Supplementary Information

Effects of hydrocarbon substituents on highly fluorescent bis(4-phenylphenyl)pyridylmethyl radical derivatives

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Table S1. Calculated torsion angles of the aryl rings of radicals in dichloromethane. Angles outside of brackets are in the D_0 state optimized using UB3LYP/6-31G(d, p). Angles inside brackets are in the D_1 state optimized using TD-UB3LYP/6-31G(d, p).

	MesPyBTM	TippPyBTM (**1**)	Mes$_2$PyBTM	Tipp$_2$PyBTM (**2**)	TippF$_2$PyBTM (**3**)	Mes$_2$F$_2$PyBTM	Tipp$_2$F$_2$PyBTM (**4**)
φ_1	48° [37°]	48° [36°]	48° [37°]	48° [37°]	32° [23°]	32° [24°]	32° [23°]
φ_2	49° [52°]	49° [52°]	49° [51°]	49° [52°]	52° [54°]	52° [53°]	52° [53°]
φ_3	49° [47°]	49° [47°]	49° [48°]	49° [48°]	52° [48°]	52° [49°]	52° [49°]
ϕ_4	83° [51°]	90° [55°]	84° [50°]	88° [55°]	89° [54°]	87° [49°]	89° [54°]
ϕ_5	-	-	84° [81°]	88° [87°]	-	87° [83°]	89° [89°]

	PyBTM	F$_2$PyBTM	PyPBTM	Ph*F$_2$PyBTM (**5**)	Ph*$_2$F$_2$PyBTM (**6**)	Xyl$_2$F$_2$PyBTM (**7**)	Biph$_2$F$_2$PyBTM (**8**)
φ_1	48° [35°]	32° [19°]	48° [43°]	32° [25°]	32° [24°]	32° [27°]	32° [25°]
φ_2	49° [51°]	53° [52°]	48° [45°]	52° [50°]	52° [52°]	52° [52°]	52° [50°]
φ_3	49° [47°]	53° [52°]	48° [45°]	53° [51°]	52° [49°]	52° [46°]	52° [48°]
ϕ_4	-	-	34° [25°]	88° [89°]	88° [88°]	48° [34°]	48° [39°]
ϕ_5	-	-	34° [25°]	-	88° [89°]	51° [50°]	50° [49°]
ϕ_6							52° [39°]
ϕ_7							52° [51°]

φ_1: Torsion angle of pyridyl ring. φ_2 and φ_3: Torsion angles of dichlorophenyl rings. ϕ_4 and ϕ_5: Dihedral angles between dichlorophenyl groups and (alkyl)phenyl groups. ϕ_6 and ϕ_7: Dihedral angles between *o*-phenylene groups and phenyl groups.

Table S2. PLQYs and photophysical parameters of radicals in chloroform.

	Φ_f / %	τ / ns	k_f / 10^7 s^{-1}	k_{nr} / 10^7 s^{-1}
MesPyBTM	28	26	1.1	2.8
TippPyBTM (**1**)	22	24	0.9	3.3
Mes$_2$PyBTM	45	39	1.2	1.4
Tipp$_2$PyBTM (**2**)	42	41	1.0	1.4
TippF$_2$PyBTM (**3**)	53	43	1.2	1.1
Mes$_2$F$_2$PyBTM	69	49	1.4	0.6
Tipp$_2$F$_2$PyBTM (**4**)	63	53	1.2	0.7
PyBTM	3	7.6	0.4	12.8
F$_2$PyBTM	6	18.1	0.3	5.2
PyPBTM	8.6	12	0.7	7.6
Ph*F$_2$PyBTM (**5**)	30	20	1.5	3.5
Ph*$_2$F$_2$PyBTM (**6**)	47	32	1.5	1.7
Xyl$_2$F$_2$PyBTM (**7**)	36	26	1.4	2.5
Biph$_2$F$_2$PyBTM (**8**)	13	14	0.9	6.2

Table S3. Stability of **1**, **2**, **3**, **4**, **7**, and **8** in dichloromethane under 370 nm UV irradiation.

Exp. no.	$t_{1/2}$ [s] PyBTM	$t_{1/2}$ [s] Mes PyBTM	$t_{1/2}$ [s] Mes_2 PyBTM	$t_{1/2}$ [s] Mes_2 F_2PyBTM	$t_{1/2}$ [s] **1**	$t_{1/2}$ [s] **2**	$t_{1/2}$ [s] **3**	$t_{1/2}$ [s] **4**	$t_{1/2}$ [s] **7**	$t_{1/2}$ [s] **8**
1	382	240	274	452	216	152	156	132	5.75×10^3	3.12×10^4
2	312	246	276	424	192	152	174	160	5.51×10^3	3.09×10^4
3	368	260	290	414	210	156	144	142	5.64×10^3	4.44×10^4
4	360									
5	254									
6	276									
7	270									
Ave.	317	249	280	430	206	153	158	145	5.63×10^3	3.55×10^4
σ	53	10	9	20	12	2	15	14	0.12×10^3	0.77×10^4

Table S4. Stability of **5**, and **6** in chloroform under 370 nm UV irradiation.

Exp. no.	$t_{1/2}$ [s] PyBTM	$t_{1/2}$ [s] **5**	$t_{1/2}$ [s] **6**
1	176	1.45×10^3	1.27×10^3
2	184	1.49×10^3	1.11×10^3
3	162	1.55×10^3	1.01×10^3
4	162		
5	188		
6	176		
7	154		
Ave.	172	1.50×10^3	1.13×10^3
σ	13	0.05×10^3	0.13×10^3

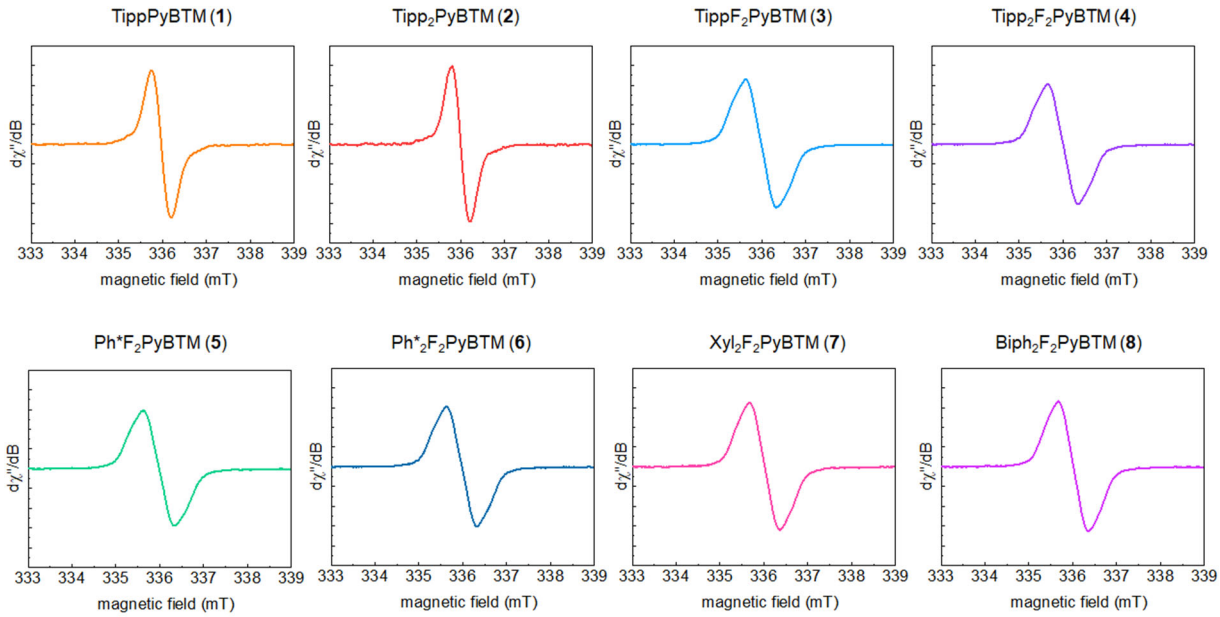


Figure S1. ESR spectra of the radicals **1**-**8** in dichloromethane. The *g* factors of the radicals were *ca.* *g* = 2.0032±0.0002.

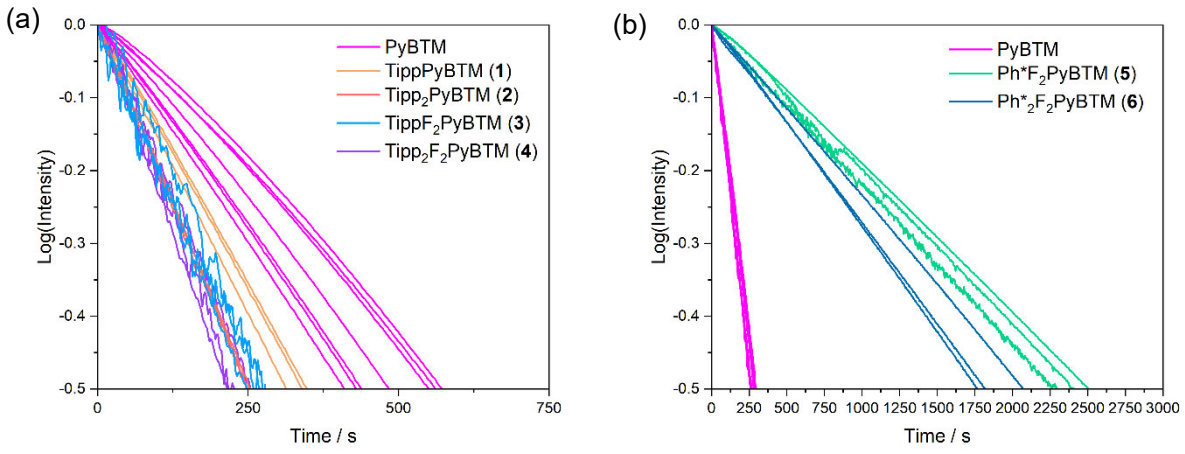


Figure S2. Plots showing the emission decay of (a) **1**, **2**, **3**, and **4** in dichloromethane under continuous excitation with light at λ_{ex} = 370 nm ± 10 nm, and (b) **5**, and **6** in chloroform under continuous excitation with light at λ_{ex} = 370 nm ± 10 nm. The emission was monitored at the peak emission.

Cartesian coordinates of the optimized geometries by DFT calculation in dichloromethane

TippPyBTM (D_0 state, UB3LYP/6-31G(d, p))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-0.588614	-1.432750	2.597282
2	17	0	-1.622899	2.242209	1.626315
3	17	0	-0.919721	0.788786	-2.465047
4	17	0	-4.485799	-0.798015	-2.006102
5	7	0	-4.057741	-4.219549	1.162406
6	6	0	1.480791	-0.670334	1.079115
7	1	0	2.062141	-1.025635	1.921725
8	6	0	-0.053364	0.258789	-1.027972
9	6	0	-4.145015	0.670351	-1.106545
10	6	0	-3.075228	-4.152870	0.261121
11	1	0	-2.762153	-5.082065	-0.206125
12	6	0	-2.839975	-1.722170	0.470552
13	6	0	-4.953146	1.761280	-1.407021
14	6	0	-4.689732	2.979713	-0.790029
15	6	0	0.095802	-0.776939	1.114561
16	6	0	-2.458679	-2.958428	-0.105952
17	6	0	-2.853624	2.003968	0.397843
18	6	0	-3.641579	3.114320	0.114299
19	6	0	1.330757	0.375215	-1.076074
20	6	0	-3.060236	0.731171	-0.194161
21	6	0	-0.744759	-0.320621	0.066863
22	6	0	-3.881973	-1.841184	1.422372
23	6	0	-4.450190	-3.076057	1.728492
24	6	0	-2.213056	-0.436189	0.113666
25	1	0	-5.243340	-3.131484	2.468484
26	6	0	2.123113	-0.089231	-0.020176
27	1	0	-5.757930	1.662712	-2.123820
28	6	0	3.617888	0.032925	-0.064539
29	6	0	4.245369	1.191938	0.450251
30	6	0	4.393587	-1.009360	-0.618828
31	6	0	5.640304	1.281163	0.397858
32	6	0	5.786838	-0.867350	-0.645647
33	6	0	6.432642	0.264563	-0.145241
34	1	0	6.120703	2.171799	0.793749
35	1	0	6.389929	-1.665789	-1.070836
36	1	0	1.795722	0.815038	-1.950476
37	1	0	-3.450224	4.058422	0.607510
38	6	0	3.766641	-2.281536	-1.187795
39	1	0	2.681386	-2.203000	-1.077035
40	6	0	3.450652	2.346246	1.060513
41	1	0	2.388699	2.089285	1.012040
42	6	0	7.950969	0.379147	-0.194109
43	1	0	8.326177	-0.540376	-0.661488
44	6	0	4.210471	-3.533417	-0.407060
45	1	0	5.290369	-3.696478	-0.489426
46	1	0	3.965693	-3.445001	0.656194
47	1	0	3.708446	-4.424841	-0.798182
48	6	0	4.056618	-2.435918	-2.693080
49	1	0	3.704566	-1.565656	-3.256079
50	1	0	5.128731	-2.548354	-2.886648
51	1	0	3.552224	-3.323678	-3.089487
52	6	0	3.796964	2.553361	2.547380
53	1	0	3.624619	1.639950	3.125509
54	1	0	4.845632	2.840159	2.679906
55	1	0	3.177884	3.348705	2.976155
56	6	0	3.635528	3.650362	0.261313
57	1	0	4.676440	3.990403	0.281776
58	1	0	3.347922	3.517199	-0.786450
59	1	0	3.016356	4.448488	0.684741
60	6	0	8.565356	0.464323	1.215668
61	1	0	9.658944	0.484642	1.157768
62	1	0	8.243106	1.372856	1.736069
63	1	0	8.272714	-0.394261	1.828205
64	6	0	8.408728	1.561516	-1.068570
65	1	0	8.004996	1.484041	-2.082968

66	1	0	8.079016	2.518087	-0.648649
67	1	0	9.501519	1.587940	-1.137899
68	17	0	-1.257195	-3.060713	-1.378006
69	17	0	-4.462726	-0.466392	2.341938
70	17	0	-5.693450	4.365773	-1.157291

Tipp$_2$PyBTM (D_0 state, UB3LYP/6-31G(d, p))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	2.114225	2.674986	-2.174737
2	17	0	-0.427116	-0.329877	-2.160154
3	17	0	0.427117	-0.329877	2.160155
4	17	0	-2.114223	2.674984	2.174739
5	7	0	-0.000003	6.239971	-0.000001
6	6	0	3.533507	0.771648	-0.936455
7	1	0	4.284874	1.036535	-1.670990
8	6	0	1.564315	0.108431	0.890419
9	6	0	-2.325933	1.459191	0.919538
10	6	0	0.774513	5.545759	0.836959
11	1	0	1.398016	6.110073	1.524423
12	6	0	-0.000001	3.375530	-0.000001
13	6	0	-3.533506	0.771646	0.936456
14	6	0	-3.773545	-0.269028	0.032133
15	6	0	2.325934	1.459193	-0.919537
16	6	0	0.801392	4.153142	0.871351
17	6	0	-1.564314	0.108430	-0.890419
18	6	0	-2.765860	-0.590281	-0.884247
19	6	0	2.765861	-0.590280	0.884247
20	6	0	-1.278597	1.167348	0.008890
21	6	0	1.278598	1.167349	-0.008889
22	6	0	-0.801395	4.153140	-0.871352
23	6	0	-0.774518	5.545757	-0.836961
24	6	0	0.000000	1.901144	0.000000
25	1	0	-1.398023	6.110070	-1.524425
26	6	0	3.773546	-0.269027	-0.032133
27	1	0	-4.284872	1.036532	1.670991
28	6	0	-5.073207	-1.018689	0.045825
29	6	0	-5.201434	-2.192147	0.826009
30	6	0	-6.164843	-0.550227	-0.718592
31	6	0	-6.423904	-2.871883	0.823053
32	6	0	-7.366301	-1.269494	-0.683751
33	6	0	-7.521047	-2.429957	0.076565
34	1	0	-6.520628	-3.772783	1.422874
35	1	0	-8.210511	-0.914005	-1.269408
36	6	0	5.073208	-1.018688	-0.045825
37	6	0	5.201435	-2.192145	-0.826012
38	6	0	6.164844	-0.550228	0.718594
39	6	0	6.423905	-2.871881	-0.823055
40	6	0	7.366301	-1.269495	0.683753
41	6	0	7.521047	-2.429957	-0.076564
42	1	0	6.520629	-3.772780	-1.422877
43	1	0	8.210510	-0.914007	1.269412
44	1	0	2.924444	-1.378897	1.610347
45	1	0	-2.924442	-1.378898	-1.610347
46	6	0	6.079681	0.709906	1.578850
47	1	0	5.067577	1.114259	1.487647
48	6	0	4.051451	-2.738177	-1.672079
49	1	0	3.192244	-2.073571	-1.545233
50	6	0	8.845300	-3.183100	-0.086223
51	1	0	9.529794	-2.635326	0.574229
52	6	0	-6.079681	0.709908	-1.578846
53	1	0	-5.067577	1.114260	-1.487644
54	6	0	-4.051449	-2.738182	1.672075
55	1	0	-3.192241	-2.073577	1.545227
56	6	0	-8.845301	-3.183099	0.086224
57	1	0	-9.529795	-2.635323	-0.574225
58	6	0	7.048608	1.801286	1.084980
59	1	0	8.091881	1.477523	1.164864
60	1	0	6.857117	2.057137	0.038014

61	1	0	6.935427	2.711732	1.683281
62	6	0	6.308720	0.399850	3.070507
63	1	0	5.595170	-0.346198	3.434530
64	1	0	7.317725	0.014242	3.251392
65	1	0	6.187273	1.307532	3.671360
66	6	0	4.400363	-2.742225	-3.172718
67	1	0	4.670600	-1.739730	-3.519440
68	1	0	5.242178	-3.408910	-3.388192
69	1	0	3.544021	-3.086277	-3.762633
70	6	0	3.612535	-4.137901	-1.201325
71	1	0	4.416590	-4.872139	-1.319628
72	1	0	3.321437	-4.128044	-0.146122
73	1	0	2.754973	-4.486136	-1.786981
74	6	0	9.479560	-3.209158	-1.489537
75	1	0	10.457005	-3.702611	-1.460708
76	1	0	8.851088	-3.757394	-2.199850
77	1	0	9.620841	-2.196317	-1.879652
78	6	0	8.698774	-4.607929	0.479960
79	1	0	8.283122	-4.591564	1.492374
80	1	0	8.036901	-5.218002	-0.144414
81	1	0	9.672495	-5.107950	0.519453
82	6	0	-9.479558	-3.209162	1.489539
83	1	0	-9.620837	-2.196323	1.879659
84	1	0	-10.457003	-3.702615	1.460710
85	1	0	-8.851084	-3.757401	2.199849
86	6	0	-8.698776	-4.607926	-0.479965
87	1	0	-8.283126	-4.591558	-1.492379
88	1	0	-8.036901	-5.218002	0.144405
89	1	0	-9.672497	-5.107947	-0.519458
90	6	0	-3.612537	-4.137907	1.201322
91	1	0	-4.416593	-4.872144	1.319628
92	1	0	-3.321442	-4.128052	0.146118
93	1	0	-2.754975	-4.486143	1.786976
94	6	0	-4.400358	-2.742226	3.172714
95	1	0	-4.670592	-1.739730	3.519436
96	1	0	-5.242175	-3.408909	3.388190
97	1	0	-3.544016	-3.086281	3.762628
98	6	0	-7.048607	1.801288	-1.084973
99	1	0	-8.091880	1.477525	-1.164855
100	1	0	-6.857114	2.057137	-0.038007
101	1	0	-6.935426	2.711734	-1.683272
102	6	0	-6.308724	0.399854	-3.070504
103	1	0	-5.595175	-0.346194	-3.434528
104	1	0	-7.317729	0.014249	-3.251387
105	1	0	-6.187277	1.307538	-3.671355
106	17	0	1.807279	3.424232	2.108505
107	17	0	-1.807281	3.424228	-2.108507

TippF$_2$PyBTM (D_0 state, UB3LYP/6-31G(d, p))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.673014	1.518112	2.614643
2	17	0	1.878548	-1.979457	1.914499
3	17	0	1.101225	-0.707149	-2.431107
4	17	0	4.540093	0.797080	-2.057651
5	7	0	4.058788	4.427135	0.978151
6	6	0	-1.371406	0.705893	1.082403
7	1	0	-1.968374	1.049388	1.918982
8	6	0	0.201206	-0.186168	-1.011071
9	6	0	4.269815	-0.599338	-1.027053
10	6	0	2.901245	4.309899	0.315561
11	1	0	2.404520	5.216843	-0.017422
12	6	0	2.916629	1.858827	0.425673
13	6	0	5.103297	-1.688523	-1.253920
14	6	0	4.900314	-2.851426	-0.517178
15	6	0	0.010451	0.839228	1.130907
16	6	0	2.323664	3.080128	0.036232
17	6	0	3.072337	-1.823304	0.636847
18	6	0	3.888083	-2.932575	0.431990

19	6	0	-1.181224	-0.327562	-1.076048
20	6	0	3.215593	-0.610370	-0.078910
21	6	0	0.867374	0.401111	0.090501
22	6	0	4.134556	2.042770	1.116395
23	6	0	4.663039	3.299247	1.372534
24	6	0	2.336169	0.556476	0.147443
25	1	0	5.599127	3.380027	1.917846
26	6	0	-1.991565	0.119631	-0.027610
27	1	0	5.882999	-1.632884	-2.002372
28	6	0	-3.484190	-0.018672	-0.092753
29	6	0	-4.106613	-1.193062	0.392024
30	6	0	-4.262884	1.025985	-0.638488
31	6	0	-5.499659	-1.295875	0.317624
32	6	0	-5.654022	0.870232	-0.688023
33	6	0	-6.294802	-0.277617	-0.218279
34	1	0	-5.976346	-2.198549	0.690109
35	1	0	-6.259498	1.670083	-1.107150
36	1	0	-1.628461	-0.772772	-1.956958
37	1	0	3.742955	-3.831605	1.016678
38	6	0	-3.640887	2.314440	-1.175828
39	1	0	-2.556758	2.246216	-1.048514
40	6	0	-3.308038	-2.349174	0.993675
41	1	0	-2.249002	-2.077062	0.970350
42	6	0	-7.810968	-0.407054	-0.291644
43	1	0	-8.189106	0.516863	-0.747876
44	9	0	4.804693	0.968343	1.570382
45	9	0	1.169728	3.064858	-0.654571
46	6	0	-4.111666	3.548308	-0.382323
47	1	0	-5.191778	3.701117	-0.480128
48	1	0	-3.883635	3.445059	0.683331
49	1	0	-3.613178	4.451489	-0.750375
50	6	0	-3.908110	2.490448	-2.682962
51	1	0	-3.536859	1.633626	-3.254173
52	1	0	-4.978204	2.593885	-2.892168
53	1	0	-3.407559	3.390227	-3.056495
54	6	0	-3.678717	-2.591472	2.469299
55	1	0	-3.530088	-1.687758	3.068859
56	1	0	-4.725365	-2.895621	2.576715
57	1	0	-3.056200	-3.386671	2.893348
58	6	0	-3.460762	-3.638881	0.164819
59	1	0	-4.497592	-3.991741	0.157968
60	1	0	-3.154686	-3.480888	-0.874233
61	1	0	-2.839952	-4.437989	0.584021
62	6	0	-8.444913	-0.524204	1.107129
63	1	0	-9.537258	-0.555230	1.032771
64	1	0	-8.120218	-1.438445	1.615863
65	1	0	-8.170672	0.326272	1.739185
66	6	0	-8.243383	-1.578016	-1.193907
67	1	0	-7.825885	-1.477858	-2.200721
68	1	0	-7.909508	-2.538579	-0.786567
69	1	0	-9.334717	-1.614619	-1.279713
70	17	0	5.938310	-4.234912	-0.790436

Tipp$_2$F$_2$PyBTM (D_0 state, UB3LYP/6-31G(d, p))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	2.061101	2.689327	-2.254380
2	17	0	-0.473788	-0.104064	-2.249045
3	17	0	0.473788	-0.104065	2.249045
4	17	0	-2.061101	2.689327	2.254381
5	7	0	-0.000001	6.334424	0.000000
6	6	0	3.512380	0.840823	-0.964799
7	1	0	4.246709	1.069507	-1.728184
8	6	0	1.590016	0.272712	0.940912
9	6	0	-2.304381	1.526840	0.953551
10	6	0	0.973536	5.639515	0.601944
11	1	0	1.765800	6.190116	1.101356
12	6	0	0.000000	3.468764	0.000000
13	6	0	-3.512380	0.840823	0.964800

14	6	0	-3.777258	-0.149637	0.011400
15	6	0	2.304381	1.526841	-0.953550
16	6	0	1.000419	4.252868	0.615687
17	6	0	-1.590016	0.272712	-0.940911
18	6	0	-2.793869	-0.424566	-0.944145
19	6	0	2.793869	-0.424567	0.944146
20	6	0	-1.281210	1.278868	0.004822
21	6	0	1.281210	1.278868	-0.004821
22	6	0	-1.000420	4.252868	-0.615687
23	6	0	-0.973537	5.639514	-0.601944
24	6	0	0.000000	2.016100	0.000000
25	1	0	-1.765801	6.190115	-1.101357
26	6	0	3.777258	-0.149637	-0.011399
27	1	0	-4.246708	1.069506	1.728185
28	6	0	-5.081304	-0.891783	0.012251
29	6	0	-5.206742	-2.097612	0.741636
30	6	0	-6.179706	-0.383849	-0.716415
31	6	0	-6.433043	-2.770230	0.724027
32	6	0	-7.384624	-1.097962	-0.698935
33	6	0	-7.536523	-2.290287	0.011090
34	1	0	-6.527517	-3.696342	1.284525
35	1	0	-8.233895	-0.712781	-1.257926
36	6	0	5.081304	-0.891783	-0.012250
37	6	0	5.206742	-2.097612	-0.741636
38	6	0	6.179707	-0.383849	0.716416
39	6	0	6.433043	-2.770230	-0.724027
40	6	0	7.384624	-1.097962	0.698935
41	6	0	7.536523	-2.290287	-0.011090
42	1	0	6.527517	-3.696342	-1.284526
43	1	0	8.233896	-0.712781	1.257926
44	1	0	2.971436	-1.173866	1.706569
45	1	0	-2.971436	-1.173865	-1.706569
46	6	0	6.096997	0.912458	1.521701
47	1	0	5.087096	1.317029	1.409421
48	6	0	4.048522	-2.687268	-1.546128
49	1	0	3.189427	-2.018476	-1.442520
50	6	0	8.865003	-3.036007	-0.004329
51	1	0	9.553019	-2.458308	0.626287
52	6	0	-6.096996	0.912458	-1.521700
53	1	0	-5.087096	1.317031	-1.409418
54	6	0	-4.048522	-2.687269	1.546128
55	1	0	-3.189428	-2.018476	1.442521
56	6	0	-8.865003	-3.036006	0.004328
57	1	0	-9.553019	-2.458308	-0.626288
58	9	0	-2.009546	3.645964	-1.266452
59	9	0	2.009546	3.645965	1.266452
60	6	0	7.072281	1.978642	0.987215
61	1	0	8.114352	1.656794	1.087484
62	1	0	6.887776	2.189777	-0.070916
63	1	0	6.957847	2.914217	1.545163
64	6	0	6.318982	0.663245	3.025822
65	1	0	5.598850	-0.061960	3.417941
66	1	0	7.324595	0.277805	3.225286
67	1	0	6.202322	1.595782	3.588375
68	6	0	4.379366	-2.766605	-3.048736
69	1	0	4.644690	-1.782786	-3.448679
70	1	0	5.218808	-3.443320	-3.241021
71	1	0	3.516120	-3.139867	-3.610137
72	6	0	3.618574	-4.062323	-1.000203
73	1	0	4.423628	-4.799543	-1.089880
74	1	0	3.338965	-3.999597	0.056295
75	1	0	2.755705	-4.441926	-1.557944
76	6	0	9.484673	-3.114659	-1.412220
77	1	0	10.465417	-3.600918	-1.374264
78	1	0	8.852026	-3.694526	-2.093109
79	1	0	9.615486	-2.117465	-1.844067
80	6	0	8.733212	-4.437803	0.619873
81	1	0	8.327558	-4.383379	1.635010
82	1	0	8.069160	-5.076458	0.027207
83	1	0	9.710450	-4.930004	0.669414
84	6	0	-9.484673	-3.114657	1.412219
85	1	0	-9.615487	-2.117462	1.844066
86	1	0	-10.465418	-3.600916	1.374264
87	1	0	-8.852027	-3.694524	2.093109
88	6	0	-8.733213	-4.437803	-0.619873
89	1	0	-8.327558	-4.383379	-1.635009
90	1	0	-8.069161	-5.076458	-0.027205

91	1	0	-9.710451	-4.930003	-0.669413
92	6	0	-3.618573	-4.062322	1.000201
93	1	0	-4.423627	-4.799543	1.089877
94	1	0	-3.338964	-3.999596	-0.056297
95	1	0	-2.755705	-4.441926	1.557942
96	6	0	-4.379366	-2.766608	3.048736
97	1	0	-4.644691	-1.782789	3.448680
98	1	0	-5.218808	-3.443324	3.241019
99	1	0	-3.516121	-3.139870	3.610136
100	6	0	-7.072283	1.978642	-0.987217
101	1	0	-8.114353	1.656793	-1.087489
102	1	0	-6.887780	2.189776	0.070913
103	1	0	-6.957848	2.914216	-1.545166
104	6	0	-6.318978	0.663244	-3.025822
105	1	0	-5.598844	-0.061960	-3.417939
106	1	0	-7.324590	0.277802	-3.225288
107	1	0	-6.202318	1.595781	-3.588376

Ph*F_2PyBTM (D_0 state, UB3LYP/6-31G(d, p))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.116884	1.694415	2.477048
2	17	0	1.433395	-1.814972	2.069317
3	17	0	0.614708	-0.937730	-2.363246
4	17	0	4.002809	0.703529	-2.129102
5	7	0	3.413888	4.555212	0.597588
6	6	0	-1.900359	0.686783	1.026506
7	1	0	-2.507899	1.080313	1.832944
8	6	0	-0.300866	-0.327808	-0.988728
9	6	0	3.777609	-0.610237	-0.985070
10	6	0	2.260595	4.348289	-0.050354
11	1	0	1.736892	5.208935	-0.456823
12	6	0	2.349840	1.916547	0.263820
13	6	0	4.644741	-1.687902	-1.123610
14	6	0	4.479384	-2.791010	-0.291679
15	6	0	-0.523719	0.869814	1.058392
16	6	0	1.720440	3.082667	-0.224854
17	6	0	2.620826	-1.728153	0.779125
18	6	0	3.471100	-2.824451	0.664540
19	6	0	-1.677738	-0.519913	-1.035989
20	6	0	2.725187	-0.575186	-0.035603
21	6	0	0.346777	0.372768	0.056478
22	6	0	3.561170	2.194128	0.934517
23	6	0	4.051592	3.482868	1.083610
24	6	0	1.809653	0.578436	0.095898
25	1	0	4.984580	3.637011	1.618334
26	6	0	-2.501864	-0.012626	-0.026321
27	1	0	5.421414	-1.670491	-1.877065
28	6	0	-3.989307	-0.206322	-0.071259
29	6	0	-4.559051	-1.353973	0.518117
30	6	0	-4.795187	0.769804	-0.693393
31	6	0	-5.956119	-1.530761	0.469000
32	6	0	-6.191113	0.583793	-0.735681
33	6	0	-6.764330	-0.577898	-0.181891
34	1	0	-2.111081	-1.053400	-1.873812
35	1	0	3.355002	-3.675789	1.322512
36	6	0	-4.176636	2.004599	-1.320814
37	1	0	-4.479210	2.918163	-0.795117
38	1	0	-3.087826	1.969612	-1.305974
39	1	0	-4.487568	2.120854	-2.364371
40	6	0	-3.686967	-2.394205	1.194968
41	1	0	-2.625918	-2.176537	1.078095
42	1	0	-3.890274	-2.451437	2.270961
43	1	0	-3.864261	-3.393864	0.784419
44	6	0	-8.260252	-0.801001	-0.284138
45	1	0	-8.510820	-1.863076	-0.302935
46	1	0	-8.796880	-0.358561	0.566293
47	1	0	-8.674156	-0.354520	-1.190257
48	9	0	4.262750	1.182055	1.476018

49	9	0	0.567666	2.975158	-0.909345
50	6	0	-7.085187	1.626760	-1.377323
51	1	0	-6.583132	2.587826	-1.486696
52	1	0	-7.414953	1.318921	-2.378546
53	1	0	-7.988138	1.798076	-0.784621
54	6	0	-6.599861	-2.743481	1.112586
55	1	0	-6.896870	-3.490574	0.364652
56	1	0	-5.931036	-3.240951	1.814424
57	1	0	-7.503886	-2.470216	1.664281
58	17	0	5.560611	-4.159105	-0.452192

Ph*$_2$F$_2$PyBTM (D_0 state, UB3LYP/6-31G(d, p))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	2.044129	2.361006	-2.269829
2	17	0	-0.490348	-0.435088	-2.244304
3	17	0	0.490350	-0.435088	2.244305
4	17	0	-2.044131	2.361006	2.269829
5	7	0	-0.000002	6.005671	-0.000002
6	6	0	3.507859	0.516921	-0.987143
7	1	0	4.237135	0.746972	-1.755005
8	6	0	1.598401	-0.055123	0.929573
9	6	0	-2.298256	1.199914	0.969147
10	6	0	0.976688	5.310630	0.596706
11	1	0	1.771614	5.861174	1.091961
12	6	0	-0.000001	3.139802	-0.000001
13	6	0	-3.507859	0.516918	0.987144
14	6	0	-3.781699	-0.471711	0.034902
15	6	0	2.298256	1.199916	-0.969147
16	6	0	1.003615	3.923980	0.610312
17	6	0	-1.598400	-0.055124	-0.929572
18	6	0	-2.804145	-0.748942	-0.925981
19	6	0	2.804146	-0.748939	0.925981
20	6	0	-1.281461	0.950625	0.014053
21	6	0	1.281461	0.950626	-0.014052
22	6	0	-1.003618	3.923979	-0.610315
23	6	0	-0.976692	5.310629	-0.596710
24	6	0	0.000000	1.686995	0.000000
25	1	0	-1.771617	5.861171	-1.091966
26	6	0	3.781700	-0.471708	-0.034902
27	1	0	-4.237135	0.746969	1.755006
28	6	0	-5.089713	-1.207393	0.043016
29	6	0	-5.207150	-2.409056	0.771901
30	6	0	-6.185329	-0.678308	-0.670534
31	6	0	-6.437583	-3.095640	0.772838
32	6	0	-7.411372	-1.372484	-0.662396
33	6	0	-7.525850	-2.592198	0.033292
34	6	0	5.089714	-1.207390	-0.043015
35	6	0	5.207154	-2.409046	-0.771909
36	6	0	6.185328	-0.678310	0.670544
37	6	0	6.437588	-3.095630	-0.772850
38	6	0	7.411368	-1.372490	0.662408
39	6	0	7.525850	-2.592197	-0.033291
40	1	0	2.988304	-1.497660	1.687490
41	1	0	-2.988302	-1.497662	-1.687490
42	6	0	6.053893	0.617192	1.448676
43	1	0	6.685617	1.407339	1.025456
44	1	0	5.030221	0.990045	1.452481
45	1	0	6.361121	0.489535	2.492003
46	6	0	4.027716	-2.967289	-1.545157
47	1	0	3.119964	-2.388013	-1.380061
48	1	0	4.219290	-2.970408	-2.624844
49	1	0	3.814021	-4.002117	-1.257406
50	6	0	8.829125	-3.365311	0.011274
51	1	0	8.665510	-4.439834	-0.088583
52	1	0	9.507887	-3.066408	-0.799240
53	1	0	9.362371	-3.204841	0.950122
54	6	0	-6.053896	0.617197	-1.448661
55	1	0	-6.685602	1.407349	-1.025423

56	1	0	-5.030220	0.990040	-1.452485
57	1	0	-6.361148	0.489549	-2.491982
58	6	0	-4.027708	-2.967301	1.545143
59	1	0	-3.119963	-2.388012	1.380063
60	1	0	-4.219288	-2.970446	2.624829
61	1	0	-3.813999	-4.002120	1.257371
62	6	0	-8.829123	-3.365315	-0.011266
63	1	0	-8.665497	-4.439842	0.088537
64	1	0	-9.507857	-3.066456	0.799289
65	1	0	-9.362404	-3.204806	-0.950087
66	9	0	-2.016191	3.317251	-1.256043
67	9	0	2.016189	3.317253	1.256040
68	6	0	8.613094	-0.816598	1.401263
69	1	0	8.498997	0.241703	1.634946
70	1	0	8.784309	-1.340425	2.351122
71	1	0	9.528142	-0.921696	0.811609
72	6	0	6.600498	-4.378027	-1.565399
73	1	0	6.571822	-5.263297	-0.916275
74	1	0	5.816652	-4.502667	-2.312117
75	1	0	7.558069	-4.402610	-2.093221
76	6	0	-6.600497	-4.378048	1.565370
77	1	0	-6.571908	-5.263303	0.916223
78	1	0	-5.816608	-4.502742	2.312032
79	1	0	-7.558036	-4.402598	2.093254
80	6	0	-8.613098	-0.816577	-1.401238
81	1	0	-8.499015	0.241738	-1.634865
82	1	0	-8.784292	-1.340358	-2.351126
83	1	0	-9.528152	-0.921718	-0.811602

Xyl_2F_2PyBTM (D_0 state, UB3LYP/6-31G(d, p))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-2.113968	2.036307	2.203699
2	17	0	0.476285	-0.730059	2.250103
3	17	0	-0.364918	-0.759528	-2.238778
4	17	0	2.120145	2.120256	-2.197228
5	7	0	-0.067926	5.710751	0.003952
6	6	0	-3.501350	0.162698	0.884871
7	1	0	-4.241938	0.372863	1.645876
8	6	0	-1.517841	-0.392729	-0.959119
9	6	0	2.350811	0.953446	-0.897229
10	6	0	-1.010017	4.998225	-0.626738
11	1	0	-1.797550	5.534327	-1.148933
12	6	0	-0.013913	2.845517	0.001943
13	6	0	3.565242	0.282187	-0.889774
14	6	0	3.824343	-0.724095	0.052693
15	6	0	-2.307069	0.869242	0.897499
16	6	0	-1.010131	3.611268	-0.642184
17	6	0	1.609801	-0.334265	0.961519
18	6	0	2.819936	-1.016922	0.984068
19	6	0	-2.707319	-1.110495	-0.986720
20	6	0	1.306304	0.679628	0.021145
21	6	0	-1.251928	0.632076	-0.019393
22	6	0	0.952745	3.647368	0.647161
23	6	0	0.900372	5.033356	0.633676
24	6	0	0.013474	1.392189	0.001207
25	1	0	1.667137	5.598030	1.156659
26	6	0	-3.728063	-0.844109	-0.064344
27	1	0	4.305204	0.520664	-1.644250
28	6	0	5.144539	-1.409144	0.071846
29	6	0	5.283156	-2.816003	0.116350
30	6	0	6.304025	-0.615261	0.023700
31	6	0	6.575765	-3.356770	0.124075
32	6	0	7.574749	-1.179302	0.040489
33	6	0	7.731887	-2.569794	0.097295
34	1	0	6.680536	-4.439416	0.139809
35	1	0	8.449591	-0.535353	0.009563
36	6	0	-4.981139	-1.645486	-0.081124
37	6	0	-4.872000	-3.046033	-0.137906

38	6	0	-6.269579	-1.062315	-0.062413
39	6	0	-5.995984	-3.864453	-0.154109
40	6	0	-7.384007	-1.911135	-0.087515
41	6	0	-7.279761	-3.305690	-0.122759
42	1	0	-5.875000	-4.943802	-0.190902
43	1	0	-8.374090	-1.460499	-0.091589
44	1	0	-2.853022	-1.860814	-1.754464
45	1	0	2.991030	-1.751936	1.760081
46	6	0	-6.499207	0.433713	-0.056120
47	1	0	-6.484666	0.845593	0.959926
48	1	0	-5.740581	0.969620	-0.632136
49	1	0	-7.478559	0.668475	-0.481477
50	6	0	-8.510827	-4.179463	-0.111997
51	1	0	-8.366101	-5.080640	-0.715375
52	1	0	-8.750727	-4.508000	0.906881
53	1	0	-9.384297	-3.645616	-0.496513
54	6	0	4.102693	-3.763240	0.116691
55	1	0	3.720378	-3.939876	1.129031
56	1	0	3.269825	-3.384169	-0.480870
57	1	0	4.397094	-4.735510	-0.287313
58	6	0	9.103711	-3.198339	0.143148
59	1	0	9.082817	-4.231846	-0.213433
60	1	0	9.819632	-2.639085	-0.466713
61	1	0	9.495119	-3.213469	1.167912
62	9	0	1.953372	3.058530	1.326764
63	9	0	-1.988042	2.986194	-1.322648
64	1	0	6.200700	0.465483	-0.008291
65	1	0	-3.883800	-3.496600	-0.150320

Biph$_2$F$_2$PyBTM (D_0 state, UB3LYP/6-31G(d, p))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	2.199038	1.547266	-2.249724
2	17	0	-0.991130	-0.497212	-2.213106
3	17	0	-0.146584	-0.607020	2.274555
4	17	0	-1.846331	2.790855	2.153088
5	7	0	1.144202	5.669787	-0.148467
6	6	0	3.099622	-0.566404	-0.874592
7	1	0	3.876703	-0.558101	-1.628206
8	6	0	1.050784	-0.570178	0.984131
9	6	0	-2.368100	1.686291	0.883589
10	6	0	1.885950	4.763225	0.500235
11	1	0	2.785895	5.101369	1.006210
12	6	0	0.383523	2.908067	-0.067601
13	6	0	-3.713400	1.342781	0.890344
14	6	0	-4.217857	0.409365	-0.025255
15	6	0	2.111996	0.406030	-0.910321
16	6	0	1.543534	3.420125	0.553820
17	6	0	-1.983835	0.204392	-0.939348
18	6	0	-3.325064	-0.154861	-0.945224
19	6	0	2.029594	-1.556537	1.032972
20	6	0	-1.431564	1.136543	-0.026230
21	6	0	1.036884	0.459560	0.014168
22	6	0	-0.359943	3.906826	-0.733518
23	6	0	0.033499	5.236629	-0.758180
24	6	0	-0.002492	1.507117	-0.026960
25	1	0	-0.573948	5.959441	-1.295614
26	6	0	3.077946	-1.568809	0.105532
27	1	0	-4.366974	1.782133	1.634388
28	6	0	-5.673003	0.093286	-0.053158
29	6	0	-6.181551	-1.228376	-0.116902
30	6	0	-6.573962	1.172131	-0.065429
31	6	0	-7.571151	-1.405933	-0.222526
32	6	0	-7.949000	0.973230	-0.160080
33	6	0	-8.450163	-0.325325	-0.247547
34	1	0	-7.963709	-2.417624	-0.255318
35	1	0	-8.619898	1.826491	-0.175996
36	6	0	4.094463	-2.656894	0.131545
37	6	0	3.631134	-3.982399	0.191827

38	6	0	5.489581	-2.417912	0.053380
39	6	0	4.508106	-5.063598	0.154940
40	6	0	6.355604	-3.523149	0.007301
41	6	0	5.879660	-4.831739	0.053844
42	1	0	4.120736	-6.076919	0.194432
43	1	0	7.425310	-3.342663	-0.035986
44	1	0	1.991779	-2.298975	1.821120
45	1	0	-3.679552	-0.856894	-1.689076
46	9	0	-1.480707	3.566193	-1.395225
47	9	0	2.342283	2.591092	1.249887
48	1	0	-6.180319	2.183524	-0.034625
49	1	0	2.561103	-4.161702	0.233953
50	1	0	-9.519204	-0.498925	-0.323864
51	1	0	6.577587	-5.662844	0.022255
52	6	0	6.092417	-1.053105	0.065023
53	6	0	7.048423	-0.694792	-0.899941
54	6	0	5.768134	-0.119116	1.063430
55	6	0	7.653847	0.562326	-0.874705
56	1	0	7.306085	-1.402398	-1.682631
57	6	0	6.375748	1.135462	1.090673
58	1	0	5.044922	-0.382858	1.828561
59	6	0	7.319297	1.482238	0.120568
60	1	0	8.384157	0.822784	-1.635200
61	1	0	6.114732	1.841231	1.873762
62	1	0	7.790016	2.460567	0.141339
63	6	0	-5.324123	-2.446289	-0.028611
64	6	0	-5.459431	-3.476078	-0.974467
65	6	0	-4.412081	-2.622439	1.025515
66	6	0	-4.698980	-4.642106	-0.875982
67	1	0	-6.155538	-3.353585	-1.799180
68	6	0	-3.655756	-3.789397	1.126400
69	1	0	-4.305737	-1.845843	1.776276
70	6	0	-3.794313	-4.802924	0.174942
71	1	0	-4.812534	-5.422766	-1.622450
72	1	0	-2.960879	-3.908843	1.952439
73	1	0	-3.203064	-5.710366	0.253283

TippPyBTM (D_1 state, UB3LYP/6-31G(d, p))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-0.634731	-1.934831	2.287712
2	17	0	-1.449383	1.835400	1.967561
3	17	0	-0.922369	1.115112	-2.314323
4	17	0	-4.622650	-0.315826	-2.026354
5	7	0	-4.135284	-4.404372	0.278158
6	6	0	1.448421	-0.942690	0.942320
7	1	0	2.020167	-1.446264	1.712313
8	6	0	-0.063635	0.376153	-0.974630
9	6	0	-4.141871	0.943411	-0.891940
10	6	0	-3.015521	-4.194961	-0.425939
11	1	0	-2.592373	-5.048524	-0.949447
12	6	0	-2.885007	-1.772837	0.103507
13	6	0	-4.879133	2.120031	-0.968020
14	6	0	-4.506097	3.201593	-0.177296
15	6	0	0.069993	-1.023607	0.966081
16	6	0	-2.402559	-2.956589	-0.542266
17	6	0	-2.729750	1.902539	0.756278
18	6	0	-3.421460	3.106733	0.686803
19	6	0	1.306233	0.553984	-0.951503
20	6	0	-3.028879	0.749678	-0.022250
21	6	0	-0.783159	-0.389668	-0.000461
22	6	0	-4.074246	-2.064554	0.849245
23	6	0	-4.641676	-3.328735	0.898626
24	6	0	-2.250015	-0.487861	0.030175
25	1	0	-5.539100	-3.480608	1.492931
26	6	0	2.105657	-0.123970	-0.002522
27	1	0	-5.709411	2.198057	-1.658226
28	6	0	3.564898	0.014019	-0.008100
29	6	0	4.172025	1.322529	0.059737

30	6	0	4.405934	-1.160417	-0.084978
31	6	0	5.552813	1.412611	0.047711
32	6	0	5.781795	-0.990852	-0.084461
33	6	0	6.387989	0.275984	-0.023060
34	1	0	6.014498	2.390731	0.128016
35	1	0	6.423198	-1.862151	-0.167647
36	1	0	1.774631	1.151431	-1.724314
37	1	0	-3.137818	3.938269	1.319128
38	6	0	3.852456	-2.567433	-0.290683
39	1	0	2.762881	-2.524147	-0.261219
40	6	0	3.365791	2.603927	0.265145
41	1	0	2.303733	2.354373	0.256610
42	6	0	7.893406	0.412132	-0.032449
43	1	0	8.311149	-0.598903	-0.097222
44	6	0	4.311002	-3.535893	0.816475
45	1	0	5.396789	-3.674250	0.811613
46	1	0	4.023446	-3.178462	1.810093
47	1	0	3.850855	-4.516542	0.662597
48	6	0	4.229889	-3.100996	-1.689902
49	1	0	3.874816	-2.431430	-2.478913
50	1	0	5.313611	-3.210572	-1.799531
51	1	0	3.774022	-4.083404	-1.845915
52	6	0	3.658238	3.216994	1.650961
53	1	0	3.449689	2.502752	2.453037
54	1	0	4.703436	3.530666	1.739599
55	1	0	3.028542	4.098163	1.807257
56	6	0	3.612341	3.627139	-0.859753
57	1	0	4.652053	3.969447	-0.876361
58	1	0	3.382970	3.208011	-1.844426
59	1	0	2.976863	4.504885	-0.708257
60	6	0	8.408059	1.049876	1.276460
61	1	0	9.501872	1.074746	1.266296
62	1	0	8.050594	2.078195	1.389849
63	1	0	8.086658	0.478209	2.151729
64	6	0	8.380229	1.204188	-1.264557
65	1	0	8.042563	0.739745	-2.195424
66	1	0	8.017781	2.236889	-1.247411
67	1	0	9.473961	1.233513	-1.273528
68	17	0	-1.019270	-2.882211	-1.638572
69	17	0	-4.843078	-0.846467	1.870866
70	17	0	-5.413815	4.704294	-0.273294

Tipp$_2$PyBTM (D_1 state, UB3LYP/6-31G(d, p))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	2.170105	2.824387	-2.034916
2	17	0	-0.317955	-0.155442	-2.112958
3	17	0	0.404312	-0.281096	2.187707
4	17	0	-2.196095	2.731670	2.219129
5	7	0	0.164124	6.370854	0.346117
6	6	0	3.530159	0.834039	-0.886917
7	1	0	4.286972	1.106439	-1.612457
8	6	0	1.536104	0.135453	0.913502
9	6	0	-2.337030	1.531130	0.931395
10	6	0	1.049443	5.589513	0.978230
11	1	0	1.811234	6.085544	1.574377
12	6	0	0.052702	3.457826	0.184119
13	6	0	-3.532396	0.822424	0.901765
14	6	0	-3.728053	-0.219215	-0.012993
15	6	0	2.345458	1.541145	-0.853483
16	6	0	1.018220	4.204094	0.934913
17	6	0	-1.509802	0.235023	-0.867008
18	6	0	-2.683936	-0.507897	-0.898343
19	6	0	2.670568	-0.645911	0.821519
20	6	0	-1.248499	1.292698	0.045444
21	6	0	1.271519	1.260522	0.063212
22	6	0	-0.855338	4.348750	-0.477944
23	6	0	-0.772475	5.728191	-0.367517
24	6	0	0.019452	2.026667	0.097068

25	1	0	-1.488033	6.343677	-0.906824
26	6	0	3.716736	-0.301864	-0.067459
27	1	0	-4.308728	1.064386	1.618665
28	6	0	-5.009824	-0.999035	-0.039721
29	6	0	-5.129361	-2.190849	0.714847
30	6	0	-6.099628	-0.544053	-0.816023
31	6	0	-6.334803	-2.899675	0.674951
32	6	0	-7.284836	-1.291105	-0.819222
33	6	0	-7.427690	-2.469244	-0.084274
34	1	0	-6.421987	-3.813759	1.256366
35	1	0	-8.125666	-0.943993	-1.415075
36	6	0	4.951075	-1.090061	-0.121366
37	6	0	4.895471	-2.513394	-0.354396
38	6	0	6.232213	-0.448469	0.064383
39	6	0	6.081705	-3.226862	-0.389132
40	6	0	7.378254	-1.227971	0.008892
41	6	0	7.340551	-2.615234	-0.211336
42	1	0	6.045779	-4.291810	-0.592333
43	1	0	8.344248	-0.761514	0.173422
44	1	0	2.794774	-1.478566	1.503347
45	1	0	-2.797168	-1.295352	-1.634714
46	6	0	6.380570	1.023916	0.438952
47	1	0	5.392173	1.485579	0.447598
48	6	0	3.599145	-3.251404	-0.685272
49	1	0	2.768156	-2.547760	-0.615029
50	6	0	8.617885	-3.423994	-0.257525
51	1	0	9.447743	-2.730820	-0.078758
52	6	0	-6.027113	0.732261	-1.653218
53	1	0	-5.028780	1.160063	-1.527238
54	6	0	-3.984824	-2.725887	1.575169
55	1	0	-3.144264	-2.032503	1.484508
56	6	0	-8.734948	-3.251273	-0.112947
57	1	0	-9.417913	-2.708732	-0.779413
58	6	0	7.245517	1.792657	-0.578505
59	1	0	8.274176	1.418942	-0.600885
60	1	0	6.840109	1.716513	-1.592233
61	1	0	7.282915	2.851921	-0.306783
62	6	0	6.942176	1.170164	1.869737
63	1	0	6.311419	0.652219	2.598339
64	1	0	7.955518	0.763305	1.947937
65	1	0	6.982073	2.228489	2.145059
66	6	0	3.616839	-3.759475	-2.142580
67	1	0	3.778624	-2.938113	-2.846983
68	1	0	4.406286	-4.501584	-2.300228
69	1	0	2.659136	-4.231042	-2.383401
70	6	0	3.320235	-4.400919	0.301430
71	1	0	4.089264	-5.178103	0.246755
72	1	0	3.278801	-4.044704	1.335523
73	1	0	2.359484	-4.868247	0.064942
74	6	0	8.829734	-4.059651	-1.648579
75	1	0	9.790330	-4.583205	-1.671261
76	1	0	8.045720	-4.787472	-1.880510
77	1	0	8.834612	-3.301062	-2.436509
78	6	0	8.650469	-4.494790	0.852992
79	1	0	8.530167	-4.045448	1.842939
80	1	0	7.858567	-5.238367	0.717807
81	1	0	9.609929	-5.020410	0.830010
82	6	0	-9.396873	-3.311363	1.276525
83	1	0	-9.568104	-2.307428	1.677525
84	1	0	-10.362472	-3.825704	1.221630
85	1	0	-8.770331	-3.855347	1.991850
86	6	0	-8.547122	-4.664371	-0.695954
87	1	0	-8.111780	-4.624566	-1.699442
88	1	0	-7.884724	-5.269329	-0.067117
89	1	0	-9.508827	-5.184614	-0.762212
90	6	0	-3.494580	-4.100017	1.080324
91	1	0	-4.280476	-4.859162	1.157853
92	1	0	-3.177174	-4.053866	0.033613
93	1	0	-2.642645	-4.440856	1.678799
94	6	0	-4.367849	-2.779332	3.066463
95	1	0	-4.676347	-1.794495	3.431360
96	1	0	-5.193614	-3.476258	3.246066
97	1	0	-3.515200	-3.112282	3.668291
98	6	0	-7.037714	1.789527	-1.169109
99	1	0	-8.069958	1.440667	-1.281914
100	1	0	-6.880600	2.033400	-0.113608
101	1	0	-6.932824	2.712560	-1.749530

102	6	0	-6.208616	0.440641	-3.155119
103	1	0	-5.464657	-0.278997	-3.511567
104	1	0	-7.201197	0.029543	-3.368912
105	1	0	-6.097179	1.360835	-3.738843
106	17	0	2.192562	3.373937	1.961175
107	17	0	-2.081739	3.748629	-1.597959

TippF$_2$PyBTM (D_1 state, UB3LYP/6-31G(d, p))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	4.684273	0.431027	-2.071261
2	17	0	1.109128	-1.102811	-2.240122
3	17	0	1.720640	-1.664291	2.111027
4	17	0	0.699928	1.962919	2.340536
5	7	0	4.002125	4.623612	0.115449
6	6	0	5.136880	-1.895308	-0.847108
7	1	0	5.958652	-1.963283	-1.548491
8	6	0	3.002604	-1.710598	0.898314
9	6	0	0.026208	1.042476	1.010766
10	6	0	4.694152	3.562041	0.566490
11	1	0	5.688292	3.736331	0.971707
12	6	0	2.915056	1.919205	0.067752
13	6	0	-1.349427	0.939693	0.968552
14	6	0	-1.978107	0.114770	0.010862
15	6	0	4.321642	-0.769035	-0.832897
16	6	0	4.202914	2.271560	0.559907
17	6	0	0.216331	-0.357929	-0.924106
18	6	0	-1.151947	-0.556902	-0.922141
19	6	0	3.774123	-2.868439	0.893480
20	6	0	0.904033	0.429446	0.050091
21	6	0	3.215230	-0.590499	0.048296
22	6	0	2.239978	3.081737	-0.396233
23	6	0	2.772752	4.355131	-0.355236
24	6	0	2.364408	0.601604	0.061663
25	1	0	2.179409	5.182037	-0.738640
26	6	0	4.852202	-2.944582	0.020358
27	1	0	-1.940985	1.434642	1.729111
28	6	0	-3.434789	-0.027633	-0.038091
29	6	0	-4.040766	-1.338634	0.003710
30	6	0	-4.276053	1.146059	-0.135556
31	6	0	-5.419914	-1.431777	-0.050139
32	6	0	-5.650471	0.972748	-0.177229
33	6	0	-6.255177	-0.296143	-0.139087
34	1	0	-5.881854	-2.411021	0.011924
35	1	0	-6.291636	1.842575	-0.275844
36	1	0	3.553833	-3.675552	1.580272
37	1	0	-1.599101	-1.162193	-1.701331
38	6	0	-3.720446	2.555505	-0.319112
39	1	0	-2.631705	2.513466	-0.269582
40	6	0	-3.237143	-2.617825	0.230338
41	1	0	-2.175132	-2.367616	0.237719
42	6	0	-7.759241	-0.435496	-0.189944
43	1	0	-8.177453	0.574511	-0.266010
44	9	0	0.994532	2.935887	-0.927352
45	9	0	4.992535	1.297420	1.079850
46	6	0	-8.307315	-1.074405	1.104932
47	1	0	-8.012496	-0.500866	1.988279
48	1	0	-9.400294	-1.103388	1.064381
49	1	0	-7.949044	-2.101201	1.228890
50	6	0	-8.210632	-1.228813	-1.434648
51	1	0	-7.848345	-0.764072	-2.356030
52	1	0	-7.847498	-2.261031	-1.407311
53	1	0	-9.303636	-1.259572	-1.473401
54	6	0	-3.464103	-3.650405	-0.889874
55	1	0	-4.501480	-3.998814	-0.917900
56	1	0	-3.223501	-3.237630	-1.874544
57	1	0	-2.826357	-4.523626	-0.722865
58	6	0	-3.551824	-3.219211	1.616601
59	1	0	-3.353698	-2.499097	2.416058

60	1	0	-4.599362	-3.528853	1.691031
61	1	0	-2.926903	-4.100667	1.789366
62	6	0	-4.201873	3.512386	0.788637
63	1	0	-5.287894	3.647125	0.764947
64	1	0	-3.931608	3.146688	1.784091
65	1	0	-3.742010	4.495732	0.652248
66	6	0	-4.072631	3.102272	-1.719695
67	1	0	-3.703479	2.440065	-2.508418
68	1	0	-5.153904	3.214666	-1.848540
69	1	0	-3.612937	4.085549	-1.857853
70	17	0	5.862719	-4.384369	0.006771

$Tipp_2F_2PyBTM$ (D_1 state, UB3LYP/6-31G(d, p))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	2.132902	2.689610	-2.335519
2	17	0	-0.432015	-0.220810	-2.193448
3	17	0	0.377559	-0.027040	2.155935
4	17	0	-2.108892	2.828366	2.105773
5	7	0	-0.220262	6.405086	-0.432292
6	6	0	3.538316	0.891754	-0.936080
7	1	0	4.298769	1.114497	-1.675949
8	6	0	1.552913	0.347539	0.887218
9	6	0	-2.326725	1.584862	0.891010
10	6	0	0.856980	5.772611	0.067604
11	1	0	1.689483	6.380733	0.414236
12	6	0	-0.072923	3.499966	-0.223091
13	6	0	-3.528492	0.908153	0.914036
14	6	0	-3.747009	-0.198618	0.064793
15	6	0	2.326485	1.570616	-0.982474
16	6	0	0.953250	4.400080	0.181738
17	6	0	-1.555544	0.205870	-0.912636
18	6	0	-2.709468	-0.550025	-0.834337
19	6	0	2.744597	-0.367786	0.937771
20	6	0	-1.267161	1.307583	-0.046194
21	6	0	1.258988	1.357898	-0.065912
22	6	0	-1.176875	4.230019	-0.745325
23	6	0	-1.227407	5.607517	-0.825840
24	6	0	-0.019670	2.078548	-0.109383
25	1	0	-2.116066	6.073840	-1.245053
26	6	0	3.771006	-0.096877	0.027594
27	1	0	-4.275616	1.180759	1.649464
28	6	0	-5.005867	-0.945847	0.087458
29	6	0	-4.999424	-2.378067	0.274080
30	6	0	-6.264210	-0.254789	-0.084526
31	6	0	-6.208622	-3.051413	0.280238
32	6	0	-7.435445	-0.996663	-0.059066
33	6	0	-7.445428	-2.391089	0.118328
34	1	0	-6.210642	-4.122688	0.450132
35	1	0	-8.384530	-0.493508	-0.213249
36	6	0	5.073729	-0.840031	0.079170
37	6	0	5.227467	-2.052869	-0.634401
38	6	0	6.149432	-0.328733	0.839899
39	6	0	6.452226	-2.726008	-0.570026
40	6	0	7.354786	-1.042177	0.869882
41	6	0	7.531347	-2.240150	0.175361
42	1	0	6.565749	-3.656641	-1.119864
43	1	0	8.184751	-0.651870	1.454166
44	1	0	2.883465	-1.118249	1.707590
45	1	0	-2.856563	-1.362896	-1.535200
46	6	0	6.039942	0.973800	1.631554
47	1	0	5.033535	1.373919	1.481537
48	6	0	4.098384	-2.649264	-1.474499
49	1	0	3.238228	-1.977841	-1.404961
50	6	0	8.859429	-2.984668	0.232270
51	1	0	9.526659	-2.400014	0.878774
52	6	0	-6.359937	1.232467	-0.414941
53	1	0	-5.355830	1.658544	-0.411072
54	6	0	-3.730389	-3.166302	0.593403

55	1	0	-2.874253	-2.492806	0.528401
56	6	0	-8.749127	-3.157061	0.135933
57	1	0	-9.555365	-2.429853	-0.012672
58	9	0	-2.249703	3.530925	-1.209055
59	9	0	2.083235	3.896247	0.740452
60	6	0	7.031046	2.036996	1.120932
61	1	0	8.069976	1.717433	1.256892
62	1	0	6.880144	2.239832	0.055870
63	1	0	6.897824	2.977074	1.667205
64	6	0	6.213135	0.737655	3.144112
65	1	0	5.481364	0.014566	3.518358
66	1	0	7.212211	0.355470	3.380283
67	1	0	6.076469	1.674469	3.695140
68	6	0	4.481399	-2.741088	-2.963900
69	1	0	4.760316	-1.760276	-3.361999
70	1	0	5.327307	-3.418889	-3.121738
71	1	0	3.638473	-3.118966	-3.552776
72	6	0	3.648729	-4.019871	-0.933426
73	1	0	4.456010	-4.758322	-0.987741
74	1	0	3.331625	-3.948208	0.111940
75	1	0	2.806054	-4.404664	-1.518238
76	6	0	9.524478	-3.077194	-1.153884
77	1	0	10.503864	-3.562263	-1.079954
78	1	0	8.914203	-3.664181	-1.848990
79	1	0	9.668367	-2.084250	-1.591346
80	6	0	8.709114	-4.380276	0.866097
81	1	0	8.271861	-4.315796	1.867474
82	1	0	8.063630	-5.024994	0.259577
83	1	0	9.684294	-4.871936	0.951163
84	6	0	-8.981013	-3.841459	1.500418
85	1	0	-8.960426	-3.115704	2.318430
86	1	0	-9.958580	-4.332994	1.503183
87	1	0	-8.221993	-4.604048	1.701614
88	6	0	-8.817948	-4.179779	-1.017804
89	1	0	-8.685595	-3.693892	-1.988741
90	1	0	-8.049743	-4.952940	-0.916184
91	1	0	-9.793741	-4.674844	-1.012898
92	6	0	-3.493516	-4.316363	-0.403204
93	1	0	-4.286502	-5.069298	-0.352399
94	1	0	-3.443211	-3.952988	-1.434383
95	1	0	-2.547809	-4.816433	-0.173350
96	6	0	-3.765568	-3.684789	2.046975
97	1	0	-3.892112	-2.863133	2.758225
98	1	0	-4.585307	-4.394423	2.199653
99	1	0	-2.827663	-4.197285	2.281833
100	6	0	-7.196752	1.999831	0.626955
101	1	0	-8.237514	1.660672	0.640396
102	1	0	-6.792996	1.880231	1.637128
103	1	0	-7.198192	3.067275	0.386595
104	6	0	-6.917228	1.441783	-1.839528
105	1	0	-6.306397	0.923398	-2.584572
106	1	0	-7.945059	1.075662	-1.928516
107	1	0	-6.917903	2.508685	-2.082680

Ph*F_2PyBTM (D_1 state, UB3LYP/6-31G(d, p))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.093604	1.861472	2.400040
2	17	0	1.314757	-1.817365	2.026554
3	17	0	0.636277	-1.058858	-2.284011
4	17	0	4.128231	0.641951	-2.067748
5	7	0	3.542110	4.588030	0.563021
6	6	0	-1.894499	0.801012	0.966036
7	1	0	-2.506620	1.258188	1.735266
8	6	0	-0.274130	-0.356541	-0.940814
9	6	0	3.803550	-0.664905	-0.927236
10	6	0	2.319771	4.380400	0.042152
11	1	0	1.749742	5.248341	-0.282495
12	6	0	2.399018	1.911923	0.251885

13	6	0	4.638995	-1.770325	-1.047260
14	6	0	4.390486	-2.885457	-0.255246
15	6	0	-0.514856	0.965779	1.005476
16	6	0	1.761170	3.128735	-0.121707
17	6	0	2.546238	-1.748949	0.759132
18	6	0	3.337225	-2.889950	0.650110
19	6	0	-1.648914	-0.567221	-0.987317
20	6	0	2.712007	-0.569768	-0.017377
21	6	0	0.389870	0.415098	0.052764
22	6	0	3.681711	2.200912	0.798586
23	6	0	4.200614	3.473124	0.929035
24	6	0	1.842137	0.607067	0.098138
25	1	0	5.189823	3.586301	1.367374
26	6	0	-2.481500	0.022130	-0.033635
27	1	0	5.446892	-1.769036	-1.767772
28	6	0	-3.967398	-0.170920	-0.077450
29	6	0	-4.566586	-1.233790	0.613668
30	6	0	-4.776193	0.710643	-0.810030
31	6	0	-6.017155	-1.413982	0.575264
32	6	0	-6.225672	0.521274	-0.850096
33	6	0	-6.818645	-0.583221	-0.221595
34	1	0	-2.068442	-1.164566	-1.788887
35	1	0	3.151698	-3.746817	1.284947
36	6	0	-4.183161	1.852618	-1.571817
37	1	0	-4.441259	2.802505	-1.084958
38	1	0	-3.099727	1.785732	-1.622080
39	1	0	-4.588561	1.902907	-2.586909
40	6	0	-3.745009	-2.209579	1.394328
41	1	0	-2.683416	-2.096087	1.191446
42	1	0	-3.902016	-2.056171	2.470348
43	1	0	-4.044803	-3.239565	1.179216
44	6	0	-8.301262	-0.846390	-0.362684
45	1	0	-8.523977	-1.910179	-0.278089
46	1	0	-8.879116	-0.322060	0.407465
47	1	0	-8.669308	-0.517283	-1.334830
48	9	0	4.449904	1.168832	1.244614
49	9	0	0.527296	3.071517	-0.697769
50	6	0	-7.067426	1.524225	-1.577835
51	1	0	-6.627303	2.520509	-1.560718
52	1	0	-7.165166	1.232855	-2.633473
53	1	0	-8.073305	1.583162	-1.163662
54	6	0	-6.634553	-2.505213	1.395189
55	1	0	-6.691505	-3.429633	0.802756
56	1	0	-6.051874	-2.731053	2.287157
57	1	0	-7.650137	-2.253771	1.699689
58	17	0	5.421472	-4.306965	-0.402042

Ph*$_2$F$_2$PyBTM (D_0 state, UB3LYP/6-31G(d, p))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-2.130558	2.429030	2.240853
2	17	0	0.407881	-0.478935	2.163743
3	17	0	-0.433791	-0.409614	-2.208296
4	17	0	2.149829	2.510966	-2.175269
5	7	0	-0.049587	6.134619	0.004805
6	6	0	-3.523677	0.540615	0.950063
7	1	0	-4.273122	0.777625	1.696828
8	6	0	-1.568394	-0.019734	-0.901501
9	6	0	2.327472	1.298049	-0.903517
10	6	0	-1.078118	5.399644	-0.457813
11	1	0	-1.943375	5.927220	-0.853671
12	6	0	-0.018644	3.204833	-0.001892
13	6	0	3.532273	0.605235	-0.916095
14	6	0	3.746982	-0.450222	-0.026894
15	6	0	-2.323609	1.242420	0.941501
16	6	0	-1.086507	4.020034	-0.477762
17	6	0	1.546619	-0.038666	0.884095
18	6	0	2.728927	-0.772053	0.873345
19	6	0	-2.747419	-0.759905	-0.899557

20	6	0	1.256112	1.039403	0.001108
21	6	0	-1.269202	1.022305	0.014134
22	6	0	1.029833	4.041161	0.479345
23	6	0	0.993417	5.420486	0.465216
24	6	0	-0.006412	1.779995	0.006217
25	1	0	1.847279	5.964531	0.863754
26	6	0	-3.756911	-0.484695	0.027445
27	1	0	4.290697	0.871693	-1.643615
28	6	0	5.037257	-1.212646	-0.041224
29	6	0	5.174306	-2.365589	-0.827013
30	6	0	6.124174	-0.781377	0.734527
31	6	0	6.435136	-3.106258	-0.835355
32	6	0	7.384297	-1.522845	0.717606
33	6	0	7.496891	-2.719684	-0.003374
34	6	0	-5.045238	-1.255797	0.031851
35	6	0	-5.147186	-2.444074	0.786335
36	6	0	-6.146283	-0.776815	-0.709811
37	6	0	-6.358619	-3.164194	0.785493
38	6	0	-7.354570	-1.502096	-0.703308
39	6	0	-7.448901	-2.707576	0.019301
40	1	0	-2.890726	-1.534780	-1.644196
41	1	0	2.863989	-1.572443	1.592077
42	6	0	-6.036853	0.502119	-1.518229
43	1	0	-6.692790	1.287295	-1.122855
44	1	0	-5.021561	0.896372	-1.515080
45	1	0	-6.327729	0.342221	-2.562090
46	6	0	-3.966541	-2.951872	1.592173
47	1	0	-3.076109	-2.346490	1.428033
48	1	0	-4.177100	-2.938012	2.668493
49	1	0	-3.717348	-3.986308	1.331396
50	6	0	-8.731409	-3.515341	-0.025153
51	1	0	-8.542001	-4.582946	0.101630
52	1	0	-9.430136	-3.216629	0.768478
53	1	0	-9.255198	-3.390522	-0.974835
54	6	0	6.021777	0.433589	1.600008
55	1	0	6.613526	1.251828	1.168017
56	1	0	4.994984	0.777177	1.693119
57	1	0	6.432031	0.245414	2.596455
58	6	0	4.042183	-2.870491	-1.663802
59	1	0	3.114598	-2.348734	-1.444534
60	1	0	4.269092	-2.726568	-2.728412
61	1	0	3.893228	-3.944997	-1.519496
62	6	0	8.754342	-3.555900	0.077987
63	1	0	8.536080	-4.612752	-0.077036
64	1	0	9.489817	-3.253552	-0.676670
65	1	0	9.226175	-3.465163	1.056639
66	9	0	2.140780	3.456387	1.011822
67	9	0	-2.184981	3.415631	-1.010704
68	6	0	-8.559341	-0.994719	-1.472272
69	1	0	-8.468714	0.060916	-1.727606
70	1	0	-8.703176	-1.542917	-2.413099
71	1	0	-9.480721	-1.110479	-0.894317
72	6	0	-6.500241	-4.432082	1.605710
73	1	0	-6.442399	-5.331820	0.978472
74	1	0	-5.722546	-4.520128	2.364076
75	1	0	-7.463251	-4.468627	2.123261
76	6	0	6.578012	-4.290815	-1.741222
77	1	0	6.290237	-5.205895	-1.203969
78	1	0	5.940421	-4.220162	-2.620894
79	1	0	7.608977	-4.421636	-2.069937
80	6	0	8.550287	-0.983758	1.488717
81	1	0	8.541934	0.104840	1.535576
82	1	0	8.515444	-1.350804	2.524413
83	1	0	9.499927	-1.303953	1.062064

Xyl_2F_2PyBTM (D_1 state, UB3LYP/6-31G(d, p))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-2.233422	2.152381	2.113132

2	17	0	0.445789	-0.719640	2.224777
3	17	0	-0.259437	-0.867175	-2.086637
4	17	0	2.130974	2.142670	-2.194593
5	7	0	0.088178	5.768827	0.096054
6	6	0	-3.551903	0.233391	0.799193
7	1	0	-4.326416	0.485596	1.512560
8	6	0	-1.486422	-0.419864	-0.894066
9	6	0	2.353173	0.963140	-0.915927
10	6	0	-0.946548	5.085115	-0.422926
11	1	0	-1.772964	5.652614	-0.844524
12	6	0	0.019920	2.860675	0.042961
13	6	0	3.561316	0.304962	-0.890617
14	6	0	3.797111	-0.761259	0.016906
15	6	0	-2.358616	0.940248	0.834107
16	6	0	-1.004224	3.705243	-0.464681
17	6	0	1.584095	-0.345864	0.941608
18	6	0	2.756702	-1.070687	0.930806
19	6	0	-2.658656	-1.161987	-0.927414
20	6	0	1.279193	0.699709	0.006559
21	6	0	-1.248798	0.677593	-0.020491
22	6	0	1.078011	3.641579	0.579048
23	6	0	1.092199	5.023062	0.585870
24	6	0	0.006571	1.428883	0.004735
25	1	0	1.945601	5.536117	1.023015
26	6	0	-3.733863	-0.839136	-0.087142
27	1	0	4.305400	0.553783	-1.636692
28	6	0	5.076018	-1.450593	0.019642
29	6	0	5.233717	-2.856165	0.307700
30	6	0	6.247484	-0.692105	-0.285354
31	6	0	6.519395	-3.386757	0.318950
32	6	0	7.502561	-1.250192	-0.252398
33	6	0	7.669137	-2.622653	0.059036
34	1	0	6.638589	-4.448178	0.515330
35	1	0	8.374820	-0.636823	-0.454715
36	6	0	-4.979970	-1.648150	-0.113749
37	6	0	-4.865216	-3.050761	-0.103168
38	6	0	-6.274362	-1.076913	-0.171131
39	6	0	-5.982467	-3.877538	-0.127799
40	6	0	-7.382530	-1.933840	-0.199059
41	6	0	-7.270424	-3.327938	-0.169431
42	1	0	-5.853962	-4.956730	-0.111467
43	1	0	-8.374283	-1.490731	-0.260226
44	1	0	-2.754856	-1.967179	-1.646322
45	1	0	2.908768	-1.818272	1.695927
46	6	0	-6.514423	0.415504	-0.244491
47	1	0	-6.541167	0.875734	0.750400
48	1	0	-5.735996	0.928711	-0.814579
49	1	0	-7.478322	0.621994	-0.717625
50	6	0	-8.495810	-4.209632	-0.167053
51	1	0	-8.332378	-5.122594	-0.747940
52	1	0	-8.756847	-4.519202	0.852712
53	1	0	-9.363900	-3.690142	-0.582304
54	6	0	4.075278	-3.799371	0.520733
55	1	0	3.762364	-3.825468	1.571268
56	1	0	3.203720	-3.528507	-0.077967
57	1	0	4.371656	-4.816602	0.254911
58	6	0	9.037168	-3.232820	0.089295
59	1	0	9.004441	-4.297566	0.326483
60	1	0	9.538671	-3.104839	-0.877333
61	1	0	9.664865	-2.728942	0.834129
62	9	0	2.139846	2.994816	1.130910
63	9	0	-2.089923	3.140034	-1.048512
64	1	0	6.145467	0.367113	-0.489321
65	1	0	-3.875092	-3.494631	-0.054722

$Biph_2F_2PyBTM$ (D_0 state, UB3LYP/6-31G(d, p))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-2.252355	-1.594054	-2.246876

2	17	0	1.018834	0.549955	-2.157840
3	17	0	0.255778	0.605190	2.174626
4	17	0	1.877901	-2.882041	2.096816
5	7	0	-1.019570	-5.774097	-0.300007
6	6	0	-3.097146	0.525141	-0.852215
7	1	0	-3.898803	0.505887	-1.579956
8	6	0	-0.992243	0.547130	0.920401
9	6	0	2.404277	-1.738921	0.877316
10	6	0	-1.853880	-4.857644	0.222352
11	1	0	-2.811917	-5.200518	0.606345
12	6	0	-0.327506	-2.948068	-0.142862
13	6	0	3.744237	-1.406027	0.893293
14	6	0	4.239120	-0.393734	0.050224
15	6	0	-2.113872	-0.450993	-0.906521
16	6	0	-1.550234	-3.513229	0.313658
17	6	0	1.995210	-0.185303	-0.890945
18	6	0	3.323052	0.209150	-0.852343
19	6	0	-1.945926	1.556475	0.976576
20	6	0	1.434919	-1.167575	-0.029492
21	6	0	-1.003781	-0.520370	-0.016342
22	6	0	0.504448	-3.964811	-0.685567
23	6	0	0.157265	-5.300785	-0.742029
24	6	0	0.025313	-1.563849	-0.063454
25	1	0	0.860323	-6.005140	-1.180747
26	6	0	-3.035077	1.555957	0.096971
27	1	0	4.394104	-1.871780	1.624138
28	6	0	5.650278	-0.012967	0.065167
29	6	0	6.081909	1.348573	-0.134722
30	6	0	6.631388	-1.016303	0.207157
31	6	0	7.459880	1.604935	-0.301673
32	6	0	7.979034	-0.725342	0.081464
33	6	0	8.397140	0.592897	-0.188710
34	1	0	7.790976	2.626988	-0.447045
35	1	0	8.712828	-1.520155	0.163741
36	6	0	-4.041902	2.651332	0.136685
37	6	0	-3.572170	3.976399	0.168733
38	6	0	-5.442127	2.424860	0.104535
39	6	0	-4.441959	5.063789	0.150409
40	6	0	-6.302130	3.535811	0.071943
41	6	0	-5.817900	4.841906	0.092440
42	1	0	-4.046297	6.074784	0.168617
43	1	0	-7.373909	3.361943	0.062443
44	1	0	-1.865621	2.319016	1.742573
45	1	0	3.677914	0.920554	-1.586170
46	9	0	1.714071	-3.606788	-1.194640
47	9	0	-2.469145	-2.703397	0.897909
48	1	0	6.316081	-2.043962	0.348154
49	1	0	-2.500069	4.148542	0.174551
50	1	0	9.453638	0.818648	-0.285361
51	1	0	-6.511098	5.677466	0.074100
52	6	0	-6.058017	1.066466	0.151734
53	6	0	-7.054085	0.709187	-0.772325
54	6	0	-5.708335	0.138545	1.147643
55	6	0	-7.674447	-0.539425	-0.710022
56	1	0	-7.331588	1.410962	-1.553567
57	6	0	-6.330588	-1.107169	1.212300
58	1	0	-4.950534	0.399914	1.879099
59	6	0	-7.314818	-1.452504	0.282685
60	1	0	-8.435632	-0.798824	-1.440118
61	1	0	-6.047707	-1.808316	1.991953
62	1	0	-7.796123	-2.424683	0.332069
63	6	0	5.157819	2.486390	-0.081163
64	6	0	5.336896	3.596980	-0.941291
65	6	0	4.107240	2.539587	0.877839
66	6	0	4.486603	4.688394	-0.869806
67	1	0	6.118505	3.570527	-1.692470
68	6	0	3.273123	3.648851	0.957141
69	1	0	3.992507	1.730143	1.587894
70	6	0	3.452266	4.721654	0.082444
71	1	0	4.615760	5.518603	-1.556069
72	1	0	2.488610	3.677966	1.705305
73	1	0	2.798399	5.585601	0.139015

Results of TD-DFT calculations in dichloromethane

TippPyBTM (Optimized ground state structure, UB3LYP/6-31G(d, p))

```
Excitation energies and oscillator strengths:

 Excited State   1:  2.059-A     2.4901 eV  497.91 nm  f=0.0003  <S**2>=0.810
    174B ->177B      -0.23212
    175B ->177B      -0.14021
    176B ->177B       0.95895
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-DFT) =  -4551.03043382
 Copying the excited state density for this state as the 1-particle RhoCI density.

 Excited State   2:  2.073-A     2.5254 eV  490.96 nm  f=0.0050  <S**2>=0.824
    173B ->177B       0.27771
    174B ->177B      -0.27667
    175B ->177B       0.90082

 Excited State   3:  2.132-A     2.5584 eV  484.61 nm  f=0.0388  <S**2>=0.886
    177A ->179A       0.17102
    171B ->177B       0.15267
    172B ->177B       0.15574
    173B ->177B       0.75021
    174B ->177B      -0.38335
    175B ->177B      -0.39601
    176B ->177B      -0.11938
```

Tipp$_2$PyBTM (Optimized ground state structure, UB3LYP/6-31G(d, p))

```
Excitation energies and oscillator strengths:

 Excited State   1:  2.124-A     2.5509 eV  486.04 nm  f=0.0388  <S**2>=0.878
    225A -> 227A     -0.15909
    217B -> 225B     -0.19443
    218B -> 225B      0.41992
    219B -> 225B      0.70405
    222B -> 225B     -0.46962
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-DFT) =  -4676.35012023
 Copying the excited state density for this state as the 1-particle RhoCI density.

 Excited State   2:  2.064-A     2.5633 eV  483.69 nm  f=0.0000  <S**2>=0.815
    220B -> 225B     -0.35186
    221B -> 225B     -0.13762
    223B -> 225B      0.60393
    224B -> 225B      0.69312

 Excited State   3:  2.060-A     2.5692 eV  482.58 nm  f=0.0007  <S**2>=0.811
    218B -> 225B      0.15402
    219B -> 225B     -0.14117
    222B -> 225B     -0.20010
    223B -> 225B      0.71901
    224B -> 225B     -0.62649
```

TippF$_2$PyBTM (Optimized ground state structure, UB3LYP/6-31G(d, p))

```
Excitation energies and oscillator strengths:

 Excited State   1:  2.058-A     2.5288 eV  490.29 nm  f=0.0004  <S**2>=0.809
    166B ->169B      -0.25734
    167B ->169B      -0.16973
    168B ->169B       0.94474
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-DFT) =  -3830.31293209
 Copying the excited state density for this state as the 1-particle RhoCI density.

 Excited State   2:  2.060-A     2.5718 eV  482.10 nm  f=0.0012  <S**2>=0.810
    165B ->169B      -0.15561
    166B ->169B      -0.11538
    167B ->169B       0.96233
    168B ->169B       0.15723
```

```
 Excited State   3:  2.143-A     2.6280 eV  471.77 nm  f=0.0295  <S**2>=0.898
    169A ->171A       0.15373
    165B ->169B       0.87121
    166B ->169B      -0.33425
    167B ->169B       0.14452
    168B ->169B      -0.14470
```

Tipp$_2$F$_2$PyBTM (Optimized ground state structure, UB3LYP/6-31G(d, p))

```
Excitation energies and oscillator strengths:

 Excited State   1:  2.065-A     2.5938 eV  478.00 nm  f=0.0003  <S**2>=0.816
    212B -> 217B     -0.44128
    216B -> 217B      0.88003
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-DFT) =  -3955.63246159
 Copying the excited state density for this state as the 1-particle RhoCI density.

 Excited State   2:  2.063-A     2.6050 eV  475.95 nm  f=0.0018  <S**2>=0.814
    210B -> 217B      0.23067
    211B -> 217B      0.18798
    214B -> 217B     -0.23431
    215B -> 217B      0.92013

 Excited State   3:  2.105-A     2.6319 eV  471.08 nm  f=0.0236  <S**2>=0.858
    217A -> 219A     -0.12184
    210B -> 217B     -0.63512
    211B -> 217B      0.19498
    214B -> 217B      0.64515
    215B -> 217B      0.30129
```

Ph*F$_2$PyBTM (Optimized ground state structure, UB3LYP/6-31G(d, p))

```
Excitation energies and oscillator strengths:

 Excited State   1:  2.054-A     2.2023 eV  562.96 nm  f=0.0000  <S**2>=0.805
    152B ->153B       0.99802
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-DFT) =  -3673.05979405
 Copying the excited state density for this state as the 1-particle RhoCI density.

 Excited State   2:  2.056-A     2.3466 eV  528.35 nm  f=0.0000  <S**2>=0.806
    151B ->153B       0.99686

 Excited State   3:  2.129-A     2.6215 eV  472.95 nm  f=0.0224  <S**2>=0.884
    153A ->155A       0.13693
    146B ->153B       0.11981
    149B ->153B       0.74169
    150B ->153B      -0.60083
```

Ph*$_2$F$_2$PyBTM (Optimized ground state structure, UB3LYP/6-31G(d, p))

```
Excitation energies and oscillator strengths:

 Excited State   1:  2.054-A     2.2869 eV  542.15 nm  f=0.0000  <S**2>=0.805
    184B ->185B       0.99745
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-DFT) =  -3641.11340266
 Copying the excited state density for this state as the 1-particle RhoCI density.

 Excited State   2:  2.054-A     2.2876 eV  541.99 nm  f=0.0001  <S**2>=0.805
    183B ->185B       0.99803

 Excited State   3:  2.057-A     2.4292 eV  510.40 nm  f=0.0000  <S**2>=0.807
    182B ->185B       0.99524
```

Xyl$_2$F$_2$PyBTM (Optimized ground state structure, UB3LYP/6-31G(d, p))

```
Excitation energies and oscillator strengths:

 Excited State   1:  2.115-A     2.3036 eV  538.23 nm  f=0.1235  <S**2>=0.868
    161A ->163A      -0.12962
    153B ->161B      -0.24800
    160B ->161B       0.93476
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-DFT) =  -3405.22248803
 Copying the excited state density for this state as the 1-particle RhoCI density.

 Excited State   2:  2.118-A     2.4007 eV  516.45 nm  f=0.0427  <S**2>=0.872
    161A ->162A      -0.14612
    152B ->161B       0.24515
    156B ->161B      -0.14156
    159B ->161B       0.92397

 Excited State   3:  2.075-A     2.6819 eV  462.30 nm  f=0.0044  <S**2>=0.827
    156B ->161B       0.95112
    158B ->161B       0.21741
    159B ->161B       0.15354
```

$Biph_2F_2PyBTM$ (Optimized ground state structure, UB3LYP/6-31G(d, p))

```
Excitation energies and oscillator strengths:

 Excited State   1:  2.109-A     2.2703 eV  546.12 nm  f=0.0941  <S**2>=0.862
    185A ->186A      -0.11569
    175B ->185B       0.14929
    182B ->185B       0.29659
    184B ->185B       0.91133
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-DFT) =  -3710.06567380
 Copying the excited state density for this state as the 1-particle RhoCI density.

 Excited State   2:  2.106-A     2.3585 eV  525.70 nm  f=0.0297  <S**2>=0.859
    185A ->187A      -0.12599
    172B ->185B      -0.15488
    181B ->185B       0.27994
    183B ->185B       0.91455

 Excited State   3:  2.097-A     2.6274 eV  471.88 nm  f=0.0038  <S**2>=0.849
    176B ->185B      -0.10199
    178B ->185B       0.41113
    180B ->185B       0.53158
    181B ->185B       0.48855
    182B ->185B       0.43330
    183B ->185B      -0.16632
    184B ->185B      -0.13913
```

TippPyBTM (Optimized first doublet excited state structure, UB3LYP/6-31G(d))

```
Excitation energies and oscillator strengths:

 Excited State   1:  2.069-A     1.8438 eV  672.42 nm  f=0.1000  <S**2>=0.820
    170B ->177B      -0.11147
    172B ->177B      -0.14699
    173B ->177B      -0.16310
    176B ->177B       0.95598
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-DFT) =  -4551.04394543
 Copying the excited state density for this state as the 1-particle RhoCI density.

 Excited State   2:  2.073-A     2.3646 eV  524.34 nm  f=0.0072  <S**2>=0.825
    171B ->177B      -0.15071
    173B ->177B      -0.21080
    174B ->177B       0.92400
    175B ->177B      -0.20069

 Excited State   3:  2.060-A     2.3847 eV  519.93 nm  f=0.0010  <S**2>=0.810
    173B ->177B       0.16383
    174B ->177B       0.23704
    175B ->177B       0.95021
```

Tipp$_2$PyBTM (Optimized first doublet excited state structure, UB3LYP/6-31G(d))

```
Excitation energies and oscillator strengths:

 Excited State   1:  2.075-A     1.8925 eV  655.13 nm  f=0.1031  <S**2>=0.826
    216B -> 225B      0.14726
    218B -> 225B      0.20947
    224B -> 225B      0.94907
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-DFT) =  -4676.36406924
 Copying the excited state density for this state as the 1-particle RhoCI density.

 Excited State   2:  2.059-A     2.3368 eV  530.57 nm  f=0.0034  <S**2>=0.810
    218B -> 225B      0.15391
    219B -> 225B     -0.29723
    220B -> 225B      0.28733
    222B -> 225B     -0.25071
    223B -> 225B      0.84713

 Excited State   3:  2.064-A     2.3774 eV  521.51 nm  f=0.0078  <S**2>=0.815
    216B -> 225B      0.14643
    217B -> 225B      0.10504
    218B -> 225B     -0.28205
    220B -> 225B     -0.39645
    222B -> 225B      0.72473
    223B -> 225B      0.42262
```

TippF$_2$PyBTM (Optimized first doublet excited state structure, UB3LYP/6-31G(d))

```
Excitation energies and oscillator strengths:

 Excited State   1:  2.075-A     1.9059 eV  650.52 nm  f=0.0957  <S**2>=0.827
    162B ->169B      -0.11062
    164B ->169B       0.19364
    168B ->169B       0.95953
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-DFT) =  -3830.32604321
 Copying the excited state density for this state as the 1-particle RhoCI density.

 Excited State   2:  2.072-A     2.4272 eV  510.80 nm  f=0.0108  <S**2>=0.823
    163B ->169B       0.14887
    166B ->169B       0.96854

 Excited State   3:  2.058-A     2.4632 eV  503.34 nm  f=0.0004  <S**2>=0.809
    167B ->169B       0.99094
```

Tipp$_2$F$_2$PyBTM (Optimized first doublet excited state structure, UB3LYP/6-31G(d))

```
Excitation energies and oscillator strengths:

 Excited State   1:  2.084-A     1.9595 eV  632.72 nm  f=0.1002  <S**2>=0.835
    217A -> 218A      0.10760
    208B -> 217B      0.14882
    210B -> 217B     -0.16943
    216B -> 217B      0.95297
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-DFT) =  -3955.64602799
 Copying the excited state density for this state as the 1-particle RhoCI density.

 Excited State   2:  2.058-A     2.4177 eV  512.82 nm  f=0.0018  <S**2>=0.808
    210B -> 217B     -0.13845
    211B -> 217B      0.31866
    212B -> 217B     -0.23284
    214B -> 217B     -0.18147
    215B -> 217B      0.88173

 Excited State   3:  2.072-A     2.4642 eV  503.13 nm  f=0.0136  <S**2>=0.823
    208B -> 217B      0.10236
    209B -> 217B      0.15581
    210B -> 217B      0.11752
    211B -> 217B      0.17872
    212B -> 217B      0.77520
    214B -> 217B      0.46218
    215B -> 217B      0.27629
```

Ph*F$_2$PyBTM (Optimized first doublet excited state structure, UB3LYP/6-31G(d))

```
Excitation energies and oscillator strengths:

 Excited State   1:  2.048-A     1.6246 eV  763.18 nm  f=0.0000  <S**2>=0.799
    152B ->153B       0.99892
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-DFT) =  -3673.07057295
 Copying the excited state density for this state as the 1-particle RhoCI density.

 Excited State   2:  2.050-A     2.2181 eV  558.95 nm  f=0.0003  <S**2>=0.800
    151B ->153B       0.99739

 Excited State   3:  2.081-A     2.4013 eV  516.33 nm  f=0.0063  <S**2>=0.833
    147B ->153B       0.13692
    148B ->153B      -0.26512
    149B ->153B      -0.21497
    150B ->153B       0.90791
```

Ph*$_2$F$_2$PyBTM (Optimized first doublet excited state structure, UB3LYP/6-31G(d))

```
Excitation energies and oscillator strengths:

 Excited State   1:  2.049-A     1.7027 eV  728.18 nm  f=0.0000  <S**2>=0.799
    184B ->185B       0.99883
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-DFT) =  -3641.12435299
 Copying the excited state density for this state as the 1-particle RhoCI density.

 Excited State   2:  2.048-A     2.0600 eV  601.86 nm  f=0.0000  <S**2>=0.799
    183B ->185B       0.99811

 Excited State   3:  2.050-A     2.2134 eV  560.16 nm  f=0.0002  <S**2>=0.801
    182B ->185B       0.99583
```

Xyl$_2$F$_2$PyBTM (Optimized first doublet excited state structure, UB3LYP/6-31G(d))

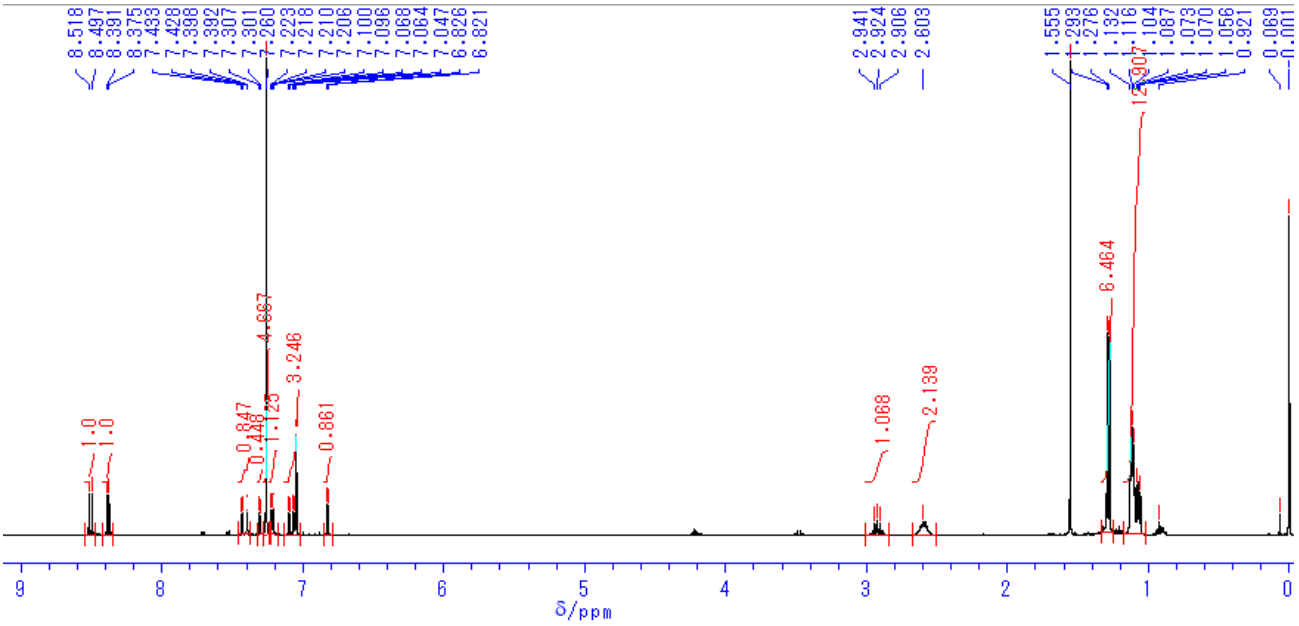
```
Excitation energies and oscillator strengths:

 Excited State   1:  2.112-A     1.9050 eV  650.84 nm  f=0.1372  <S**2>=0.865
    161A ->162A       0.15043
```

```
   153B ->161B       0.15865
   160B ->161B       0.95544
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-DFT) =  -3405.22990239
 Copying the excited state density for this state as the 1-particle RhoCI density.

 Excited State   2:  2.101-A     2.2212 eV  558.18 nm  f=0.0864  <S**2>=0.853
   161A ->163A       0.14709
   152B ->161B       0.20617
   155B ->161B      -0.11667
   159B ->161B       0.93101

 Excited State   3:  2.080-A     2.5109 eV  493.78 nm  f=0.0091  <S**2>=0.831
   154B ->161B       0.24704
   155B ->161B       0.26875
   156B ->161B       0.90174
   157B ->161B      -0.11643
   158B ->161B       0.10932
```

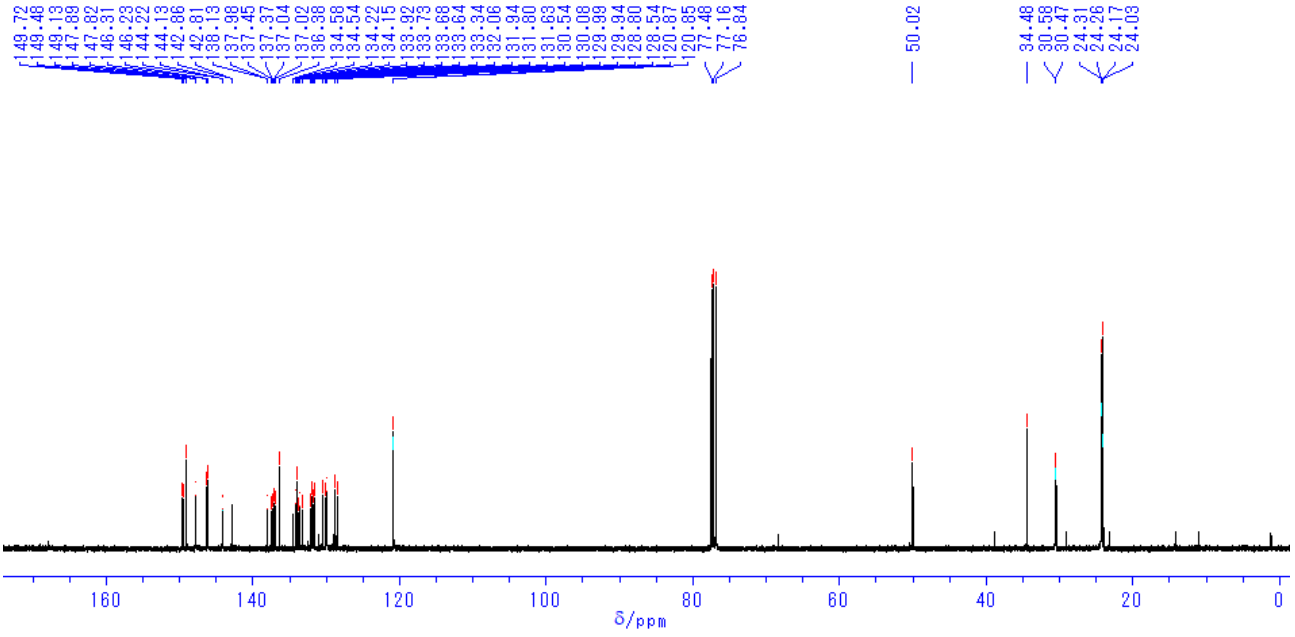
$Biph_2F_2PyBTM$ (Optimized first doublet excited state structure, UB3LYP/6-31G(d))

```
Excitation energies and oscillator strengths:

 Excited State   1:  2.100-A     1.8147 eV  683.22 nm  f=0.0895  <S**2>=0.853
   185A ->186A       0.12262
   182B ->185B       0.19439
   184B ->185B       0.95374
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-DFT) =  -3710.07389682
 Copying the excited state density for this state as the 1-particle RhoCI density.

 Excited State   2:  2.085-A     2.1640 eV  572.95 nm  f=0.0674  <S**2>=0.837
   185A ->187A      -0.11043
   173B ->185B      -0.10488
   181B ->185B       0.25849
   183B ->185B       0.92645

 Excited State   3:  2.085-A     2.4548 eV  505.06 nm  f=0.0037  <S**2>=0.836
   173B ->185B      -0.11584
   176B ->185B       0.12897
   178B ->185B       0.40200
   179B ->185B       0.55797
   180B ->185B       0.20058
   181B ->185B       0.61296
   182B ->185B       0.10235
   183B ->185B      -0.16573
```

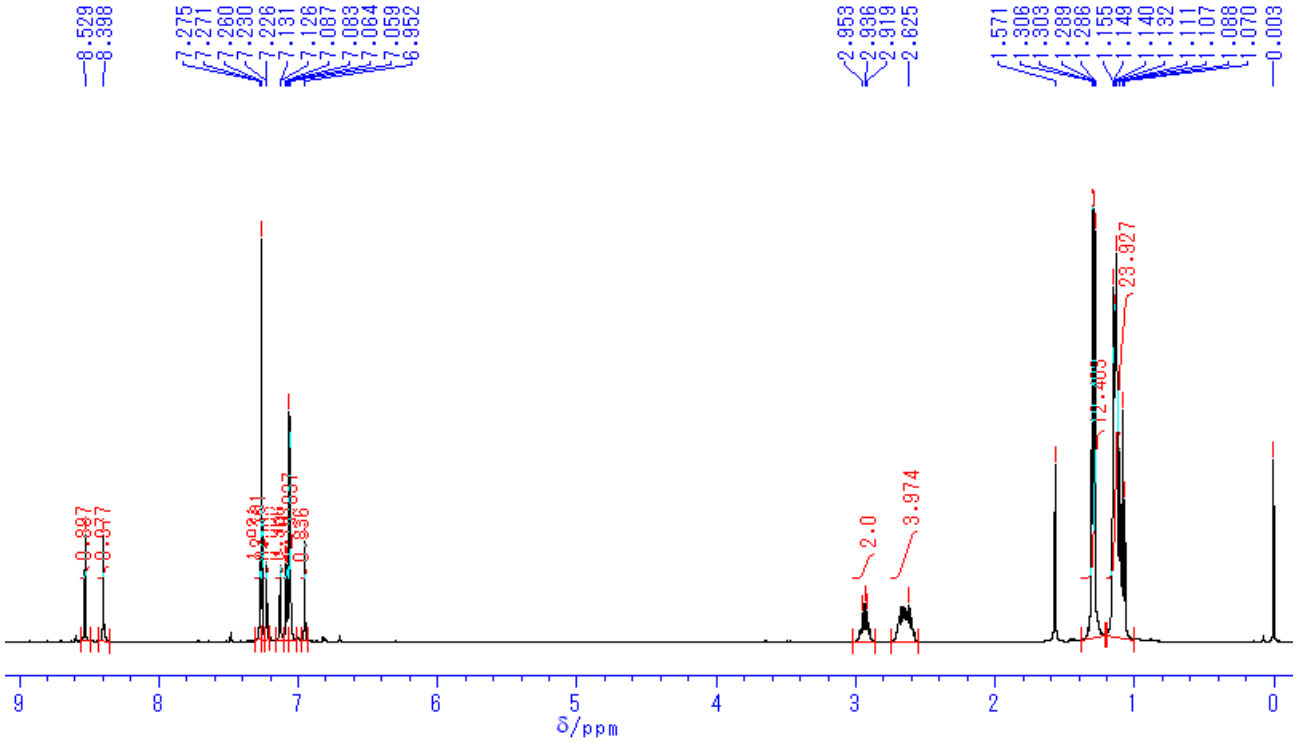
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of αH-TippPyBTM (**1H**)



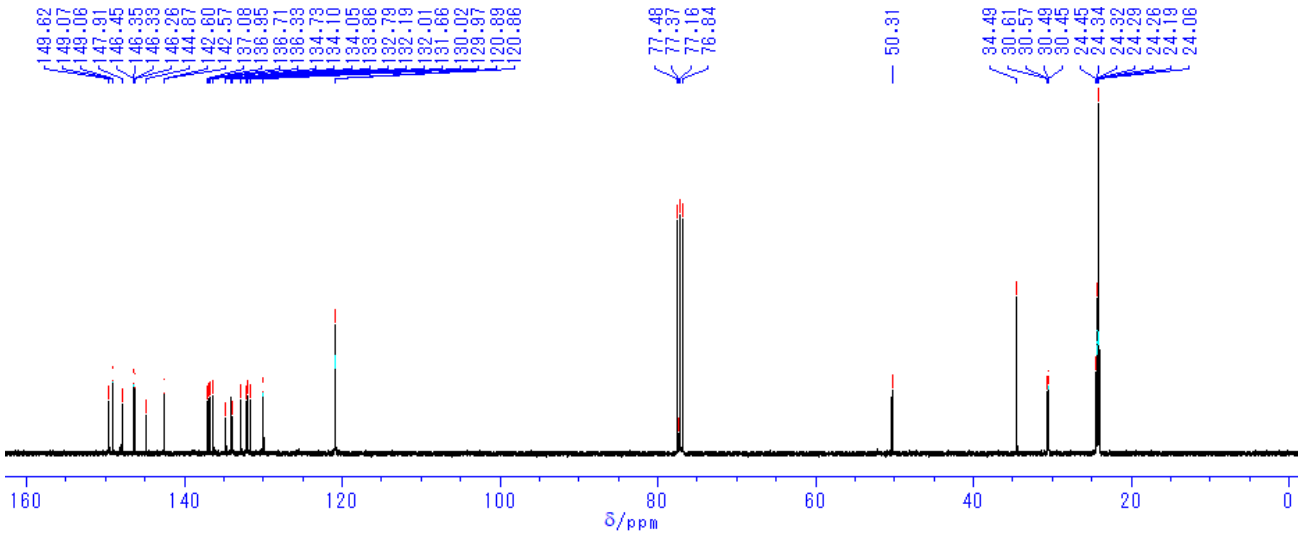
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of αH-TippPyBTM (**1H**)



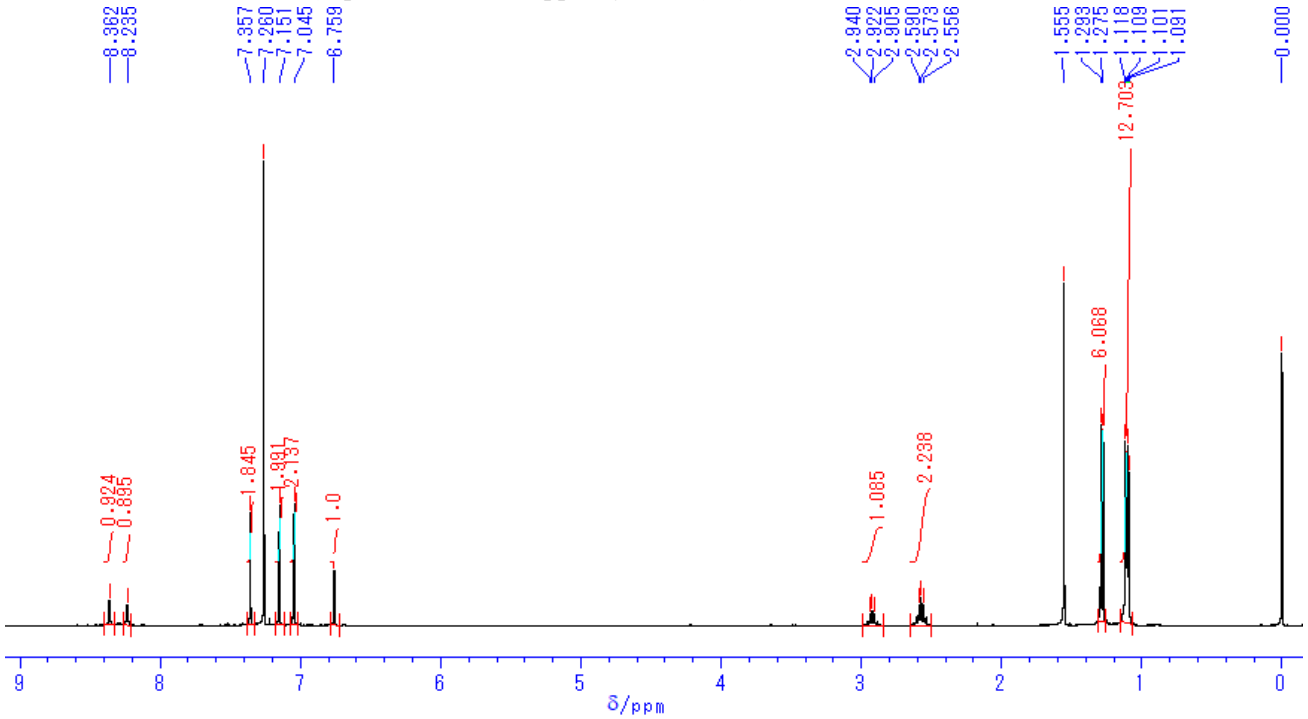
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of αH-TippPyBTM (**2H**)



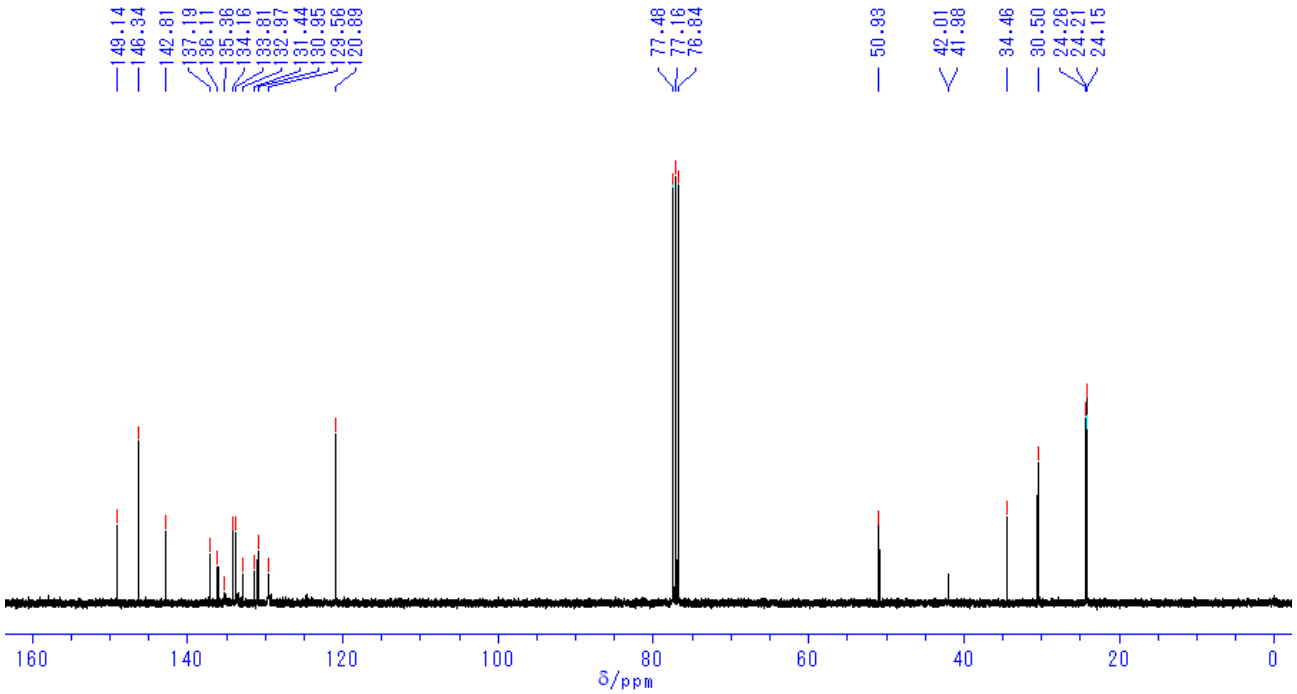
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of αH-Tipp$_2$PyBTM (**2H**)



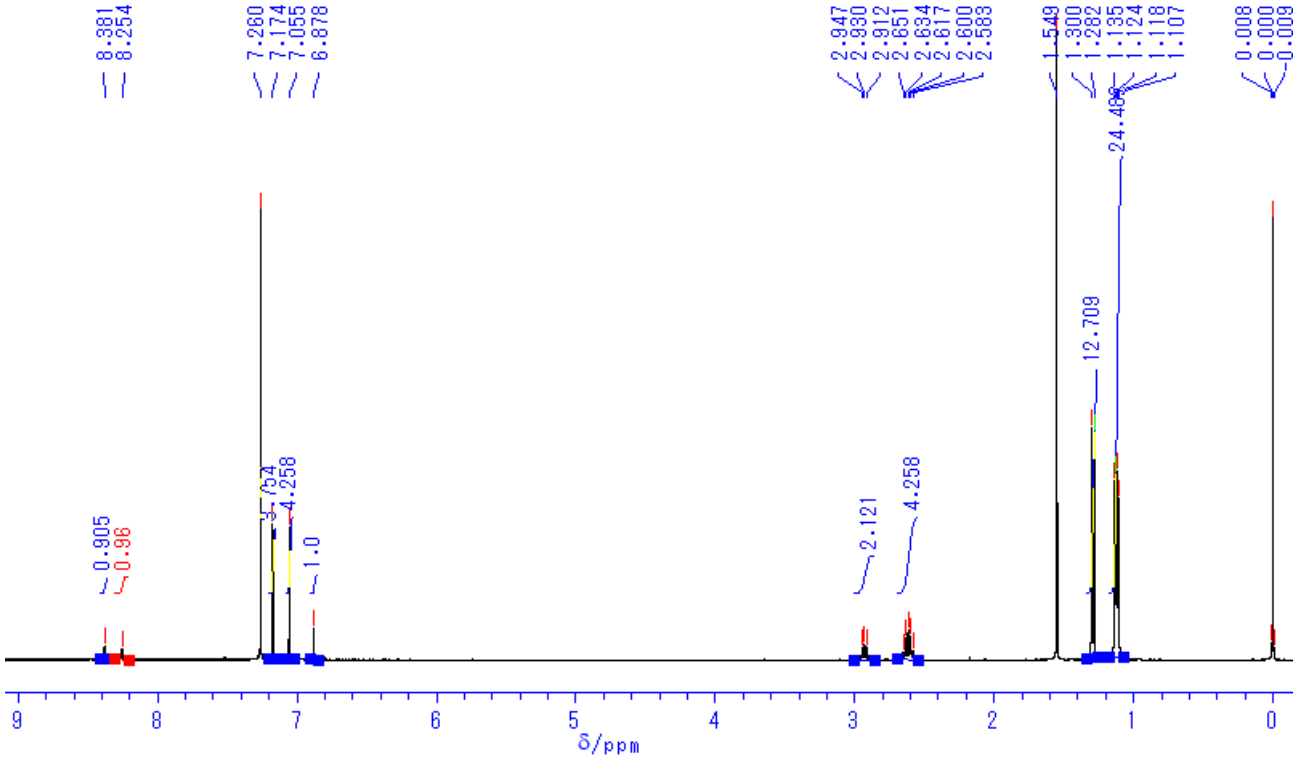
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of αH-TippF_2PyBTM (**3H**)



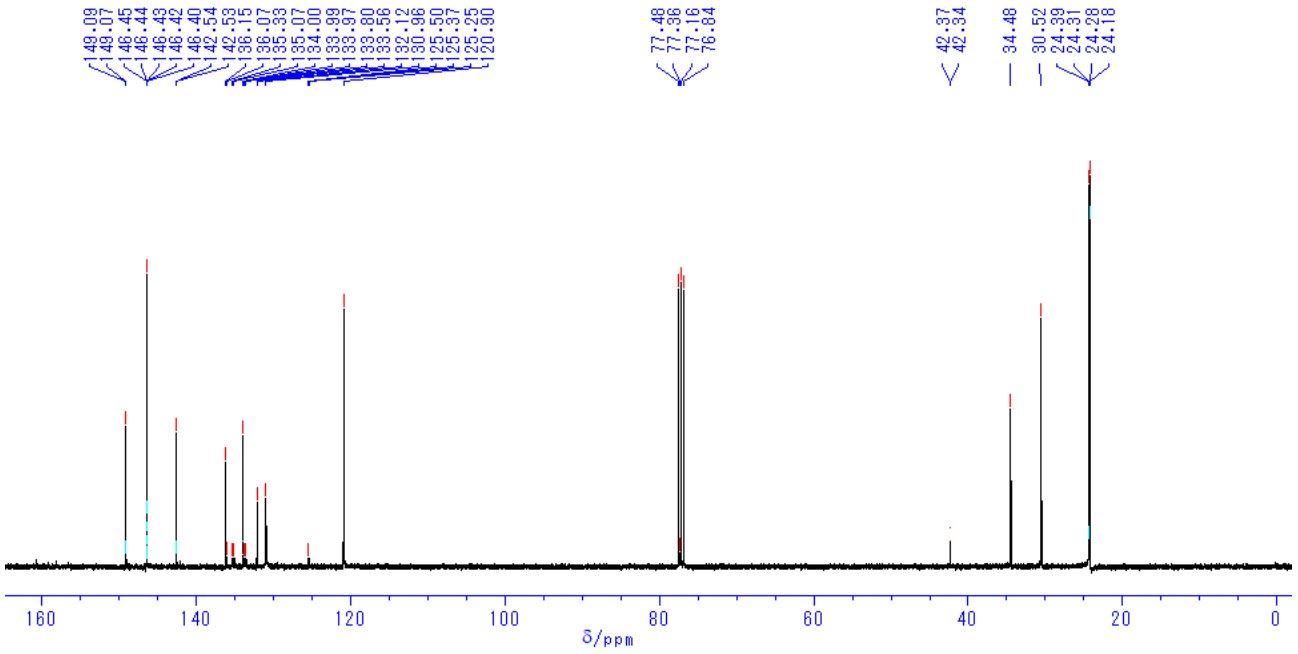
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of αH-TippF_2PyBTM (**3H**)



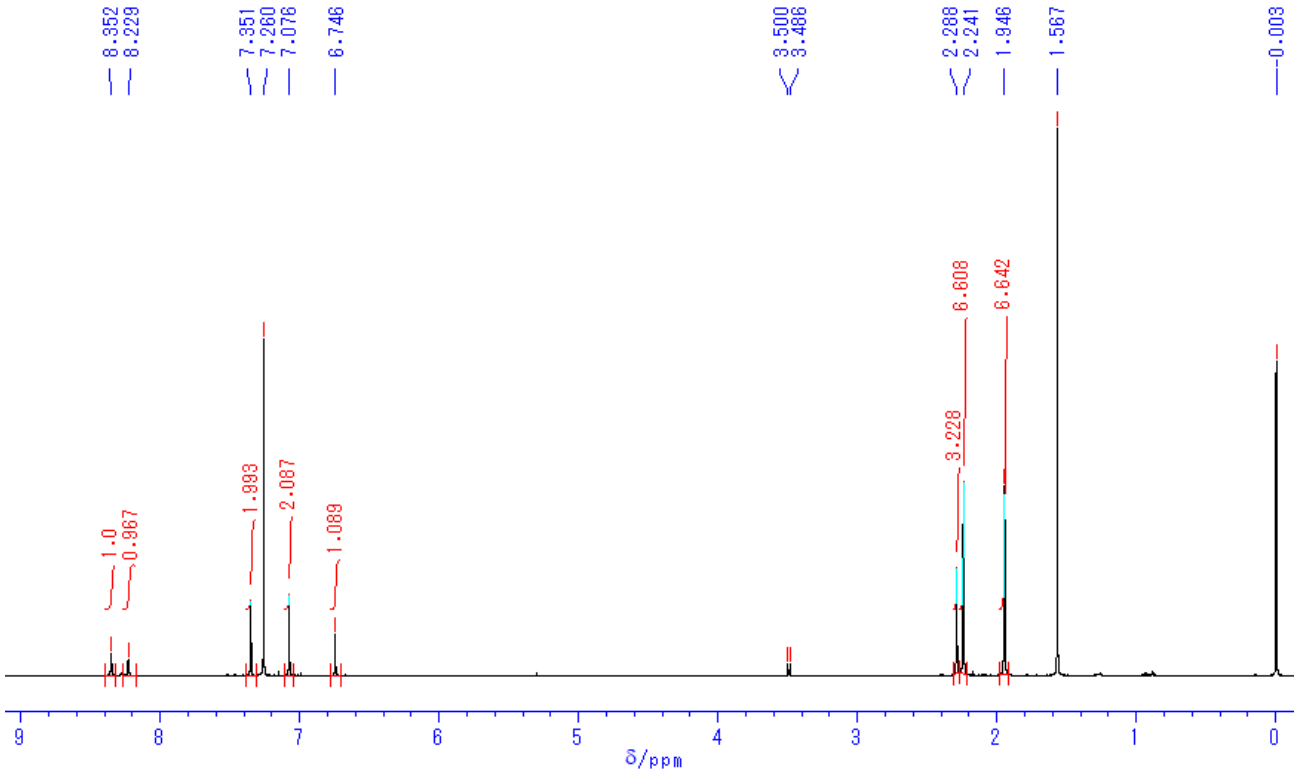
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of αH-Tipp$_2$F$_2$PyBTM (**4H**)



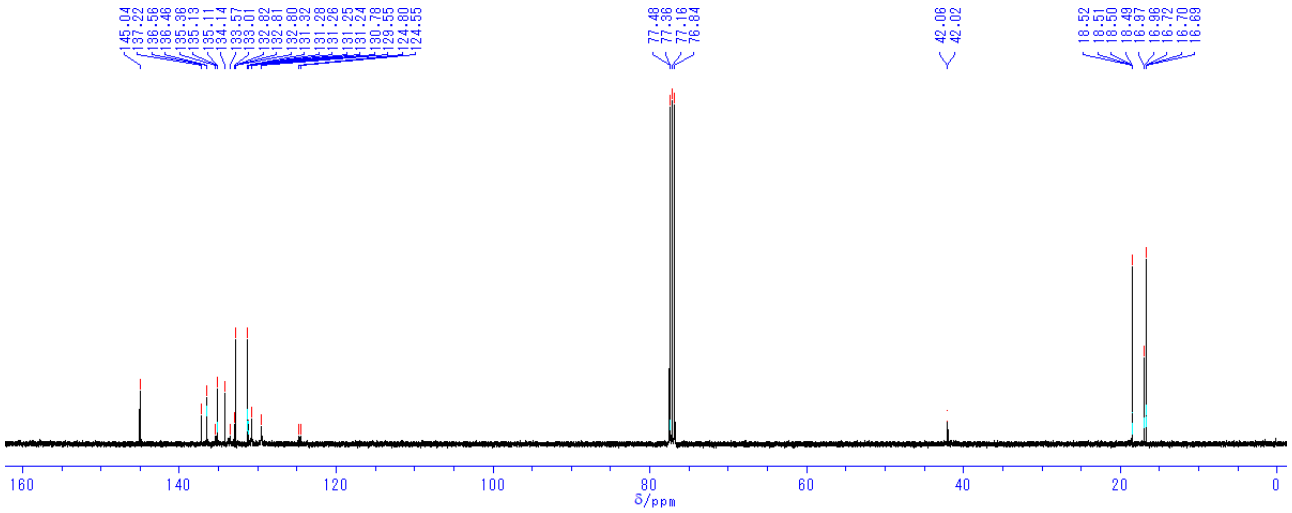
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of αH-Tipp$_2$F$_2$PyBTM (**4H**)



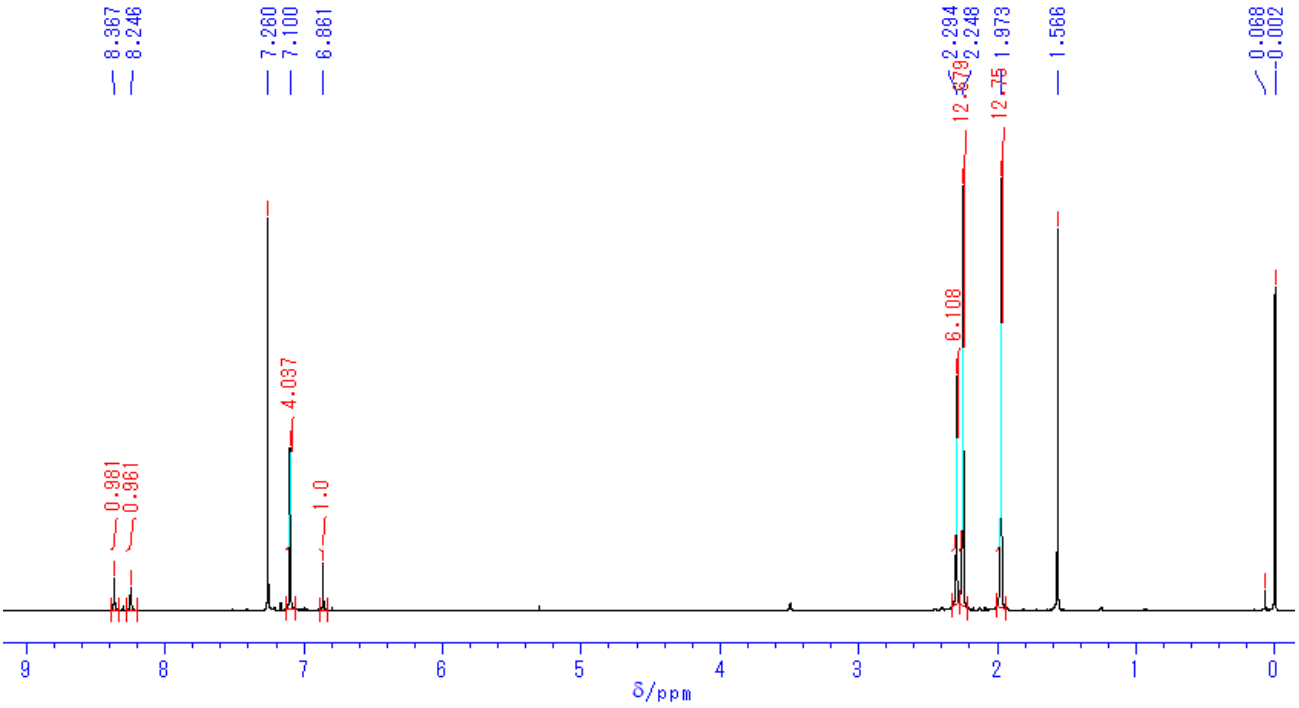
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of αH-Ph*F_2PyBTM (**5H**)



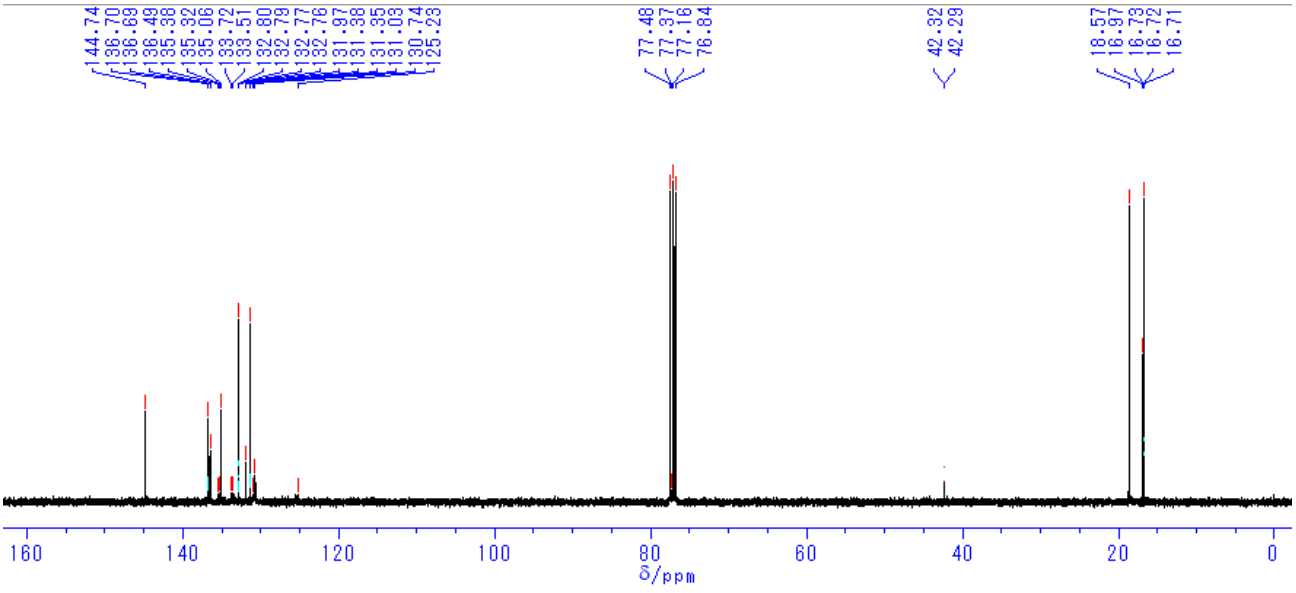
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of αH-Ph*F_2PyBTM (**5H**)



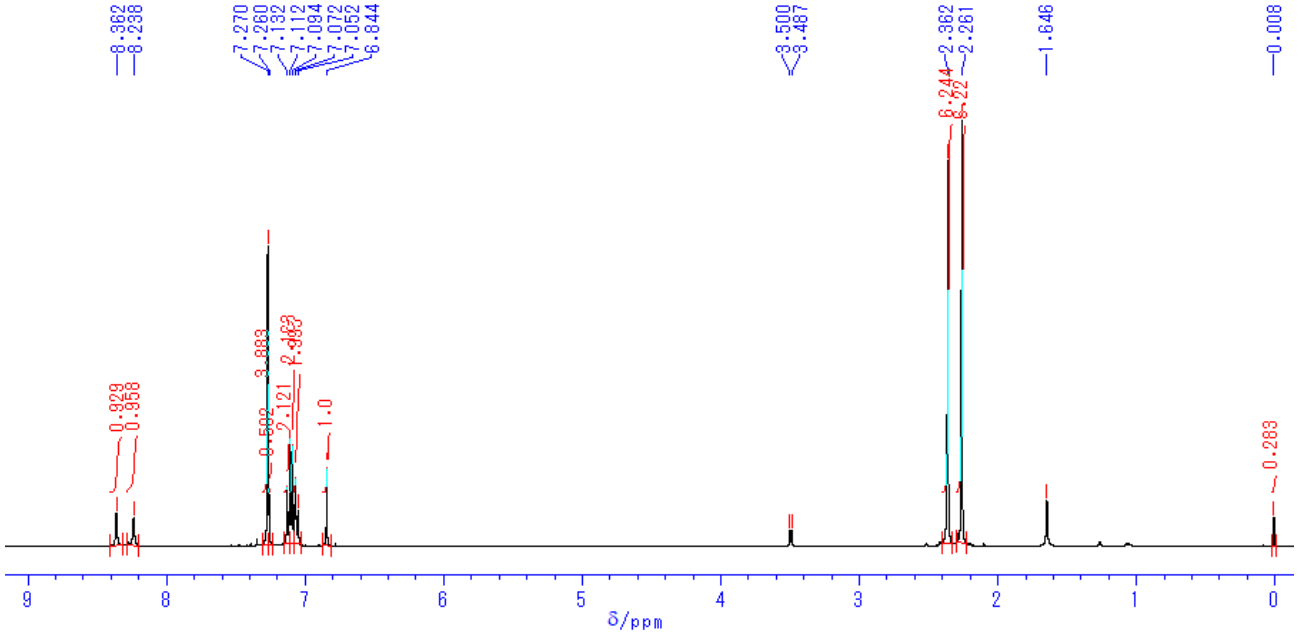
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of αH-Ph*$_2$F$_2$PyBTM (**6H**)



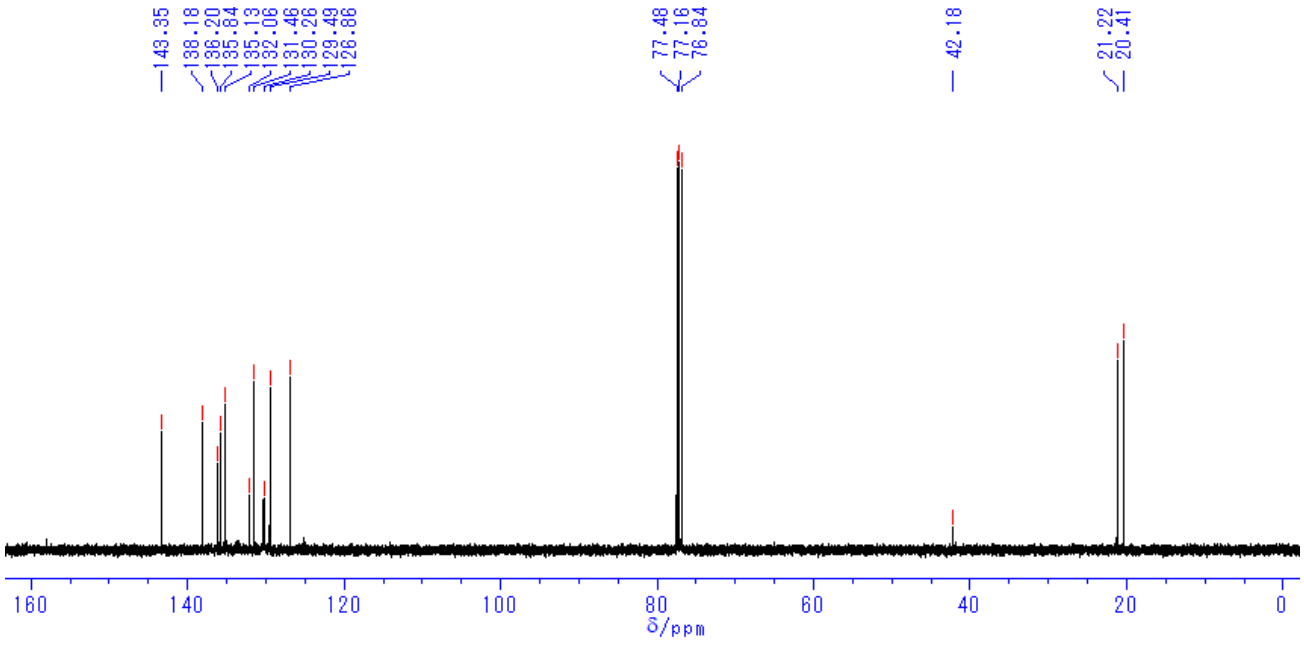
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of αH-Ph*$_2$F$_2$PyBTM (**6H**)



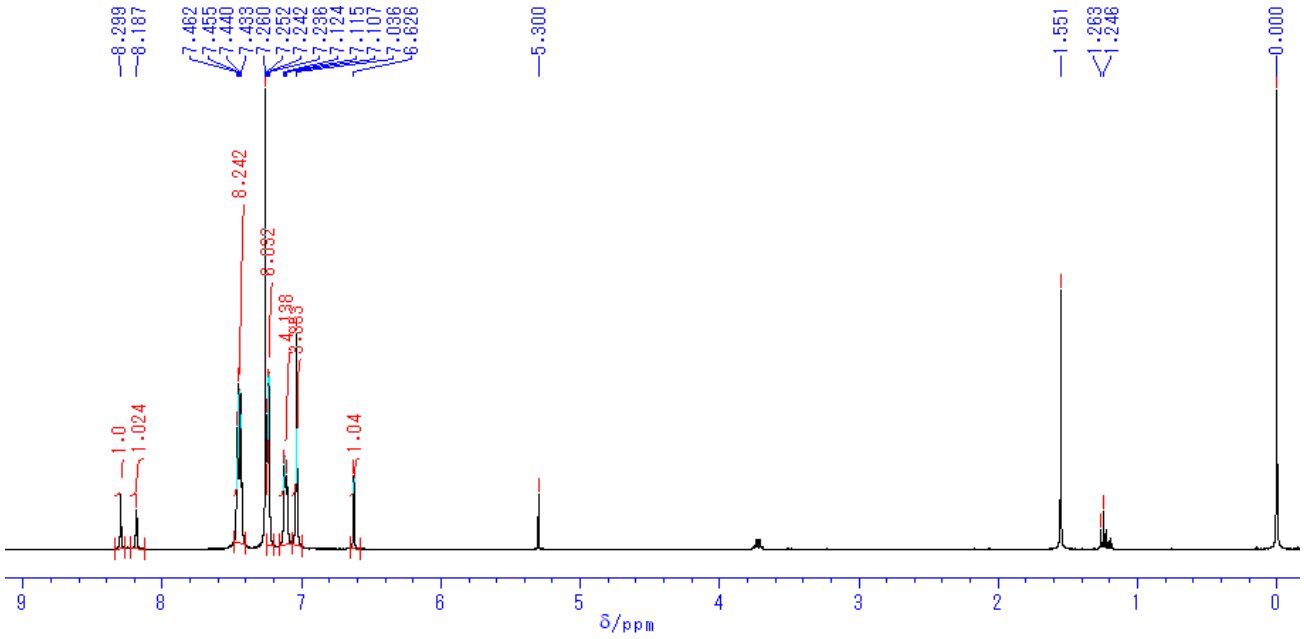
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of αH-Xyl$_2$F$_2$PyBTM (**7H**)



^{13}C NMR (100 MHz, $CDCl_3$) spectrum of αH-Xyl$_2$F$_2$PyBTM (**7H**)



^{1}H NMR (400 MHz, $CDCl_3$) spectrum of αH-Biph$_2$F$_2$PyBTM (**8H**)



^{13}C NMR (100 MHz, $CDCl_3$) spectrum of αH-Biph$_2$F$_2$PyBTM (**8H**)