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Supplementary Information

Synthesis, Computational and Optical Studies of Tetraphenylethene linked Pd(II)Dipyrrinato Complexes

Neha Manav,[a] Rajvir Singh,[a] Anu Janaagal,[a] Amit Kumar Singh Yadav,[a] Vijayalakshmi Pandey[a] and Iti Gupta*[a]

[a]Indian Institute of Technology Gandhinagar, Palaj Campus, Gandhinagar, Gujarat-382355, India.

*Corresponding author, e-mail: iti@iitgn.ac.in

Sr. No.	Data
Figure S1	^{1}H NMR spectrum of compound **DPM1** in $CDCl_3$
Figure S2	^{13}C NMR spectrum of compound **DPM1** in $CDCl_3$
Figure S3	^{1}H NMR spectrum of compound **DPM2** in $CDCl_3$
Figure S4	^{13}C NMR spectrum of compound **DPM2** in $CDCl_3$
Figure S5	^{1}H NMR spectrum of compound of **(Z)-2-(naphthalen-2-yl(2H-pyrrol-2-ylidene)methyl)-1H-pyrrole** in $CDCl_3$.
Figure S6	^{13}C NMR spectrum of compound of **(Z)-2-(naphthalen-2-yl(2H-pyrrol-2-ylidene)methyl)-1H-pyrrole** in $CDCl_3$
Figure S7	^{1}H NMR spectrum of compound of **DPM3** in $CDCl_3$
Figure S8	^{13}C NMR spectrum of compound of **DPM3** in $CDCl_3$
Figure S9	^{1}H NMR spectrum of compound **DPM4** in $CDCl_3$
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Figure S11	^{1}H NMR spectrum of compound **Pd1** in $CDCl_3$
Figure S12	^{13}C NMR spectrum of compound **Pd1** in $CDCl_3$
Figure S13	IR spectrum of compound **Pd1**
Figure S14	MALDI-MS of compound **Pd1**
Figure S15	^{1}H NMR spectrum of compound **Pd2** in $CDCl_3$
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Figure S19	^{1}H NMR spectrum of compound **Pd3** in $CDCl_3$
Figure S20	^{13}C NMR spectrum of compound **Pd3** in $CDCl_3$
Figure S21	IR spectrum of compound **Pd3**
Figure S22	MALDI-MS of compound **Pd3**
Figure S23	^{1}H NMR spectrum of compound **Pd4** in $CDCl_3$

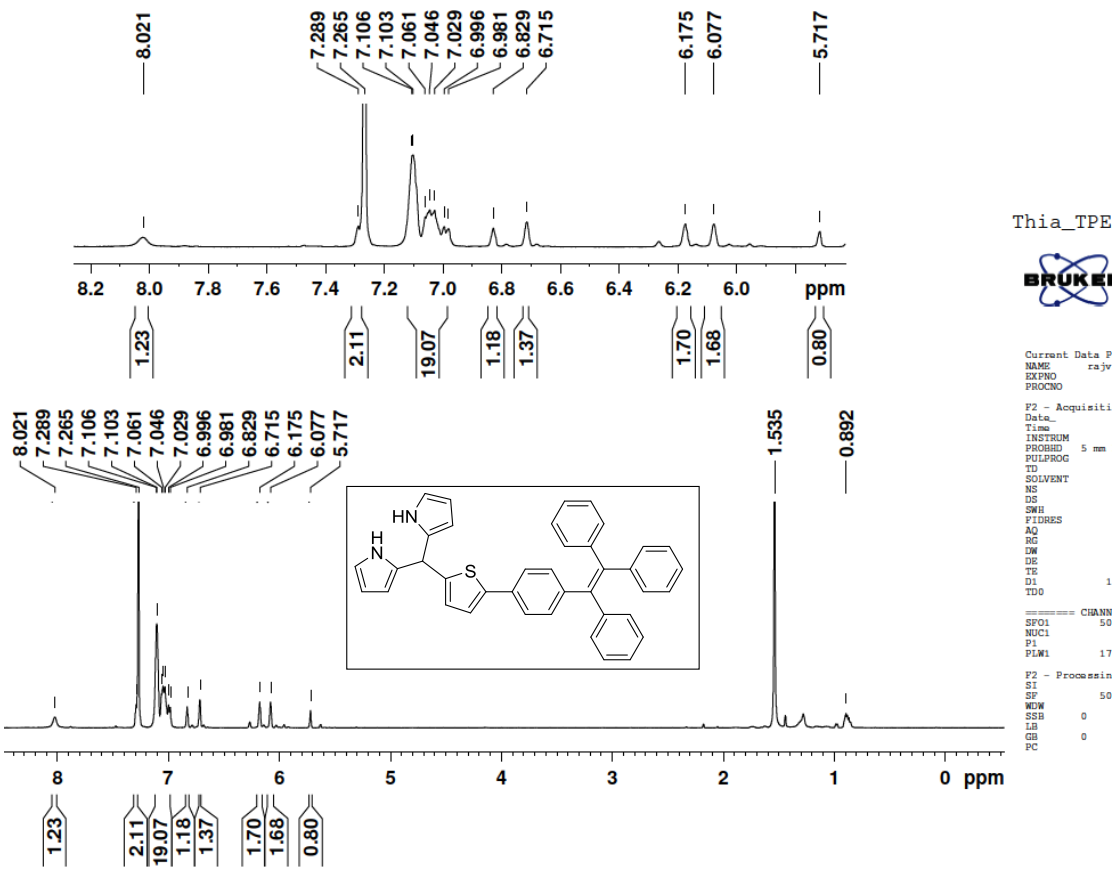


Figure S1. ^{1}H NMR spectrum of compound **DPM1** in $CDCl_3$.

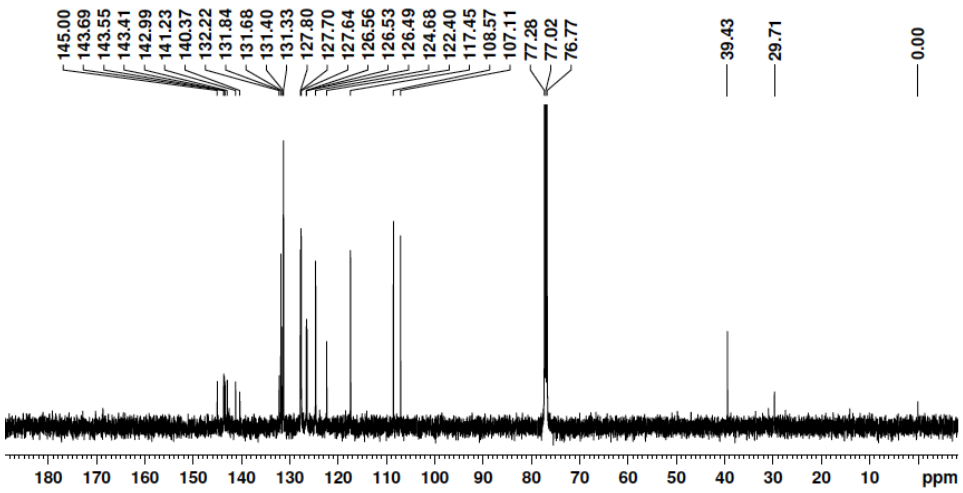


Figure S1. ^{13}C NMR spectrum of compound **DPM1** in $CDCl_3$

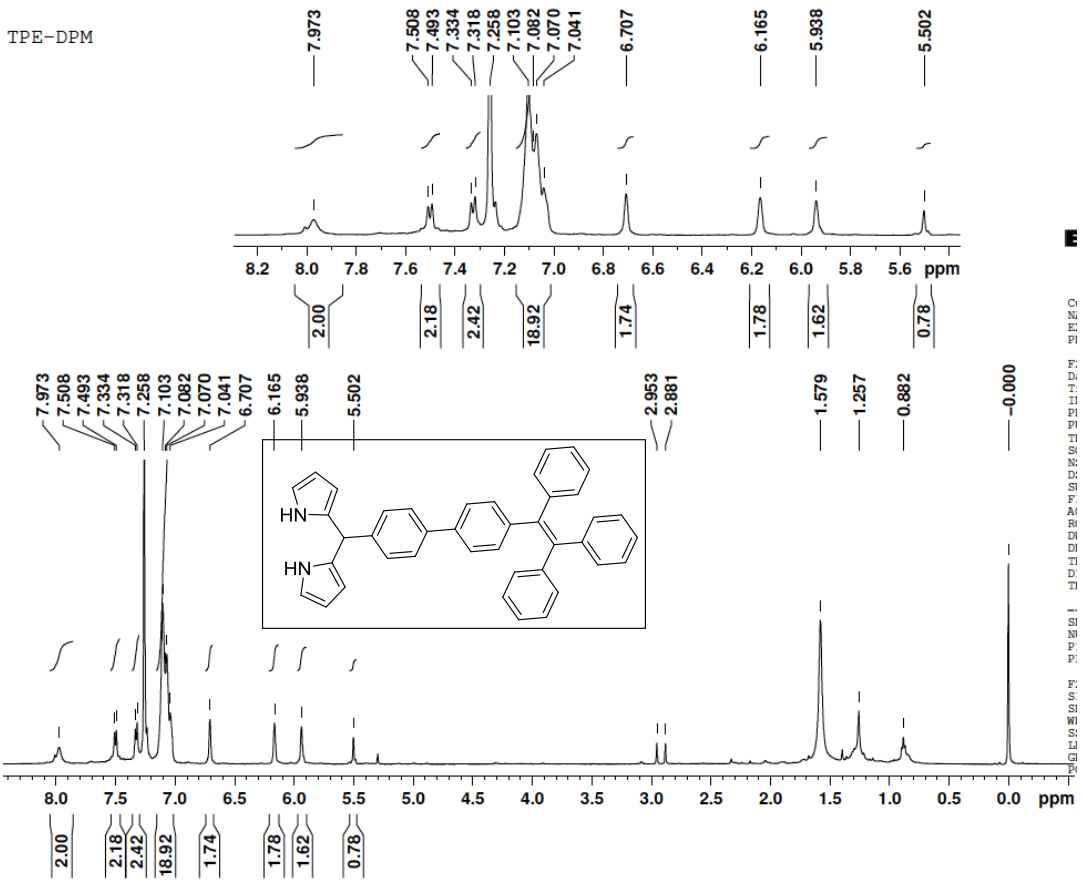


Figure S3. ^{1}H NMR spectrum of compound **DPM2** in $CDCl_3$.

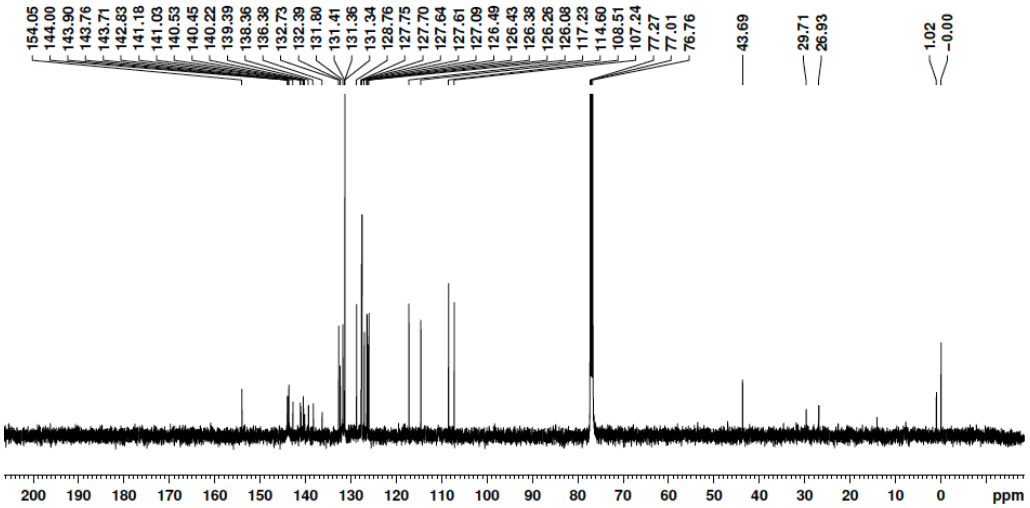


Figure S4. ^{13}C NMR spectrum of compound **DPM2** in $CDCl_3$.

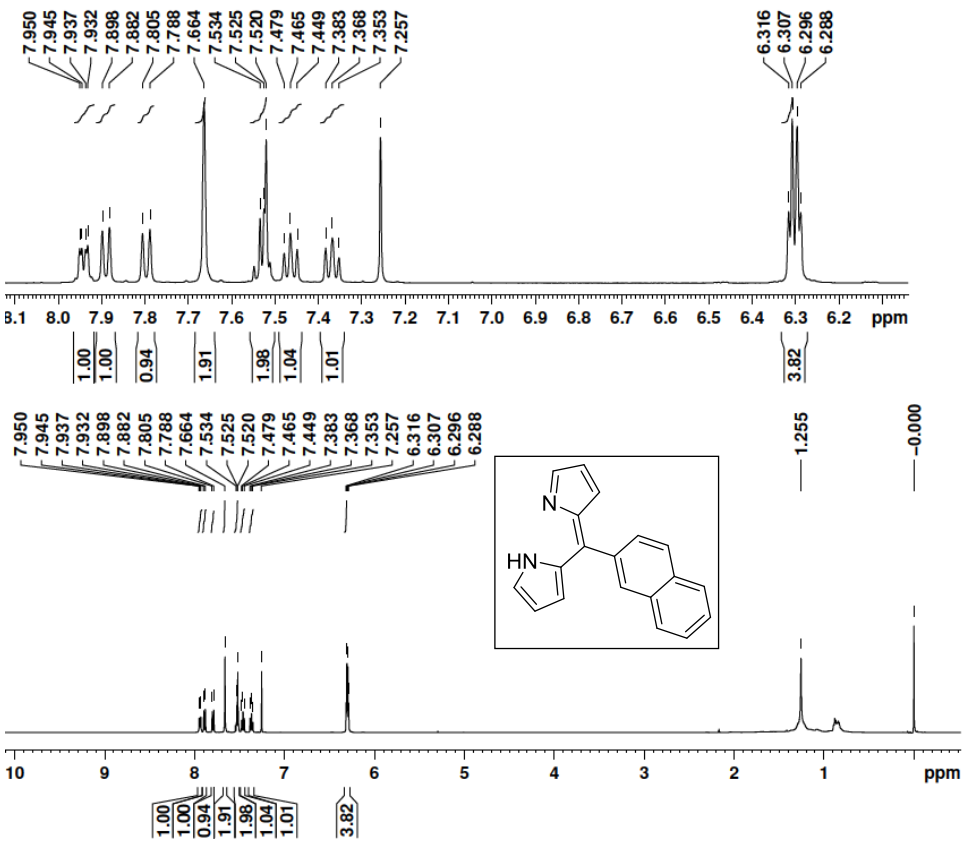


Figure S5. ^{1}H NMR spectrum of compound of **(Z)-2-(naphthalen-2-yl(2H-pyrrol-2-ylidene)methyl)-1H-pyrrole** in $CDCl_3$.

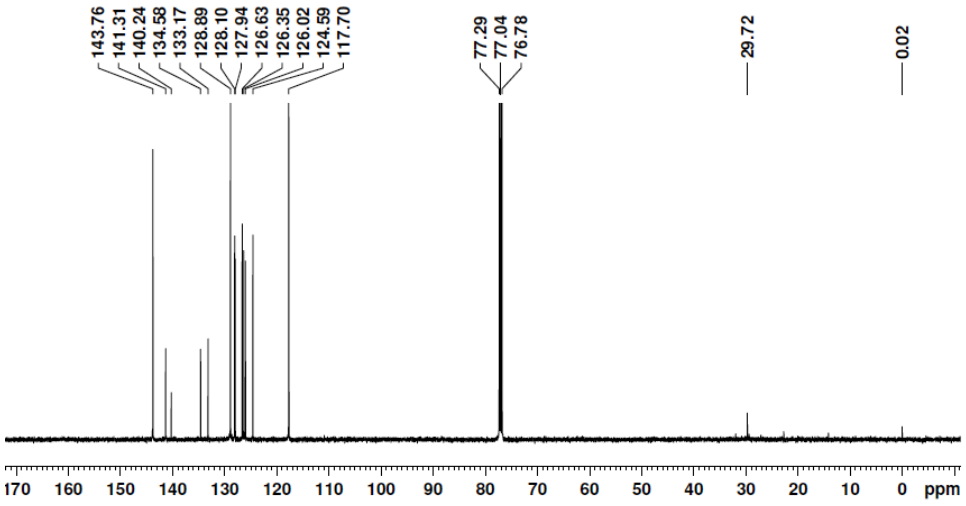


Figure S6. ^{13}C NMR spectrum of compound of **(Z)-2-(naphthalen-2-yl(2H-pyrrol-2-ylidene)methyl)-1H-pyrrole** in $CDCl_3$.

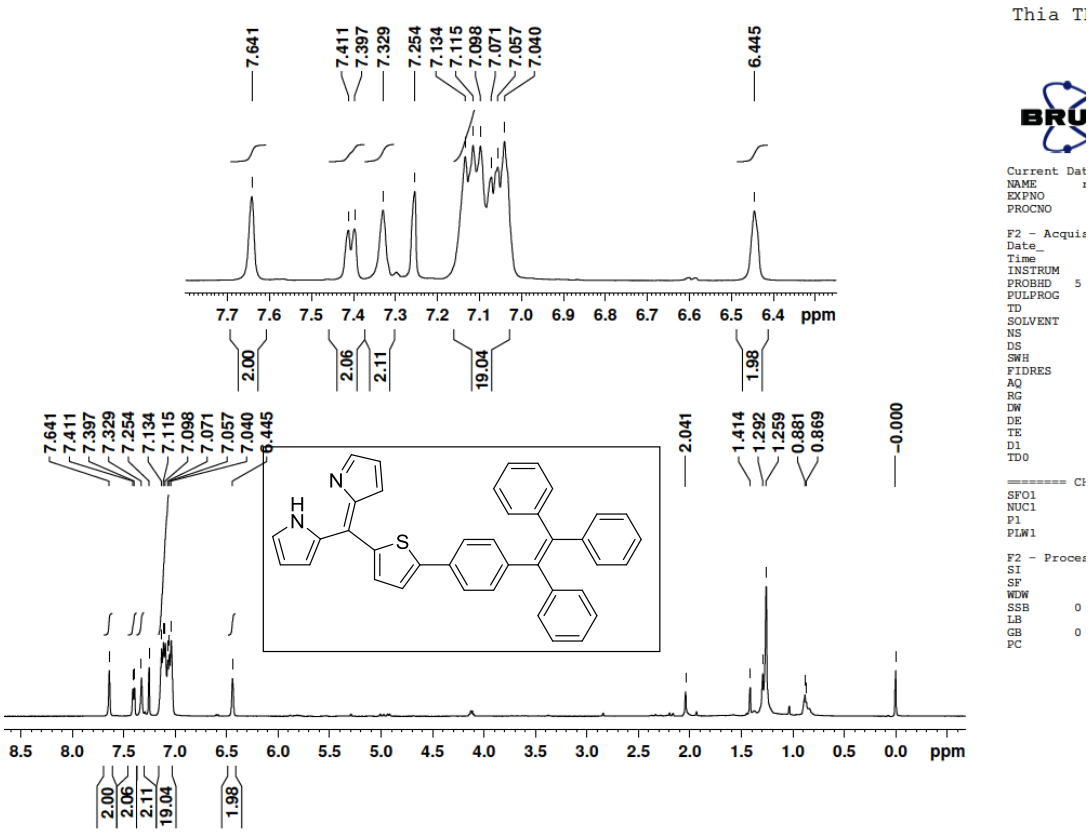


Figure S7. ^{1}H NMR spectrum of compound of **DPM3** in $CDCl_3$.

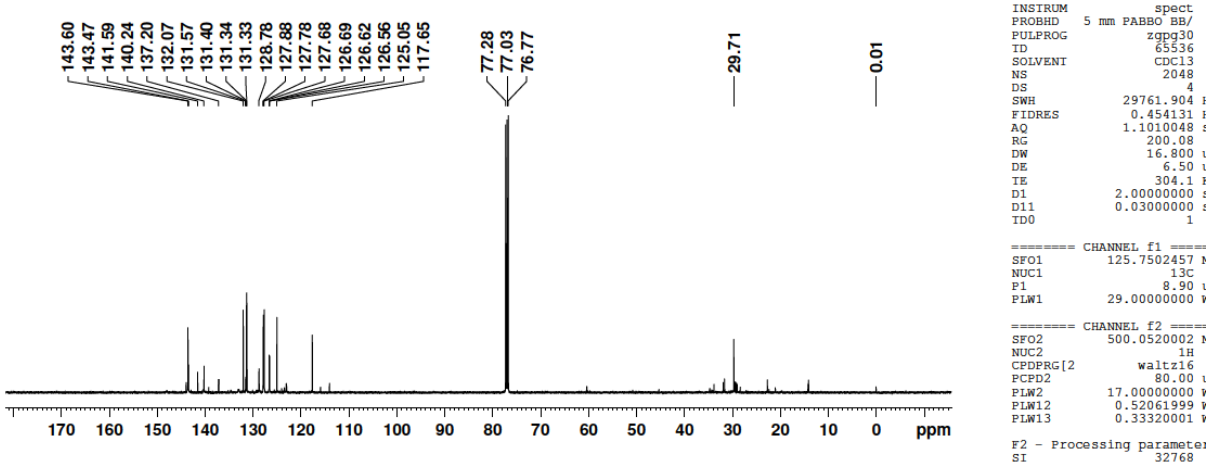


Figure S8. ^{13}C NMR spectrum of compound of **DPM3** in $CDCl_3$.

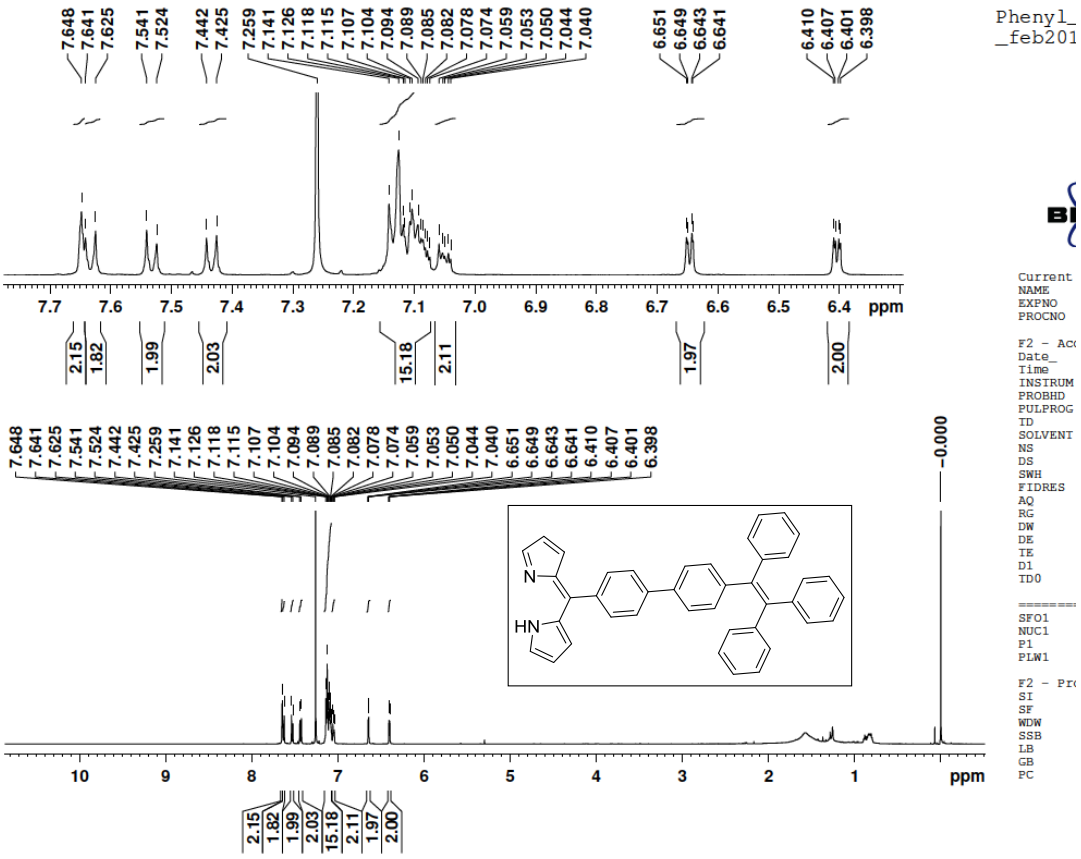


Figure S9. ^{1}H NMR spectrum of compound **DPM4** in $CDCl_3$.

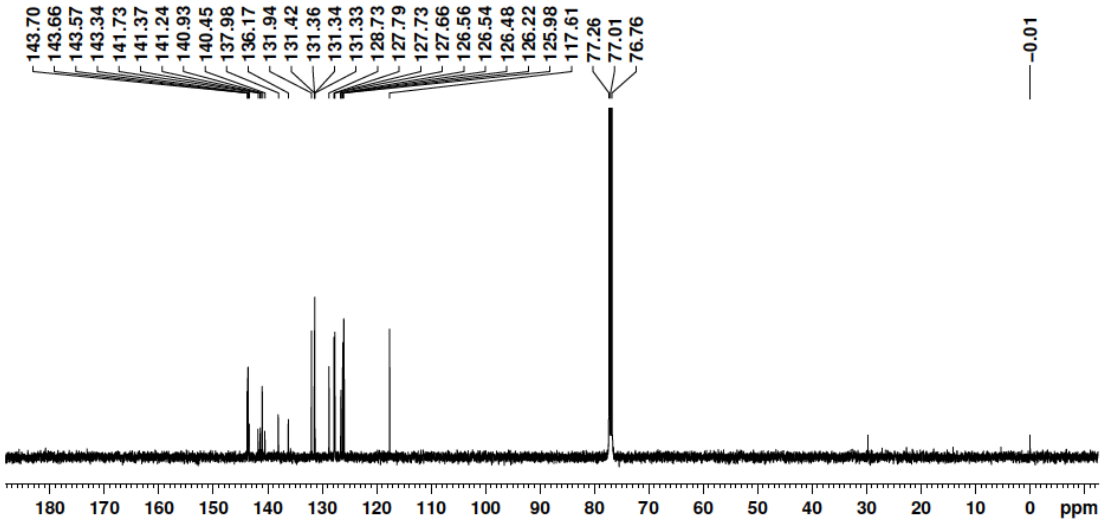


Figure S10. ^{13}C NMR spectrum of compound **DPM4** in $CDCl_3$.

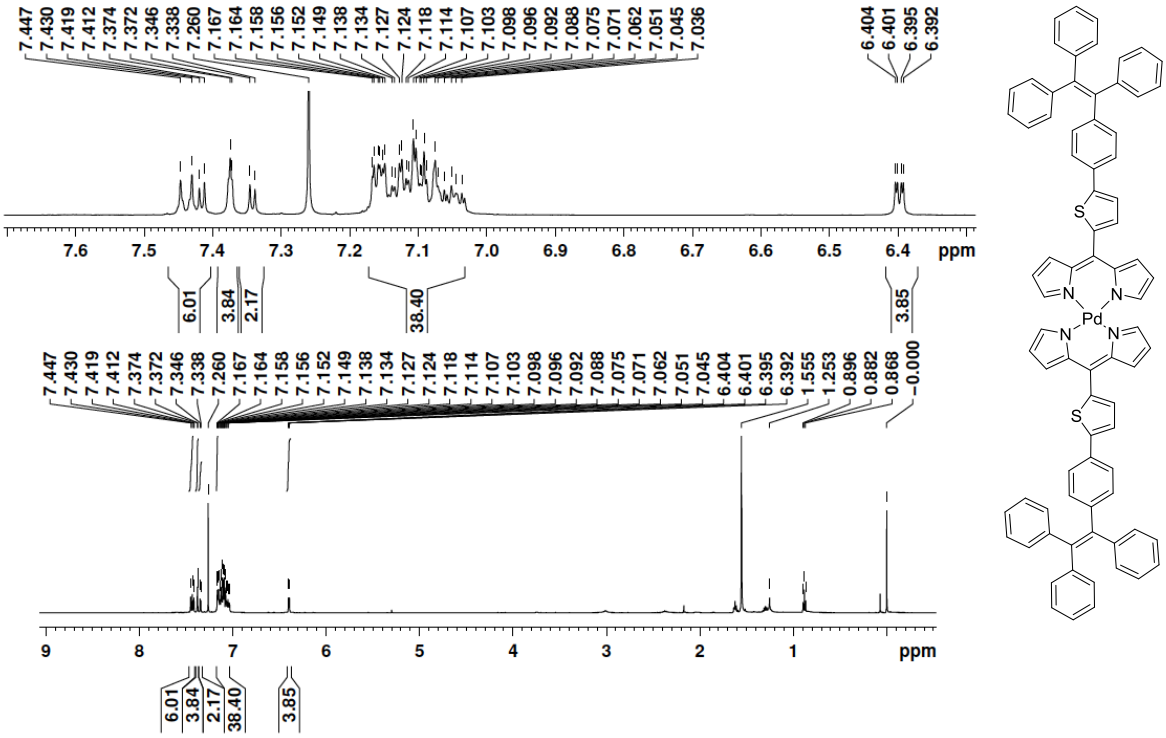


Figure S11. ^{1}H NMR spectrum of compound **Pd1** in $CDCl_3$.

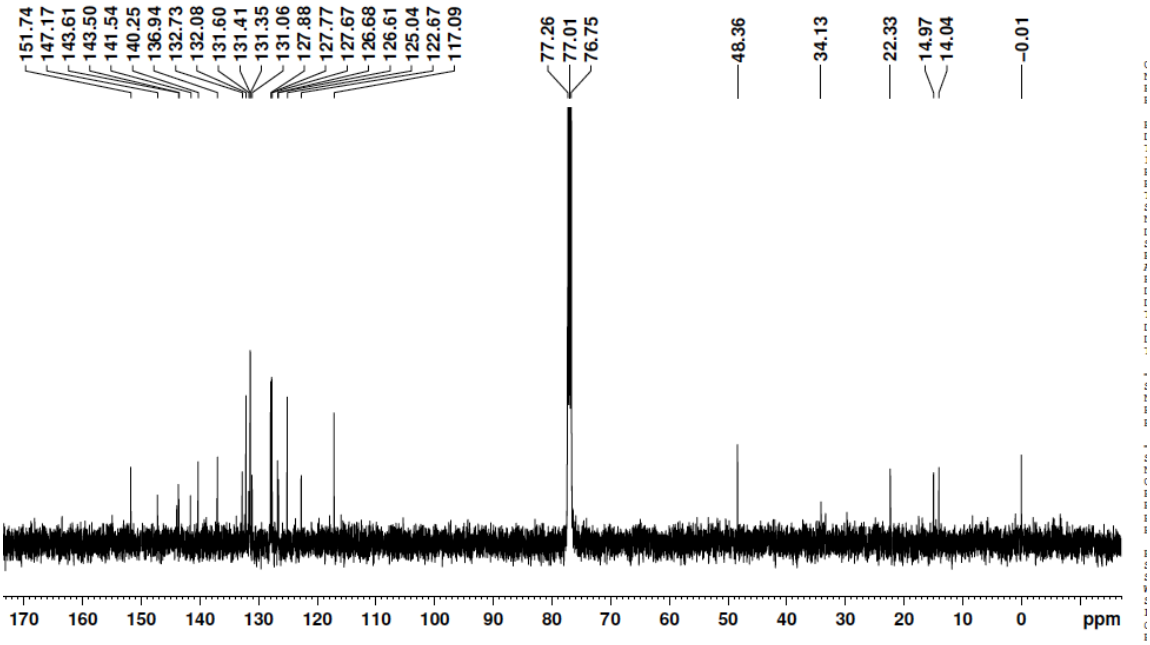


Figure S12. ^{13}C NMR spectrum of compound **Pd1** in $CDCl_3$.

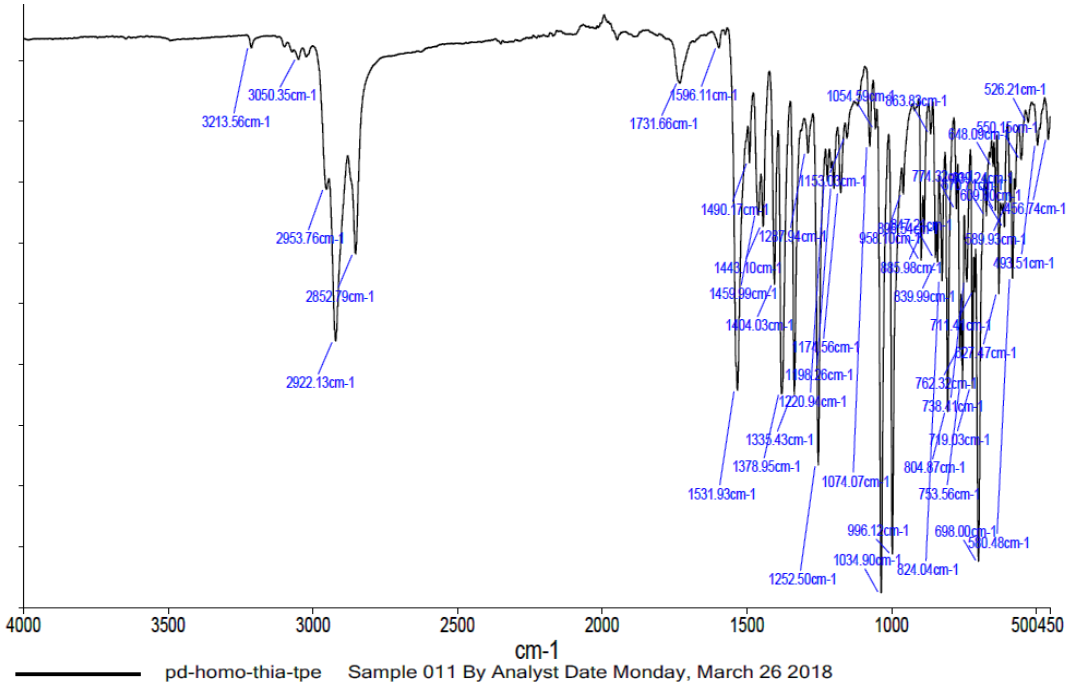


Figure S23. IR spectrum of compound **Pd1**.

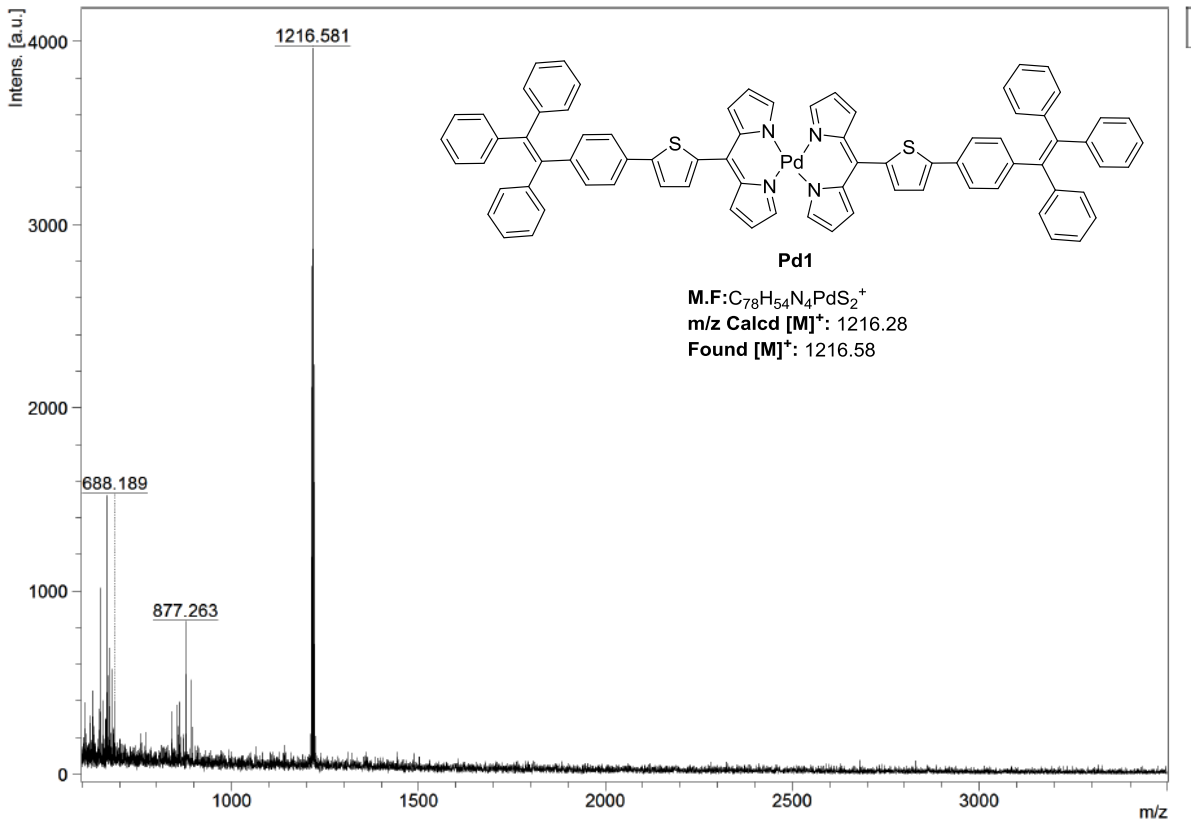


Figure S14. MALDI-MS of compound **Pd1**.

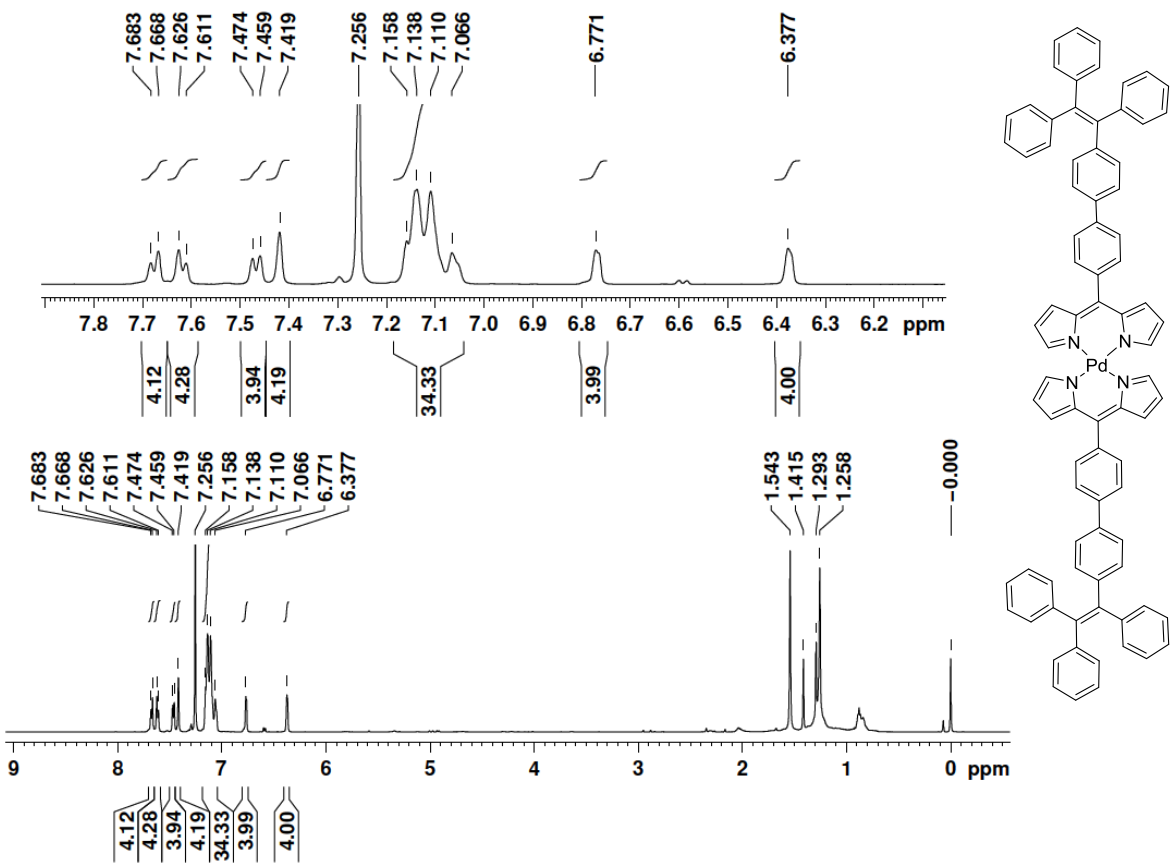


Figure S15. ^{1}H NMR spectrum of compound **Pd2** in $CDCl_3$.

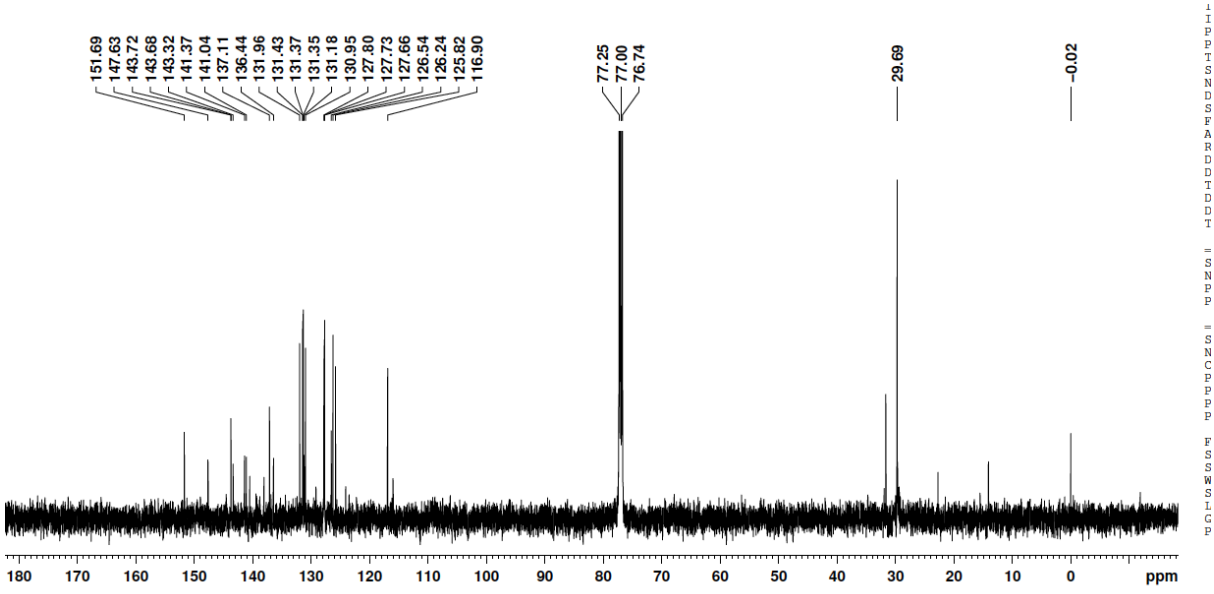


Figure S16. ^{13}C NMR spectrum of compound **Pd2** in $CDCl_3$.

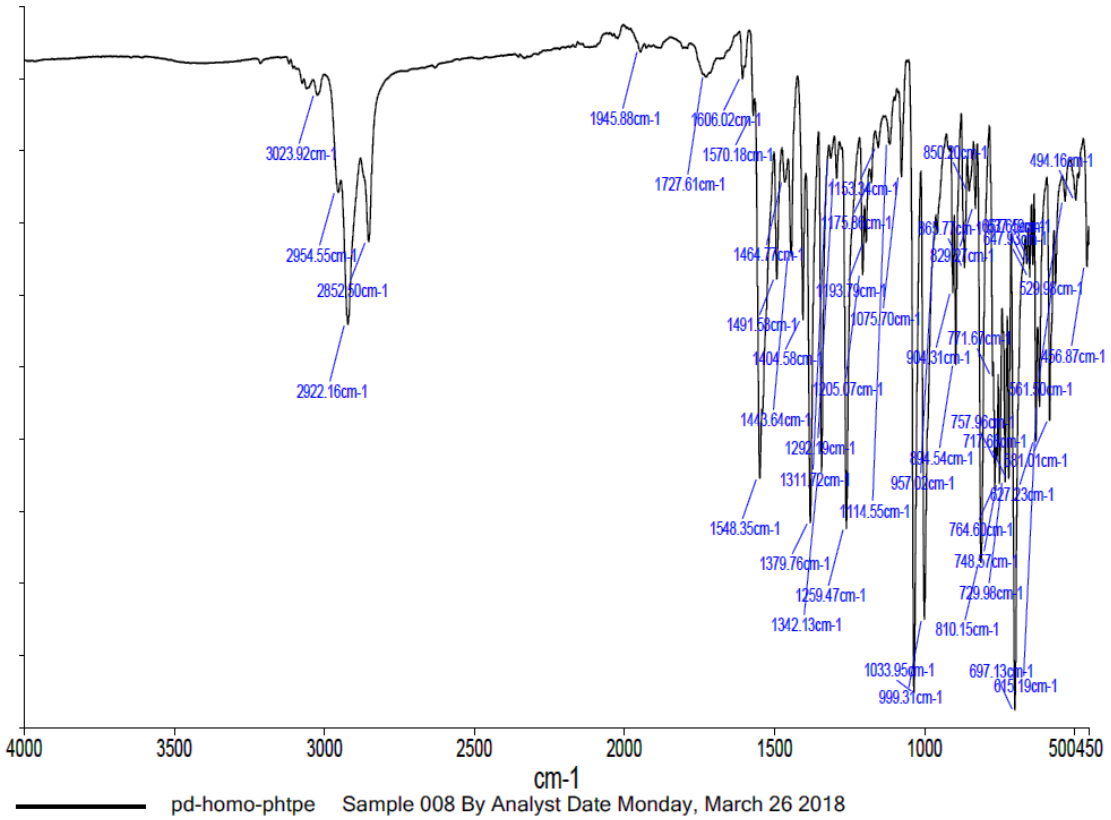


Figure S17. IR spectrum of compound **Pd2**.

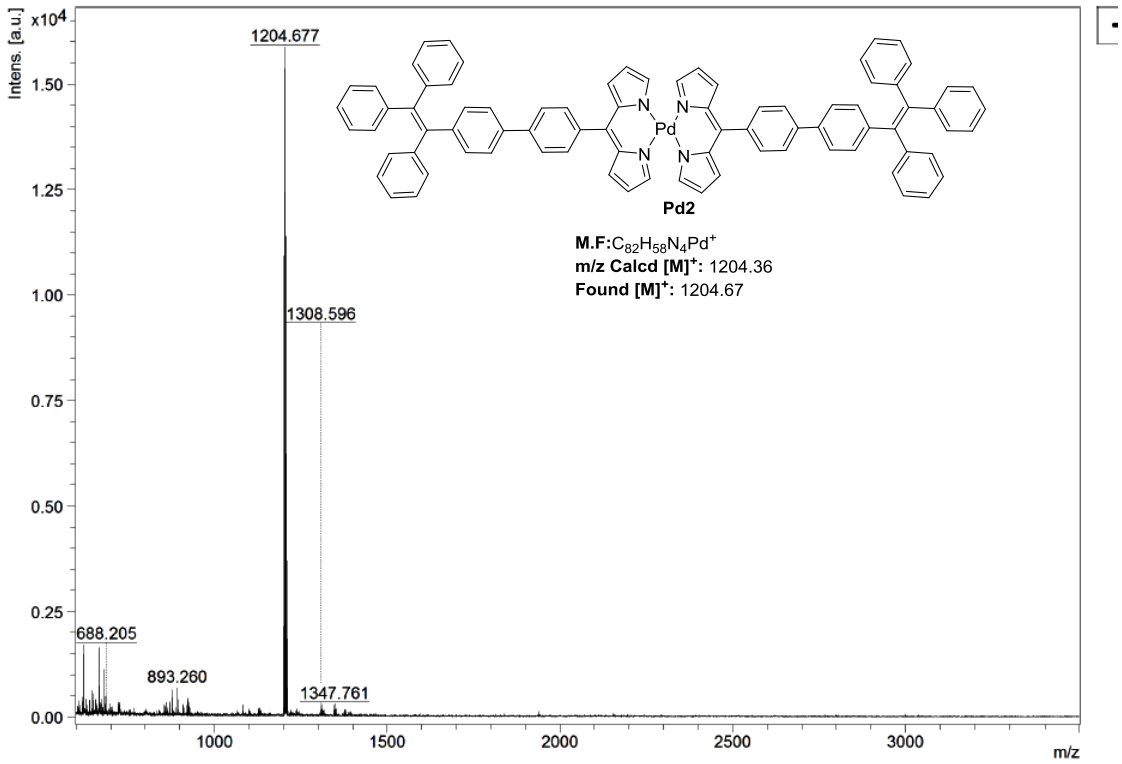


Figure S18. MALDI-MS of compound **Pd2**.

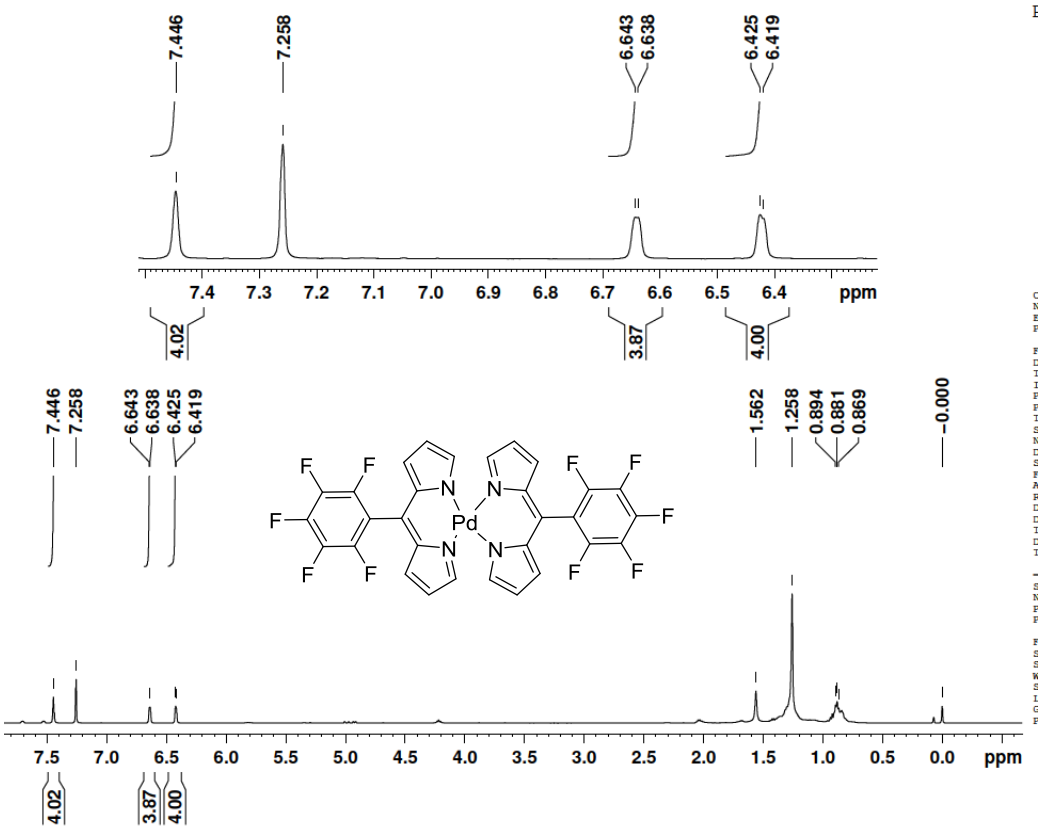


Figure S19. ^{1}H NMR spectrum of compound **Pd3** in $CDCl_3$.

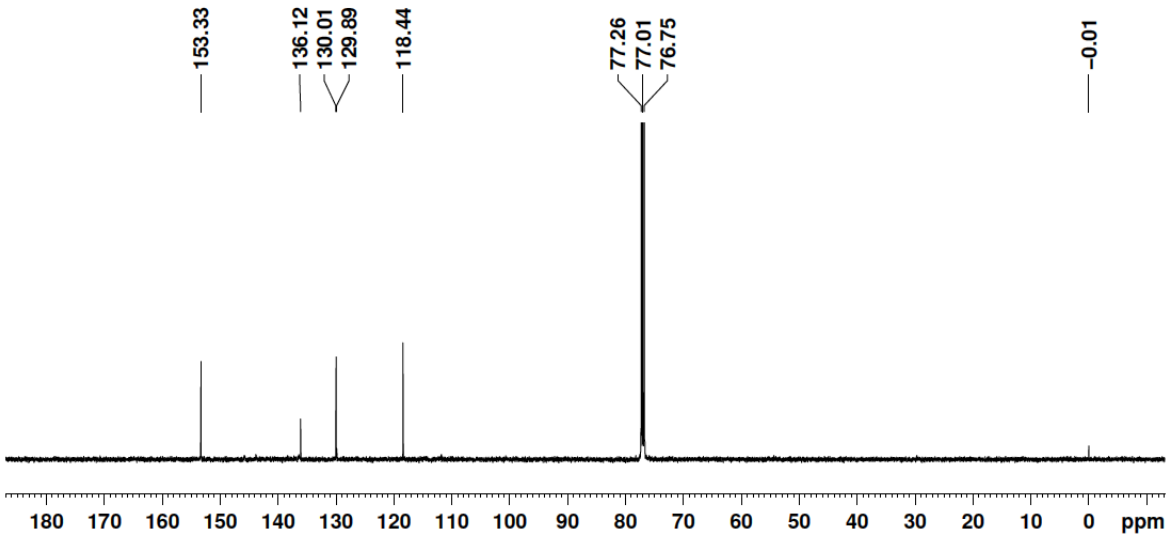


Figure S20. ^{13}C NMR spectrum of compound **Pd3** in $CDCl_3$.

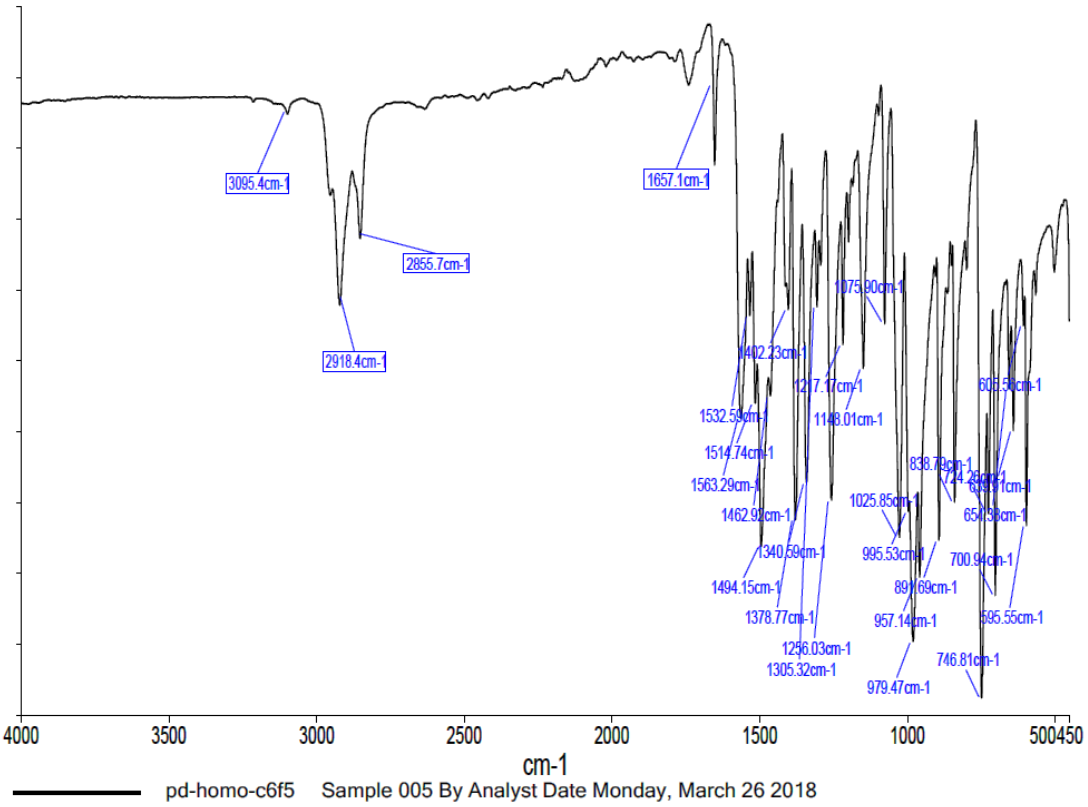


Figure S21. IR spectrum of compound **Pd3**.

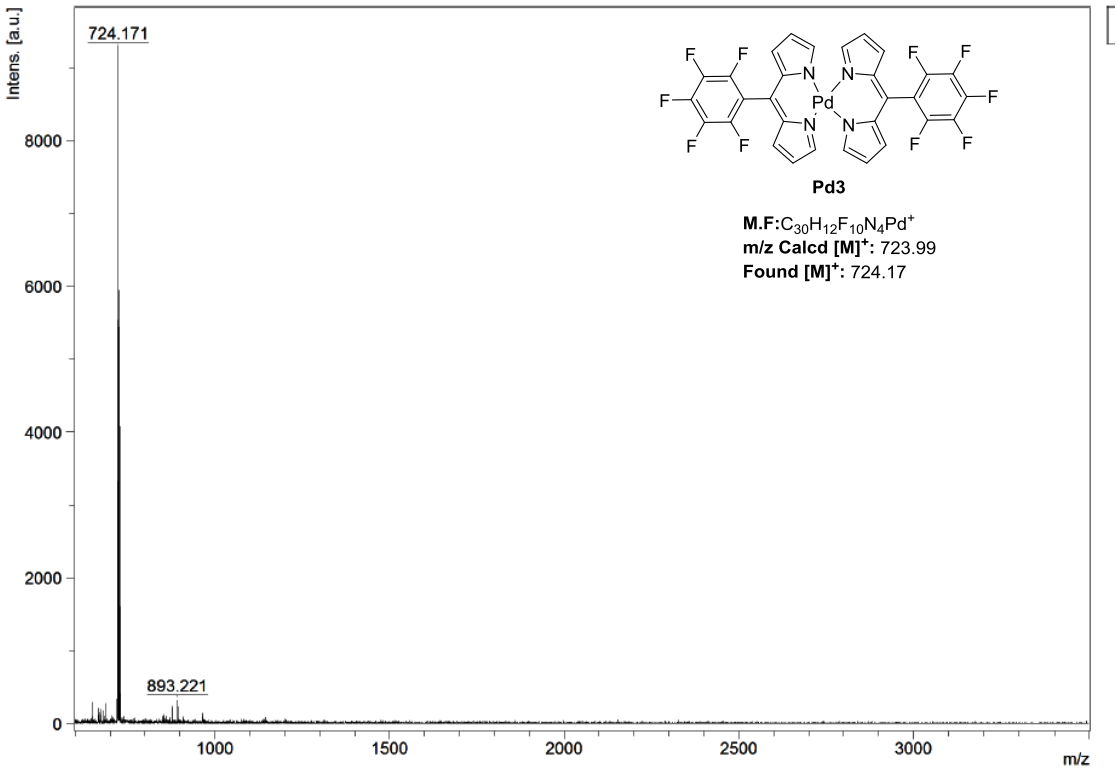


Figure S22. MALDI-MS of compound **Pd3**.

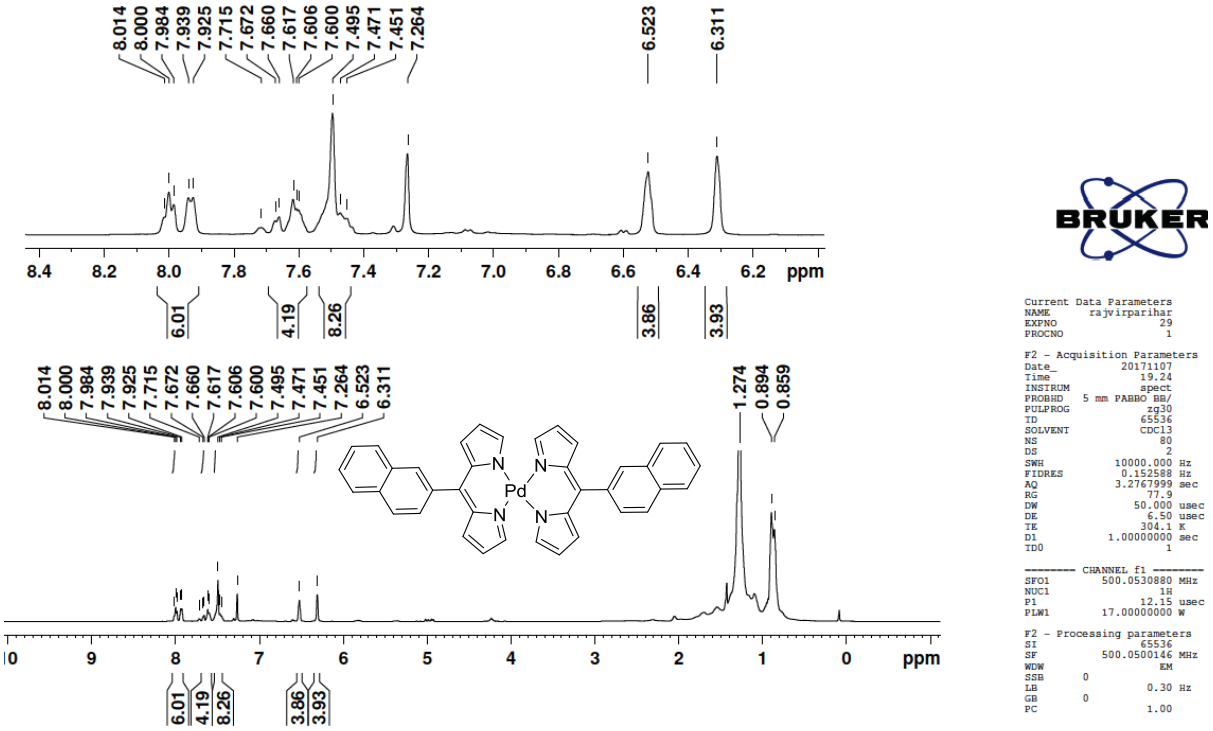


Figure S3. ^{1}H NMR spectrum of compound **Pd4** in $CDCl_3$.

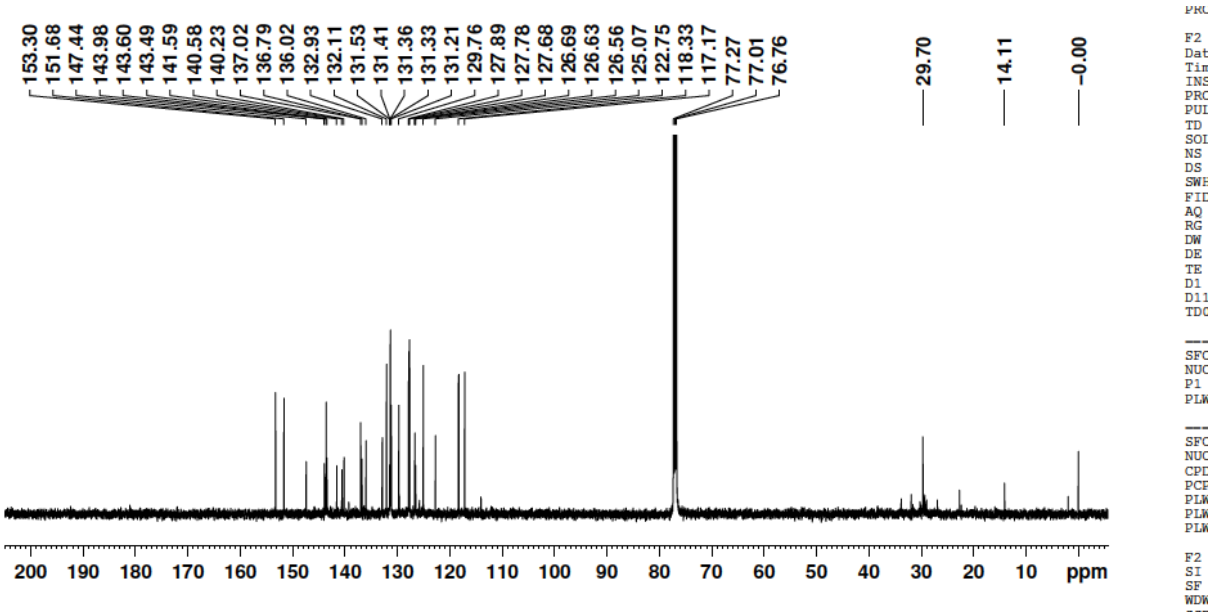


Figure S4. ^{13}C NMR spectrum of compound **Pd4** in $CDCl_3$.

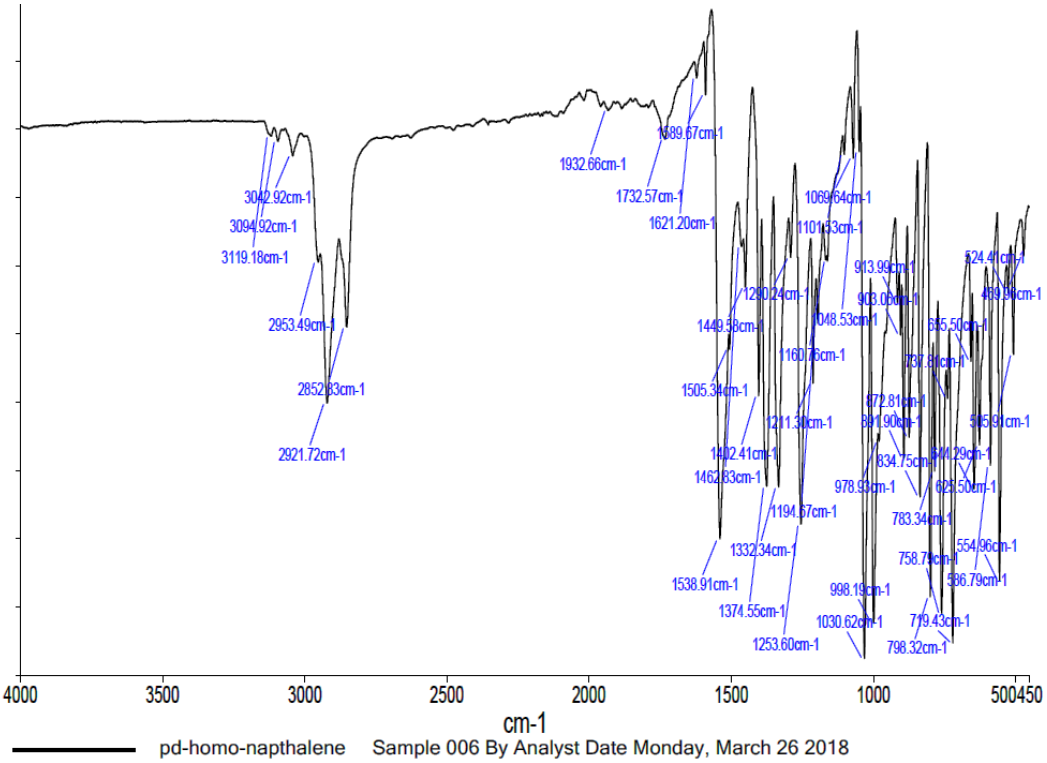


Figure S25. IR spectrum of compound **Pd4**.

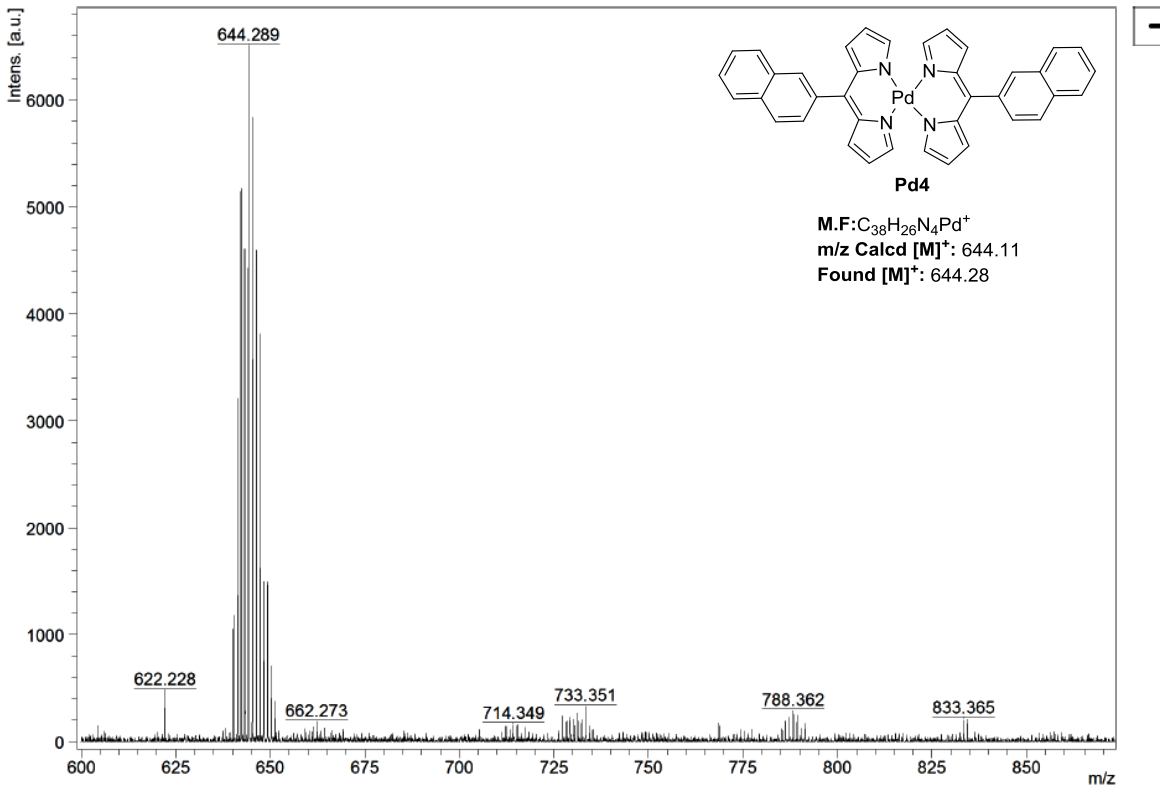


Figure S26. MALDI-MS of compound **Pd4**.

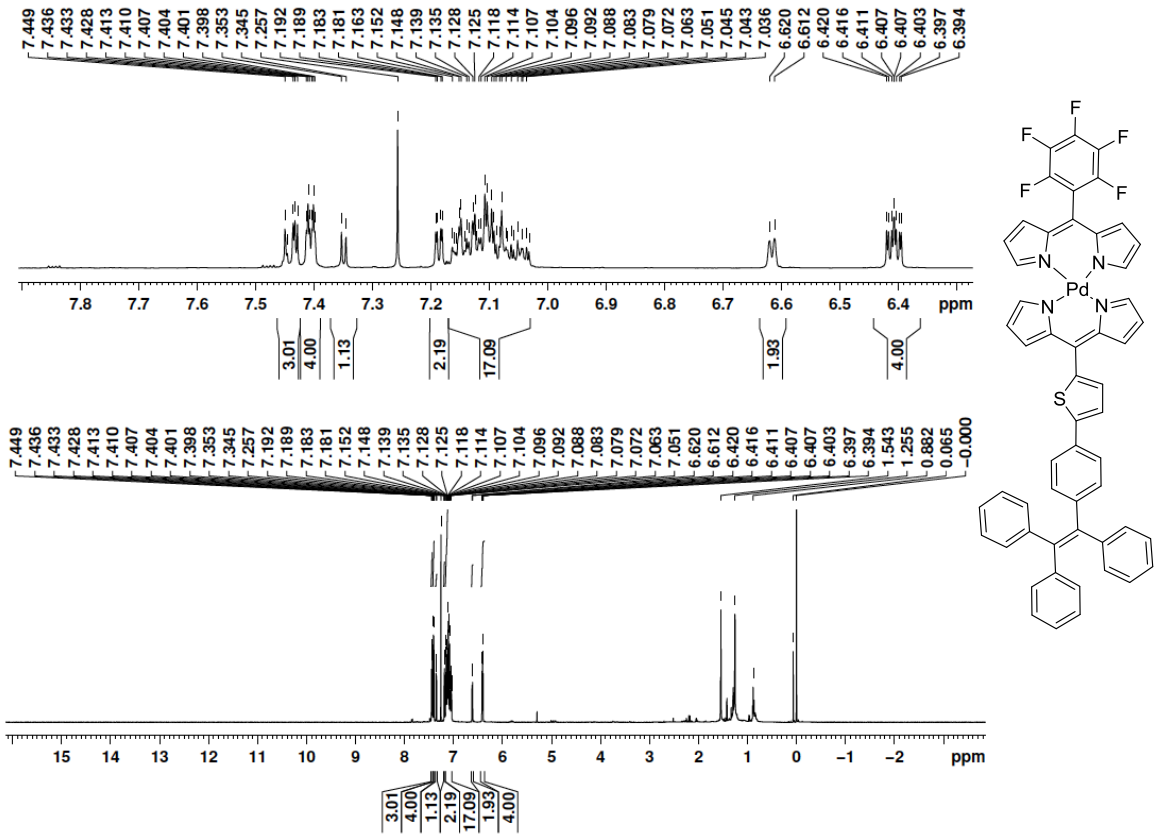


Figure S27. ^{1}H NMR spectrum of compound **Pd5** in $CDCl_3$.

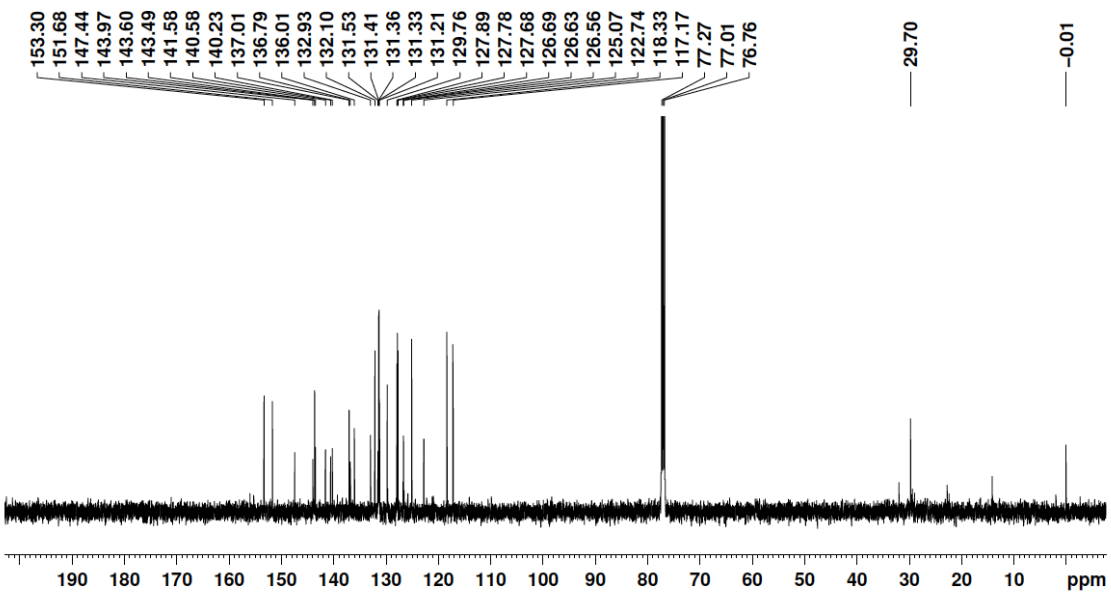


Figure S5. ^{13}C NMR spectrum of compound **Pd5** in $CDCl_3$.

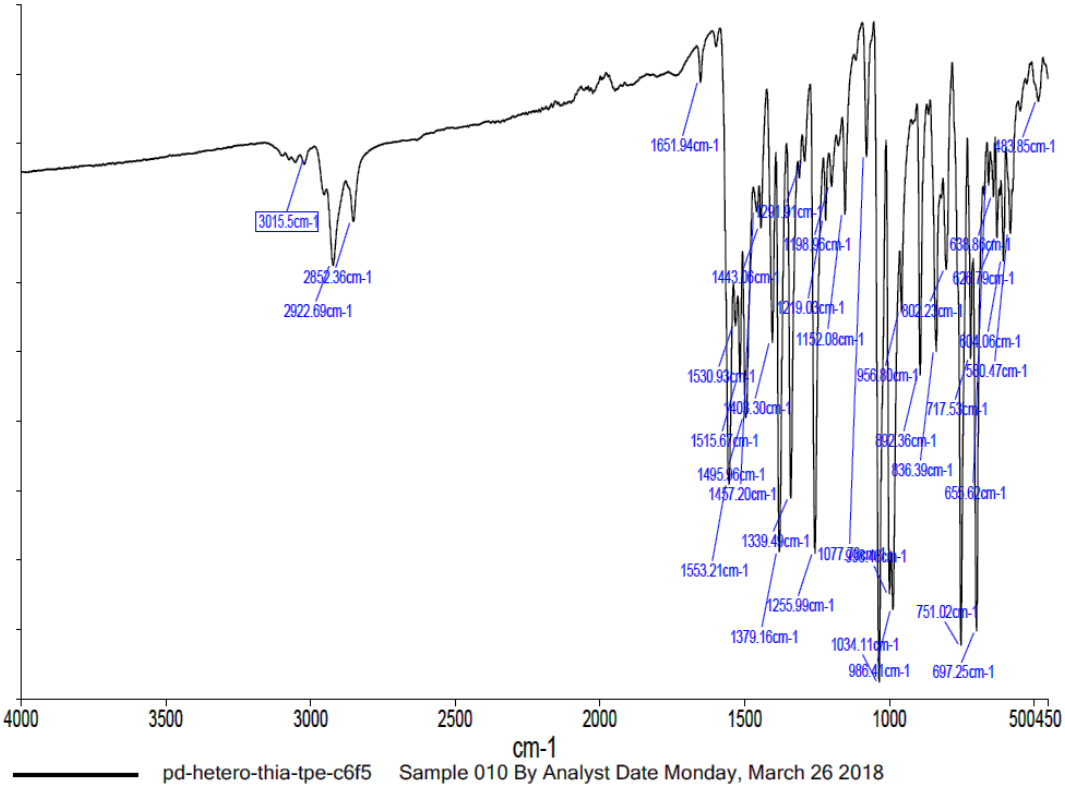


Figure S26. IR spectrum of compound **Pd5**.

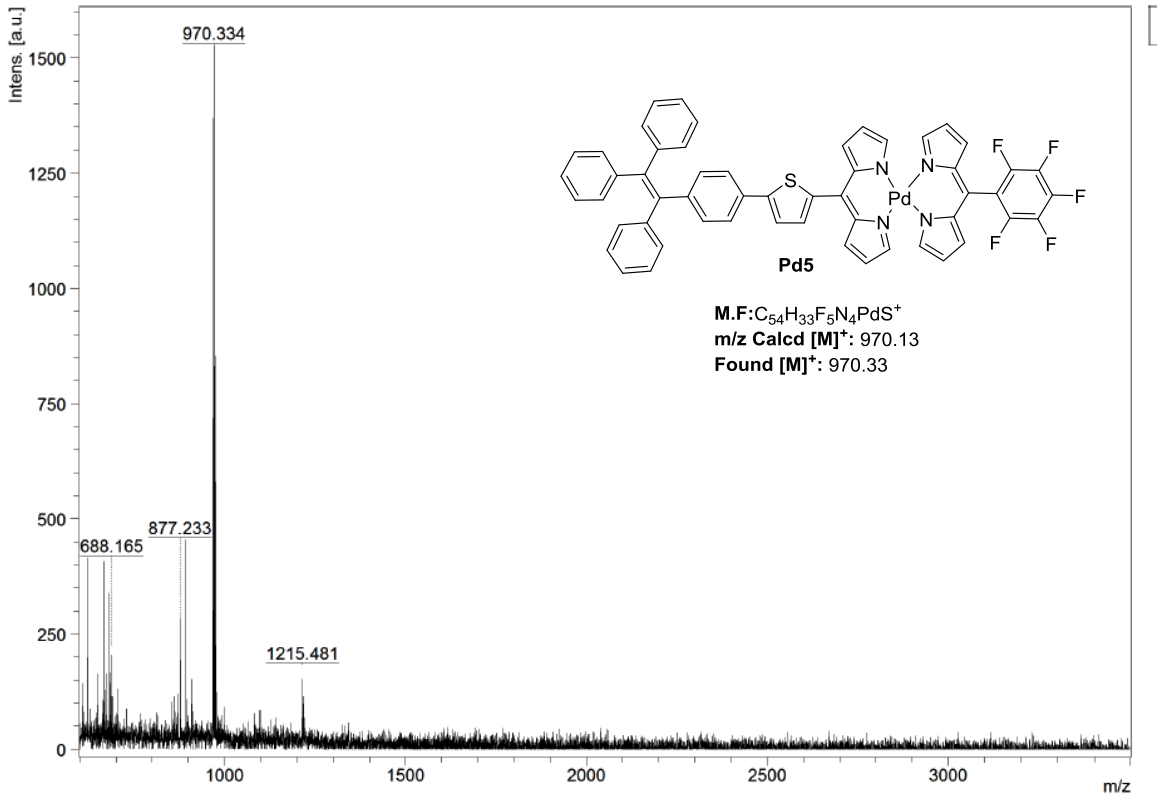


Figure S7. MALDI-MS of compound **Pd5**.

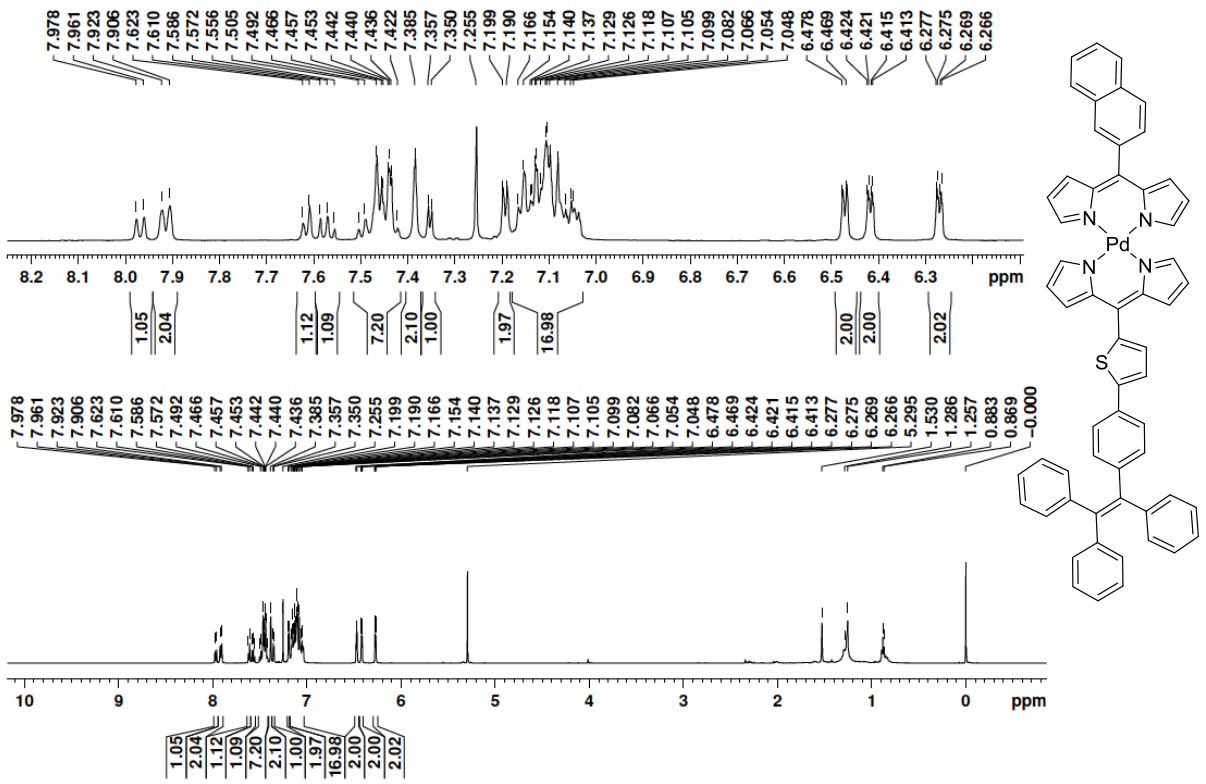


Figure S8. ^{1}H NMR spectrum of compound **Pd6** in $CDCl_3$.

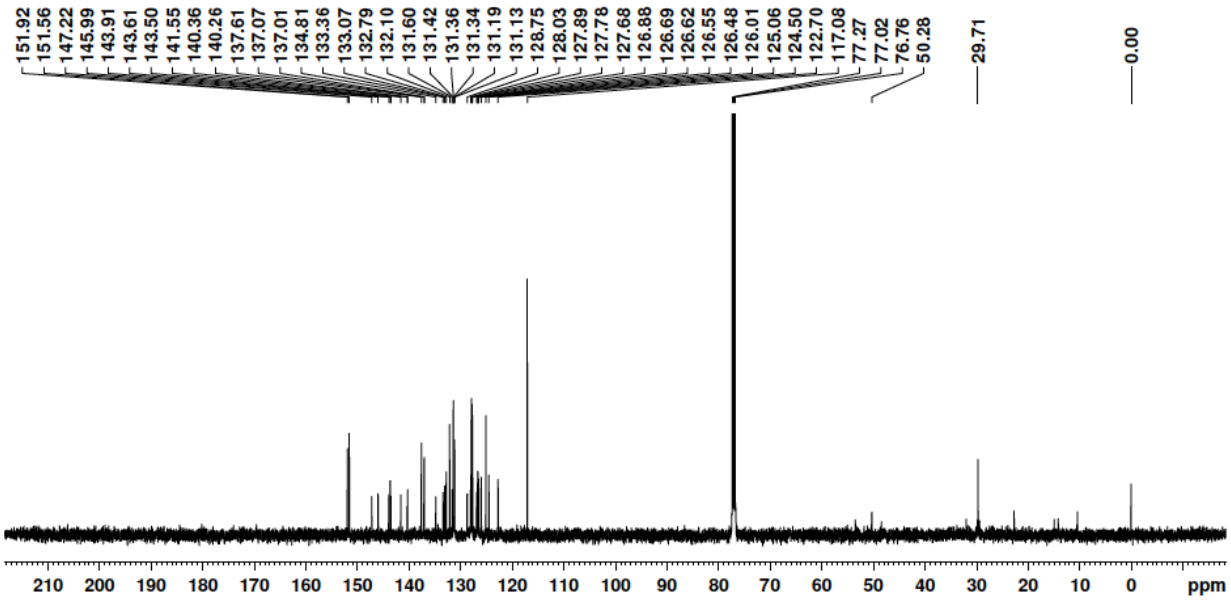


Figure S9. ^{13}C NMR spectrum of compound **Pd6** in $CDCl_3$.

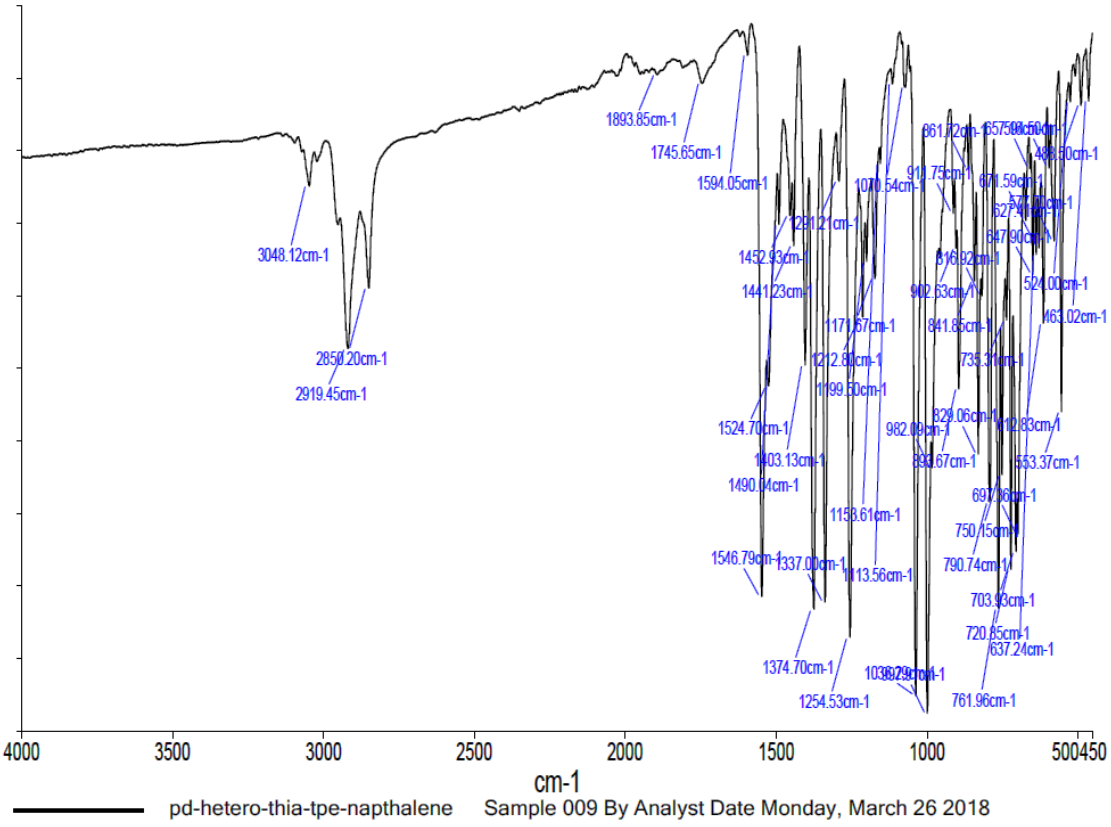


Figure S33. IR spectrum of compound **Pd6**.

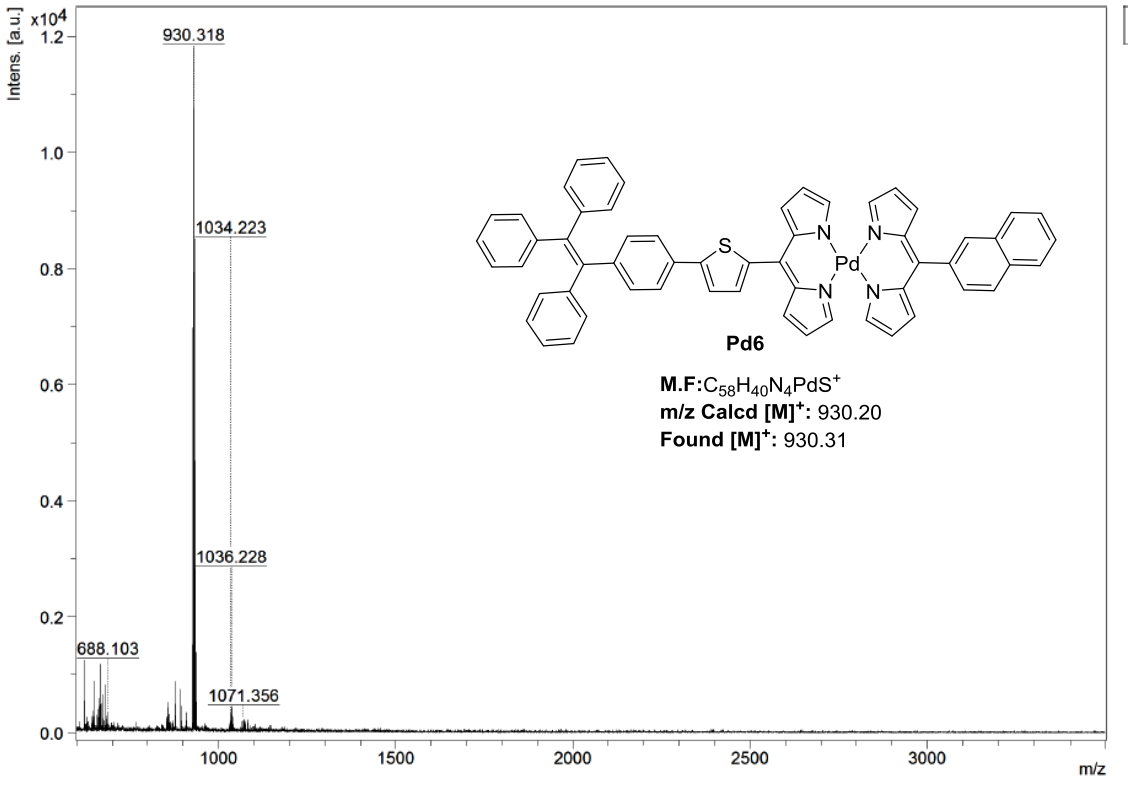


Figure S34. MALDI-MS of compound **Pd6**.

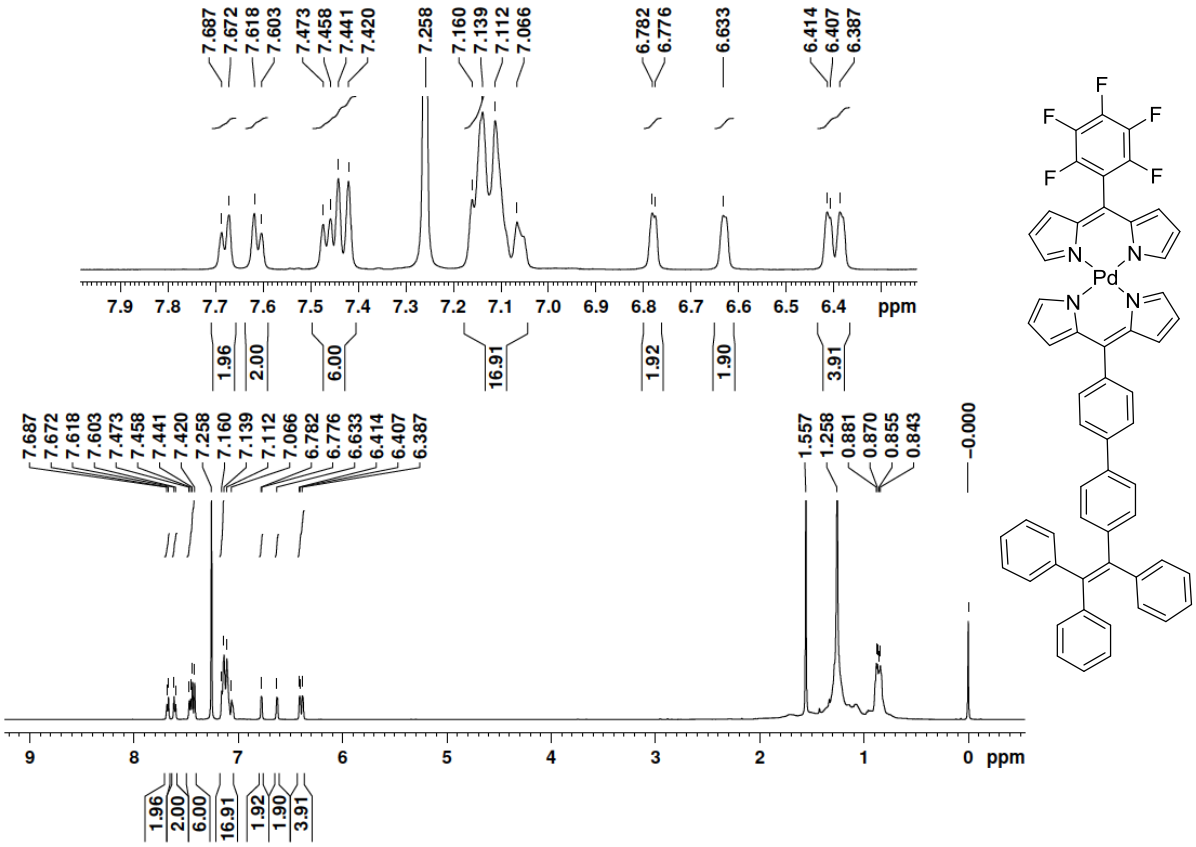


Figure S35. ^{1}H NMR spectrum of compound **Pd7** in $CDCl_3$.

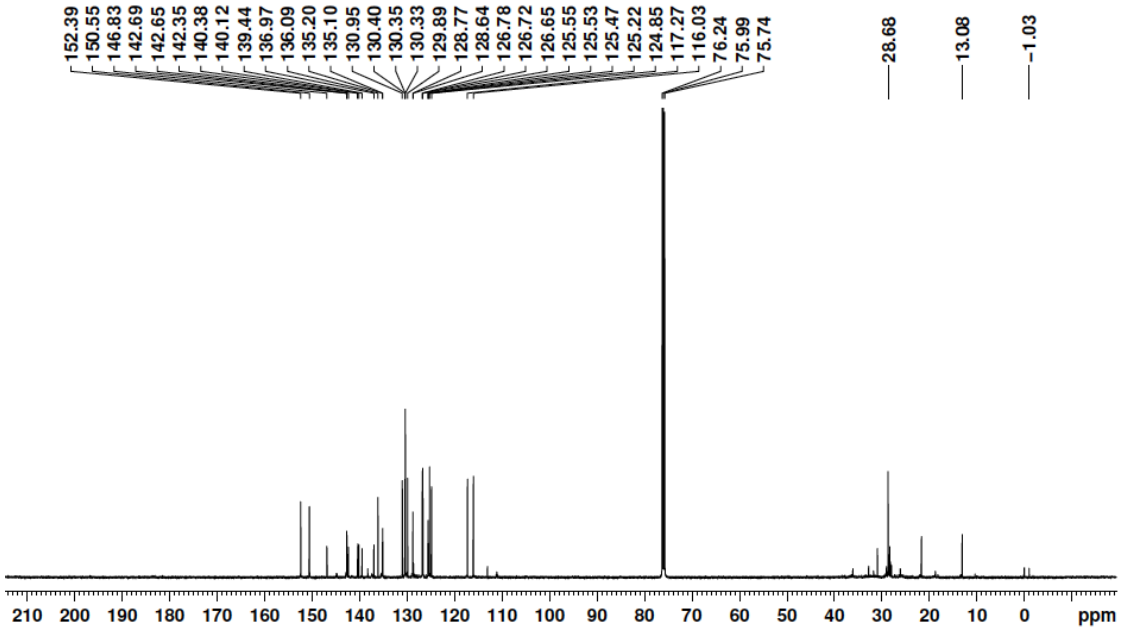


Figure S36. ^{13}C NMR spectrum of compound **Pd7** in $CDCl_3$.

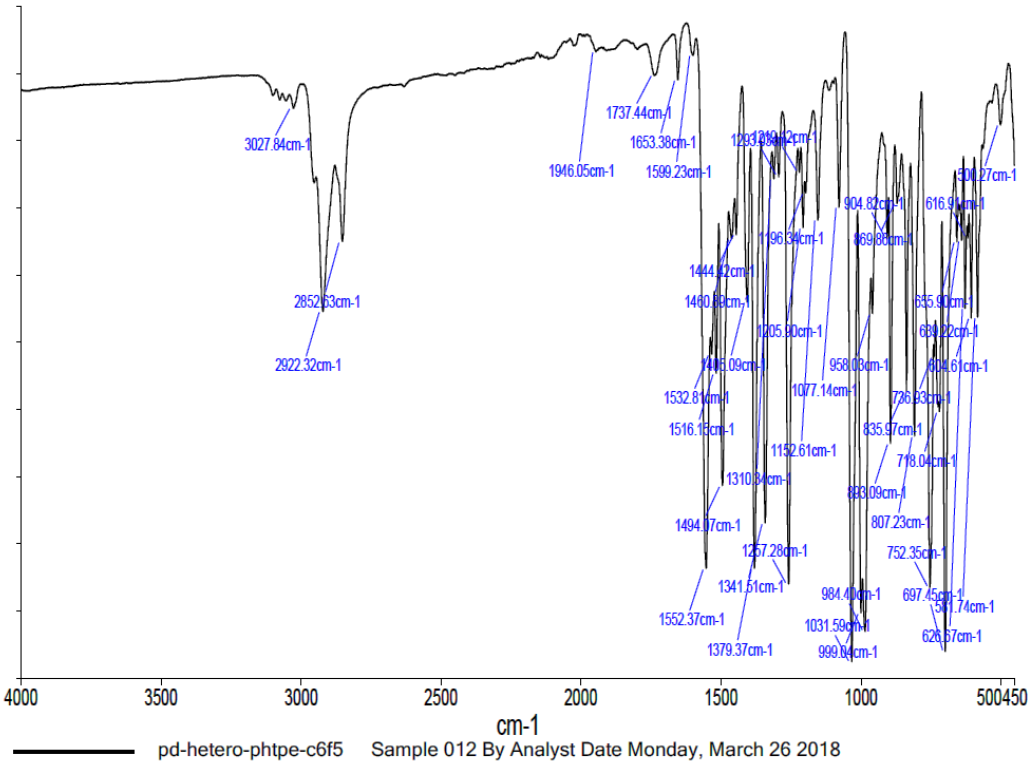


Figure S37. IR spectrum of compound **Pd7**.

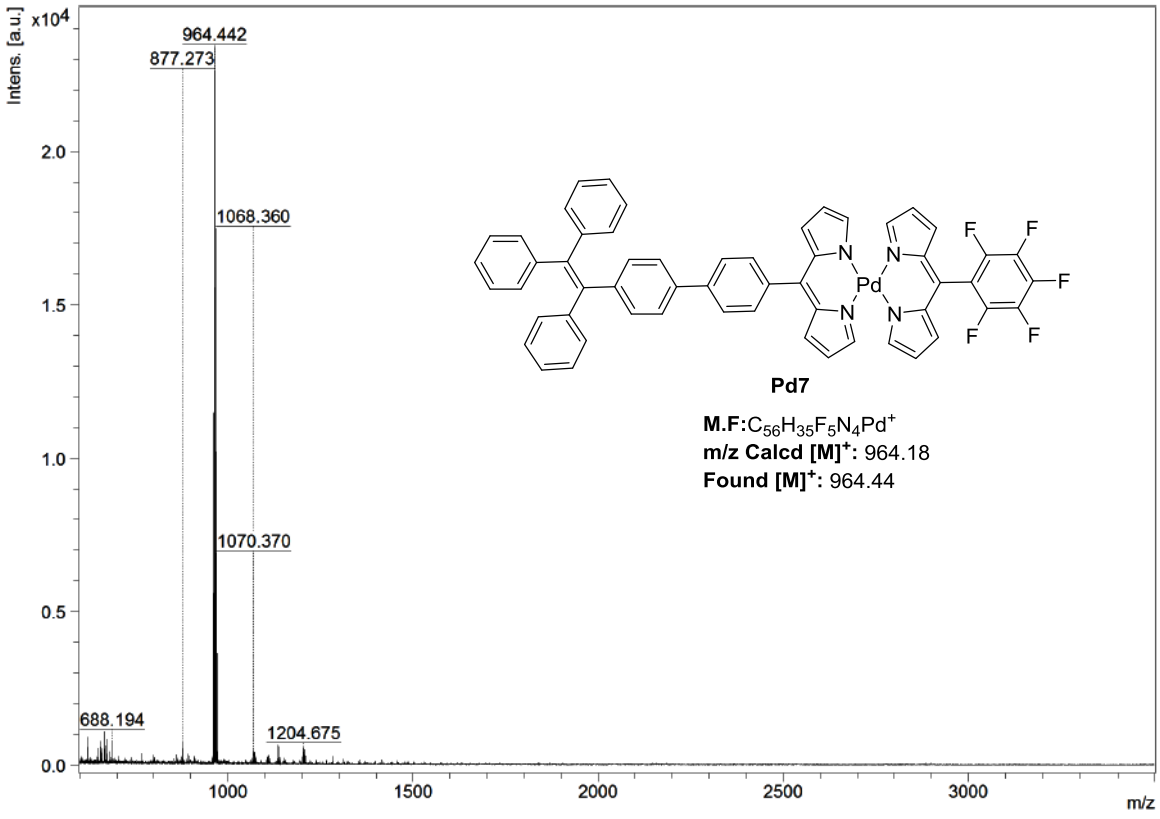


Figure S38. MALDI-MS of compound **Pd7**.

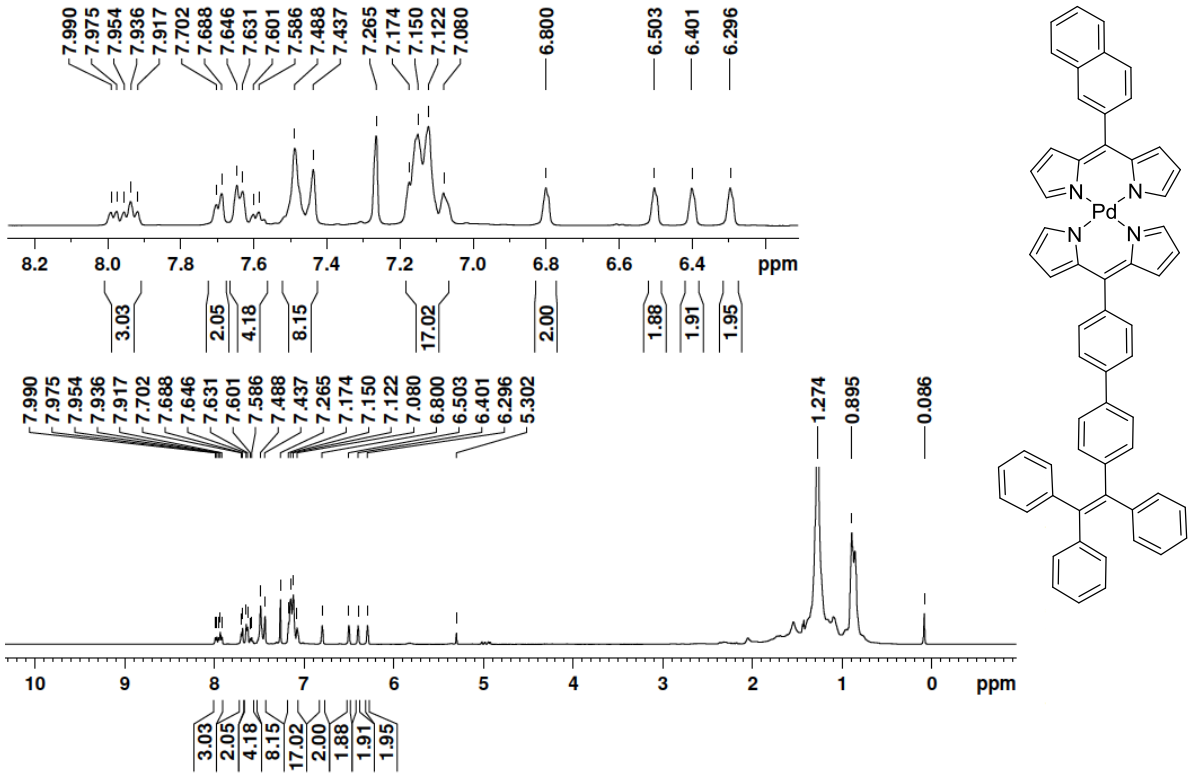


Figure S39. ^{1}H NMR spectrum of compound **Pd8** in $CDCl_3$.

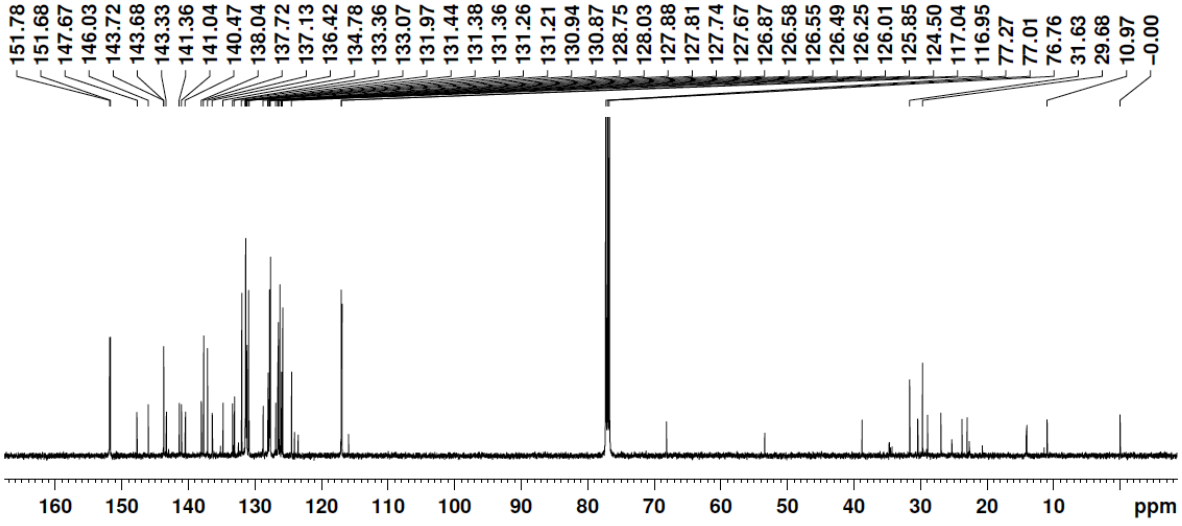


Figure S40. ^{13}C NMR spectrum of compound **Pd8** in $CDCl_3$.

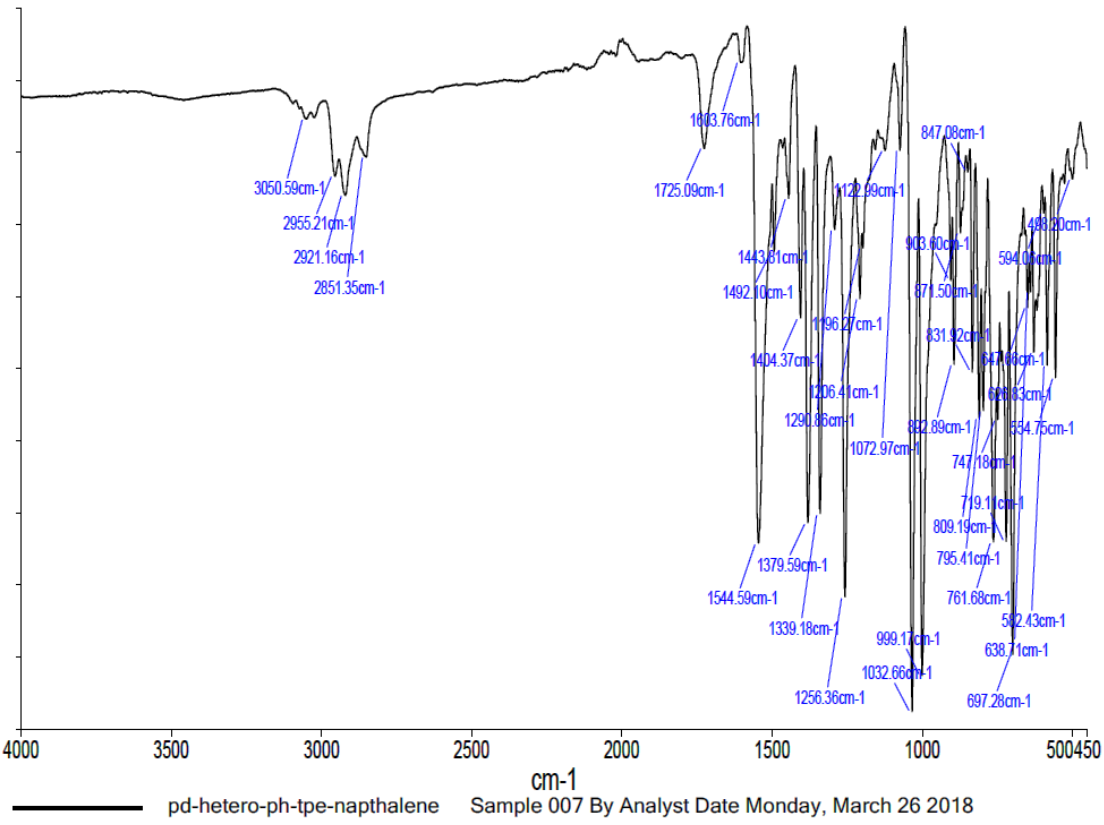


Figure S41. IR spectrum of compound **Pd8**.

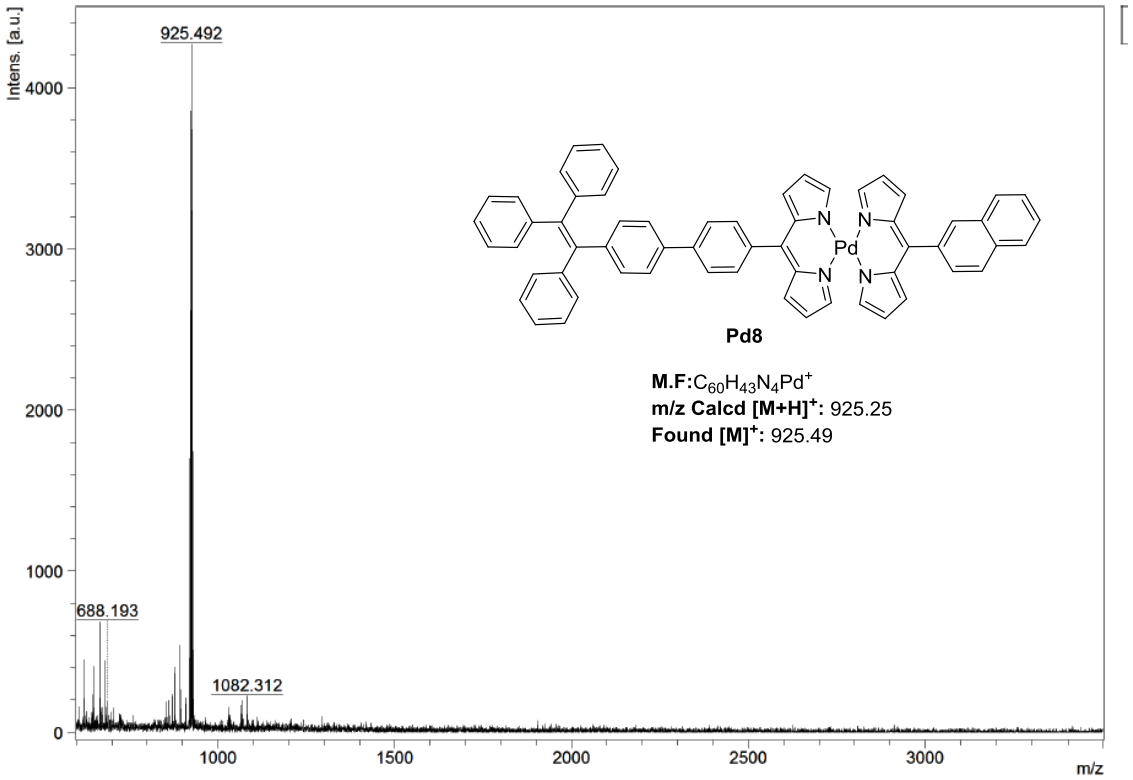


Figure S42. MALDI-MS of compound **Pd8**.

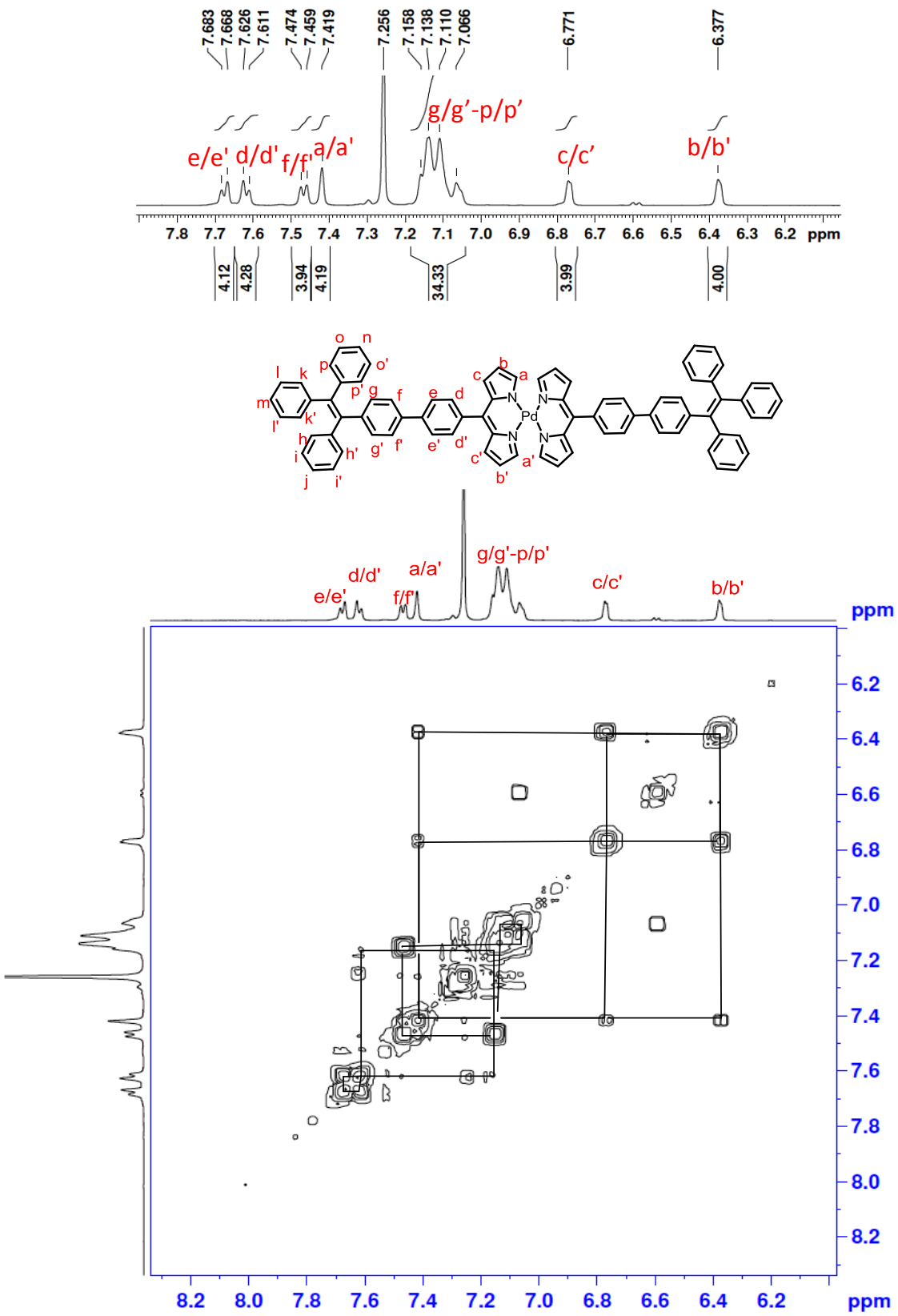


Figure S10. ^{1}H-^{1}H and COSY spectrum of compound **Pd2**.

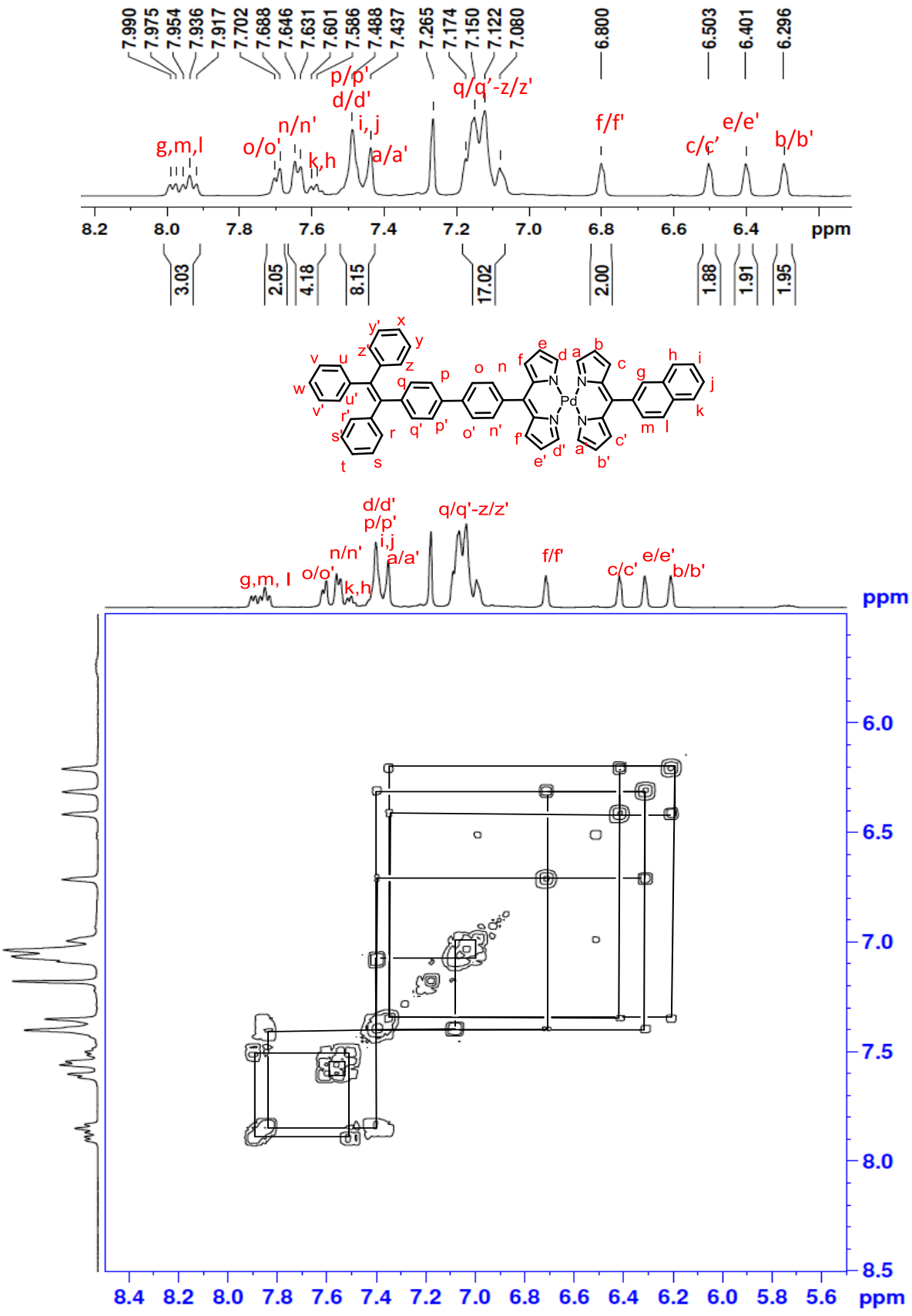


Figure S11. ^{1}H-^{1}H and COSY spectrum of compound **Pd8**.

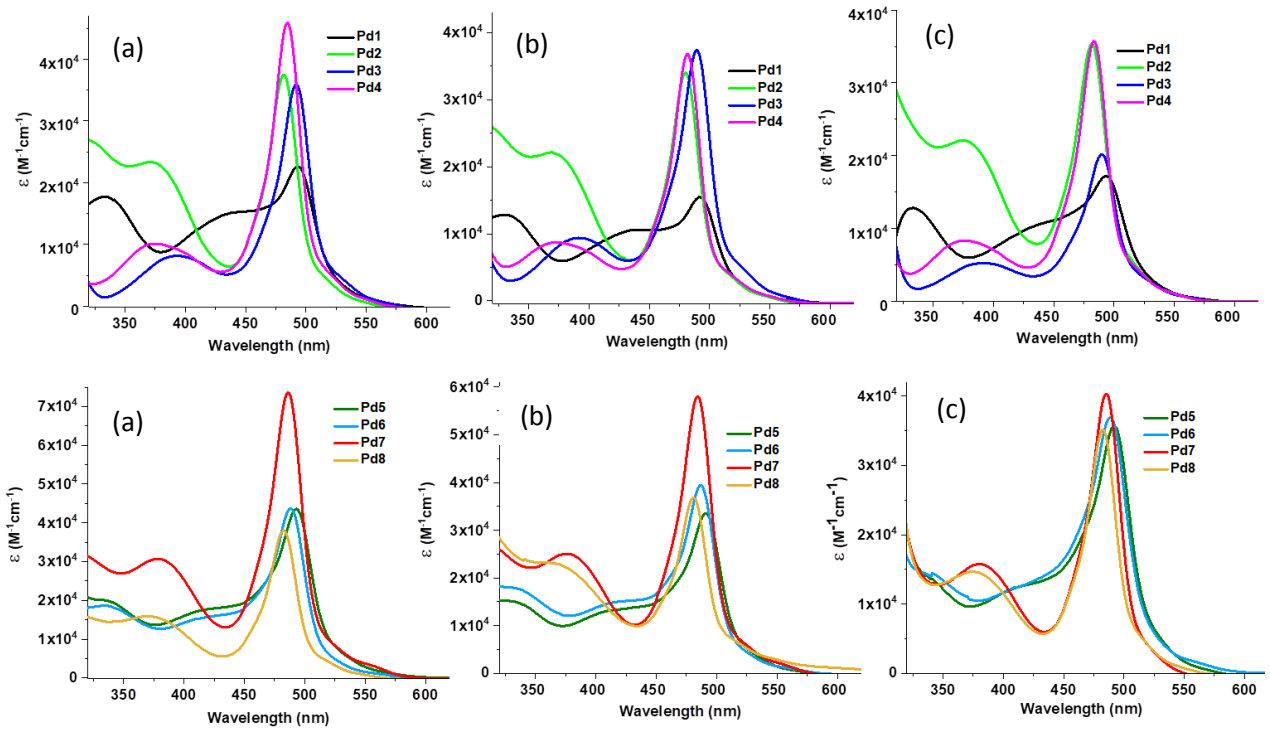


Figure S12. Absorption spectra of compound **Pd1-Pd8** in (a) $CHCl_3$ (b) THF (c) DMSO.

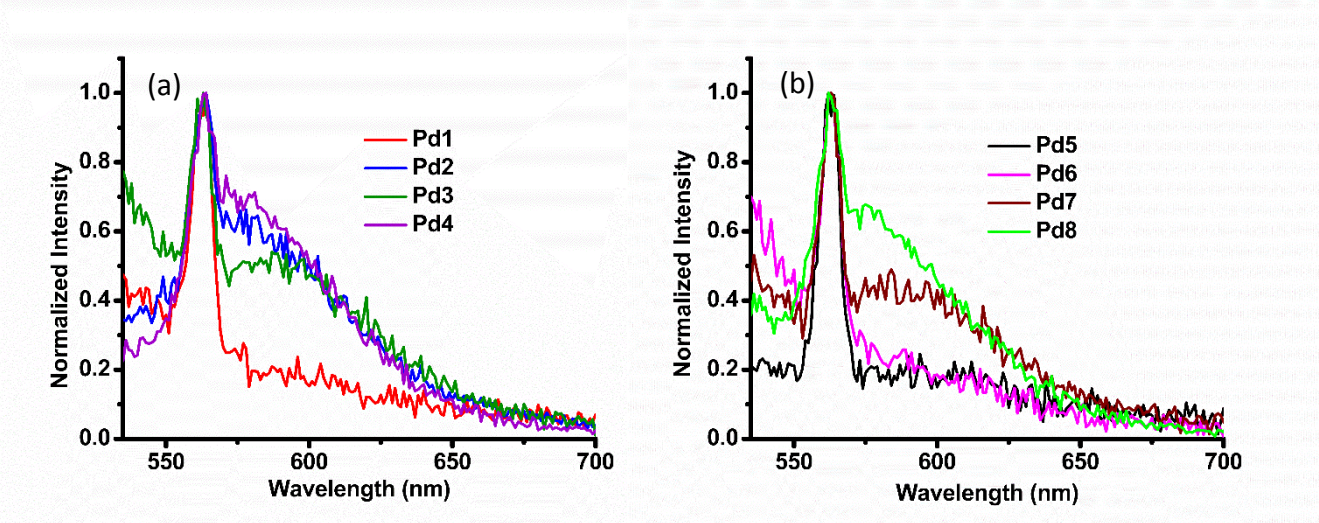


Figure S13. Emission spectra of compound (a) **Pd1-Pd4**; (b) **Pd5-Pd8**.

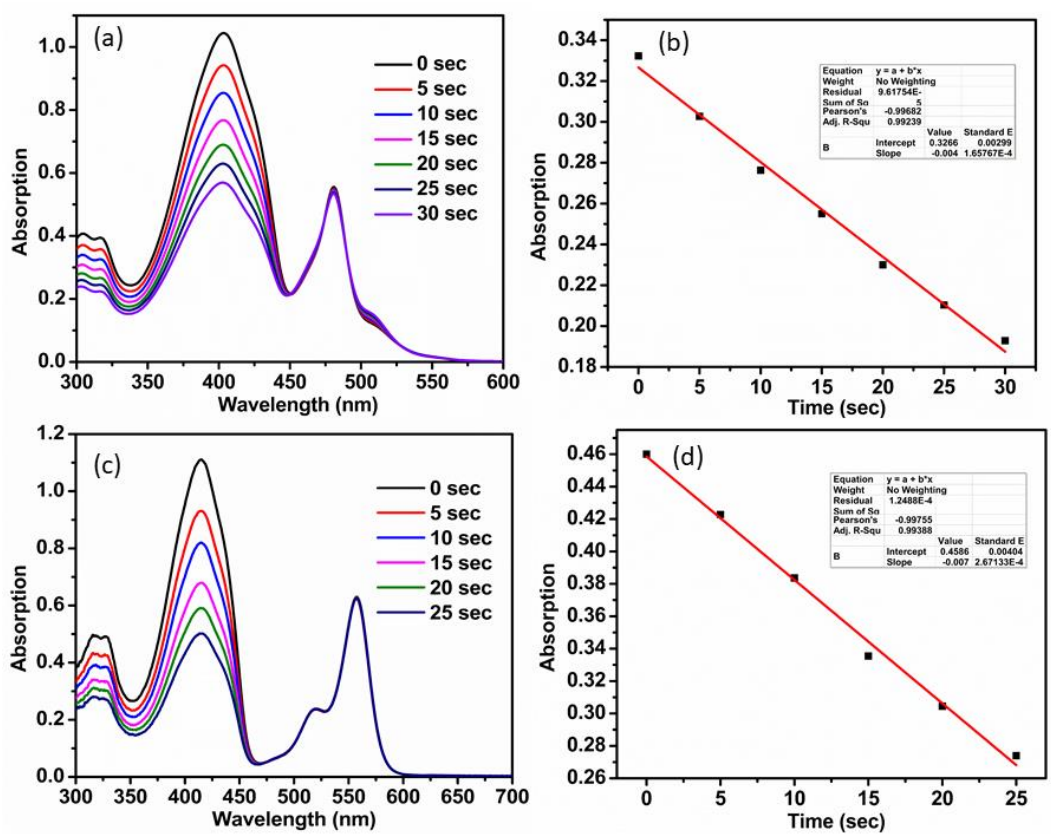


Figure S47. Absorbance spectral changes in chloroform: (a) **Pd3 complex** and (c) Rose Bengal upon irradiation of light (λ = 400-700 nm, 15 J cm^{-2}); rate of decrease of absorbance at 324 nm: (b) **Pd3 Complex** (d) Rose Bengal.

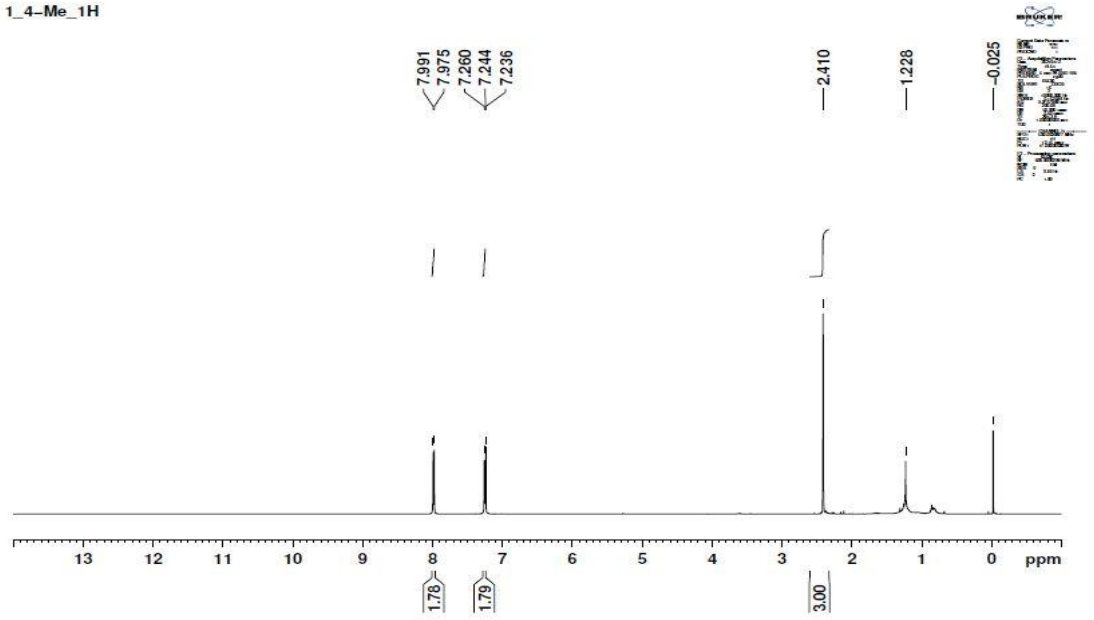


Figure S48. ^{1}H NMR spectrum of compound **4-Methylbenzoic acid** in $CDCl_3$

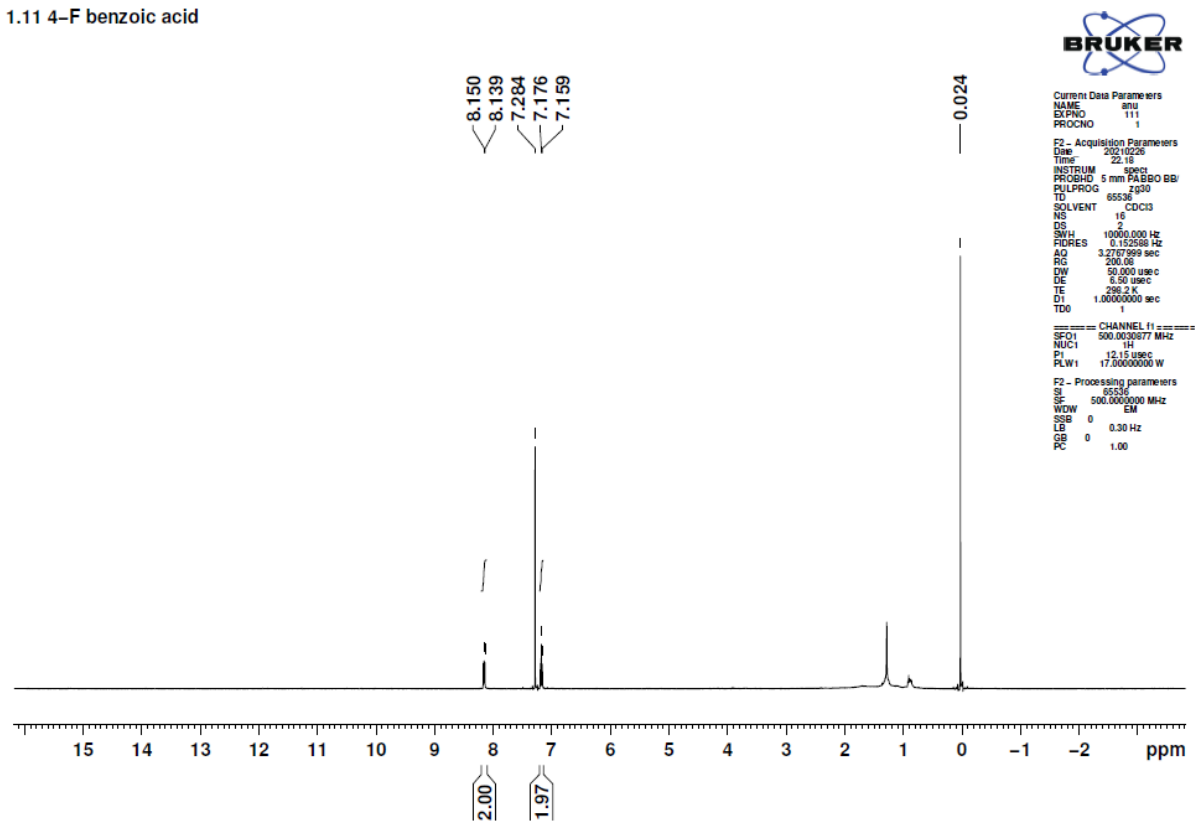


Figure S49. ^{1}H NMR spectrum of compound **4-Fluorobenzoic acid** in $CDCl_3$

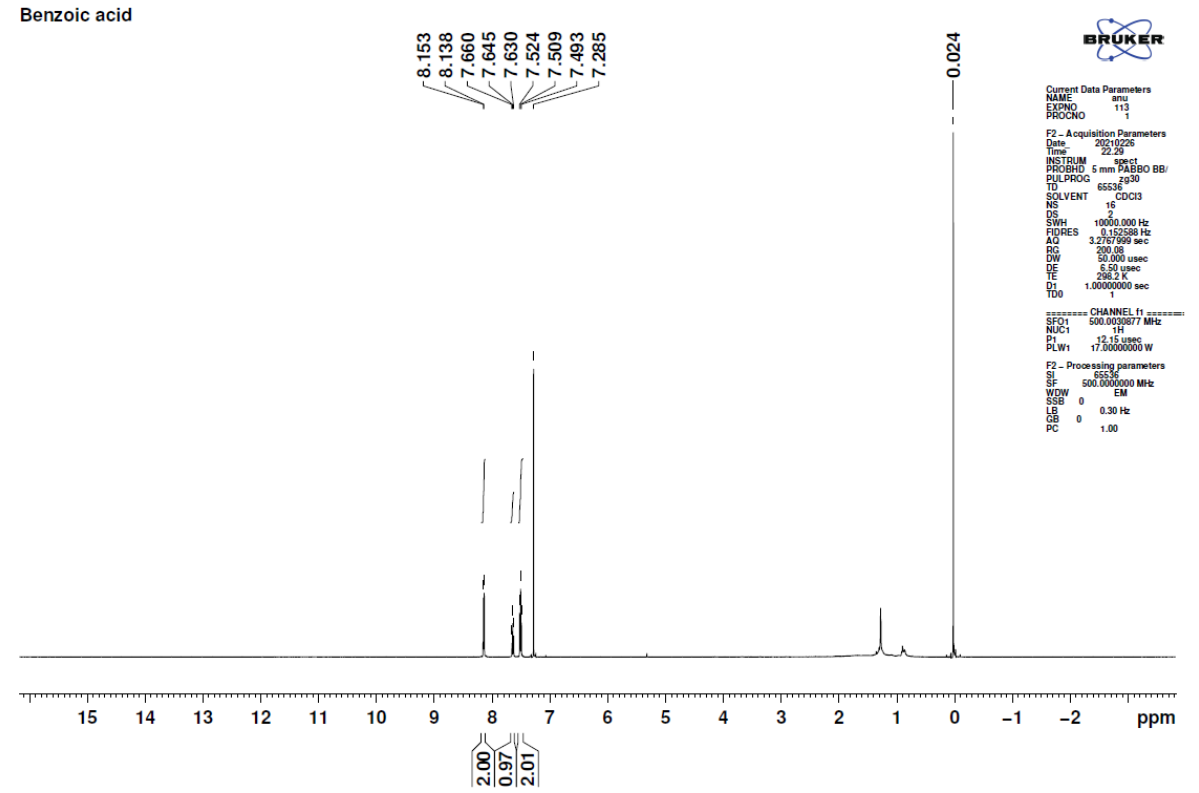


Figure S50. ^{1}H NMR spectrum of compound **Benzoic acid** in $CDCl_3$

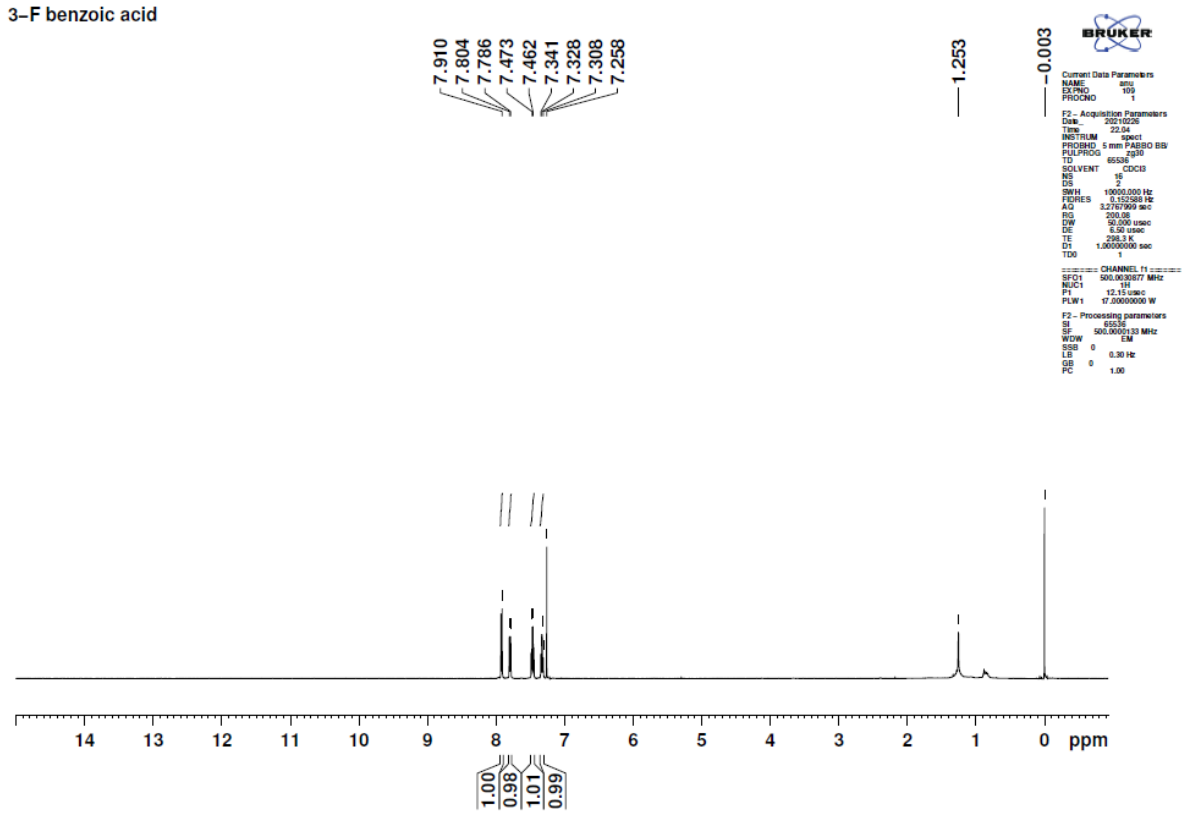


Figure S51. ^{1}H NMR spectrum of compound **3-Fluorobenzoic acid** in $CDCl_3$

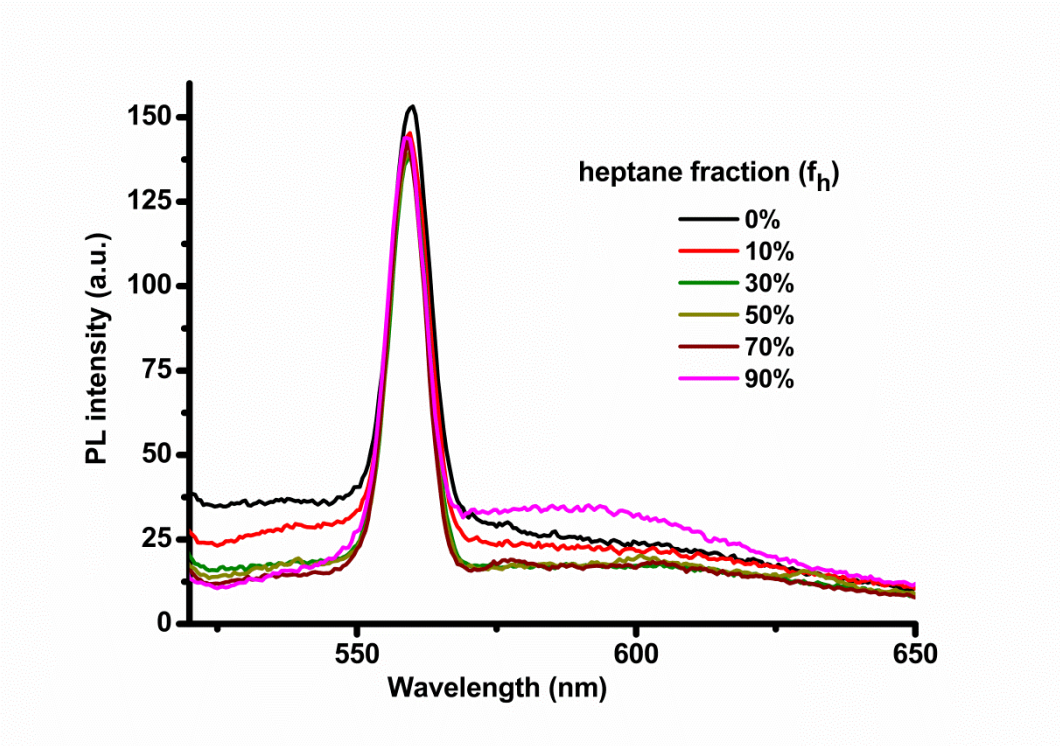


Figure S52. Aggregation based emission study of complex **Pd1** in THF/heptane.

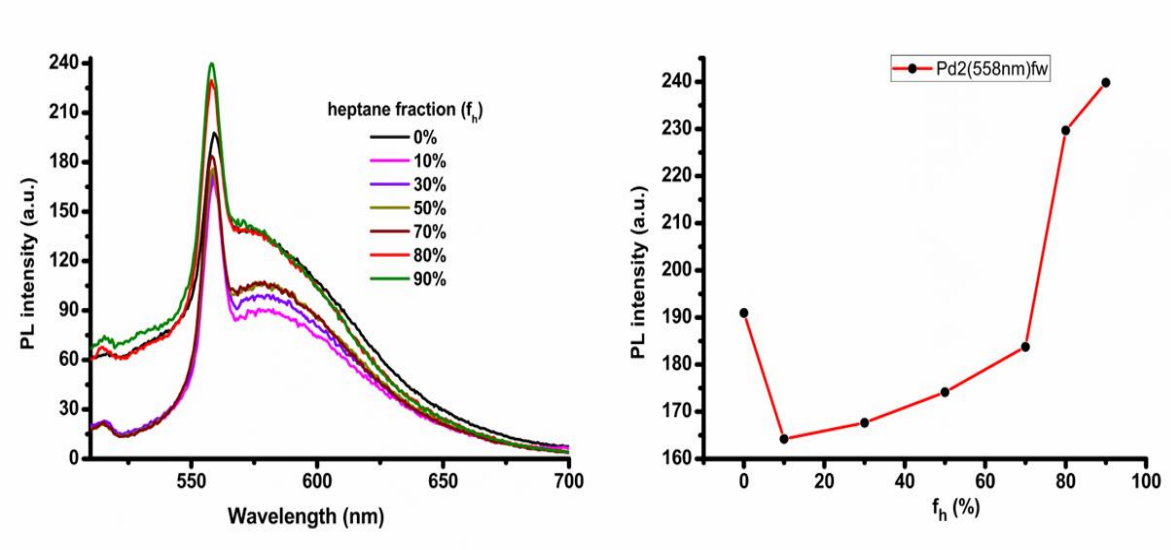


Figure S53. Aggregation based emission study of complex **Pd2** in THF/heptane.

Table S1. White light induced catalytic oxidation reactions, using palladium complexes as catalysts.

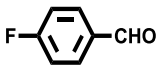
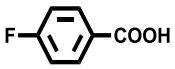
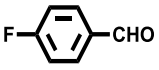
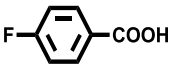
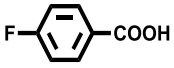
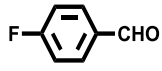
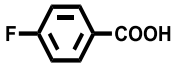
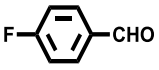
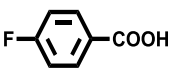
Entry	Aldehyde	Acid	Catalyst (effective conc.)	Yield (%)	Time(h)	TON	TOF(h^{-1})
1.			Pd3 (36.6 uM)	80	3	3636	1212
2.			Pd3 (73.3 uM)	91	1.5	2068	1378
3.			Pd3 (110 uM)	84	1	1272	1272
4.			Pd5 (73.3 uM)	31	6	713	118
5.			Pd7 (73.3 uM)	29	6	655	109

Table S2. B3LYP/6-31G+(d) gas phase optimised coordinates

Compound **Pd1**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.924120	-0.504068	-1.163576
2	6	0	-3.605244	-0.074337	-2.341966
3	6	0	-2.662090	0.496834	-3.175137
4	6	0	-1.428379	0.402873	-2.497657
5	7	0	-1.570995	-0.179512	-1.293141
6	1	0	-2.816318	0.919688	-4.158871
7	6	0	1.165667	1.590371	-1.119573
8	6	0	2.339055	2.313889	-1.416092
9	7	0	1.431187	0.288118	-0.937368
10	6	0	3.372548	1.396799	-1.402146
11	1	0	2.397681	3.375243	-1.616647
12	6	0	2.811219	0.127991	-1.063185
13	6	0	2.919527	-2.245399	-0.292326
14	6	0	3.570238	-3.503348	-0.086047
15	7	0	1.568291	-2.399583	0.039046
16	6	0	2.607394	-4.404641	0.323952
17	6	0	1.390797	-3.687354	0.371701
18	1	0	2.737786	-5.450433	0.568434
19	6	0	-1.004885	-2.535449	2.097097
20	6	0	-2.139545	-2.765244	2.906749
21	7	0	-1.348692	-2.018514	0.904274
22	6	0	-3.231177	-2.345957	2.168736
23	1	0	-2.133233	-3.166062	3.911583
24	6	0	-2.734813	-1.867473	0.917159
25	1	0	-4.266535	-2.322462	2.476601
26	6	0	3.502671	-1.068090	-0.799786
27	6	0	-3.481127	-1.231589	-0.094279
28	1	0	4.624135	-3.688405	-0.228814
29	1	0	4.418695	1.591372	-1.584304
30	1	0	-4.656453	-0.216736	-2.545667
31	6	0	8.849665	-0.393164	-0.878180
32	6	0	9.840605	-0.584335	-1.859590
33	6	0	9.237291	0.220260	0.326817
34	6	0	11.154096	-0.188997	-1.640219
35	1	0	9.568584	-1.023629	-2.815129
36	6	0	10.552722	0.613696	0.544324
37	1	0	8.501698	0.379716	1.110958
38	1	0	11.891959	-0.334785	-2.423915
39	1	0	10.818571	1.084981	1.484717
40	6	0	11.547027	0.406877	-0.427335

41	6	0	13.623136	0.697397	0.962504
42	6	0	12.955020	0.860880	-0.220254
43	6	0	13.584194	1.495955	-1.415970
44	6	0	14.805289	1.030939	-1.934434
45	6	0	12.928747	2.538785	-2.094636
46	6	0	15.361694	1.603221	-3.077349
47	1	0	15.316214	0.213042	-1.436387
48	6	0	13.490654	3.119225	-3.231129
49	1	0	11.974019	2.898296	-1.721226
50	6	0	14.710109	2.653649	-3.727602
51	1	0	16.304505	1.224131	-3.463097
52	1	0	12.972508	3.932981	-3.731941
53	1	0	15.145082	3.100222	-4.617810
54	6	0	14.922688	1.376981	1.244924
55	6	0	15.085191	2.756526	1.035381
56	6	0	16.000920	0.651443	1.782984
57	6	0	16.291512	3.387062	1.337446
58	1	0	14.257166	3.333084	0.633576
59	6	0	17.211128	1.279722	2.073280
60	1	0	15.884387	-0.413185	1.967003
61	6	0	17.360860	2.651062	1.852635
62	1	0	16.394496	4.456602	1.173494
63	1	0	18.036676	0.698749	2.476388
64	1	0	18.301105	3.143331	2.086693
65	6	0	13.126237	-0.153965	2.088186
66	6	0	13.152347	0.336697	3.406717
67	6	0	12.677704	-1.469258	1.879044
68	6	0	12.714817	-0.447745	4.472660
69	1	0	13.515018	1.345059	3.588053
70	6	0	12.251657	-2.258688	2.946957
71	1	0	12.668703	-1.872099	0.871597
72	6	0	12.262745	-1.749858	4.246873
73	1	0	12.730975	-0.043310	5.481470
74	1	0	11.913478	-3.274981	2.761997
75	1	0	11.928098	-2.364673	5.078163
76	1	0	-0.457315	0.712599	-2.853348
77	46	0	0.024345	-1.076231	-0.315429
78	1	0	0.411801	-4.062472	0.629624
79	1	0	0.154726	1.963508	-1.043452
80	1	0	0.032483	-2.697547	2.350068
81	6	0	-4.938364	-1.358435	-0.001095
82	6	0	-5.665418	-2.516012	0.187307
83	16	0	-6.006298	0.030403	-0.039601
84	6	0	-7.061640	-2.300776	0.270151
85	1	0	-5.197231	-3.493610	0.227577
86	6	0	-7.425701	-0.971568	0.170651
87	1	0	-7.781217	-3.105425	0.372858
88	6	0	-8.769472	-0.392734	0.223845
89	6	0	-9.059173	0.868066	-0.329809
90	6	0	-9.823991	-1.091648	0.841590

91	6	0	-10.341553	1.401397	-0.270681
92	1	0	-8.274866	1.433171	-0.826613
93	6	0	-11.109041	-0.565568	0.879931
94	1	0	-9.629556	-2.048792	1.316416
95	6	0	-11.403857	0.689109	0.315594
96	1	0	-10.530561	2.379726	-0.701995
97	1	0	-11.899310	-1.126910	1.367508
98	6	0	-12.773664	1.276559	0.389600
99	6	0	-12.826313	2.691433	0.873303
100	6	0	-13.523336	3.681251	0.159448
101	6	0	-12.126063	3.076944	2.030608
102	6	0	-13.535094	5.005416	0.596559
103	1	0	-14.056673	3.405629	-0.744992
104	6	0	-12.147151	4.398352	2.474828
105	1	0	-11.566458	2.330352	2.587089
106	6	0	-12.851657	5.368921	1.758952
107	1	0	-14.076691	5.754768	0.025312
108	1	0	-11.609333	4.670891	3.379192
109	1	0	-12.862198	6.400483	2.100572
110	6	0	-13.897064	0.569857	0.067555
111	6	0	-15.269430	1.052985	0.410742
112	6	0	-16.297942	1.042507	-0.548373
113	6	0	-15.583107	1.471161	1.715162
114	6	0	-17.585069	1.469413	-0.223988
115	1	0	-16.082095	0.701654	-1.556771
116	6	0	-16.872844	1.887141	2.043193
117	1	0	-14.808194	1.464850	2.475483
118	6	0	-17.878313	1.894261	1.073849
119	1	0	-18.360580	1.465616	-0.985579
120	1	0	-17.092728	2.202359	3.059829
121	1	0	-18.882890	2.220397	1.329564
122	6	0	-13.843444	-0.743078	-0.644195
123	6	0	-14.564687	-1.851515	-0.164849
124	6	0	-13.120196	-0.889962	-1.840427
125	6	0	-14.535542	-3.071942	-0.838547
126	1	0	-15.148096	-1.753368	0.745898
127	6	0	-13.099731	-2.106764	-2.520550
128	1	0	-12.574667	-0.039847	-2.238548
129	6	0	-13.802316	-3.205212	-2.019934
130	1	0	-15.090789	-3.918074	-0.442043
131	1	0	-12.537479	-2.194272	-3.446533
132	1	0	-13.785183	-4.153810	-2.549843
133	6	0	4.961583	-1.118001	-1.084428
134	6	0	5.602636	-1.931910	-1.988832
135	16	0	6.127051	-0.123172	-0.241627
136	6	0	7.013593	-1.760348	-2.014608
137	1	0	5.066796	-2.628967	-2.622863
138	6	0	7.475508	-0.819374	-1.120466
139	1	0	7.671214	-2.331862	-2.660078

Compound **Pd2**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.616347	-0.941751	-0.432268
2	6	0	-3.281730	-2.027961	-1.284771
3	6	0	-2.330550	-2.914447	-1.604510
4	6	0	-1.049163	-2.421514	-0.940937
5	7	0	-1.316292	-1.282394	-0.265484
6	1	0	-2.445124	-3.790808	-2.206608
7	6	0	1.079900	-1.793964	-1.506926
8	6	0	2.331582	-2.091723	-2.329144
9	7	0	1.390756	-0.940259	-0.506680
10	6	0	3.325301	-1.393816	-1.770810
11	1	0	2.398482	-2.737393	-3.182846
12	6	0	2.716296	-0.648316	-0.570597
13	6	0	2.763353	0.886015	1.301962
14	6	0	3.424229	1.917512	2.210157
15	7	0	1.451086	0.850611	1.628135
16	6	0	2.446950	2.409366	2.977958
17	6	0	1.252246	1.755419	2.620466
18	1	0	2.552066	3.168576	3.726997
19	6	0	-0.890064	2.489099	1.389843
20	6	0	-2.048222	3.270162	1.444555
21	7	0	-1.205951	1.252900	0.962647
22	6	0	-3.063564	2.503522	1.006598
23	1	0	-2.114499	4.286516	1.777457
24	6	0	-2.533574	1.250425	0.658382
25	1	0	-4.085056	2.803170	0.938501
26	6	0	4.983325	0.221860	0.254302
27	6	0	5.708797	-0.197585	-0.875416
28	6	0	5.682186	0.698126	1.372419
29	6	0	7.118770	-0.171990	-0.865792
30	6	0	7.079304	0.656288	1.408280
31	6	0	7.806506	0.219014	0.294772
32	6	0	3.433441	0.154219	0.319413
33	6	0	-4.817160	0.279366	-0.051628
34	6	0	-5.536910	-0.863296	-0.433590
35	6	0	-5.516283	1.466255	0.224885
36	6	0	-6.936156	-0.838878	-0.493163
37	6	0	-6.917528	1.500363	0.123792
38	6	0	-7.631384	0.340591	-0.213599
39	6	0	-3.273205	0.198128	0.068375
40	1	0	4.456197	2.200079	2.227851
41	1	0	4.344279	-1.367259	-2.095920
42	1	0	-4.308132	-2.070708	-1.574126
43	1	0	5.192658	-0.532922	-1.745197
44	1	0	7.664914	-0.458280	-1.742412

45	1	0	7.597959	0.968162	2.292904
46	1	0	5.145163	1.084699	2.212356
47	1	0	-4.984711	2.346118	0.511670
48	1	0	-5.016721	-1.764539	-0.670980
49	1	0	-7.472396	-1.725802	-0.754208
50	1	0	-7.442461	2.413309	0.312481
51	6	0	9.349287	0.181662	0.378514
52	6	0	9.957749	0.218231	1.640125
53	6	0	10.148491	0.113198	-0.774566
54	6	0	11.353330	0.198942	1.755710
55	1	0	9.352114	0.260023	2.522932
56	6	0	11.553246	0.164881	-0.660455
57	1	0	9.691792	0.034781	-1.741892
58	1	0	11.807421	0.183549	2.723627
59	1	0	12.160703	0.163147	-1.543126
60	6	0	-9.173318	0.358367	-0.275700
61	6	0	-9.867143	1.571187	-0.198823
62	6	0	-9.893485	-0.839098	-0.404653
63	6	0	-11.269171	1.590349	-0.250908
64	1	0	-9.326561	2.489909	-0.103057
65	6	0	-11.299710	-0.819855	-0.414095
66	1	0	-9.370300	-1.769410	-0.490197
67	6	0	-11.999640	0.394000	-0.333737
68	1	0	-11.775732	2.524438	-0.216527
69	6	0	-13.554752	0.395349	-0.322838
70	6	0	-14.227464	-0.787113	-0.168508
71	6	0	-13.398567	-2.103361	-0.184113
72	6	0	-12.009278	-2.015446	-0.375070
73	6	0	-13.976346	-3.373397	-0.025640
74	6	0	-11.212654	-3.171784	-0.402428
75	6	0	-13.183318	-4.529079	-0.053008
76	1	0	-15.021977	-3.473287	0.118459
77	6	0	-11.801655	-4.429559	-0.241074
78	1	0	-10.155112	-3.091434	-0.548113
79	1	0	-13.637495	-5.491060	0.070171
80	1	0	-11.196488	-5.313290	-0.263331
81	6	0	-15.774422	-0.752953	0.023407
82	6	0	-16.446475	0.487545	-0.002521
83	6	0	-16.536625	-1.916596	0.230267
84	6	0	-17.837789	0.553823	0.193466
85	6	0	-17.923323	-1.847581	0.428852
86	1	0	-16.068021	-2.865964	0.242812
87	6	0	-18.572877	-0.612319	0.414412
88	1	0	-18.334961	1.501608	0.174923
89	1	0	-18.485661	-2.745010	0.593215
90	1	0	-19.631012	-0.558192	0.570478
91	6	0	-14.359973	1.710946	-0.474128
92	6	0	-13.722814	2.945731	-0.671276
93	6	0	-15.763463	1.671453	-0.421293
94	6	0	-14.472145	4.118922	-0.838353

95	1	0	-12.662646	3.001281	-0.702519
96	6	0	-16.513078	2.848121	-0.585764
97	6	0	-15.867905	4.069555	-0.799943
98	1	0	-13.973723	5.054152	-0.996619
99	1	0	-17.582677	2.810201	-0.548610
100	1	0	-16.441281	4.963905	-0.931416
101	6	0	12.156396	0.209474	0.609383
102	6	0	14.291876	0.609642	-0.410388
103	6	0	13.690393	0.286458	0.781074
104	6	0	14.130730	-1.072123	1.355249
105	6	0	14.780098	-1.158650	2.593161
106	6	0	13.862276	-2.242525	0.622936
107	6	0	15.169881	-2.412231	3.092196
108	1	0	14.981720	-0.270911	3.157421
109	6	0	14.249454	-3.491888	1.122984
110	1	0	13.360351	-2.177637	-0.320203
111	6	0	14.904266	-3.576653	2.358099
112	1	0	15.669481	-2.479790	4.037237
113	1	0	14.044528	-4.380606	0.561195
114	1	0	15.200806	-4.531738	2.741011
115	6	0	15.433447	-0.212861	-1.096846
116	6	0	15.919640	-1.409465	-0.543158
117	6	0	16.014853	0.246878	-2.294284
118	6	0	16.958363	-2.121096	-1.162763
119	1	0	15.503581	-1.784636	0.360191
120	6	0	17.051912	-0.461898	-2.913262
121	1	0	15.669736	1.146058	-2.742722
122	6	0	17.525043	-1.647748	-2.349002
123	1	0	17.318756	-3.029257	-0.724240
124	1	0	17.483143	-0.092337	-3.821308
125	1	0	18.318877	-2.189890	-2.822834
126	6	0	13.745969	1.920749	-1.028115
127	6	0	14.250124	2.496118	-2.204950
128	6	0	12.688254	2.556291	-0.357629
129	6	0	13.700032	3.685890	-2.701668
130	1	0	15.052754	2.036986	-2.728061
131	6	0	12.135600	3.740959	-0.854822
132	1	0	12.299817	2.128752	0.544208
133	6	0	12.640896	4.306318	-2.029510
134	1	0	14.091599	4.122193	-3.598140
135	1	0	11.326487	4.213294	-0.335180
136	1	0	12.218064	5.212201	-2.413572
137	1	0	-0.092234	-2.901606	-1.001187
138	46	0	0.029222	-0.320755	0.820783
139	1	0	0.554553	2.488046	2.289982
140	1	0	0.337012	-1.350659	-2.138279
141	1	0	-16.092017	0.984127	-1.177036
142	1	0	-15.998462	1.108072	0.749644
143	1	0	-11.853172	-1.504892	-1.308371
144	1	0	-11.627156	-1.425778	0.412142

145	1	0	-0.467993	2.428954	2.367350

Compound **Pd3**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.795029	-1.232553	-0.134409
2	6	0	3.380660	-2.464201	-0.564086
3	6	0	2.355308	-3.380688	-0.704191
4	6	0	1.167487	-2.698721	-0.357550
5	7	0	1.418656	-1.428910	0.002173
6	1	0	2.424988	-4.411256	-1.026161
7	6	0	-1.308229	-2.252555	1.592326
8	6	0	-2.514211	-2.738672	2.145212
9	7	0	-1.536831	-1.256269	0.720408
10	6	0	-3.527178	-1.980309	1.587603
11	1	0	-2.604297	-3.537354	2.869495
12	6	0	-2.915322	-1.037099	0.704716
13	6	0	-2.900116	1.073350	-0.623798
14	6	0	-3.488990	2.020713	-1.518343
15	7	0	-1.523711	1.309847	-0.582865
16	6	0	-2.465770	2.800604	-2.023875
17	6	0	-1.275897	2.321248	-1.431622
18	1	0	-2.538119	3.609234	-2.739049
19	6	0	1.211252	2.714274	0.516837
20	6	0	2.418408	3.382352	0.821552
21	7	0	1.437188	1.446405	0.134124
22	6	0	3.429414	2.459026	0.628388
23	1	0	2.510463	4.408545	1.151783
24	6	0	2.815298	1.236994	0.212079
25	1	0	4.487825	2.599640	0.793268
26	6	0	-5.048350	-0.002139	-0.015137
27	6	0	-5.797167	1.100029	0.430475
28	6	0	-5.744779	-1.119757	-0.505068
29	6	0	-7.188233	1.082787	0.389110
30	6	0	-7.135384	-1.128326	-0.558586
31	6	0	-7.889040	-0.028541	-0.111870
32	6	0	-3.559156	0.012655	0.024061
33	6	0	3.456758	-0.000930	0.022637
34	1	0	-4.539075	2.073485	-1.766303
35	1	0	-4.585570	-2.042647	1.795118
36	1	0	4.429868	-2.616138	-0.771450
37	1	0	0.156932	-3.080177	-0.374447
38	46	0	-0.051134	0.019110	0.072297
39	1	0	-0.266141	2.663346	-1.606022
40	1	0	-0.301115	-2.580071	1.806984
41	1	0	0.205086	3.103783	0.576450
42	9	0	-5.048764	-2.182989	-0.960703

43	9	0	-7.768723	-2.197903	-1.085262
44	9	0	-9.238060	-0.039226	-0.162192
45	9	0	-7.875551	2.140486	0.870116
46	9	0	-5.153787	2.175856	0.931634
47	6	0	5.196143	-0.009503	-0.022843
48	6	0	5.903782	1.183051	0.127518
49	6	0	5.883003	-1.209464	-0.209194
50	6	0	7.298452	1.175916	0.091245
51	6	0	7.277325	-1.216608	-0.245943
52	6	0	7.985228	-0.023455	-0.096026
53	9	0	7.982965	2.330483	0.235868
54	9	0	9.334733	-0.030348	-0.131909
55	9	0	7.942353	-2.377389	-0.427124
56	9	0	5.197793	-2.363573	-0.354183
57	9	0	5.239243	2.344182	0.308252

Compound **Pd4**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.872002	1.359016	0.282427
2	6	0	3.505359	2.474927	0.912379
3	6	0	2.505750	3.336819	1.323828
4	6	0	1.285607	2.739309	0.934949
5	7	0	1.492459	1.575725	0.296535
6	1	0	2.613594	4.276387	1.849357
7	6	0	-1.285638	2.739257	-0.934934
8	6	0	-2.505788	3.336731	-1.323847
9	7	0	-1.492476	1.575693	-0.296478
10	6	0	-3.505385	2.474830	-0.912385
11	1	0	-2.613643	4.276277	-1.849415
12	6	0	-2.872015	1.358970	-0.282358
13	6	0	-2.834879	-0.987949	0.560917
14	6	0	-3.405312	-2.101735	1.253568
15	7	0	-1.461328	-1.209807	0.435568
16	6	0	-2.372709	-2.967861	1.560133
17	6	0	-1.196048	-2.374435	1.049611
18	1	0	-2.429891	-3.906770	2.094683
19	6	0	1.196074	-2.374445	-1.049433
20	6	0	2.372746	-2.967882	-1.559918
21	7	0	1.461338	-1.209803	-0.435410
22	6	0	3.405343	-2.101754	-1.253337
23	1	0	2.429939	-3.906800	-2.094449
24	6	0	2.834888	-0.987941	-0.560748

25	1	0	4.448845	-2.205521	-1.512509
26	6	0	-3.502721	0.186536	0.171346
27	6	0	3.502716	0.186568	-0.171226
28	1	0	-4.448805	-2.205493	1.512778
29	1	0	-4.569947	2.585002	-1.061545
30	1	0	4.569921	2.585130	1.061520
31	1	0	0.284104	3.105588	1.108331
32	46	0	-0.000002	0.182485	0.000054
33	1	0	-0.183387	-2.744020	1.122635
34	1	0	-0.284138	3.105546	-1.108319
35	1	0	0.183414	-2.744033	-1.122468
36	6	0	4.991955	0.192246	-0.249137
37	6	0	5.741669	-0.754785	0.428011
38	6	0	5.667347	1.181580	-1.022901
39	6	0	7.159884	-0.755888	0.374896
40	1	0	5.239374	-1.507067	1.030001
41	6	0	7.039582	1.195875	-1.106117
42	1	0	5.078118	1.916949	-1.561466
43	6	0	7.827618	0.238035	-0.412405
44	6	0	7.940090	-1.714745	1.077656
45	1	0	7.540441	1.946955	-1.712352
46	6	0	9.246849	0.229742	-0.470301
47	6	0	9.314606	-1.695484	1.002050
48	1	0	7.430724	-2.466170	1.676251
49	6	0	9.974147	-0.714285	0.220148
50	1	0	9.750896	0.983842	-1.070151
51	1	0	9.900363	-2.433876	1.542622
52	1	0	11.059522	-0.710016	0.168699
53	6	0	-4.991963	0.192192	0.249191
54	6	0	-5.741644	-0.754750	-0.428120
55	6	0	-5.667398	1.181442	1.023027
56	6	0	-7.159860	-0.755857	-0.375083
57	1	0	-5.239320	-1.506947	-1.030190
58	6	0	-7.039637	1.195731	1.106167
59	1	0	-5.078197	1.916757	1.561697
60	6	0	-7.827637	0.237972	0.412299
61	6	0	-7.940029	-1.714620	-1.078012
62	1	0	-7.540529	1.946747	1.712452
63	6	0	-9.246871	0.229678	0.470111
64	6	0	-9.314549	-1.695363	-1.002486
65	1	0	-7.430631	-2.465969	-1.676676
66	6	0	-9.974133	-0.714261	-0.220499
67	1	0	-9.750951	0.983706	1.070024
68	1	0	-9.900277	-2.433683	-1.543188
69	1	0	-11.059511	-0.709994	-0.169115

Compound **Pd5**

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	1.385623	0.277465	0.795068
2	6	0	0.846809	1.578958	0.991636
3	6	0	1.884027	2.496251	0.936756
4	6	0	3.046939	1.752732	0.711229
5	7	0	2.777495	0.437366	0.666617
6	1	0	1.816199	3.570595	1.045559
7	6	0	5.550719	0.687186	2.446132
8	6	0	6.750012	1.013805	3.123102
9	7	0	5.827937	0.126499	1.253513
10	6	0	7.777995	0.705252	2.261689
11	1	0	6.829666	1.453717	4.108655
12	6	0	7.204453	0.181583	1.061987
13	6	0	7.307094	-1.372417	-0.852987
14	6	0	7.837805	-2.265653	-1.841820
15	7	0	5.925684	-1.683728	-0.754855
16	6	0	6.799139	-2.975450	-2.400308
17	6	0	5.627340	-2.551466	-1.729544
18	1	0	6.852131	-3.671287	-3.227219
19	6	0	3.170073	-3.629922	0.682483
20	6	0	2.066689	-4.364660	1.174526
21	7	0	2.830598	-2.352922	0.429493
22	6	0	1.000349	-3.482283	1.194549
23	1	0	2.092502	-5.369959	1.576382
24	6	0	1.470215	-2.218862	0.704709
25	1	0	0.037002	-3.677084	1.642509
26	6	0	7.881308	-0.293581	-0.099136
27	6	0	0.734899	-0.991340	0.685529
28	1	0	8.862696	-2.404108	-2.108035
29	1	0	8.832357	0.730117	2.505210
30	1	0	-0.179292	1.846142	1.172938
31	1	0	4.058706	2.108818	0.573927
32	46	0	4.320581	-0.825502	0.213193
33	1	0	4.661750	-3.039840	-1.737620
34	1	0	4.567905	0.576727	2.887152
35	1	0	4.101106	-4.037580	0.309209
36	6	0	-0.707113	-1.144221	0.479653
37	6	0	-1.344755	-2.250996	-0.084333
38	16	0	-1.953194	0.103306	0.722555
39	6	0	-2.733048	-2.142146	-0.248741
40	1	0	-0.803668	-3.114192	-0.441380
41	6	0	-3.254437	-0.921933	0.154534
42	1	0	-3.330673	-2.937202	-0.678089
43	6	0	-4.627105	-0.464791	0.128453
44	6	0	-5.006724	0.830088	0.554986
45	6	0	-5.666997	-1.300944	-0.347056
46	6	0	-6.319258	1.255175	0.530323
47	1	0	-4.249269	1.515959	0.923813
48	6	0	-6.976994	-0.875130	-0.396330

49	1	0	-5.432723	-2.297636	-0.706421
50	6	0	-7.377757	0.423502	0.052883
51	1	0	-6.546862	2.258361	0.869638
52	1	0	-7.725971	-1.540893	-0.805705
53	6	0	-8.745369	0.871080	-0.041480
54	6	0	-9.118080	2.271824	0.340243
55	6	0	-9.803148	3.206802	-0.456700
56	6	0	-8.840057	2.653112	1.674124
57	6	0	-10.161695	4.460706	0.041245
58	1	0	-10.076026	2.954626	-1.473379
59	6	0	-9.191339	3.908610	2.168129
60	1	0	-8.341881	1.948279	2.333139
61	6	0	-9.853471	4.826527	1.351302
62	1	0	-10.683213	5.156176	-0.610813
63	1	0	-8.952488	4.161317	3.197399
64	1	0	-10.130483	5.805729	1.730219
65	6	0	-9.837761	-0.027024	-0.442080
66	6	0	-10.017432	-1.230505	0.361705
67	6	0	-10.430482	-2.505087	-0.110969
68	6	0	-9.705815	-1.154610	1.748029
69	6	0	-10.547514	-3.598181	0.740131
70	1	0	-10.575758	-2.681073	-1.167741
71	6	0	-9.794972	-2.255776	2.590741
72	1	0	-9.438141	-0.191962	2.165752
73	6	0	-10.234733	-3.487961	2.099164
74	1	0	-10.857533	-4.555054	0.329017
75	1	0	-9.552423	-2.140375	3.643200
76	1	0	-10.331299	-4.344792	2.758768
77	6	0	-10.565346	0.326786	-1.662002
78	6	0	-11.974295	0.352297	-1.832002
79	6	0	-9.789427	0.646405	-2.808521
80	6	0	-12.556241	0.639108	-3.061025
81	1	0	-12.624876	0.250705	-0.974828
82	6	0	-10.374735	0.936406	-4.038801
83	1	0	-8.708393	0.597183	-2.736655
84	6	0	-11.763182	0.925855	-4.178673
85	1	0	-13.639300	0.667140	-3.141909
86	1	0	-9.738663	1.154133	-4.891923
87	1	0	-12.223482	1.150104	-5.136068
88	6	0	9.173024	0.465572	-0.391975
89	6	0	10.340261	0.094942	-1.121498
90	6	0	9.207719	1.876772	-0.128732
91	6	0	11.446651	0.919344	-1.343704
92	6	0	10.295377	2.721536	-0.351187
93	6	0	11.456545	2.243996	-0.935999
94	9	0	8.117519	2.585261	0.210498
95	9	0	10.188600	4.017531	-0.042287
96	9	0	12.504195	3.030559	-1.154063
97	9	0	12.510007	0.416435	-1.979259
98	9	0	10.541021	-1.109957	-1.672939

Compound **Pd6**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.331120	0.123937	-0.444872
2	6	0	-0.538137	1.342719	-0.430110
3	6	0	-1.367531	2.396124	-0.157399
4	6	0	-2.663993	1.839870	0.002359
5	7	0	-2.641639	0.517262	-0.198222
6	1	0	-1.104469	3.439861	-0.067584
7	6	0	-4.961175	1.799337	-1.669240
8	6	0	-5.961239	2.614851	-2.308503
9	7	0	-5.585559	0.851679	-0.920871
10	6	0	-7.174170	2.130574	-1.932501
11	1	0	-5.767033	3.450469	-2.966683
12	6	0	-6.961496	1.028377	-0.987076
13	6	0	-7.468183	-0.922010	0.450224
14	6	0	-8.287800	-1.926666	1.128308
15	7	0	-6.149370	-1.362928	0.588707
16	6	0	-7.460878	-2.844595	1.694978
17	6	0	-6.133177	-2.482320	1.351208
18	1	0	-7.749009	-3.694285	2.298792
19	6	0	-3.734895	-3.438177	-0.966583
20	6	0	-2.714778	-4.297351	-1.430507
21	7	0	-3.214611	-2.230759	-0.617263
22	6	0	-1.542714	-3.602363	-1.338440
23	1	0	-2.852617	-5.302176	-1.805997
24	6	0	-1.827412	-2.289111	-0.839100
25	1	0	-0.602146	-4.002832	-1.641210
26	6	0	-7.910004	0.272135	-0.224074
27	6	0	-0.883580	-1.205148	-0.665149
28	1	0	-9.352178	-1.978404	1.218004
29	1	0	-8.096369	2.527164	-2.312016
30	1	0	0.518867	1.430999	-0.589488
31	1	0	-3.564089	2.375059	0.252474
32	46	0	-4.350817	-0.540861	0.027807
33	1	0	-5.525242	-3.278847	0.973163
34	1	0	-4.181138	1.421986	-2.326529
35	1	0	-4.411704	-3.883195	-0.259399
36	6	0	0.613073	-1.434633	-0.644295
37	6	0	1.363546	-2.610735	-0.704181
38	16	0	1.758449	-0.126357	-0.442002
39	6	0	2.761240	-2.449276	-0.622396
40	1	0	0.963685	-3.599644	-0.782485
41	6	0	3.152730	-1.132573	-0.480940
42	1	0	3.443724	-3.290717	-0.659174
43	6	0	4.512839	-0.592430	-0.364198

44	6	0	4.750520	0.791426	-0.217513
45	6	0	5.629998	-1.446830	-0.395089
46	6	0	6.034498	1.293707	-0.110911
47	1	0	3.912064	1.484049	-0.192571
48	6	0	6.919641	-0.951717	-0.277516
49	1	0	5.488847	-2.518628	-0.505600
50	6	0	7.168994	0.437749	-0.125398
51	1	0	6.173814	2.363730	-0.005684
52	1	0	7.752713	-1.646423	-0.301650
53	6	0	8.534843	0.958299	-0.008902
54	6	0	8.705815	2.305752	0.717798
55	6	0	9.115727	2.625032	2.026525
56	6	0	8.445710	3.401428	-0.137225
57	6	0	9.228110	3.951250	2.450656
58	1	0	9.375482	1.853056	2.735521
59	6	0	8.552308	4.726396	0.285878
60	1	0	8.146455	3.203018	-1.164489
61	6	0	8.942580	5.010889	1.591829
62	1	0	9.546686	4.152701	3.471832
63	1	0	8.333010	5.534075	-0.410085
64	1	0	9.032016	6.040234	1.932752
65	6	0	9.627905	-0.014697	0.150739
66	6	0	10.373399	-0.247458	-1.126556
67	6	0	11.405083	-1.186542	-1.383014
68	6	0	10.009858	0.570043	-2.233409
69	6	0	12.011696	-1.293496	-2.630206
70	1	0	11.752005	-1.868197	-0.622907
71	6	0	10.602538	0.451445	-3.484647
72	1	0	9.243589	1.324026	-2.088379
73	6	0	11.618799	-0.480443	-3.694822
74	1	0	12.799898	-2.030335	-2.771800
75	1	0	10.281789	1.104326	-4.293872
76	1	0	12.100430	-0.568819	-4.666374
77	6	0	9.878247	-0.688083	1.448980
78	6	0	11.003792	-1.500532	1.740494
79	6	0	8.900198	-0.612199	2.481410
80	6	0	11.151897	-2.157199	2.955281
81	1	0	11.798789	-1.623091	1.023842
82	6	0	9.050012	-1.270395	3.700486
83	1	0	7.993327	-0.052033	2.324207
84	6	0	10.178645	-2.046460	3.951791
85	1	0	12.040427	-2.761669	3.125366
86	1	0	8.269499	-1.179337	4.452905
87	1	0	10.297219	-2.562933	4.901915
88	6	0	-9.374011	0.768367	-0.061959
89	6	0	-10.348063	0.081603	0.657347
90	6	0	-9.822985	2.031584	-0.569951
91	6	0	-11.680320	0.533303	0.837308
92	1	0	-10.136126	-0.847822	1.141954
93	6	0	-11.101547	2.508946	-0.420574

94	1	0	-9.138119	2.685543	-1.071919
95	6	0	-12.089183	1.776884	0.280111
96	6	0	-12.626535	-0.234349	1.574408
97	1	0	-11.360341	3.480787	-0.837725
98	6	0	-13.423973	2.223592	0.466183
99	6	0	-13.915162	0.217127	1.739168
100	1	0	-12.314073	-1.185318	2.003206
101	6	0	-14.318200	1.457422	1.179186
102	1	0	-13.724084	3.178711	0.038422
103	1	0	-14.635353	-0.373412	2.301364
104	1	0	-15.341458	1.798583	1.321988

Compound **Pd7**

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000122897	-0.000008560	0.000121011
2	6	0.000197523	0.000029390	0.000303766
3	6	0.000355229	0.000120259	-0.000001293
4	6	0.000096945	-0.000059789	-0.000526780
5	7	0.000032310	-0.000069651	0.000628247
6	1	0.000038266	0.000016884	0.000026745
7	6	-0.000243270	-0.001452955	0.001218636
8	6	0.002831265	0.000447970	0.000662871
9	7	0.000053335	0.000177728	0.000200494
10	6	-0.001693857	0.000608312	-0.000733400
11	1	0.000059608	-0.000139945	0.000041367
12	6	0.001038976	0.001919783	0.002135204
13	6	0.001005104	-0.001929799	-0.002052121
14	6	-0.001700039	-0.000636405	0.000679403
15	7	0.000049137	-0.000141531	0.000020122
16	6	0.002855228	-0.000401347	-0.000701275
17	6	-0.000340509	0.001464307	-0.001263447
18	1	0.000056268	0.000139083	-0.000037396
19	6	0.000015762	0.000082781	0.000578537
20	6	0.000403829	-0.000096448	-0.000009895
21	7	0.000151460	0.000029501	-0.000906886
22	6	0.000214623	-0.000029328	-0.000317949
23	1	0.000039083	-0.000002383	-0.000027132
24	6	-0.000150414	-0.000035591	0.000010750
25	1	0.000039308	-0.000021076	-0.000110614
26	6	-0.001398880	0.000071714	0.000058747
27	6	-0.007585920	0.000347567	-0.003925056
28	6	-0.007545257	-0.000435992	0.004022602
29	6	0.013786112	0.004719897	0.008129841
30	6	0.013736016	-0.004967759	-0.008409101
31	6	-0.007373157	0.000079450	0.000079829
32	6	-0.007173174	0.000006556	0.000071022

33	6	0.000228091	0.000027380	-0.000018344
34	6	-0.000066657	0.000008161	0.000153602
35	6	-0.000014554	-0.000005515	-0.000103913
36	6	0.000256106	-0.000089382	0.000050613
37	6	0.000209719	0.000122264	-0.000008656
38	6	-0.000382617	0.000036914	-0.000120276
39	6	-0.000602546	-0.000048748	-0.000156199
40	1	0.000186965	-0.000520309	0.000590207
41	1	0.000162217	0.000506496	-0.000544773
42	1	-0.000003142	0.000043482	0.000094364
43	1	0.000011016	0.000063826	-0.000004909
44	1	0.000018400	-0.000055984	0.000038892
45	1	-0.000075312	0.000026579	-0.000035659
46	1	-0.000032700	-0.000061911	-0.000016272
47	6	0.000447502	-0.000870649	0.001530220
48	6	-0.001859668	-0.000346883	-0.000592965
49	6	0.001831940	0.001315499	-0.002101620
50	6	0.001004695	-0.002188262	0.001037846
51	1	0.000003538	0.000108629	-0.000032115
52	6	0.002766495	0.004906221	-0.001153210
53	1	0.000039055	0.000233285	0.000216537
54	6	0.002020237	-0.004124364	-0.003579168
55	1	0.001647249	0.001023465	0.000297968
56	1	0.000094113	-0.000084684	-0.000109079
57	46	-0.001344931	0.000030438	0.000051278
58	1	0.000096986	0.000155712	0.000093442
59	1	0.000040227	-0.000237297	-0.000121347
60	1	0.010953750	0.002898372	-0.004786168
61	1	-0.000019455	0.000149933	0.000156150
62	9	0.011906415	0.000807123	0.007323037
63	9	-0.003104159	0.003979195	0.007652141
64	9	-0.017600333	0.000173585	0.000176646
65	9	-0.003288715	-0.003907439	-0.007613809
66	9	0.011537352	-0.000902864	-0.007593598
67	6	0.014620580	0.041504676	0.010586431
68	1	-0.003813362	-0.008071000	-0.011137980
69	6	0.005558549	-0.015597438	0.002634827
70	6	-0.001199858	-0.002355244	-0.005150162
71	6	0.002455767	0.008560063	0.003181316
72	6	-0.001913721	0.000844260	-0.010199856
73	1	-0.002081964	0.006123318	0.004505986
74	6	-0.000070610	0.006820610	0.005477834
75	1	-0.001869165	0.002220399	-0.011677510
76	6	-0.004363797	0.008316874	-0.005632032
77	1	0.001688648	0.000261921	0.008052450
78	1	0.001330546	-0.007073300	-0.004230333
79	1	0.003113299	-0.006847018	0.003813067
80	6	-0.022120611	-0.035068437	-0.012129761
81	1	0.004827575	0.009901198	0.010142854
82	6	0.014168130	-0.000401699	0.007037709

83	6	-0.003582779	-0.005421515	-0.004580853
84	6	-0.001618588	0.002603547	0.005581421
85	6	-0.003172686	-0.006200220	-0.005884236
86	1	-0.006647534	0.006562863	0.005442658
87	6	-0.005148298	0.006137526	0.005239151
88	1	-0.004449938	-0.005466934	-0.004539930
89	6	-0.010924517	0.001677137	0.000556045
90	1	0.004453397	0.005195256	0.004746875
91	1	0.003958799	-0.005712088	-0.004500356
92	1	0.008421862	-0.000514749	0.000239424
93	6	-0.010406937	0.011700426	-0.003290160
94	6	-0.003231858	-0.001565810	0.009273811
95	6	-0.001330837	-0.007497543	-0.003080737
96	6	0.001676848	0.000588843	0.009650742
97	1	0.000160490	-0.006006681	-0.004844449
98	6	-0.000130192	-0.007481213	-0.004627857
99	1	0.004050469	-0.005182647	0.011679064
100	6	0.003084669	-0.010517309	0.003680777
101	1	-0.001861176	0.000538298	-0.008068168
102	1	-0.000326991	0.006915083	0.004732926
103	1	-0.002099507	0.007503657	-0.003418698

Compound **Pd8**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.966032	-1.177782	-1.474551
2	6	0	-3.750832	-1.050592	-2.662143
3	6	0	-2.880534	-0.789426	-3.704648
4	6	0	-1.587545	-0.759590	-3.139702
5	7	0	-1.627906	-0.969325	-1.811840
6	1	0	-3.121066	-0.648893	-4.750035
7	6	0	1.026029	0.839311	-2.331632
8	6	0	2.169028	1.541050	-2.783233
9	7	0	1.360393	-0.341732	-1.790639
10	6	0	3.255673	0.743765	-2.481456
11	1	0	2.169014	2.508254	-3.267887
12	6	0	2.754555	-0.425093	-1.827054
13	6	0	3.001515	-2.527565	-0.502052
14	6	0	3.725655	-3.669247	-0.036646
15	7	0	1.657156	-2.695662	-0.165396
16	6	0	2.806654	-4.535491	0.523961
17	6	0	1.547232	-3.899894	0.416285
18	1	0	2.991726	-5.506000	0.964829
19	6	0	-0.756943	-2.414843	2.007909
20	6	0	-1.808937	-2.397406	2.949375
21	7	0	-1.207615	-2.179681	0.763035
22	6	0	-2.958854	-2.113303	2.236729

23	1	0	-1.710471	-2.556272	4.015012
24	6	0	-2.584147	-1.965418	0.865000
25	1	0	-3.955949	-1.977094	2.628149
26	6	0	3.515475	-1.453554	-1.248783
27	6	0	-3.422654	-1.571595	-0.199081
28	1	0	4.791621	-3.811525	-0.137222
29	1	0	4.297819	0.949670	-2.677446
30	1	0	-4.820382	-1.184742	-2.723627
31	6	0	8.784663	-0.387774	-0.935153
32	6	0	9.868592	-0.533596	-1.821865
33	6	0	9.018688	0.289237	0.275617
34	6	0	11.127343	-0.038317	-1.502592
35	1	0	9.715104	-1.020303	-2.780532
36	6	0	10.279415	0.781975	0.592430
37	1	0	8.207107	0.418306	0.986796
38	1	0	11.940947	-0.154714	-2.212654
39	1	0	10.427751	1.298024	1.535403
40	6	0	11.368613	0.616514	-0.280562
41	6	0	13.320974	0.987195	1.252991
42	6	0	12.718857	1.166942	0.038296
43	6	0	13.364422	1.926980	-1.076325
44	6	0	14.681582	1.648960	-1.480237
45	6	0	12.644272	2.903922	-1.786903
46	6	0	15.265078	2.337086	-2.543331
47	1	0	15.247362	0.886381	-0.954167
48	6	0	13.231220	3.600795	-2.842375
49	1	0	11.618147	3.119406	-1.502183
50	6	0	14.544730	3.319956	-3.225643
51	1	0	16.283664	2.101948	-2.840989
52	1	0	12.660052	4.361075	-3.368925
53	1	0	15.000300	3.857624	-4.052947
54	6	0	14.538207	1.746996	1.671174
55	6	0	14.603101	3.146020	1.551312
56	6	0	15.631046	1.079259	2.252663
57	6	0	15.728295	3.849954	1.978536
58	1	0	13.761727	3.680869	1.122031
59	6	0	16.761577	1.781356	2.668393
60	1	0	15.591092	0.000264	2.372770
61	6	0	16.815030	3.170647	2.533479
62	1	0	15.753723	4.932203	1.881058
63	1	0	17.599781	1.242887	3.103135
64	1	0	17.692600	3.719494	2.864710
65	6	0	12.814532	0.012172	2.266679
66	6	0	12.658729	0.394774	3.611112
67	6	0	12.535077	-1.320873	1.919424
68	6	0	12.205808	-0.513836	4.566799
69	1	0	12.890553	1.415310	3.902958
70	6	0	12.094428	-2.233240	2.877326
71	1	0	12.667566	-1.639179	0.889978
72	6	0	11.921713	-1.832523	4.203932

73	1	0	12.079187	-0.192451	5.597409
74	1	0	11.888731	-3.260182	2.586686
75	1	0	11.575501	-2.543023	4.949790
76	1	0	-0.646212	-0.613624	-3.649176
77	46	0	0.047094	-1.549089	-0.752630
78	1	0	0.585916	-4.273790	0.738661
79	1	0	-0.006471	1.153783	-2.380213
80	1	0	0.295772	-2.565552	2.197277
81	6	0	-4.870644	-1.588284	0.059628
82	6	0	-5.615122	-2.597780	0.634892
83	16	0	-5.897695	-0.211436	-0.291717
84	6	0	-6.988869	-2.283776	0.777437
85	1	0	-5.179346	-3.549841	0.915271
86	6	0	-7.318868	-1.019163	0.330292
87	1	0	-7.722527	-2.979743	1.168907
88	6	0	-8.630217	-0.365290	0.341678
89	6	0	-8.956378	0.665088	-0.559365
90	6	0	-9.610993	-0.752935	1.275009
91	6	0	-10.204040	1.277420	-0.527347
92	1	0	-8.229976	0.979754	-1.303988
93	6	0	-10.864101	-0.153595	1.289750
94	1	0	-9.376038	-1.513097	2.014002
95	6	0	-11.195770	0.870005	0.383378
96	1	0	-10.423038	2.076580	-1.229308
97	1	0	-11.597139	-0.469642	2.024785
98	6	0	-12.523089	1.550984	0.420961
99	6	0	-12.461165	3.044148	0.361210
100	6	0	-13.240594	3.769671	-0.556037
101	6	0	-11.572733	3.756382	1.186590
102	6	0	-13.149244	5.158933	-0.632108
103	1	0	-13.920382	3.236120	-1.212983
104	6	0	-11.489318	5.146596	1.119053
105	1	0	-10.947624	3.212449	1.889359
106	6	0	-12.277271	5.854299	0.208431
107	1	0	-13.758123	5.698378	-1.352953
108	1	0	-10.804230	5.676950	1.775396
109	1	0	-12.207218	6.937171	0.149735
110	6	0	-13.703160	0.863842	0.498530
111	6	0	-15.007289	1.529428	0.797413
112	6	0	-16.148596	1.237316	0.028891
113	6	0	-15.145360	2.415600	1.879836
114	6	0	-17.375699	1.835732	0.311490
115	1	0	-16.066549	0.539346	-0.799530
116	6	0	-16.375163	3.004773	2.170305
117	1	0	-14.280229	2.638972	2.496142
118	6	0	-17.494497	2.722371	1.384181
119	1	0	-18.241300	1.605338	-0.304259
120	1	0	-16.459375	3.682840	3.015573
121	1	0	-18.452416	3.183299	1.609947
122	6	0	-13.791073	-0.612743	0.282475

123	6	0	-14.504817	-1.425420	1.181574
124	6	0	-13.216241	-1.219149	-0.847843
125	6	0	-14.610288	-2.800342	0.975720
126	1	0	-14.974404	-0.971284	2.049683
127	6	0	-13.332540	-2.592290	-1.060960
128	1	0	-12.678389	-0.604623	-1.563180
129	6	0	-14.024493	-3.389999	-0.147092
130	1	0	-15.155533	-3.411254	1.690549
131	1	0	-12.884964	-3.038593	-1.945184
132	1	0	-14.113553	-4.460411	-0.312342
133	6	0	4.990631	-1.417686	-1.439027
134	6	0	5.763051	-2.235697	-2.225817
135	16	0	5.996623	-0.280512	-0.570731
136	6	0	7.155639	-1.957997	-2.139508
137	1	0	5.339218	-3.017455	-2.846816
138	6	0	7.465083	-0.929904	-1.276248
139	1	0	7.908979	-2.522042	-2.678387
