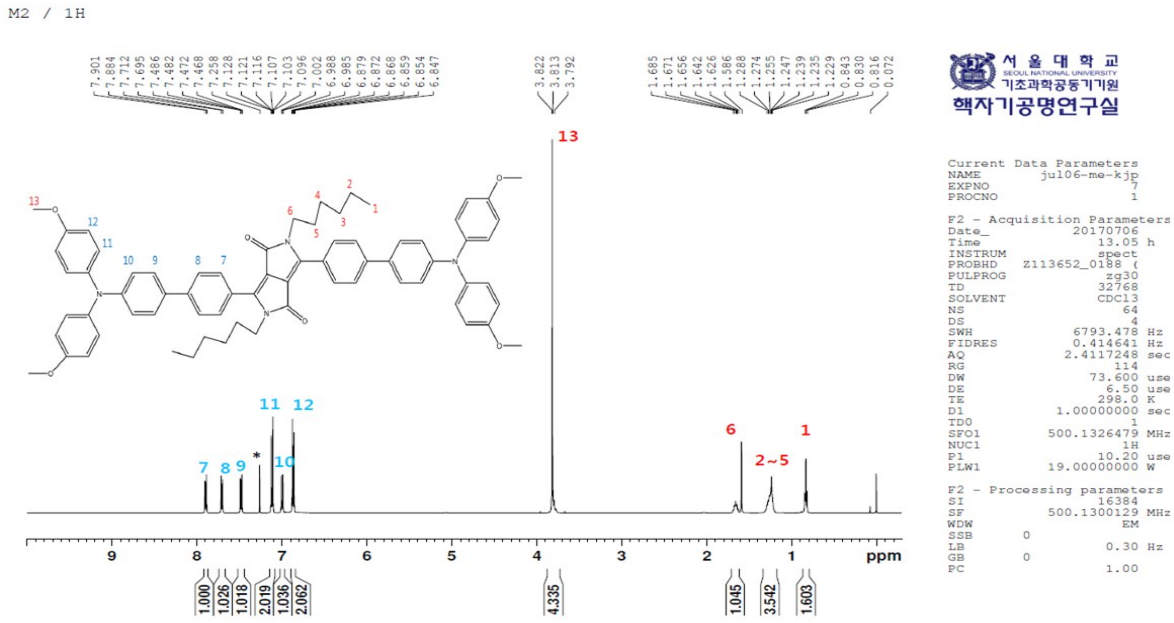

Figure S8. ^{1}H NMR spectrum of M2 in $CDCl_3$. The solvent peak is marked with asterisk.

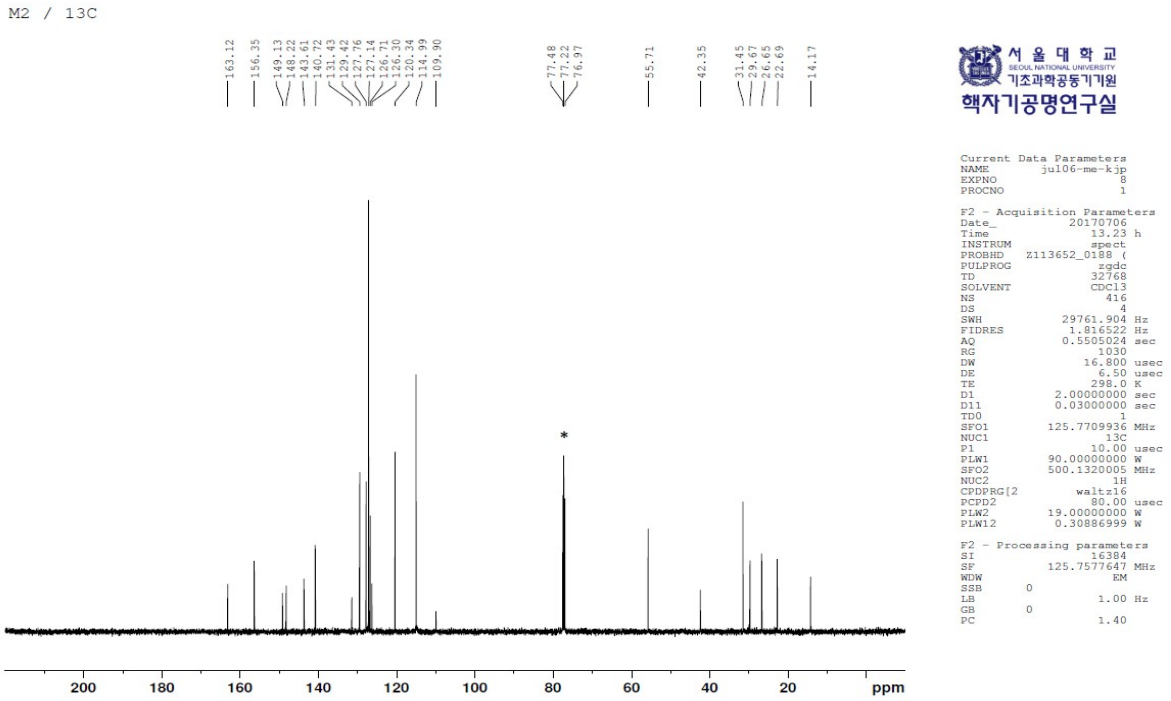

Figure S9. ^{13}C NMR spectrum of M2 in $CDCl_3$. The solvent peak is marked with asterisk

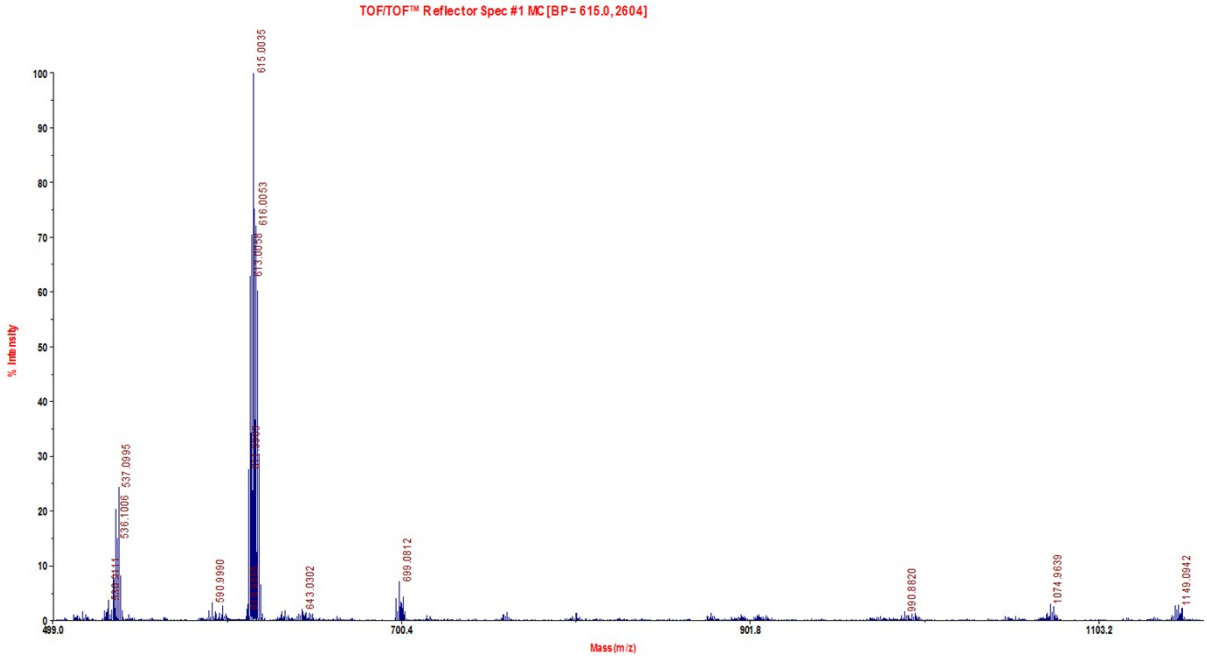

Figure S10. MALDI-TOF mass spectrum of D6C.

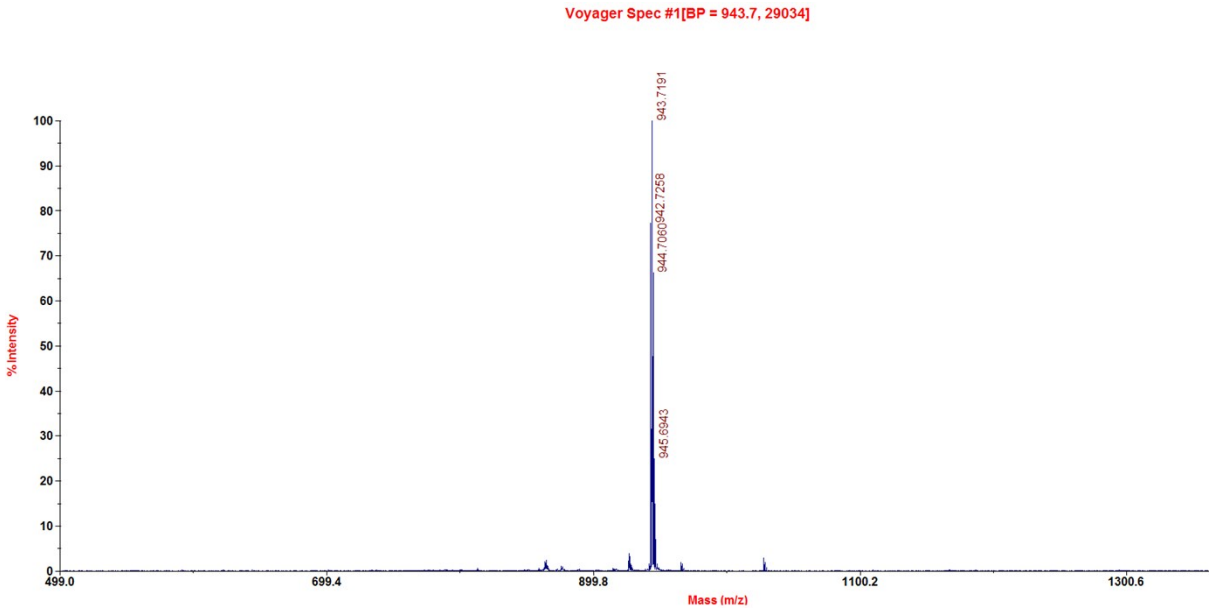

Figure S11. MALDI-TOF mass spectrum of T2.

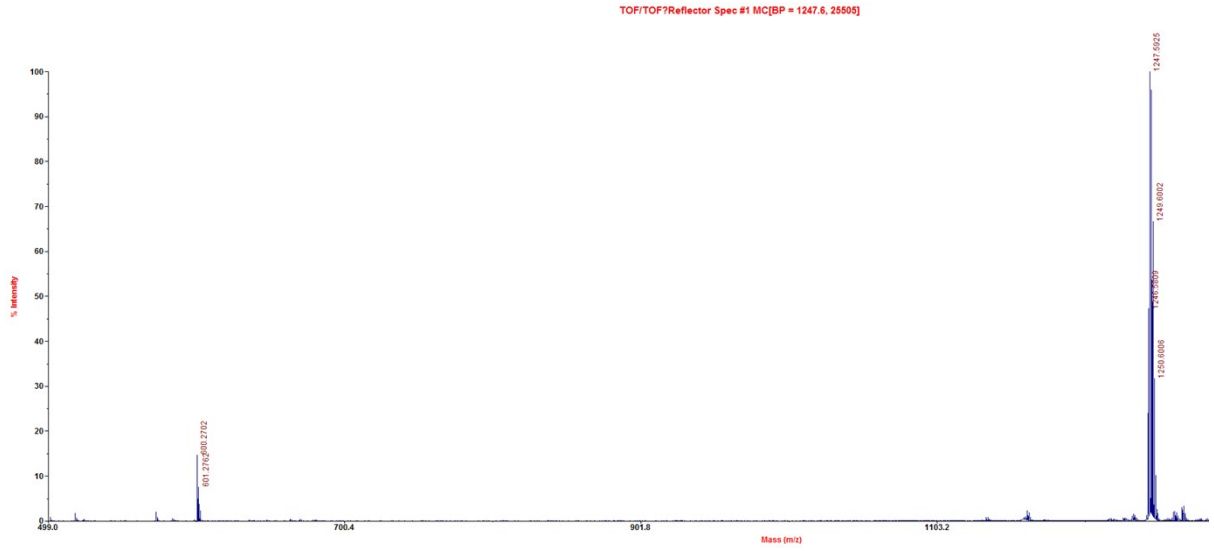

Figure S12. MALDI-TOF mass spectrum of D2.

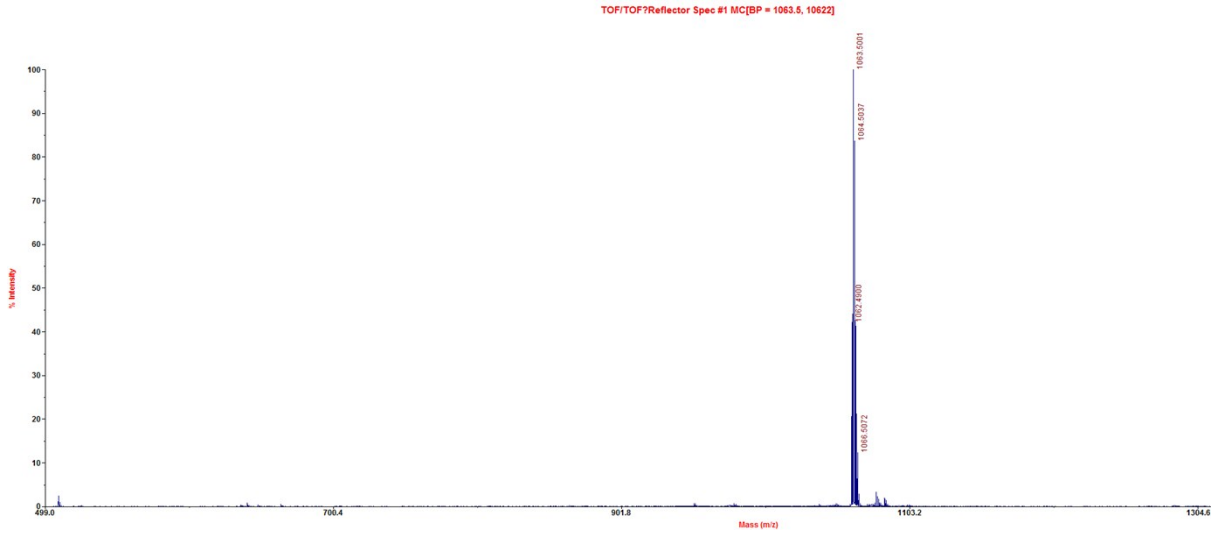

Figure S13. MALDI-TOF mass spectrum of M2.

서울대학교 기초과학공동기기원

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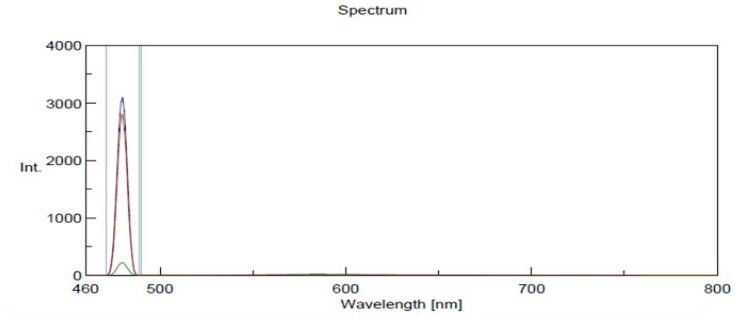
본 공동기기원의 분석결과는 광고, 선전, 홍보 및 법적 수단으로 이용될 수 없습니다.

Operator ID: SNU-EA2000
Company name: Thermo Fisher

(Unit: wt%)

Sample name	Nitrogen	Carbon	Hydrogen	Sulphur	Oxygen
T2	5.9707	84.0411	6.6186	n.d.	3.3798
D2	4.4197	86.0800	6.4452	n.d.	3.1238
D6C	4.5255	58.6215	5.5714	n.d.	5.2373
M2	5.2562	79.0506	6.7356	n.d.	8.9788

Figure S14. Elemental analysis of compounds. (n.d. = not detected)



[Calculation Results]

Absorptance	92.0757 %
External quantum yield	10.2522 %
Internal quantum yield	11.1345 %
Scattering region	471.0 - 489.0 nm
Fluorescence region	490.0 - 800.0 nm
Incident light	20385.80
Sample scattering	1432.96
Sample fluorescence	2110.68
Indirect Ex. scattering	18083.18
Indirect Ex. fluorescence	261.08
2nd order light correction	Off

[Comments]

Sample name	
Comment	
User	
Division	
Company	UNIST

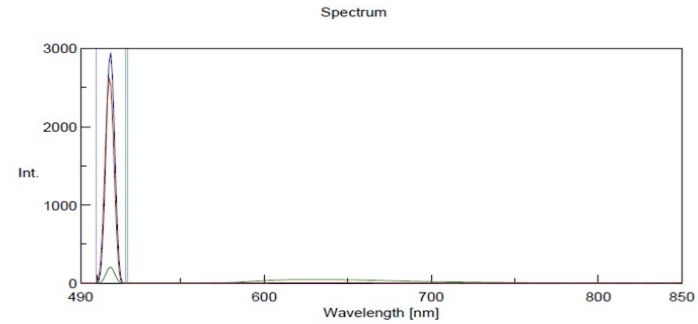
[Detailed Information]

Creation date	2017-11-07 오후 4:11

[Measurement Information]

Model name	FP-8500
Serial No.	C003961452
Ex filter holder	None
Em filter holder	None
Accessory	ILF-835
Accessory S/N	A001361507
Measurement date	2017-11-07 오후 4:10
Mode	Emission
Ex bandwidth	5 nm
Em bandwidth	5 nm
Response	0.1 sec
Sensitivity	Manual
PMT voltage	300 V
Measurement range	460 - 800 nm
Data interval	1 nm
Ex wavelength	480.0 nm
Scan speed	500 nm/min
Auto gain	Off
Shutter control	Open only for measurement
Light source	Xe lamp
Filter	Continue scan for exchanging filter
Blank correction	Off
Spectral correction	On
Ex correction data	20150319_Ex_ILF_combined
Em correction data	20150319_Em_ILF_combined

Figure S15. Fluorescence quantum yield measurement of D6C/PMMA thin film.



[Calculation Results]

Absorptance	92.3428 %
External quantum yield	28.9019 %
Internal quantum yield	31.2985 %
Scattering region	499.0 - 517.0 nm
Fluorescence region	518.0 - 850.0 nm
Incident light	18438.00
Sample scattering	1291.31
Sample fluorescence	5388.91
Indirect Ex. scattering	16864.02
Indirect Ex. fluorescence	783.41
2nd order light correction	Off

[Comments]

Sample name	
Comment	
User	
Division	
Company	UNIST

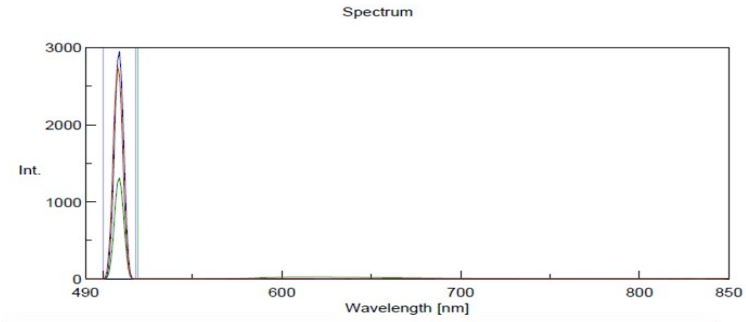
[Detailed Information]

Creation date	2017-10-23 오후 4:38

[Measurement Information]

Model name	FP-8500
Serial No.	C003961452
Ex filter holder	None
Em filter holder	None
Accessory	ILF-835
Accessory S/N	A001361507
Measurement date	2017-10-23 오후 4:37
Mode	Emission
Ex bandwidth	5 nm
Em bandwidth	5 nm
Response	0.1 sec
Sensitivity	Manual
PMT voltage	300 V
Measurement range	490 - 850 nm
Data interval	1 nm
Ex wavelength	508.0 nm
Scan speed	500 nm/min
Auto gain	Off
Shutter control	Open only for measurement
Light source	Xe lamp
Filter	Continue scan for exchanging filter
Blank correction	Off
Spectral correction	On
Ex correction data	20150319_Ex_ILF_combined
Em correction data	20150319_Em_ILF_combined

Figure S16. Fluorescence quantum yield measurement of T2/PMMA thin film.



[Calculation Results]

Absorptance	53.2884 %
External quantum yield	13.6349 %
Internal quantum yield	25.5870 %
Scattering region	500.0 - 518.0 nm
Fluorescence region	519.0 - 850.0 nm
Incident light	18513.34
Sample scattering	8226.63
Sample fluorescence	2711.77
Indirect Ex. scattering	17611.55
Indirect Ex. fluorescence	401.38
2nd order light correction	Off

[Comments]

Sample name	
Comment	
User	
Division	
Company	UNIST

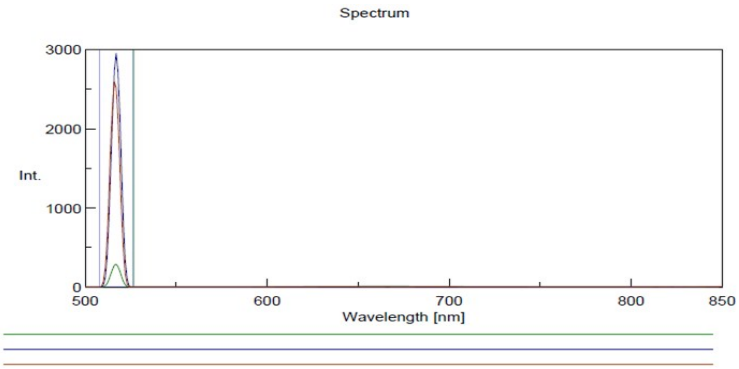
[Detailed Information]

Creation date	2017-10-23 오후 5:17

[Measurement Information]

Model name	FP-8500
Serial No.	C003961452
Ex filter holder	None
Em filter holder	None
Accessory	ILF-835
Accessory S/N	A001361507
Measurement date	2017-10-23 오후 5:16
Mode	Emission
Ex bandwidth	5 nm
Em bandwidth	5 nm
Response	0.1 sec
Sensitivity	Manual
PMT voltage	300 V
Measurement range	490 - 850 nm
Data interval	1 nm
Ex wavelength	509.0 nm
Scan speed	500 nm/min
Auto gain	Off
Shutter control	Open only for measurement
Light source	Xe lamp
Filter	Continue scan for exchanging filter
Blank correction	Off
Spectral correction	On
Ex correction data	20150319_Ex_ILF_combined
Em correction data	20150319_Em_ILF_combined

Figure S17. Fluorescence quantum yield measurement of D2/PMMA thin film.



[Calculation Results]

Absorptance	89.0894 %
External quantum yield	7.6772 %
Internal quantum yield	8.6174 %
Scattering region	508.0 - 526.0 nm
Fluorescence region	527.0 - 850.0 nm
Incident light	18252.66
Sample scattering	1796.57
Sample fluorescence	1433.64
Indirect Ex. scattering	16466.39
Indirect Ex. fluorescence	296.47
2nd order light correction	Off

[Comments]

Sample name	
Comment	
User	
Division	
Company	UNIST

[Detailed Information]

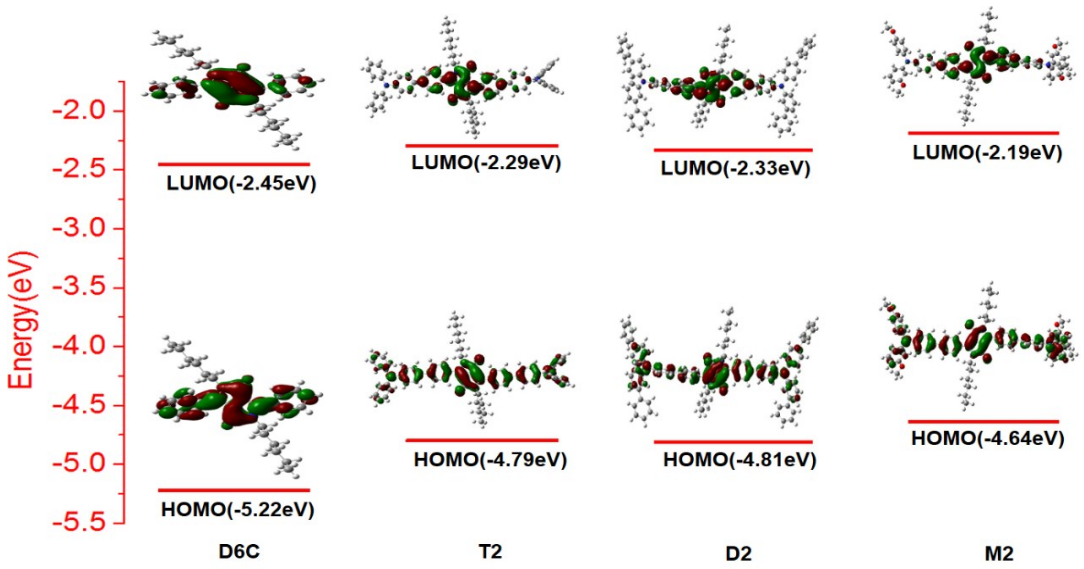
Creation date	2017-10-23 오후 4:55

[Measurement Information]

Model name	FP-8500
Serial No.	C003961452
Ex filter holder	None
Em filter holder	None
Accessory	ILF-835
Accessory S/N	A001361507
Measurement date	2017-10-23 오후 4:53
Mode	Emission
Ex bandwidth	5 nm
Em bandwidth	5 nm
Response	0.1 sec
Sensitivity	Manual
PMT voltage	300 V
Measurement range	500 - 850 nm
Data interval	1 nm
Ex wavelength	517.0 nm
Scan speed	500 nm/min
Auto gain	Off
Shutter control	Open only for measurement
Light source	Xe lamp
Filter	Continue scan for exchanging filter
Blank correction	Off
Spectral correction	On
Ex correction data	20150319_Ex_ILF_combined
Em correction data	20150319_Em_ILF_combined

Figure S18. Fluorescence quantum yield measurement of M2/PMMA thin film.

DFT Calculations for the optimized structures



(Figure 2 in the manuscript)

Table S1. Coordinates of D6C at B3LYP/6-31G(d.p), Gaussian 09 program package

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.417586	-0.809782	-0.538152
2	6	0	0.160043	-0.452818	-0.086077
3	6	0	-0.031507	0.948993	-0.268051
4	6	0	-1.351409	1.270792	0.007358
5	7	0	-1.993187	0.092196	0.398439
6	7	0	2.053240	0.356292	-0.974915
7	6	0	-3.275744	-0.073063	1.083547
8	1	0	-3.614106	0.905898	1.425479
9	1	0	-3.082751	-0.690267	1.967580
10	6	0	-4.339798	-0.766943	0.223494
11	1	0	-3.948958	-1.747000	-0.068897
12	1	0	-4.498395	-0.203484	-0.704878

13	6	0	-5.669560	-0.932000	0.968682
14	1	0	-6.056245	0.056946	1.255516
15	1	0	-5.493304	-1.473787	1.908425
16	6	0	-6.734352	-1.673496	0.151407
17	1	0	-6.349574	-2.664278	-0.127869
18	1	0	-6.906039	-1.137755	-0.793224
19	6	0	-8.069102	-1.837552	0.888292
20	6	0	-9.123620	-2.587860	0.069317
21	1	0	-8.455264	-0.846090	1.161849
22	1	0	-7.895923	-2.366937	1.835039
23	1	0	-10.064906	-2.684472	0.619861
24	1	0	-9.340364	-2.066826	-0.870286
25	1	0	-8.782522	-3.597704	-0.185342
26	6	0	3.484606	0.585861	-1.175988
27	6	0	4.311716	0.460626	0.110326
28	1	0	3.545537	1.605519	-1.561320
29	1	0	3.874575	-0.078601	-1.950682
30	1	0	3.924402	1.179431	0.843475
31	1	0	4.175889	-0.538188	0.542104
32	6	0	5.803376	0.718282	-0.133722
33	1	0	5.930470	1.702209	-0.606666
34	1	0	6.187261	-0.018653	-0.853800
35	6	0	6.645445	0.659218	1.146411
36	1	0	6.509577	-0.320390	1.626324
37	1	0	6.267339	1.402650	1.862451
38	6	0	8.140850	0.902034	0.908567
39	6	0	8.972530	0.855868	2.193806
40	1	0	8.274874	1.876736	0.420210
41	1	0	8.520191	0.153234	0.199893
42	1	0	10.034063	1.030482	1.991163
43	1	0	8.640686	1.618258	2.907771
44	1	0	8.884495	-0.118490	2.687963

45	6	0	-2.001172	2.577310	-0.124266
46	6	0	-1.216097	3.739627	0.021570
47	6	0	-3.366903	2.725067	-0.438768
48	6	0	-1.788353	4.999929	-0.114533
49	1	0	-0.154691	3.645675	0.214948
50	6	0	-3.930063	3.991260	-0.578230
51	1	0	-3.982829	1.854112	-0.612359
52	6	0	-3.147500	5.133610	-0.406672
53	1	0	-1.167526	5.882561	0.004477
54	1	0	-4.982243	4.082970	-0.830514
55	1	0	-3.589955	6.119521	-0.512904
56	6	0	1.981399	-2.160911	-0.624929
57	6	0	2.863590	-2.552173	-1.650758
58	6	0	1.577693	-3.126012	0.319066
59	6	0	3.347027	-3.856214	-1.712135
60	1	0	3.138115	-1.849303	-2.428084
61	6	0	2.069838	-4.425985	0.254654
62	1	0	0.860363	-2.855035	1.084744
63	6	0	2.961860	-4.795446	-0.753851
64	1	0	4.018408	-4.141204	-2.516515
65	1	0	1.750565	-5.154480	0.993624
66	1	0	3.343356	-5.810977	-0.801425
67	6	0	-1.090035	-1.019056	0.388139
68	8	0	-1.409969	-2.134626	0.785542
69	6	0	1.199178	1.502034	-0.803369
70	8	0	1.566960	2.647262	-1.040993

Zero-point correction= 0.601543 (Hartree/Particle)

Thermal correction to Energy= 0.635010

Thermal correction to Enthalpy= 0.635955

Thermal correction to Gibbs Free Energy= 0.531753

Sum of electronic and zero-point Energies= -1424.323683

Sum of electronic and thermal Energies= -1424.290216

Sum of electronic and thermal Enthalpies= -1424.289272

Sum of electronic and thermal Free Energies= -1424.393473

Table S2. Coordinates of T2 at B3LYP/6-31G(d.p), Gaussian 09 program package

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.598114	-0.900735	0.317562
2	6	0	0.678514	0.069725	-0.049246
3	6	0	-0.642973	-0.446488	0.088121
4	6	0	-1.562726	0.531399	-0.266669
5	7	0	-0.832215	1.658463	-0.651987
6	7	0	0.873322	-2.042139	0.680954
7	6	0	0.581288	1.428989	-0.547786
8	8	0	1.408585	2.283571	-0.847453
9	6	0	-0.542645	-1.800374	0.596615
10	8	0	-1.376394	-2.638715	0.925622
11	6	0	3.056657	-0.775985	0.319876
12	6	0	3.628211	0.491081	0.555200
13	6	0	3.929812	-1.846348	0.046711
14	6	0	5.004747	0.664576	0.551001
15	1	0	2.984422	1.343475	0.733185
16	6	0	5.306857	-1.662752	0.035836
17	1	0	3.531400	-2.817735	-0.212706
18	6	0	5.881571	-0.406672	0.298763
19	1	0	5.409582	1.647281	0.771034
20	1	0	5.947610	-2.501528	-0.218044
21	6	0	-3.021579	0.445636	-0.221100
22	6	0	-3.636822	-0.817791	-0.341390
23	6	0	-3.856211	1.560211	-0.003822

24	6	0	-5.016483	-0.948281	-0.277453
25	1	0	-3.023562	-1.701184	-0.470818
26	6	0	-5.235805	1.419171	0.069761
27	1	0	-3.426130	2.539310	0.163151
28	6	0	-5.854375	0.164294	-0.074502
29	1	0	-5.455596	-1.932134	-0.408530
30	1	0	-5.843004	2.293428	0.282494
31	6	0	-7.324049	0.021350	0.006042
32	6	0	-7.920087	-1.129650	0.552021
33	6	0	-8.184510	1.035316	-0.451818
34	6	0	-9.299877	-1.259098	0.649731
35	1	0	-7.291837	-1.919978	0.951112
36	6	0	-9.565757	0.909784	-0.373720
37	1	0	-7.765961	1.922789	-0.916751
38	6	0	-10.149327	-0.239731	0.186253
39	1	0	-9.728410	-2.147451	1.100641
40	1	0	-10.203161	1.699454	-0.756318
41	6	0	7.349326	-0.217656	0.295164
42	6	0	8.218280	-1.229891	0.739065
43	6	0	7.932889	0.980538	-0.152894
44	6	0	9.597658	-1.061862	0.731543
45	1	0	7.806779	-2.163245	1.111226
46	6	0	9.310198	1.164612	-0.152116
47	1	0	7.298541	1.779952	-0.523088
48	6	0	10.169118	0.143027	0.288096
49	1	0	10.241513	-1.862675	1.078375
50	1	0	9.729430	2.101544	-0.502127
51	7	0	11.574115	0.322746	0.285880
52	7	0	-11.556013	-0.364809	0.282882
53	6	0	-12.180835	-1.625824	0.070262
54	6	0	-13.208274	-2.062304	0.921273
55	6	0	-11.783415	-2.447675	-0.996316

56	6	0	-13.826655	-3.291579	0.702106
57	1	0	-13.516539	-1.433863	1.750071
58	6	0	-12.395369	-3.683385	-1.196079
59	1	0	-10.996358	-2.112274	-1.663442
60	6	0	-13.422489	-4.111915	-0.352881
61	1	0	-14.619956	-3.614463	1.370187
62	1	0	-12.075775	-4.307203	-2.025915
63	1	0	-13.901709	-5.072219	-0.516030
64	6	0	-12.354085	0.768316	0.607361
65	6	0	-13.551929	1.014255	-0.081918
66	6	0	-11.958192	1.651818	1.624012
67	6	0	-14.337166	2.117332	0.247121
68	1	0	-13.860193	0.337355	-0.871662
69	6	0	-12.741118	2.762089	1.933275
70	1	0	-11.038146	1.462098	2.166603
71	6	0	-13.936139	3.000373	1.251545
72	1	0	-15.261329	2.293394	-0.295870
73	1	0	-12.420773	3.435727	2.722916
74	1	0	-14.547205	3.862500	1.500196
75	6	0	12.204130	1.038937	-0.770623
76	6	0	11.828253	0.819439	-2.105356
77	6	0	13.215573	1.971310	-0.491622
78	6	0	12.446233	1.527585	-3.134003
79	1	0	11.052583	0.094477	-2.328268
80	6	0	13.840379	2.660936	-1.528667
81	1	0	13.506371	2.148461	0.538331
82	6	0	13.458043	2.448300	-2.854546
83	1	0	12.143327	1.346107	-4.161245
84	1	0	14.621324	3.378998	-1.295355
85	1	0	13.942161	2.992593	-3.659426
86	6	0	12.365699	-0.206607	1.343737
87	6	0	11.949314	-0.081684	2.678661

88	6	0	13.578834	-0.856074	1.065953
89	6	0	12.727625	-0.605581	3.708817
90	1	0	11.016918	0.426470	2.900640
91	6	0	14.359237	-1.360030	2.104396
92	1	0	13.903286	-0.960068	0.036025
93	6	0	13.938199	-1.243299	3.430467
94	1	0	12.391087	-0.500015	4.736203
95	1	0	15.295561	-1.859345	1.872170
96	1	0	14.545578	-1.643479	4.236336
97	6	0	-1.286106	2.876697	-1.323304
98	6	0	-1.259257	4.120978	-0.425439
99	1	0	-2.283161	2.697690	-1.730977
100	1	0	-0.604991	3.039871	-2.164856
101	1	0	-1.902631	3.967738	0.451040
102	1	0	-0.238560	4.241879	-0.047774
103	6	0	-1.693386	5.384764	-1.177416
104	6	0	-1.672985	6.646033	-0.305233
105	1	0	-2.704973	5.243210	-1.585446
106	1	0	-1.034506	5.533163	-2.044214
107	1	0	-2.341031	6.503509	0.556242
108	1	0	-0.665421	6.780970	0.112345
109	6	0	-2.083428	7.917530	-1.058286
110	6	0	-2.071350	9.170786	-0.177968
111	1	0	-3.086754	7.778374	-1.483708
112	1	0	-1.409730	8.063497	-1.913338
113	1	0	-2.369012	10.060302	-0.742564
114	1	0	-2.760935	9.067352	0.667553
115	1	0	-1.072542	9.356571	0.232876
116	6	0	1.329194	-3.221784	1.429524
117	6	0	1.059071	-4.563805	0.727563
118	1	0	0.787491	-3.223830	2.382100
119	1	0	2.388337	-3.091631	1.654888

120	1	0	1.314707	-5.354408	1.446073
121	1	0	-0.018544	-4.636475	0.556173
122	6	0	1.812692	-4.807446	-0.584082
123	6	0	1.395586	-6.110709	-1.278930
124	1	0	2.894968	-4.842755	-0.392501
125	1	0	1.642832	-3.966180	-1.269491
126	1	0	1.545527	-6.955030	-0.590694
127	1	0	0.317217	-6.078947	-1.487807
128	6	0	2.157983	-6.379040	-2.581843
129	6	0	1.735964	-7.679088	-3.273012
130	1	0	3.235660	-6.410435	-2.370544
131	1	0	2.009074	-5.534441	-3.268136
132	1	0	2.297662	-7.841532	-4.198636
133	1	0	1.905893	-8.546223	-2.624596
134	1	0	0.670532	-7.663717	-3.529126

Zero-point correction=	1.119000 (Hartree/Particle)
Thermal correction to Energy=	1.183202
Thermal correction to Enthalpy=	1.184146
Thermal correction to Gibbs Free Energy=	1.004864
Sum of electronic and zero-point Energies=	-2920.859081
Sum of electronic and thermal Energies=	-2920.794879
Sum of electronic and thermal Enthalpies=	-2920.793935
Sum of electronic and thermal Free Energies=	-2920.973217

Table S3. Coordinates of D2 at B3LYP/6-31G(d.p), Gaussian 09 program package

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

1	6	0	1.600138	0.213401	0.993295
2	6	0	0.648893	-0.652780	0.471997
3	6	0	-0.654532	-0.206220	0.842436
4	6	0	-1.609177	-0.958736	0.173024
5	6	0	-0.503516	0.961310	1.690656
6	8	0	-1.293155	1.644188	2.336652
7	6	0	0.496140	-1.783557	-0.424534
8	8	0	1.288042	-2.570819	-0.934795
9	7	0	0.912404	1.183850	1.728626
10	7	0	-0.922885	-1.910137	-0.588007
11	6	0	-1.439183	-3.121655	-1.228061
12	1	0	-2.457020	-3.293865	-0.872397
13	1	0	-0.816872	-3.951701	-0.877139
14	6	0	-1.379126	-3.077582	-2.760209
15	1	0	-1.942610	-2.212140	-3.133593
16	1	0	-0.335456	-2.921481	-3.052686
17	6	0	-1.917294	-4.364415	-3.396814
18	1	0	-1.354297	-5.224055	-3.007076
19	1	0	-2.961302	-4.519864	-3.087466
20	6	0	-1.838450	-4.362423	-4.928246
21	1	0	-2.397546	-3.500935	-5.320834
22	1	0	-0.794423	-4.211104	-5.236277
23	6	0	-2.374732	-5.647475	-5.570822
24	1	0	-3.418544	-5.797812	-5.262967
25	1	0	-1.816390	-6.507835	-5.177637
26	6	0	-2.289421	-5.639197	-7.099957
27	1	0	-2.677515	-6.569101	-7.528085
28	1	0	-2.867769	-4.810939	-7.525018
29	1	0	-1.253313	-5.524561	-7.438065
30	6	0	1.434404	2.141272	2.705655
31	1	0	0.838001	2.016981	3.615668
32	1	0	2.464909	1.868636	2.941701

33	6	0	1.329839	3.601025	2.245527
34	1	0	1.859036	3.732967	1.292369
35	1	0	0.274501	3.817992	2.049608
36	6	0	1.882911	4.578902	3.288869
37	1	0	1.358670	4.426259	4.242673
38	1	0	2.940955	4.350584	3.484267
39	6	0	1.751227	6.048352	2.870352
40	1	0	2.266936	6.201760	1.911476
41	1	0	0.692614	6.276883	2.683933
42	6	0	2.307785	7.032976	3.905999
43	1	0	1.794928	6.876932	4.864759
44	1	0	3.366918	6.805549	4.088959
45	6	0	2.165784	8.498140	3.483292
46	1	0	1.114370	8.765395	3.328313
47	1	0	2.572362	9.175297	4.241432
48	1	0	2.696542	8.693221	2.544426
49	6	0	-3.059731	-0.784976	0.192572
50	6	0	-3.662543	-0.196987	1.324262
51	6	0	-3.893946	-1.129766	-0.889541
52	6	0	-5.034783	0.002295	1.376446
53	1	0	-3.041166	0.135952	2.147437
54	6	0	-5.266164	-0.923964	-0.829356
55	1	0	-3.468576	-1.535563	-1.798680
56	6	0	-5.874373	-0.363290	0.307812
57	1	0	-5.461443	0.480421	2.252490
58	1	0	-5.880068	-1.221290	-1.673774
59	6	0	3.046361	0.179555	0.789301
60	6	0	3.665381	-1.052442	0.490520
61	6	0	3.860223	1.329850	0.823753
62	6	0	5.033183	-1.126440	0.269543
63	1	0	3.062103	-1.949663	0.417298
64	6	0	5.227284	1.247162	0.594287

65	1	0	3.418114	2.305683	0.979744
66	6	0	5.852203	0.016852	0.321264
67	1	0	5.480552	-2.096089	0.075335
68	1	0	5.815808	2.159254	0.587553
69	6	0	-7.338203	-0.155239	0.372145
70	6	0	-8.042786	-0.289753	1.581794
71	6	0	-8.082084	0.183422	-0.771928
72	6	0	-9.416766	-0.093460	1.649869
73	1	0	-7.507832	-0.565257	2.485434
74	6	0	-9.458408	0.368349	-0.717924
75	1	0	-7.573331	0.318869	-1.721409
76	6	0	-10.150730	0.234042	0.497107
77	1	0	-9.931834	-0.200915	2.598270
78	1	0	-10.004873	0.625419	-1.618763
79	6	0	7.308842	-0.065957	0.080483
80	6	0	7.849317	-0.990850	-0.831015
81	6	0	8.211315	0.779682	0.749678
82	6	0	9.215523	-1.062023	-1.072627
83	1	0	7.183950	-1.636109	-1.396449
84	6	0	9.581119	0.704711	0.529843
85	1	0	7.838521	1.480948	1.490091
86	6	0	10.108430	-0.215511	-0.392486
87	1	0	9.598769	-1.766523	-1.802589
88	1	0	10.252725	1.353140	1.081627
89	7	0	11.501960	-0.290762	-0.630438
90	7	0	-11.554161	0.422748	0.558850
91	6	0	12.298686	0.886311	-0.630370
92	6	0	11.846453	2.063352	-1.247362
93	6	0	13.561370	0.894314	-0.017762
94	6	0	12.630406	3.211857	-1.236958
95	1	0	10.873093	2.075665	-1.726092
96	6	0	14.344860	2.043143	-0.029421

97	1	0	13.929001	-0.007879	0.459258
98	6	0	13.899083	3.231416	-0.632571
99	1	0	12.244582	4.115687	-1.698672
100	1	0	15.328331	2.013225	0.429630
101	6	0	12.118031	-1.553495	-0.865018
102	6	0	11.804543	-2.653263	-0.055458
103	6	0	13.053062	-1.704955	-1.899494
104	6	0	12.393056	-3.907304	-0.271603
105	1	0	11.110369	-2.519153	0.766857
106	6	0	13.657584	-2.942702	-2.106154
107	1	0	13.296836	-0.857710	-2.531222
108	6	0	13.331050	-4.038823	-1.309662
109	1	0	14.373437	-3.058355	-2.914793
110	1	0	13.781328	-5.005877	-1.508569
111	6	0	-12.170639	1.450336	-0.206053
112	6	0	-11.595691	2.728196	-0.287241
113	6	0	-13.371038	1.211167	-0.892877
114	6	0	-12.201746	3.728554	-1.039437
115	1	0	-10.666837	2.930382	0.235518
116	6	0	-13.978080	2.224046	-1.627390
117	1	0	-13.831120	0.230213	-0.838905
118	6	0	-13.408848	3.505170	-1.723556
119	1	0	-11.722128	4.700449	-1.105077
120	1	0	-14.919965	2.018927	-2.127083
121	6	0	-12.353170	-0.425158	1.375766
122	6	0	-12.108160	-1.804653	1.414064
123	6	0	-13.401908	0.106686	2.141377
124	6	0	-12.876684	-2.659334	2.216614
125	1	0	-11.322157	-2.216480	0.790894
126	6	0	-14.183685	-0.740482	2.923001
127	1	0	-13.595324	1.173530	2.120034
128	6	0	-13.926388	-2.109472	2.971605

129	1	0	-14.987949	-0.321977	3.521162
130	1	0	-14.519125	-2.749817	3.616694
131	6	0	-12.588506	-4.116868	2.252716
132	6	0	-13.628745	-5.058365	2.325433
133	6	0	-11.266228	-4.590702	2.216962
134	6	0	-13.356582	-6.424926	2.362160
135	1	0	-14.659065	-4.715479	2.327760
136	6	0	-10.993830	-5.957151	2.252338
137	1	0	-10.445853	-3.879884	2.185468
138	6	0	-12.037825	-6.880694	2.325568
139	1	0	-14.177066	-7.135205	2.410315
140	1	0	-9.963416	-6.300271	2.231320
141	1	0	-11.825808	-7.945409	2.353634
142	6	0	-14.056815	4.580018	-2.515351
143	6	0	-14.708318	4.293712	-3.727541
144	6	0	-14.037285	5.914732	-2.075148
145	6	0	-15.317847	5.303142	-4.470473
146	1	0	-14.714008	3.274406	-4.102119
147	6	0	-14.644517	6.924805	-2.819036
148	1	0	-13.563902	6.157151	-1.128376
149	6	0	-15.288504	6.624069	-4.020377
150	1	0	-15.808528	5.058209	-5.408201
151	1	0	-14.622489	7.947789	-2.454220
152	1	0	-15.762506	7.410827	-4.599714
153	6	0	12.039215	-5.064643	0.590912
154	6	0	10.721707	-5.252983	1.041277
155	6	0	13.012654	-6.001482	0.976486
156	6	0	10.389470	-6.339733	1.848348
157	1	0	9.948384	-4.554608	0.735416
158	6	0	12.680377	-7.089080	1.782308
159	1	0	14.042410	-5.860668	0.662013
160	6	0	11.367172	-7.263103	2.222074

161	1	0	9.362865	-6.469690	2.178557
162	1	0	13.450881	-7.796797	2.074612
163	1	0	11.108182	-8.110100	2.850456
164	6	0	14.734163	4.458030	-0.631560
165	6	0	14.755079	5.320440	-1.741349
166	6	0	15.527105	4.792660	0.479809
167	6	0	15.537371	6.473844	-1.739289
168	1	0	14.172369	5.069768	-2.622759
169	6	0	16.311940	5.944339	0.481061
170	1	0	15.506854	4.157100	1.360099
171	6	0	16.320399	6.791422	-0.628277
172	1	0	15.542662	7.120848	-2.611907
173	1	0	16.910533	6.185474	1.354919
174	1	0	16.930818	7.689587	-0.627075

Zero-point correction=	1.442578 (Hartree/Particle)
Thermal correction to Energy=	1.525727
Thermal correction to Enthalpy=	1.526671
Thermal correction to Gibbs Free Energy=	1.301346
Sum of electronic and zero-point Energies=	-3844.795180
Sum of electronic and thermal Energies=	-3844.712031
Sum of electronic and thermal Enthalpies=	-3844.711087
Sum of electronic and thermal Free Energies=	-3844.936413

Table S4. Coordinates of M2 at B3LYP/6-31G(d.p), Gaussian 09 program package

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.577040	0.828552	0.584698
2	6	0	0.661586	-0.157271	0.926270

3	6	0	-0.662426	0.362597	0.813427
4	6	0	-1.579691	-0.667041	0.973977
5	6	0	-0.563113	1.762160	0.444473
6	8	0	-1.386134	2.665393	0.323605
7	6	0	0.562100	-1.571221	1.235598
8	8	0	1.387241	-2.433996	1.522796
9	7	0	0.845688	1.984937	0.295392
10	7	0	-0.848047	-1.831085	1.230493
11	6	0	-1.314663	-3.114557	1.757712
12	1	0	-2.336541	-2.988855	2.121080
13	1	0	-0.679470	-3.349593	2.618370
14	6	0	-1.214081	-4.262652	0.745309
15	1	0	-1.784068	-4.015033	-0.160015
16	1	0	-0.166177	-4.351924	0.440195
17	6	0	-1.708372	-5.593176	1.324655
18	1	0	-1.139670	-5.825807	2.235902
19	1	0	-2.757425	-5.491474	1.639317
20	6	0	-1.586623	-6.763537	0.341211
21	1	0	-2.150196	-6.530237	-0.573606
22	1	0	-0.537346	-6.867268	0.031360
23	6	0	-2.080929	-8.098256	0.911919
24	1	0	-3.129232	-7.992679	1.223207
25	1	0	-1.516519	-8.332122	1.824809
26	6	0	-1.956947	-9.261220	-0.076955
27	1	0	-2.315242	-10.198933	0.360123
28	1	0	-2.540942	-9.073322	-0.985132
29	1	0	-0.915148	-9.412989	-0.381298
30	6	0	1.316183	3.366627	0.180875
31	1	0	0.701493	3.965139	0.861652
32	1	0	2.348000	3.412331	0.534734
33	6	0	1.180550	3.941543	-1.234814
34	1	0	1.749376	3.327739	-1.945877

35	1	0	0.128176	3.867462	-1.528355
36	6	0	1.646059	5.400005	-1.314535
37	1	0	1.081938	5.999749	-0.586554
38	1	0	2.701274	5.468669	-1.011942
39	6	0	1.478185	6.013132	-2.710198
40	1	0	2.042391	5.416193	-3.441115
41	1	0	0.423586	5.941405	-3.011027
42	6	0	1.930601	7.475810	-2.795534
43	1	0	1.367743	8.070848	-2.063611
44	1	0	2.985342	7.547109	-2.496367
45	6	0	1.753461	8.082167	-4.190775
46	1	0	0.702972	8.059066	-4.502052
47	1	0	2.085633	9.125008	-4.219748
48	1	0	2.330780	7.528489	-4.940016
49	6	0	-3.033578	-0.595516	0.852884
50	6	0	-3.679046	0.635090	1.097110
51	6	0	-3.832936	-1.685283	0.451799
52	6	0	-5.055961	0.753390	0.974934
53	1	0	-3.089319	1.502718	1.368701
54	6	0	-5.209746	-1.555604	0.325754
55	1	0	-3.374230	-2.628741	0.184081
56	6	0	-5.859968	-0.337141	0.593623
57	1	0	-5.522260	1.706567	1.203239
58	1	0	-5.788795	-2.403790	-0.025812
59	6	0	3.029063	0.705128	0.484420
60	6	0	3.686816	-0.272139	1.260612
61	6	0	3.813591	1.482526	-0.391155
62	6	0	5.062533	-0.434130	1.183960
63	1	0	3.104727	-0.928099	1.897376
64	6	0	5.190034	1.311647	-0.462505
65	1	0	3.345671	2.208468	-1.044221
66	6	0	5.853418	0.357852	0.330284

67	1	0	5.531440	-1.212947	1.776925
68	1	0	5.764111	1.943546	-1.132987
69	6	0	-7.326323	-0.205436	0.461330
70	6	0	-8.189753	-1.270621	0.775169
71	6	0	-7.917910	0.988694	0.013443
72	6	0	-9.568326	-1.152076	0.657837
73	1	0	-7.776427	-2.197891	1.160784
74	6	0	-9.294527	1.113019	-0.126486
75	1	0	-7.286104	1.823791	-0.273623
76	6	0	-10.148825	0.043565	0.196233
77	1	0	-10.206086	-1.984318	0.933549
78	1	0	-9.716317	2.039411	-0.499838
79	6	0	7.320934	0.184748	0.261087
80	6	0	8.068906	-0.177382	1.395930
81	6	0	8.028077	0.372692	-0.939212
82	6	0	9.445931	-0.348858	1.338607
83	1	0	7.564851	-0.315505	2.347520
84	6	0	9.407155	0.215594	-1.006179
85	1	0	7.487889	0.630253	-1.845152
86	6	0	10.143907	-0.150293	0.133849
87	1	0	9.991169	-0.630805	2.232322
88	1	0	9.921665	0.367602	-1.948444
89	7	0	11.544639	-0.332605	0.062322
90	7	0	-11.550378	0.175734	0.077111
91	6	0	12.126250	-0.866323	-1.127234
92	6	0	11.625427	-2.047743	-1.700330
93	6	0	13.208572	-0.230579	-1.742389
94	6	0	12.186575	-2.565897	-2.858400
95	1	0	10.788383	-2.554289	-1.231026
96	6	0	13.793988	-0.757910	-2.895396
97	1	0	13.602838	0.683940	-1.311484
98	6	0	13.279894	-1.928456	-3.464166

99	1	0	11.803720	-3.476575	-3.306917
100	1	0	14.634682	-0.240947	-3.342422
101	6	0	12.391738	0.027995	1.144214
102	6	0	12.149337	1.193477	1.877675
103	6	0	13.494448	-0.780572	1.478811
104	6	0	12.979730	1.543373	2.949327
105	1	0	11.316988	1.843301	1.634690
106	6	0	14.321200	-0.409363	2.531421
107	1	0	13.687325	-1.687299	0.917500
108	6	0	14.079557	0.744748	3.283203
109	1	0	15.168577	-1.038512	2.788732
110	1	0	14.736132	1.001583	4.104993
111	6	0	-12.164674	1.444953	0.303562
112	6	0	-11.901283	2.169325	1.478540
113	6	0	-13.046105	1.988649	-0.635104
114	6	0	-12.495530	3.403812	1.696587
115	1	0	-11.222259	1.756996	2.217706
116	6	0	-13.665713	3.220296	-0.413525
117	1	0	-13.255313	1.439868	-1.547566
118	6	0	-13.387265	3.938814	0.754519
119	1	0	-12.295781	3.969473	2.600586
120	1	0	-14.346863	3.609480	-1.160714
121	6	0	-12.367525	-0.922181	-0.305778
122	6	0	-11.949069	-1.806225	-1.304739
123	6	0	-13.618477	-1.117154	0.309200
124	6	0	-12.755460	-2.888853	-1.676885
125	1	0	-10.998169	-1.671654	-1.806628
126	6	0	-14.415781	-2.184364	-0.084083
127	1	0	-13.947745	-0.436659	1.085806
128	6	0	-14.001767	-3.084795	-1.070680
129	1	0	-15.378908	-2.333691	0.395642
130	1	0	-14.641134	-3.913346	-1.348262

131	8	0	-13.925484	5.153960	1.069474
132	8	0	-12.238135	-3.686845	-2.658477
133	8	0	12.636891	2.698119	3.595146
134	8	0	13.764991	-2.525462	-4.593028
135	6	0	14.867515	-1.920225	-5.248721
136	1	0	15.089309	-2.551106	-6.110632
137	1	0	14.626853	-0.907230	-5.596308
138	1	0	15.751090	-1.874388	-4.598962
139	6	0	13.449271	3.127697	4.675469
140	1	0	13.005206	4.057111	5.035008
141	1	0	13.459837	2.394413	5.492057
142	1	0	14.481352	3.321292	4.355983
143	6	0	-13.019797	-4.778651	-3.115469
144	1	0	-12.432712	-5.262665	-3.897340
145	1	0	-13.216288	-5.501872	-2.313553
146	1	0	-13.976464	-4.444635	-3.537253
147	6	0	-14.826886	5.745800	0.147825
148	1	0	-15.129522	6.696034	0.590006
149	1	0	-14.349223	5.935742	-0.822031
150	1	0	-15.716241	5.121526	-0.008006

Zero-point correction= 1.249157 (Hartree/Particle)

Thermal correction to Energy= 1.323876

Thermal correction to Enthalpy= 1.324820

Thermal correction to Gibbs Free Energy= 1.123230

Sum of electronic and zero-point Energies= -3378.831768

Sum of electronic and thermal Energies= -3378.757049

Sum of electronic and thermal Enthalpies= -3378.756104

Sum of electronic and thermal Free Energies= -3378.957694