Supplementary Information (SI) for Physical Chemistry Chemical Physics.

Role of peripheral F-/H-atoms and tert-butyl substituent in charge transfer of axially substituted titanium phthalocyanines

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Table S1. Optimized cartesian coordinate of structure CYLY6-2.

Charge	0	Multiplicity	1

Tag	Symbol	X	Y	Z
1	Ti	-4.76832	-0.089331	-0.026178
2	N	-5.583958	-0.560357	1.830108
3	C	-5.79137	0.344882	2.857468
4	N	-5.907505	1.654524	2.769437
5	C	-5.906105	2.301205	1.616238
6	N	-5.777492	1.773888	0.350917
7	C	-5.763143	2.815799	-0.549501
8	N	-5.602313	2.754316	-1.860251
9	C	-5.44016	1.619478	-2.5105
10	N	-5.338415	0.34444	-1.980359
11	C	-5.349383	-0.566281	-3.023152
12	N	-5.409382	-1.880647	-2.947474
13	C	-5.538252	-2.530421	-1.803512
14	N	-5.615153	-2.001783	-0.534142
15	C	-5.678411	-3.044744	0.36252
16	N	-5.709558	-2.979974	1.682675
17	C	-5.697697	-1.840775	2.344988
18	C	-5.895718	-1.757422	3.780814
19	C	-5.95466	-0.38271	4.103134
20	C	-6.175157	0.033108	5.413313
21	F	-6.243227	1.318159	5.75576
22	C	-6.322758	-0.941461	6.397673
23	F	-6.522854	-0.586829	7.668001
24	C	-6.264266	-2.306723	6.077561
25	F	-6.410838	-3.203121	7.054521
26	C	-6.056808	-2.727785	4.765984
27	F	-6.013936	-4.032092	4.501355
28	C	-5.700198	-4.306334	-0.35988
29	C	-5.611549	-3.980685	-1.73117
30	C	-5.610911	-4.977193	-2.701474
31	F	-5.531015	-4.711844	-4.004376
32	C	-5.695995	-6.304443	-2.283302
33	F	-5.69382	-7.291504	-3.181167
34	C	-5.784007	-6.627802	-0.921589
35	F	-5.862719	-7.912029	-0.568019
36	C	-5.789019	-5.631382	0.053513
37	F	-5.876368	-5.979958	1.336145
38	C	-5.368712	0.15662	-4.281997

39	C	-5.425351	1.531525	-3.959517
40	C	-5.490682	2.496073	-4.961305
41	F	-5.550659	3.800178	-4.697955
42	C	-5.485791	2.069987	-6.287464
43	F	-5.533999	2.961585	-7.278668
44	C	-5.429749	0.704598	-6.60772
45	F	-5.426748	0.345064	-7.892367
46	C	-5.377192	-0.264885	-5.608852
47	F	-5.33114	-1.55045	-5.952884
48	C	-5.947942	4.072256	0.158276
49	C	-6.038784	3.74644	1.529408
50	C	-6.222858	4.738457	2.486829
51	F	-6.315423	4.47262	3.788801
52	C	-6.310977	6.061569	2.056564
53	F	-6.482695	7.044588	2.942474
54	C	-6.220551	6.385152	0.69503
55	F	-6.308996	7.665601	0.329775
56	C	-6.040138	5.393115	-0.267668
57	F	-5.960931	5.741793	-1.550975
58	O	-3.257808	-1.222743	-0.21139
59	O	-3.362081	1.127214	0.347248
60	C	-2.030003	-0.692699	-0.022172
61	C	-2.089207	0.673983	0.301659
62	C	-0.940921	1.409895	0.533363
63	H	-0.996949	2.46249	0.785613
64	C	0.310042	0.764749	0.424007
65	C	0.356007	-0.597	0.114798
66	H	1.301854	-1.109242	0.055587
67	C	-0.810651	-1.343241	-0.111952
68	H	-0.7629	-2.399237	-0.35345
69	C	2.710088	3.552338	0.595328
70	H	2.644767	3.815991	1.656338
71	H	2.941402	4.453437	0.024943
72	C	1.531678	1.602284	0.735417
73	H	1.545504	1.746219	1.826294
74	N	1.465218	2.949073	0.176217
75	C	1.167616	3.062451	-1.254273
76	H	0.174866	2.655021	-1.449258
77	H	1.156956	4.123401	-1.516594
78	H	1.879496	2.551694	-1.913106
79	C	9.115146	1.2101	2.368904
80	C	8.46695	2.419024	1.896881
81	C	7.138703	2.676896	2.248441

82	C	6.405972	1.74058	3.071036
83	C	7.025887	0.588233	3.522342
84	C	8.404938	0.311812	3.171544
85	C	9.969672	0.70759	1.303585
86	C	9.843336	1.610106	0.166599
87	C	8.913112	2.667334	0.537358
88	C	8.008214	3.160195	-0.407282
89	C	6.203923	3.185982	1.261738
90	C	5.014022	1.704932	2.574556
91	C	4.299315	0.45353	2.581914
92	C	4.986997	-0.753147	3.089122
93	C	6.297523	-0.690852	3.531422
94	C	7.237952	-1.73941	3.188005
95	C	8.534824	-1.121445	2.955552
96	C	9.361399	-1.600031	1.939943
97	C	10.087958	-0.664994	1.093451
98	C	9.842657	1.099903	-1.12976
99	C	9.970928	-0.334786	-1.350798
100	C	10.092095	-1.19882	-0.261427
101	C	9.374646	-2.46114	-0.250863
102	C	8.923378	-2.713103	1.110503
103	C	7.685152	-3.311004	1.337317
104	C	6.823719	-2.819021	2.401916
105	C	5.450201	-2.885249	1.939748
106	C	4.551958	-1.871161	2.284675
107	C	4.896492	2.580738	1.505848
108	C	3.510126	-0.919664	-1.121784
109	C	3.340276	0.439409	-0.912947
110	C	4.111697	1.348422	-1.718503
111	C	4.923471	0.881513	-2.771813
112	C	5.051828	-0.537068	-3.007788
113	C	5.015152	-2.638587	-1.711891
114	C	4.563567	-2.899794	-0.356336
115	C	3.628646	-1.852204	0.013267
116	C	3.628857	-1.339421	1.298584
117	C	3.46655	0.095445	1.529556
118	C	3.011798	1.051105	0.461449
119	C	4.526604	2.470104	-0.92772
120	C	5.764974	3.041801	-1.156324
121	C	6.624595	2.550128	-2.210913
122	C	6.207112	1.496031	-3.023491
123	C	7.146246	0.4519	-3.398968
124	C	6.427043	-0.814379	-3.389387

125	C	7.056998	-1.97068	-2.928794
126	C	6.333627	-2.905879	-2.077582
127	C	5.45565	-3.414889	0.587934
128	C	6.837045	-3.67868	0.210753
129	C	7.265665	-3.433673	-1.092075
130	C	8.562361	-2.812663	-1.330109
131	C	8.431487	-1.913615	-2.462512
132	C	9.122974	-0.696277	-2.472371
133	C	8.465768	0.508129	-2.949309
134	C	8.905914	1.618691	-2.115532
135	C	8.005577	2.620781	-1.756703
136	C	3.84859	2.463869	0.442652
137	C	6.631826	3.432682	-0.030817
138	C	4.366443	-1.420712	-2.174853

Table S2. Optimized cartesian coordinate of structure CYLY6-3.

Charge	0	Multiplicity	1

Tag	Symbol	X	Y	Z
1	C	-6.967146	0.307206	-4.135333
2	C	-6.908281	1.684375	-3.851014
3	C	-7.054641	2.638127	-4.859237
4	C	-7.246076	2.176177	-6.158367
5	C	-7.305108	0.797071	-6.443073
6	C	-7.174147	-0.154798	-5.435824
7	H	-7.458286	0.475313	-7.468351
8	H	-7.226592	-1.218043	-5.641589
9	H	-7.016249	3.696517	-4.627064
10	H	-7.354937	2.888411	-6.970185
11	C	-6.812475	-0.38803	-2.869466
12	C	-6.718794	1.807196	-2.416183
13	N	-6.612353	0.541513	-1.859832
14	C	-6.732553	4.346223	0.225482
15	C	-6.655769	4.058231	1.599906
16	C	-6.655381	5.075504	2.553414
17	C	-6.731111	6.388432	2.093167
18	C	-6.807988	6.676765	0.716904
19	C	-6.811152	5.65975	-0.235457
20	H	-6.868637	5.870235	-1.297598
21	H	-6.864298	7.712184	0.395947
22	H	-6.59448	4.842082	3.610559
23	H	-6.7297	7.207359	2.805656
24	C	-6.708894	3.065611	-0.464202
25	C	-6.587234	2.609513	1.712655
26	N	-6.655612	2.040992	0.457547
27	C	-6.452519	-0.01396	4.266083
28	C	-6.511295	-1.391264	3.981749
29	C	-6.586083	-2.33835	5.004089
30	C	-6.585139	-1.870746	6.315203
31	C	-6.526106	-0.491587	6.599901
32	C	-6.466655	0.454556	5.580612
33	C	-6.416859	0.675526	2.988222
34	H	-6.529961	-0.165114	7.635076
35	H	-6.429741	1.518264	5.787357
36	H	-6.640259	-3.396294	4.772924
37	H	-6.63342	-2.578267	7.136964
38	C	-6.510658	-1.519714	2.535019

39	N	-6.400924	-0.260408	1.965272
40	C	-7.000798	-4.04376	-0.075525
41	C	-7.077809	-3.755659	-1.449947
42	C	-7.254916	-4.767644	-2.392616
43	C	-7.350055	-6.075579	-1.921993
44	C	-7.273015	-6.364074	-0.545731
45	C	-7.098769	-5.35223	0.3961
46	H	-7.311694	-4.534133	-3.449973
47	H	-7.350152	-7.395601	-0.216619
48	H	-7.037112	-5.562969	1.457973
49	H	-7.48495	-6.890479	-2.626292
50	C	-6.817043	-2.769344	0.60132
51	C	-6.93899	-2.313063	-1.575449
52	N	-6.818591	-1.746158	-0.323891
53	N	-6.731354	2.96513	-1.783662
54	N	-6.470792	1.989153	2.875708
55	N	-6.930639	-1.696329	-2.746433
56	N	-6.669234	-2.672632	1.91287
57	Ti	-5.815815	0.119466	0.010138
58	C	-3.07042	0.717705	0.016843
59	C	-3.130341	-0.654648	-0.28766
60	C	-1.980051	-1.393882	-0.501872
61	C	-0.727965	-0.750101	-0.393334
62	C	-0.681141	0.615109	-0.102542
63	C	-1.848882	1.365436	0.105344
64	H	-2.038339	-2.449641	-0.740479
65	H	0.264863	1.127038	-0.043837
66	H	-1.801805	2.424839	0.332259
67	O	-4.293965	1.25569	0.188672
68	O	-4.399514	-1.10925	-0.334371
69	C	8.087788	-1.234974	-2.287324
70	C	7.435781	-2.436164	-1.800869
71	C	6.108686	-2.697058	-2.154631
72	C	5.380848	-1.771845	-2.994083
73	C	6.004469	-0.626996	-3.459368
74	C	7.38235	-0.347411	-3.106012
75	C	8.937994	-0.718238	-1.225381
76	C	8.805173	-1.604146	-0.076067
77	C	7.875471	-2.665565	-0.435905
78	C	6.965215	-3.143303	0.511535
79	C	5.168459	-3.190442	-1.165021
80	C	3.986555	-1.727506	-2.504866
81	C	3.273269	-0.475693	-2.534306

82	C	3.965651	0.722575	-3.054605
83	C	5.27796	0.652679	-3.490617
84	C	6.21822	1.704837	-3.157601
85	C	7.513162	1.088621	-2.910094
86	C	8.33591	1.58083	-1.897748
87	C	9.057271	0.657128	-1.034516
88	C	8.799394	-1.0753	1.212868
89	C	8.928503	0.362326	1.413731
90	C	9.055868	1.210414	0.312561
91	C	8.34016	2.473377	0.280478
92	C	7.895636	2.706328	-1.086515
93	C	6.659129	3.302299	-1.327662
94	C	5.801935	2.79638	-2.389209
95	C	4.426423	2.870926	-1.934349
96	C	3.528528	1.852844	-2.268247
97	C	3.86288	-2.587673	-1.423999
98	C	2.469292	0.952129	1.14639
99	C	2.298677	-0.40948	0.955683
100	C	3.065164	-1.307501	1.778351
101	C	3.872553	-0.826816	2.828775
102	C	4.001771	0.594835	3.045134
103	C	3.974332	2.677138	1.718493
104	C	3.529435	2.919306	0.3572
105	C	2.595074	1.867562	-0.001414
106	C	2.60021	1.336577	-1.279076
107	C	2.437531	-0.101461	-1.489686
108	C	1.975836	-1.040553	-0.411039
109	C	3.482731	-2.440706	1.005417
110	C	4.718815	-3.011516	1.248545
111	C	5.574247	-2.505661	2.29989
112	C	5.154367	-1.439343	3.095143
113	C	6.093217	-0.391161	3.45965
114	C	5.375703	0.875819	3.428611
115	C	6.009535	2.024648	2.954612
116	C	5.291393	2.948362	2.086616
117	C	4.42643	3.41998	-0.590231
118	C	5.806331	3.687346	-0.210422
119	C	6.228636	3.460665	1.09789
120	C	7.523382	2.841485	1.350835
121	C	7.386106	1.959008	2.495531
122	C	8.075988	0.741068	2.526155
123	C	7.414922	-0.455529	3.017261
124	C	7.857413	-1.578538	2.20167

125	C	6.957117	-2.584422	1.853061
126	C	2.81082	-2.4533	-0.367484
127	C	5.590257	-3.419722	0.132829
128	C	3.321574	1.466994	2.195957
129	C	1.670327	-3.543189	-0.50722
130	C	0.493423	-1.594236	-0.685746
131	H	1.898349	-4.434942	0.07914
132	H	1.610625	-3.82371	-1.564268
133	H	0.516872	-1.757317	-1.773759
134	N	0.426567	-2.930713	-0.104153
135	C	0.115848	-3.022242	1.324456
136	H	-0.875614	-2.6052	1.503706
137	H	0.096904	-4.079355	1.601994
138	H	0.82559	-2.506027	1.98184

Table S3. Optimized cartesian coordinate of structure CYLY6-4.

Charge	0	Multiplicity	1
Tag	**Symbol**	**X**	**Y**	**Z**
1	C	-5.93909	0.624532	-4.064956
2	C	-5.874525	1.972856	-3.669442
3	C	-6.021215	3.007322	-4.587803
4	C	-6.22224	2.695269	-5.938587
5	C	-6.285217	1.333967	-6.317225
6	C	-6.154431	0.293409	-5.400423
7	C	-5.780549	-0.174045	-2.863919
8	C	-5.677379	1.976953	-2.229787
9	N	-5.572128	0.66873	-1.7809
10	H	-5.97454	4.033981	-4.243095
11	H	-6.443277	1.081127	-7.35797
12	H	-6.214457	-0.743771	-5.711398
13	C	-6.368609	3.835984	-6.956189
14	C	-7.581993	4.708946	-6.567794
15	C	-5.087566	4.698413	-6.936693
16	C	-6.582893	3.324002	-8.389782
17	H	-8.503507	4.118642	-6.572733
18	H	-7.466851	5.141984	-5.570558
19	H	-7.69911	5.532816	-7.27981
20	H	-4.211774	4.100362	-7.206601
21	H	-5.174349	5.521856	-7.65355
22	H	-4.905883	5.131182	-5.949319
23	H	-6.679549	4.174769	-9.070795
24	H	-5.739513	2.718146	-8.735386
25	H	-7.495667	2.726261	-8.476098
26	C	-5.66502	4.290916	0.61075
27	C	-5.578684	3.893262	1.956114
28	C	-5.564612	4.822732	2.989266
29	C	-5.635147	6.188108	2.677935
30	C	-5.722469	6.56882	1.319867
31	C	-5.739893	5.640319	0.279868
32	C	-5.651693	3.072836	-0.181598
33	C	-5.515258	2.439416	1.950966
34	N	-5.595792	1.975286	0.65402
35	H	-5.805529	5.955155	-0.755891
36	H	-5.776599	7.620176	1.067158
37	H	-5.494983	4.477689	4.014593
38	C	-5.611648	7.216958	3.817674

39	C	-6.81104	6.96118	4.75637
40	C	-4.295804	7.062336	4.611344
41	C	-5.69947	8.664512	3.3078
42	H	-7.756992	7.063761	4.215674
43	H	-6.779715	5.957669	5.189104
44	H	-6.807756	7.68227	5.580734
45	H	-3.42958	7.237165	3.965888
46	H	-4.261884	7.784908	5.433739
47	H	-4.196931	6.061483	5.040014
48	H	-5.679901	9.353247	4.157658
49	H	-4.856626	8.918128	2.657371
50	H	-6.62744	8.845704	2.756496
51	C	-5.362458	-0.385434	4.278131
52	C	-5.425857	-1.733925	3.882538
53	C	-5.489923	-2.762793	4.81664
54	C	-5.475313	-2.445873	6.181051
55	C	-5.411747	-1.084531	6.559624
56	C	-5.362779	-0.048753	5.629533
57	C	-5.339336	0.408341	3.063774
58	C	-5.440843	-1.742745	2.429609
59	N	-5.335514	-0.439998	1.965626
60	H	-5.322919	0.988966	5.941949
61	H	-5.402757	-0.82774	7.611303
62	H	-5.547344	-3.789198	4.472767
63	C	-5.530999	-3.581327	7.213513
64	C	-6.830787	-4.38972	7.008213
65	C	-4.312037	-4.508096	7.01211
66	C	-5.508994	-3.064193	8.661025
67	H	-7.710437	-3.752991	7.143927
68	H	-6.883424	-4.82461	6.00654
69	H	-6.885838	-5.208997	7.732953
70	H	-3.377028	-3.956609	7.150727
71	H	-4.336245	-5.329	7.736699
72	H	-4.297384	-4.945476	6.010228
73	H	-5.54981	-3.911219	9.352259
74	H	-4.594507	-2.503718	8.878684
75	H	-6.367674	-2.420514	8.875988
76	C	-5.955119	-4.043442	-0.375026
77	C	-6.040666	-3.645839	-1.720482
78	C	-6.221349	-4.571081	-2.7417
79	C	-6.317027	-5.932124	-2.4185
80	C	-6.23017	-6.312817	-1.060376
81	C	-6.051772	-5.388448	-0.03195

82	C	-5.766022	-2.83072	0.402799
83	C	-5.902305	-2.197214	-1.729743
84	N	-5.773407	-1.73434	-0.436663
85	H	-6.280314	-4.22625	-3.767758
86	H	-6.302121	-7.360913	-0.798705
87	H	-5.985984	-5.703229	1.003833
88	C	-6.507862	-6.956662	-3.546295
89	C	-7.813115	-6.636407	-4.30713
90	C	-5.311114	-6.867116	-4.518423
91	C	-6.597004	-8.399705	-3.023909
92	H	-8.677123	-6.691937	-3.637736
93	H	-7.791815	-5.63445	-4.744042
94	H	-7.963432	-7.354054	-5.120724
95	H	-4.372566	-7.088247	-4.000947
96	H	-5.430723	-7.587779	-5.334479
97	H	-5.222565	-5.871241	-4.960695
98	H	-6.732991	-9.085362	-3.865574
99	H	-5.68489	-8.698683	-2.498112
100	H	-7.445899	-8.535179	-2.346463
101	N	-5.683014	3.079114	-1.504851
102	N	-5.390745	1.727138	3.059054
103	N	-5.900304	-1.488107	-2.847102
104	N	-5.607213	-2.8404	1.716742
105	Ti	-4.766201	0.095701	0.04358
106	C	-2.019077	0.692034	0.063574
107	C	-2.081757	-0.664387	-0.306375
108	C	-0.932682	-1.393465	-0.558828
109	C	0.320658	-0.756611	-0.425315
110	C	0.370142	0.593566	-0.072426
111	C	-0.796273	1.333845	0.175849
112	H	-0.993099	-2.437462	-0.84432
113	H	1.316772	1.10156	0.006287
114	H	-0.747376	2.381376	0.452258
115	O	-3.240071	1.221276	0.271383
116	O	-3.350791	-1.114705	-0.373284
117	C	9.116119	-1.191403	-2.424091
118	C	8.468201	-2.405642	-1.965358
119	C	7.137205	-2.655527	-2.312341
120	C	6.401304	-1.706071	-3.117041
121	C	7.020992	-0.548746	-3.555932
122	C	8.402835	-0.280269	-3.209398
123	C	9.978086	-0.705904	-1.356906
124	C	9.85671	-1.62439	-0.232132

125	C	8.922223	-2.674421	-0.612373
126	C	8.02164	-3.178626	0.330595
127	C	6.207105	-3.176478	-1.327296
128	C	5.012391	-1.674893	-2.611887
129	C	4.29986	-0.422415	-2.598115
130	C	4.987788	0.789869	-3.091077
131	C	6.295364	0.731734	-3.542924
132	C	7.240084	1.773303	-3.189745
133	C	8.536998	1.149438	-2.973723
134	C	9.370972	1.611881	-1.956534
135	C	10.100627	0.663342	-1.127909
136	C	9.865106	-1.132789	1.071449
137	C	9.997617	0.298416	1.312112
138	C	10.114121	1.17773	0.234448
139	C	9.399241	2.441544	0.246218
140	C	8.940387	2.713916	-1.108722
141	C	7.701838	3.31719	-1.319476
142	C	6.832944	2.842568	-2.385981
143	C	5.462381	2.904884	-1.914554
144	C	4.559983	1.8974	-2.267941
145	C	4.899443	-2.565709	-1.554919
146	C	3.536923	0.899316	1.130459
147	C	3.362778	-0.456117	0.902551
148	C	4.136839	-1.377858	1.691106
149	C	4.955914	-0.927936	2.746173
150	C	5.088774	0.486816	3.001877
151	C	5.049218	2.606339	1.735776
152	C	4.589966	2.887778	0.386896
153	C	3.650802	1.847396	0.008197
154	C	3.641602	1.353505	-1.284189
155	C	3.475936	-0.077807	-1.534042
156	C	3.024729	-1.047261	-0.478299
157	C	4.54517	-2.488652	0.881497
158	C	5.783327	-3.066892	1.095028
159	C	6.65036	-2.591919	2.151326
160	C	6.239929	-1.54862	2.981282
161	C	7.183582	-0.511871	3.36568
162	C	6.466947	0.755923	3.378539
163	C	7.096756	1.917525	2.931013
164	C	6.370279	2.866305	2.097627
165	C	5.477228	3.415048	-0.555243
166	C	6.861311	3.670538	-0.182652
167	C	7.297376	3.40623	1.114071

168	C	8.594159	2.779174	1.335306
169	C	8.468267	1.864251	2.455577
170	C	9.157401	0.645561	2.444038
171	C	8.500502	-0.564288	2.907616
172	C	8.933243	-1.663644	2.05539
173	C	8.028347	-2.658581	1.687674
174	C	3.85882	-2.461109	-0.483995
175	C	6.642524	-3.443337	-0.041144
176	C	4.400553	1.383347	2.185207
177	C	2.715746	-3.545942	-0.643262
178	C	1.538863	-1.591364	-0.755159
179	H	2.948525	-4.453916	-0.084249
180	H	2.646207	-3.796628	-1.707202
181	H	1.552379	-1.722835	-1.847584
182	N	1.476689	-2.944157	-0.211913
183	C	1.176487	-3.076156	1.215527
184	H	0.186939	-2.662904	1.413256
185	H	1.158113	-4.140708	1.463163
186	H	1.891941	-2.579529	1.881993

Table S4. Excited states information of structure CYLY6-2.

Excited State	Excitation Energy [eV]	Absorption Wavelength [nm]	Oscillator Strength
1	1.5965	776.60	0.01280
2	1.7632	703.18	0.58830
3	**1.7980**	**689.57**	**0.61450**
4	2.0446	606.40	0.00070
5	2.1433	578.47	0.00780
6	2.2390	553.75	0.00040
7	2.3426	529.26	0.00370
8	2.3602	525.31	0.00480
9	2.3696	523.23	0.00080
10	2.4036	515.83	0.00940
11	2.5499	486.23	0.00010
12	**2.6004**	**476.79**	**0.10730**
13	2.6361	470.33	0.00460
14	2.6879	461.27	0.00000
15	2.6966	459.78	0.00250
16	2.7044	458.45	0.00000
17	2.7151	456.65	0.00000
18	2.7546	450.10	0.01400
19	2.7851	445.17	0.00000
20	2.8538	434.45	0.00050
21	2.9102	426.03	0.00410
22	2.9675	417.81	0.00030
23	3.0195	410.61	0.03580
24	3.0215	410.34	0.02070
25	3.0863	401.72	0.01850
26	3.1283	396.33	0.00560
27	3.1325	395.80	0.00320
28	3.1560	392.85	0.00030
29	3.2797	378.04	0.04210
30	3.3395	371.27	0.00010
31	3.3583	369.19	0.02970
32	3.3898	365.76	0.00050
33	3.4089	363.71	0.00010
34	3.4212	362.40	0.05290
35	3.4381	360.62	0.00820
36	3.4480	359.58	0.00030
37	3.4507	359.30	0.00250
38	3.4576	358.58	0.00010
39	3.4652	357.80	0.00060

40	3.4723	357.07	0.00120
41	3.4844	355.83	0.02360
42	3.4907	355.18	0.00170
43	3.4981	354.43	0.00000
44	3.5077	353.46	0.00000
45	3.5373	350.51	0.00050
46	3.5432	349.92	0.03020
47	3.5563	348.63	0.00010
48	3.5598	348.29	0.00800
49	3.5840	345.94	0.00330
50	3.5895	345.41	0.08700
51	3.6431	340.33	0.01740
52	3.6925	335.77	0.00620
53	3.6945	335.59	0.00290
54	3.7077	334.40	0.05710
55	3.7115	334.05	0.01160
56	3.7175	333.51	0.00010
57	3.7575	329.96	0.06690
58	3.7616	329.60	0.00000
59	3.8110	325.33	0.02690
60	3.8444	322.51	0.38520
61	3.8564	321.50	0.19650
62	3.8684	320.51	0.06500
63	3.8696	320.41	0.14170
64	3.8898	318.74	0.00180
65	**3.8945**	**318.36**	**0.79020**
66	3.9256	315.84	0.01410
67	3.9379	314.85	0.03440
68	3.9587	313.19	0.33930
69	3.9600	313.09	0.21860
70	3.9621	312.93	0.00110
71	3.9722	312.13	0.00660
72	3.9866	311.00	0.04250
73	4.0074	309.39	0.00020
74	4.0311	307.57	0.06150
75	4.0528	305.92	0.04460
76	4.0623	305.21	0.00000
77	4.0689	304.71	0.07050
78	4.0940	302.84	0.15230
79	4.0965	302.66	0.02120
80	4.0977	302.57	0.05010
81	4.1193	300.98	0.06560
82	4.1468	298.99	0.06300

83	4.1503	298.74	0.00060
84	4.1879	296.05	0.00960
85	4.1932	295.68	0.00660
86	4.1939	295.63	0.02930
87	4.2118	294.37	0.00420
88	4.2170	294.01	0.00230
89	4.2197	293.82	0.00340
90	4.2242	293.51	0.00990
91	4.2251	293.45	0.05420
92	4.2274	293.29	0.00100
93	4.2339	292.84	0.00000
94	4.2505	291.69	0.02670
95	4.2574	291.22	0.01330
96	4.2732	290.14	0.00080
97	4.2844	289.39	0.00170
98	4.3221	286.86	0.00190
99	4.3272	286.52	0.03260
100	4.3328	286.15	0.31630

Table S5. Excited states information of structure CYLY6-3.

Excited State	Excitation Energy [eV]	Absorption Wavelength [nm]	Oscillator Strength
1	1.5944	777.62	0.01310
2	1.7941	691.07	0.55360
3	**1.8301**	**677.47**	**0.58710**
4	1.9335	641.24	0.00080
5	2.1387	579.72	0.00780
6	2.3433	529.10	0.00340
7	2.3601	525.33	0.00510
8	2.3663	523.96	0.00050
9	2.3720	522.70	0.00080
10	2.4006	516.47	0.00850
11	2.5489	486.42	0.00010
12	2.5778	480.97	0.00000
13	2.6336	470.78	0.00990
14	2.6958	459.92	0.00350
15	2.7498	450.88	0.02500
16	2.7724	447.21	0.00050
17	**2.8160**	**440.28**	**0.11620**
18	2.8536	434.48	0.00060
19	2.9085	426.28	0.00300
20	2.9116	425.83	0.00000
21	2.9773	416.43	0.02930
22	3.0157	411.13	0.03460
23	3.0184	410.76	0.02060
24	3.0825	402.22	0.00050
25	3.1287	396.28	0.00240
26	3.1302	396.09	0.00090
27	3.1522	393.33	0.00040
28	3.1615	392.17	0.00000
29	3.1985	387.63	0.00000
30	3.2559	380.80	0.05750
31	3.2992	375.80	0.00470
32	3.3725	367.63	0.01630
33	3.4162	362.93	0.00000
34	3.4287	361.61	0.02230
35	3.4478	359.60	0.00020
36	3.4516	359.21	0.00000
37	3.4601	358.33	0.00970
38	3.4844	355.83	0.02570
39	3.5383	350.41	0.02870

40	3.5734	346.96	0.09520
41	3.5967	344.72	0.01870
42	3.6395	340.66	0.01560
43	3.7049	334.65	0.06390
44	3.7101	334.18	0.00720
45	3.7152	333.72	0.00000
46	3.7396	331.54	0.00170
47	3.7533	330.33	0.02280
48	3.7968	326.55	0.01770
49	3.7998	326.29	0.00410
50	3.8159	324.91	0.00060
51	3.8323	323.52	0.02810
52	3.8346	323.33	0.00530
53	3.8444	322.51	0.03200
54	3.8482	322.19	0.00080
55	3.8519	321.88	0.04650
56	3.8557	321.56	0.00070
57	3.8651	320.78	0.01780
58	3.8704	320.34	0.00060
59	3.8905	318.68	0.00330
60	3.8931	318.47	0.02560
61	3.9129	316.86	0.00430
62	3.9186	316.40	0.01460
63	3.9200	316.29	0.01870
64	3.9383	314.82	0.06070
65	3.9637	312.80	0.83040
66	3.9714	312.19	0.01790
67	3.9763	311.81	0.06710
68	3.9770	311.75	0.46710
69	3.9825	311.32	0.07130
70	4.0015	309.84	0.02000
71	4.0116	309.06	0.00310
72	4.0441	306.58	0.03470
73	4.0654	304.97	0.03550
74	**4.0721**	**304.47**	**0.97090**
75	4.0815	303.77	0.05450
76	4.1005	302.36	0.02690
77	4.1091	301.73	0.00330
78	4.1147	301.32	0.02630
79	4.1368	299.71	0.03660
80	4.1960	295.48	0.01730
81	4.1964	295.45	0.00040
82	4.2023	295.04	0.01110

83	4.2241	293.52	0.07860
84	4.2273	293.29	0.00260
85	4.2755	289.99	0.13660
86	4.2810	289.62	0.00100
87	4.3251	286.66	0.05100
88	4.3328	286.15	0.01720
89	4.3391	285.74	0.07830
90	4.3421	285.54	0.03920
91	4.3472	285.20	0.00050
92	4.3528	284.84	0.00010
93	4.3607	284.32	0.00010
94	4.3646	284.07	0.00000
95	4.3726	283.55	0.01060
96	4.3852	282.73	0.09500
97	4.3916	282.32	0.00010
98	4.4280	280.00	0.02340
99	4.4281	279.99	0.02190
100	4.4466	278.83	0.08710

Table S6. Excited states information of structure CYLY6-4.

Excited State	Excitation Energy [eV]	Absorption Wavelength [nm]	Oscillator Strength
1	1.5934	778.11	0.01270
2	1.7541	706.83	0.60480
3	**1.7942**	**691.03**	**0.64460**
4	1.8646	664.94	0.00080
5	2.1372	580.12	0.00770
6	2.3432	529.12	0.00340
7	2.3598	525.40	0.00520
8	2.3724	522.61	0.00070
9	2.3798	520.99	0.00060
10	2.3994	516.73	0.00840
11	2.5058	494.79	0.00000
12	2.5484	486.52	0.00010
13	2.6331	470.87	0.00990
14	2.6519	467.53	0.00040
15	2.6954	459.98	0.00340
16	2.7494	450.95	0.02270
17	2.8527	434.62	0.02300
18	**2.8557**	**434.16**	**0.10500**
19	2.9049	426.81	0.03760
20	2.9081	426.34	0.00220
21	2.9563	419.39	0.00000
22	3.0149	411.24	0.03330
23	3.0177	410.86	0.02020
24	3.0397	407.88	0.00000
25	3.0943	400.69	0.00070
26	3.1283	396.33	0.00320
27	3.1516	393.40	0.00040
28	3.2011	387.32	0.00010
29	3.2452	382.05	0.05260
30	3.2726	378.86	0.00000
31	3.2874	377.15	0.00480
32	3.2945	376.34	0.00000
33	3.3705	367.85	0.01730
34	3.3799	366.83	0.00000
35	3.4279	361.69	0.02280
36	3.4474	359.65	0.00020
37	3.4593	358.41	0.01020
38	3.4843	355.84	0.02550
39	3.5377	350.47	0.02830

40	3.5707	347.23	0.09630
41	3.6134	343.12	0.01870
42	3.6290	341.65	0.00080
43	3.6390	340.71	0.01450
44	3.6694	337.89	0.03390
45	3.7042	334.71	0.06230
46	3.7096	334.23	0.00770
47	3.7707	328.81	0.07920
48	3.7882	327.29	0.01420
49	3.8022	326.09	0.00110
50	3.8042	325.91	0.00240
51	3.8227	324.34	0.02150
52	3.8492	322.10	0.05020
53	3.8498	322.05	0.00580
54	3.8677	320.56	0.01120
55	3.8757	319.90	0.03380
56	3.8801	319.54	0.03340
57	3.8907	318.67	0.00680
58	3.8948	318.33	0.00740
59	3.9063	317.40	0.03680
60	3.9165	316.57	0.01650
61	3.9347	315.10	0.59220
62	3.9360	315.00	0.40630
63	3.9435	314.40	0.03210
64	3.9596	313.12	0.10950
65	3.9789	311.60	0.31300
66	3.9829	311.29	0.20000
67	3.9885	310.85	0.00020
68	3.9905	310.70	0.01840
69	3.9938	310.44	0.01690
70	3.9999	309.97	0.04310
71	4.0363	307.17	0.30320
72	**4.0380**	**307.04**	**0.73000**
73	4.0452	306.50	0.13650
74	4.0625	305.19	0.05150
75	4.0707	304.58	0.00870
76	4.0730	304.41	0.06840
77	4.0959	302.70	0.00850
78	4.0965	302.66	0.01480
79	4.1051	302.02	0.02870
80	4.1260	300.49	0.05730
81	4.1291	300.27	0.00580
82	4.1853	296.24	0.04290

83	4.1944	295.59	0.01560
84	4.2001	295.19	0.01390
85	4.2114	294.40	0.00420
86	4.2193	293.85	0.00180
87	4.2236	293.55	0.08100
88	4.2705	290.33	0.00070
89	4.2843	289.39	0.00000
90	4.3210	286.93	0.00040
91	4.3247	286.69	0.05040
92	4.3317	286.23	0.05580
93	4.3420	285.55	0.03140
94	4.3502	285.01	0.02860
95	4.3717	283.61	0.07530
96	4.3718	283.60	0.00350
97	4.3842	282.80	0.00210
98	4.3846	282.77	0.08710
99	4.3928	282.24	0.15150
100	4.3949	282.11	0.00830

Table S7. Transition dipole moments of the ground state to the excited state and between excited states of three titanium phthalocyanine derivatives.

Molecules	Process	Components			Tol.	Process	Components			Tol.
		X	Y	Z			X	Y	Z	
CYLY6-2	$\mu_{0\to3}$	-0.33	1.22	-5.08	5.23	$\mu_{3\to73}$	-0.32	1.06	-4.78	4.91
CYLY6-3	$\mu_{0\to2}$	-0.22	-4.95	-1.09	5.08	$\mu_{2\to51}$	0.03	1.72	0.34	1.75
CYLY6-4	$\mu_{0\to2}$	-0.26	-5.34	-1.59	5.57	$\mu_{2\to49}$	0.15	1.97	0.44	2.03

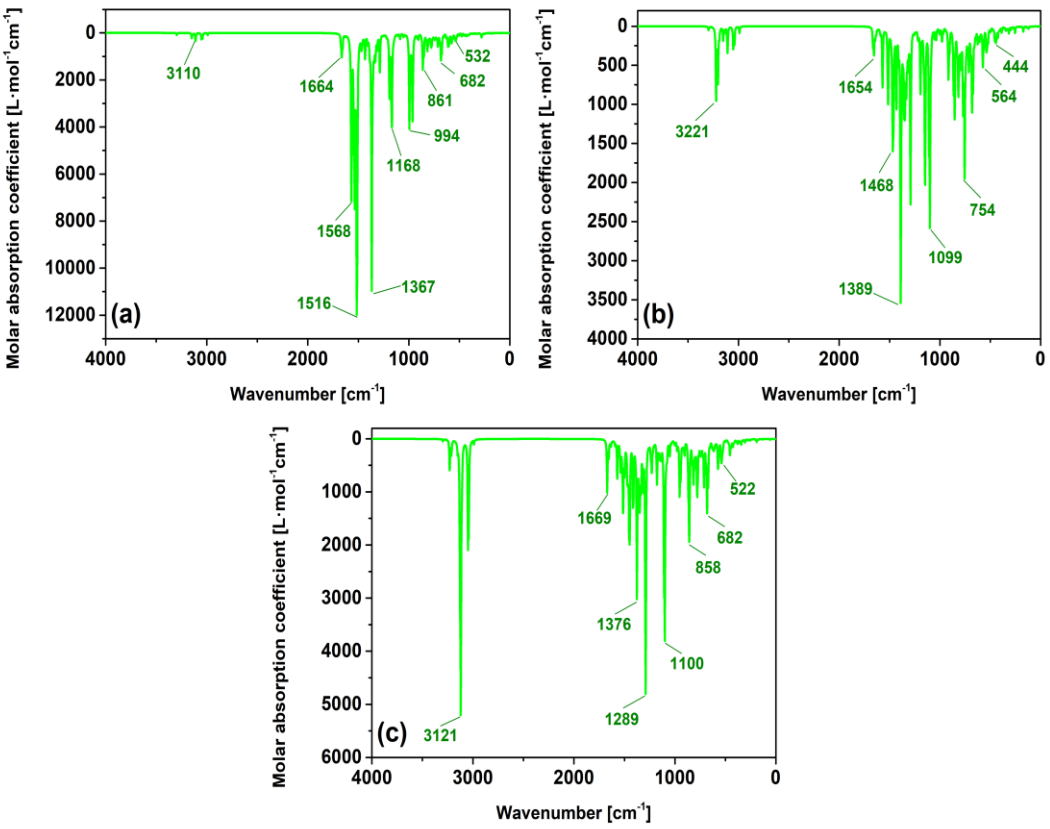

Fig. S1. Infrared (IR) spectra of three titanium phthalocyanine derivatives by DFT simulating.