Supporting Information For:

Mechano-Responsive Color Changes of a Pt(II) Complex Possessing Triethylene Glycol Towards Pressure Sensors

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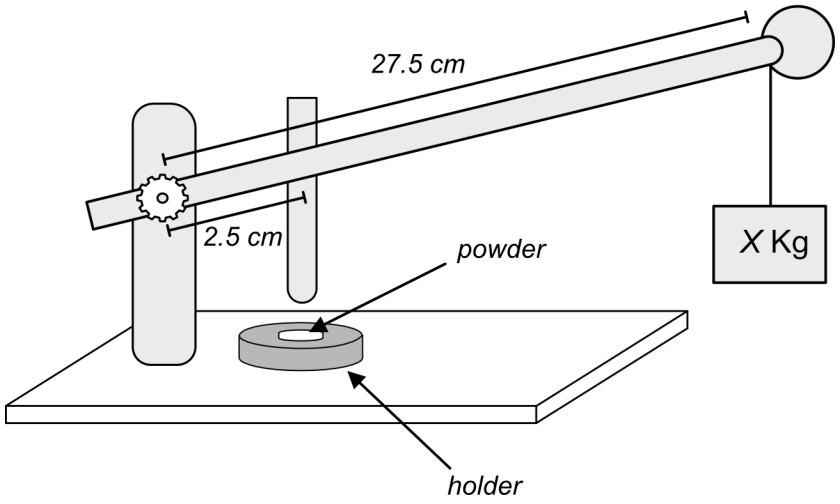
Contents

Method



Pressure responsive color change (Fig. 6): Powder **1** (2.2 mg) was placed on the specimen holder, which was pressed using a hand-press machine (JASCO, mini press MP-1). The resulting powder was subjected to luminescence measurement. The external forces "X kg" applied were converted to "X MPa" based on the relation of 1 kgf/cm^2 = 0.098 MPa using the diameter of the sample holder (φ = 5 mm).

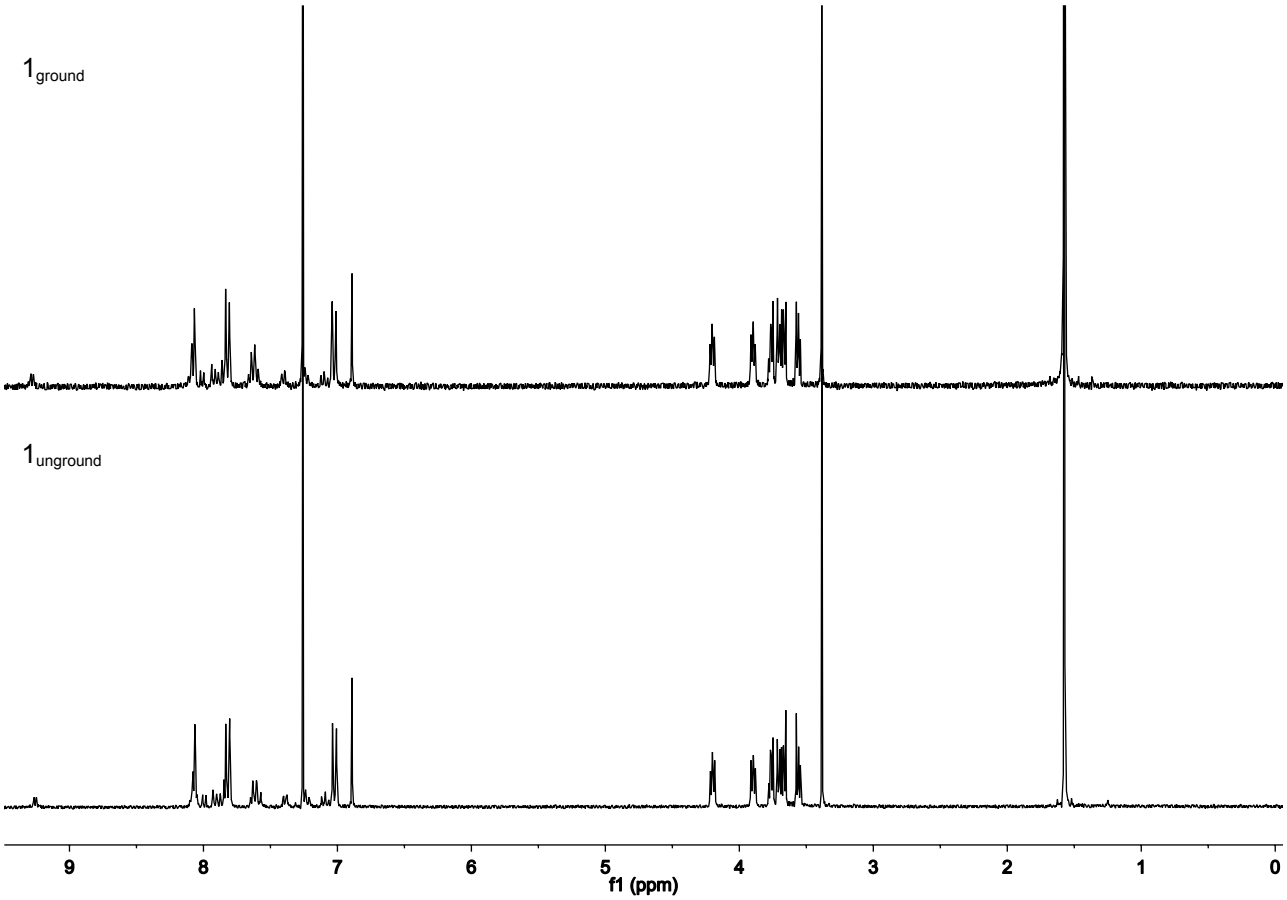


Figure S1. ^{1}H NMR spectra of complex **1** before and after grinding ($CDCl_3$).

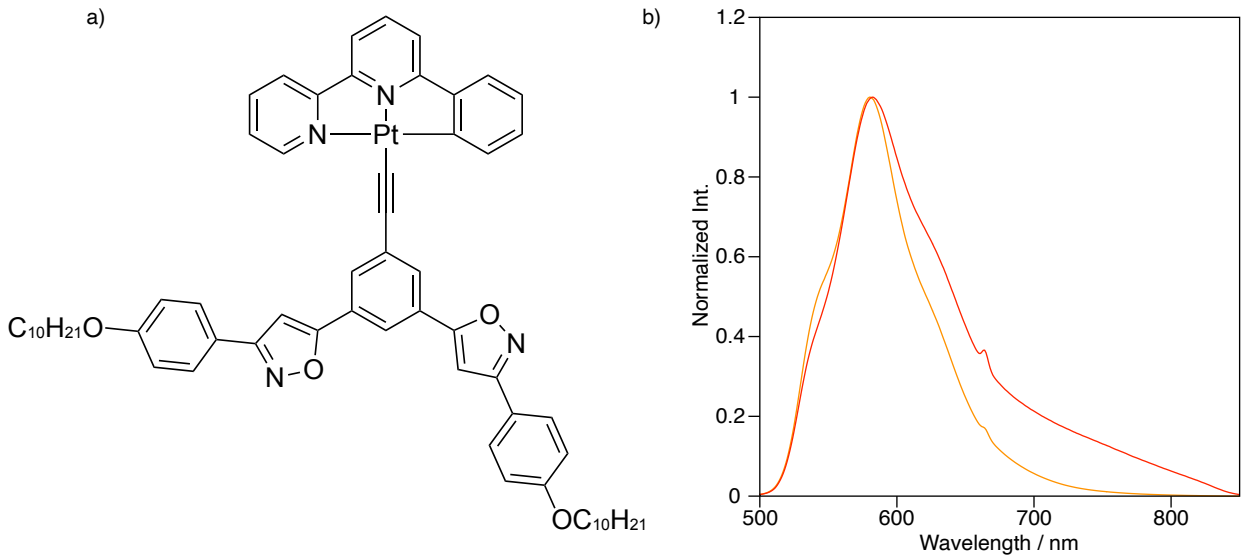


Figure S2. Emission spectra of **2** (λ_{ex} = 444 nm) in the solid state. The orange line and the red line represent the spectrum before grinding and after grinding, respectively.

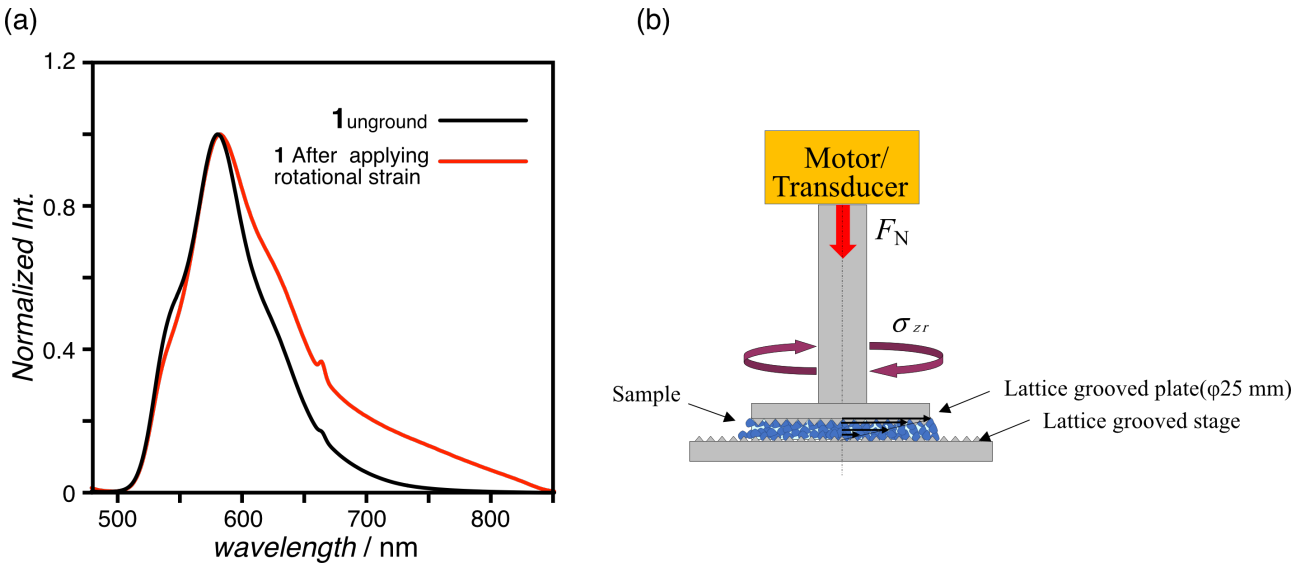


Figure S3. (a) Solid-state emission spectra (λ_{ex} = 444 nm) of **1**$_{\textbf{unground}}$ (black line) and **1** after applying shear stress (red line). (b) Schematic illustration of applying rotational strain to the powder **1**$_{\textbf{unground}}$ using a rotational rheometer.

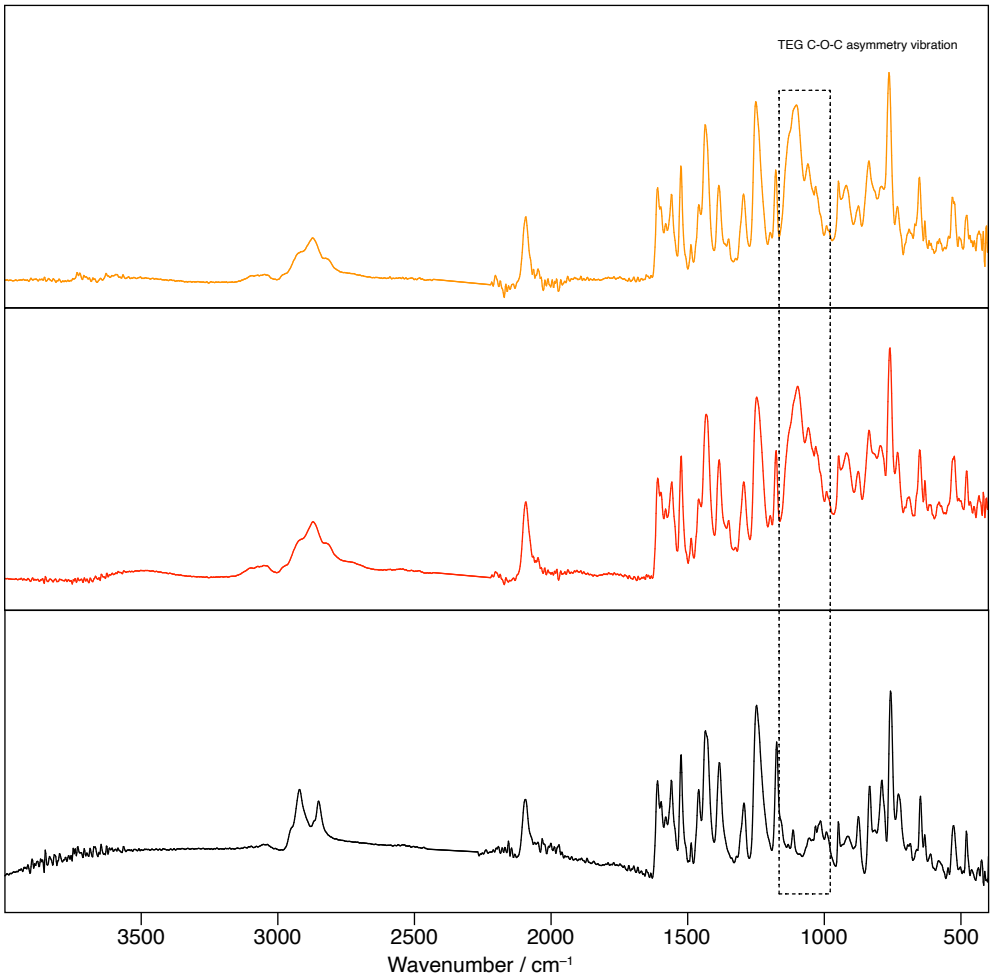


Figure S4. IR spectra of $\mathbf{1}_{\mathbf{unground}}$ (orange line), $\mathbf{1}_{\mathbf{ground}}$ (red line), and $\mathbf{2}_{\mathbf{unground}}$ (black line).

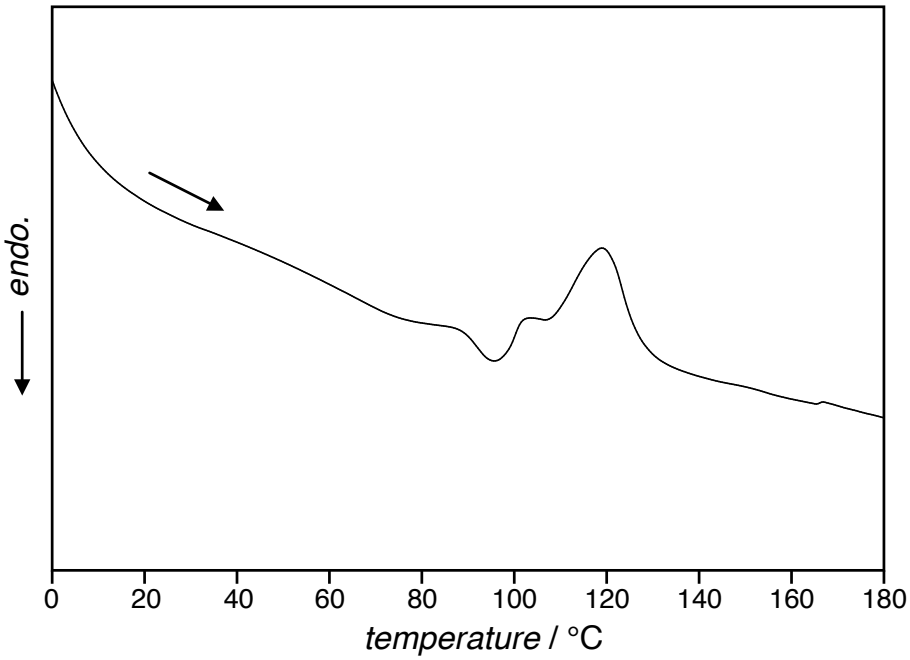


Figure S5. DSC curve of decyl side chain equipped platinum complex $\mathbf{2}_{\mathbf{ground}}$.

Note S1. The exothermic peak at approximately 120 °C suggests the formation of ordered structure of **2** in bulk. Considering the fact that the ordered structure was formed without relying on Pt–Pt interactions, **2** presumably formed benzene-centered assemblies as previously reported [*Chem. Commun.*, **2022**, *58*, 8356-8359].

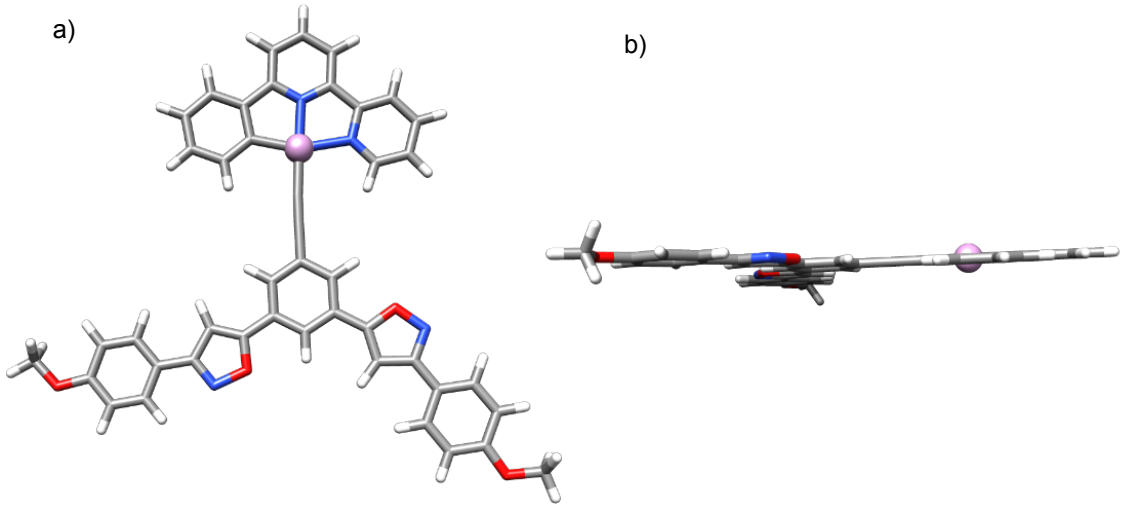


Figure S6. (a) Top view and (b) side view of the calculated structure of monomeric **1**.

Table S1. DFT calculated vibrations of the monomeric **1** as per Fig. S6.

#	Frequency	Infrared	#	Frequency	Infrared	#	Frequency	Infrared
1	1.65	0.6494	31	224.71	0.0153	61	510.93	3.9243
2	8.68	0.7379	32	233.95	0.5238	62	517.46	12.6043
3	9.27	3.335	33	236.06	0.1981	63	528.17	5.6317
4	11.08	0.0391	34	238.57	0.1638	64	541.64	4.7807
5	12.34	0.0447	35	241.04	8.3416	65	542.17	7.7872
6	17.36	0.2728	36	263.74	1.9793	66	549	0.139
7	18.92	0.2536	37	272.48	1.9942	67	549.91	0.2203
8	21.07	0.0871	38	274.72	1.1701	68	565.41	1.2978
9	31.56	0.2252	39	290.98	0.1458	69	606.5	3.027
10	40.81	0.0608	40	293.54	0.0038	70	609.18	2.4817
11	50.51	10.0452	41	302.55	2.6582	71	620.37	44.3477
12	55.66	1.0602	42	317.46	0.0016	72	621.23	0.5449
13	61.33	0.751	43	342.62	1.245	73	627.24	40.2781
14	64.59	0.1636	44	354.29	0.1357	74	662.18	0.5654
15	87.8	2.7466	45	364.43	6.1266	75	662.81	5.5115
16	89.41	0.3723	46	365.52	0.1722	76	667.14	1.8111
17	92.23	0.4562	47	384.17	2.9566	77	667.38	2.423
18	95.97	5.0828	48	397.82	0.0047	78	669.35	1.5634
19	111.92	7.7101	49	401.39	0.6072	79	684.45	3.3244
20	113.23	0.5306	50	410.96	0.1429	80	688.1	1.4975
21	119.25	2.3092	51	433.3	0.0693	81	693.7	0.1709
22	125.04	0.3202	52	434.19	0.0086	82	698.32	0.226
23	131.92	0.0167	53	439.7	2.2238	83	710.23	4.0012
24	143.13	1.4101	54	440.66	0.0749	84	717.15	0.6144
25	175.17	1.7154	55	451.14	1.0579	85	727	0.1122
26	189.39	1.9458	56	467.48	1.6699	86	755.95	3.8806
27	197.84	0.0094	57	472.6	2.3722	87	762.38	0.3775
28	200.5	0.9384	58	480.84	0.4798	88	763.06	2.0744
29	201.99	0.6651	59	486.53	0.5566	89	763.28	5.5645
30	205.62	1.3854	60	495.45	10.5538	90	763.6	4.3152

#	Frequency	Infrared	#	Frequency	Infrared	#	Frequency	Infrared
91	771.39	2.1305	121	1006.59	0.3197	151	1205.49	1.5216
92	784.53	27.8872	122	1015.54	0.3159	152	1222.37	2.1959
93	793.9	134.6239	123	1018.32	0.1828	153	1224.57	1.3888
94	807.35	2.4923	124	1020.65	0.6646	154	1226.22	16.0876
95	811.17	4.232	125	1024.34	84.7761	155	1230.68	268.523
96	818.44	12.075	126	1025.04	73.2103	156	1231.9	97.0735
97	847.29	41.1179	127	1028.52	6.7213	157	1240.12	7.5785
98	849.65	78.7115	128	1031.28	1.8676	158	1247.35	3.0823
99	850.68	8.382	129	1033.97	0.4316	159	1272.86	85.3263
100	853.77	0.9297	130	1046.44	0.0023	160	1275.03	54.6012
101	854.05	10.6371	131	1049.01	2.3153	161	1286.06	206.7807
102	856.38	42.3261	132	1049.15	1.8621	162	1287.29	178.061
103	856.77	71.2785	133	1051.32	2.8332	163	1301.53	29.3082
104	859.26	2.5787	134	1071.27	8.8675	164	1315.44	20.8677
105	878.64	28.0617	135	1074.34	9.8489	165	1328.48	0.7986
106	883.63	24.1745	136	1083.4	15.4401	166	1334.49	14.9042
107	901.42	47.1065	137	1087.67	4.0217	167	1339.23	5.6851
108	914.82	0.3684	138	1096.88	5.7048	168	1344.58	2.1206
109	929.92	1.0372	139	1100.46	3.8184	169	1345.15	0.4062
110	932.6	10.1873	140	1118.91	2.1234	170	1355.67	40.9322
111	935.53	0.1535	141	1128.83	0.2228	171	1357.12	6.5877
112	938.08	17.4093	142	1130.99	4.522	172	1361.68	27.7294
113	956.64	10.3568	143	1131.05	1.6939	173	1372.45	0.2414
114	975.84	0.0099	144	1161.85	7.2353	174	1374.82	13.5086
115	976.77	13.738	145	1162.53	1.6665	175	1376.13	25.1139
116	977.01	4.555	146	1162.68	13.5685	176	1376.24	40.008
117	981.09	0.7472	147	1164.92	0.2674	177	1420.61	85.7372
118	990.41	15.2485	148	1165.12	0.265	178	1426.32	87.2081
119	991.89	0.0288	149	1184.15	0.8701	179	1437.58	76.8217
120	997.93	4.9235	150	1205.25	0.7582	180	1454.3	17.3129

#	Frequency	Infrared	#	Frequency	Infrared	#	Frequency	Infrared
181	1476.51	62.4443	211	1673.99	115.0783	241	3254.19	15.2152
182	1480.41	179.7858	212	1674.92	107.3784	242	3318.4	2.2407
183	1484.07	40.1616	213	2210.93	139.8478	243	3318.44	1.8824
184	1492.11	171.6494	214	3034.37	56.4771			
185	1495.78	26.1819	215	3035.09	61.243			
186	1496.21	0.2907	216	3105.96	42.0172			
187	1498.98	42.6525	217	3106.98	42.0639			
188	1501.74	16.5309	218	3180.99	4.7286			
189	1504.94	67.2623	219	3182.2	25.3106			
190	1505.75	18.3384	220	3182.47	26.1237			
191	1515.22	47.3357	221	3189.51	18.6682			
192	1532.25	19.3473	222	3209.9	17.707			
193	1533.04	0.6592	223	3213.98	15.1113			
194	1533.04	17.6623	224	3214.5	47.4221			
195	1543.49	70.7618	225	3216.39	3.8024			
196	1543.73	24.6812	226	3220.01	5.5749			
197	1582.96	138.7446	227	3223.97	7.8529			
198	1584.2	48.2151	228	3226.48	3.5908			
199	1597.51	23.7663	229	3226.91	5.5876			
200	1610.96	88.7063	230	3230.14	23.3059			
201	1611.08	152.4904	231	3235.61	2.3535			
202	1615.72	9.7993	232	3237.79	12.7085			
203	1622.25	161.4962	233	3238.41	8.7636			
204	1632.49	61.6141	234	3240.62	1.1836			
205	1636.38	89.7179	235	3241.33	8.8593			
206	1642.13	2.7594	236	3243.03	4.693			
207	1645.34	82.9529	237	3243.9	0.2274			
208	1649.45	22.6399	238	3244.49	5.7178			
209	1654.57	1.6591	239	3248.12	1.0755			
210	1660.63	63.6289	240	3249.09	16.9256			

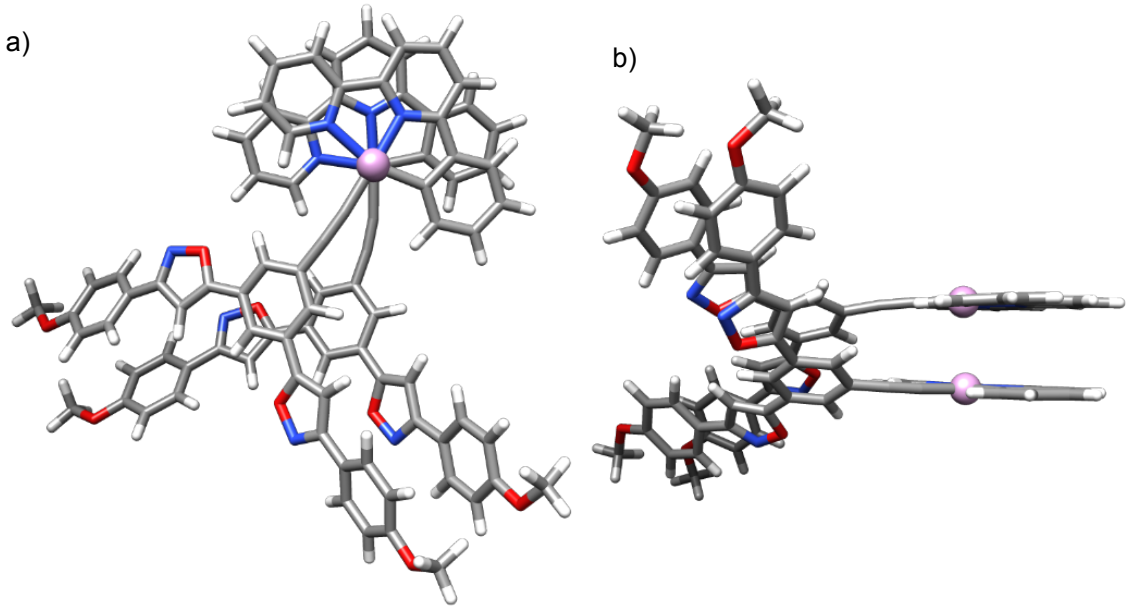


Figure S7. (a) Top view and (b) side view of the calculated structure of dimeric **1**.

Table S2. DFT calculated vibrations of dimeric **1** as per Fig. S7.

#	Frequency	Infrared	#	Frequency	Infrared	#	Frequency	Infrared
1	5.33	0.5851	31	84.24	0.7199	61	207.17	0.6712
2	7.98	0.9266	32	90.48	1.2966	62	211.53	2.4237
3	11.84	0.9711	33	90.76	6.7761	63	213.97	1.9493
4	12.19	0.2591	34	96.77	0.0402	64	217.01	1.8869
5	16.47	0.2139	35	98.79	1.0986	65	218.5	2.6172
6	17.47	0.4305	36	104.37	4.0932	66	219.87	0.0679
7	19.42	0.7589	37	107.5	1.5576	67	225.3	0.1629
8	22.54	0.6162	38	111.87	0.2283	68	227.71	0.7652
9	22.66	0.2519	39	116.37	2.3632	69	230.82	2.7635
10	27.32	0.5491	40	118.96	0.1403	70	239.38	3.5757
11	30.42	0.0836	41	119.93	3.4981	71	242.87	0.1092
12	32.69	0.4061	42	121.37	0.7493	72	244.67	0.6355
13	38.52	0.708	43	122.72	0.7514	73	248.61	0.5349
14	41.15	0.7104	44	124.52	5.2401	74	251.06	5.3819
15	44.77	0.2571	45	128.71	1.1507	75	253.06	2.794
16	48.72	0.4597	46	133.08	5.4411	76	254	1.3091
17	50.7	1.6859	47	138.13	2.7029	77	267.95	3.5651
18	53.33	0.8051	48	141.98	2.8316	78	275.06	1.9845
19	55.08	1.1919	49	143.69	5.1501	79	275.56	1.9406
20	58.55	0.6253	50	144.61	4.4341	80	276.39	0.6641
21	59.76	0.4425	51	146.87	7.1126	81	280.14	1.3041
22	63.47	0.1149	52	148.51	0.7025	82	282.54	0.482
23	65.93	0.6766	53	150.98	1.5211	83	293.58	5.7831
24	70.9	3.2197	54	153.6	2.7227	84	295.75	0.3136
25	72.74	1.5544	55	165.99	4.0147	85	296.25	0.3533
26	74.56	0.6224	56	168.51	0.1065	86	297.86	1.5084
27	76.64	0.4277	57	194.05	1.9258	87	304.83	1.235
28	78.69	0.7313	58	196.87	1.4432	88	309.09	1.0464
29	81.77	1.4814	59	197.44	0.6518	89	316.62	0.4761
30	83.52	3.1974	60	203.24	0.4913	90	323.11	0.0814

#	Frequency	Infrared	#	Frequency	Infrared	#	Frequency	Infrared
91	346.23	2.1151	121	478.69	1.246	151	631.3	35.4528
92	349.43	1.9856	122	479.76	0.4045	152	638.91	9.9446
93	359.6	1.0988	123	484.92	2.5697	153	659.22	0.6877
94	359.84	0.1294	124	485.89	1.0195	154	661.33	1.2139
95	363.49	3.2952	125	492.52	6.1041	155	664.44	0.7322
96	365.3	2.3951	126	494.66	14.7248	156	665.1	5.9634
97	368.65	0.0876	127	507.81	12.1085	157	666.22	2.6147
98	368.93	1.6587	128	509.02	3.1603	158	667.49	1.8337
99	388.41	0.2296	129	509.34	2.0659	159	667.76	1.6909
100	388.5	5.265	130	510.29	2.1851	160	668.64	2.5769
101	402.42	2.0114	131	521.18	4.858	161	673.68	0.2999
102	403.53	0.076	132	524.76	4.6239	162	676.44	0.7341
103	404.58	0.8728	133	541.65	7.0353	163	683.87	3.7029
104	406.49	0.4724	134	544.98	7.6016	164	686.01	0.4056
105	409.69	0.9474	135	546.87	1.7128	165	689.24	1.7905
106	413.86	0.1185	136	548.39	15.9953	166	691.5	2.0775
107	432.97	0.3938	137	548.67	2.4344	167	698.47	0.0671
108	433.01	0.1687	138	550.18	0.5481	168	698.96	0.1737
109	434.17	0.3471	139	556.82	3.6549	169	701.3	0.277
110	435.73	0.0592	140	566.76	1.5968	170	702.2	0.3062
111	438.29	0.3477	141	568.51	0.2371	171	712.63	9.3071
112	439.18	3.7315	142	569.12	1.1682	172	714.94	0.5457
113	439.62	1.7593	143	592.1	2.5859	173	717.97	4.0458
114	441.04	0.555	144	598.03	1.151	174	721.91	3.588
115	453.86	1.5312	145	612.71	0.556	175	728.41	1.4381
116	457.56	4.0542	146	614.55	0.7145	176	730.57	1.2565
117	466.27	3.0989	147	621.59	6.6473	177	755.96	11.9998
118	468.88	2.3501	148	623.37	65.6513	178	757.27	8.2314
119	475.32	1.3205	149	625.52	28.2381	179	759.19	1.2465
120	477.66	1.1596	150	627.86	21.8568	180	759.62	3.0037

#	Frequency	Infrared	#	Frequency	Infrared	#	Frequency	Infrared
181	760.22	2.5537	211	858.31	0.4203	241	989.35	8.9736
182	760.72	3.7361	212	859.17	159.5427	242	990.57	3.2187
183	761	0.8195	213	859.62	0.2267	243	992.72	10.5077
184	761.47	0.8505	214	866.5	39.1435	244	993.84	2.9241
185	762.06	6.6106	215	875.07	20.4046	245	995.13	3.4658
186	763.95	3.1657	216	876.32	49.2149	246	999.12	1.2279
187	767.47	7.5099	217	880.2	6.613	247	1000.01	1.5296
188	770.21	20.971	218	880.81	0.2431	248	1002.24	2.3068
189	786.41	151.6486	219	905.77	1.8221	249	1006.7	0.3648
190	786.8	40.698	220	906.77	5.3372	250	1007.56	0.1378
191	791	24.0367	221	907.02	12.788	251	1008.8	0.2548
192	794.78	24.2416	222	908.78	41.7718	252	1009.59	1.0426
193	805.59	0.2009	223	919.76	2.0369	253	1011.1	0.2038
194	809.27	2.0384	224	921.48	1.3972	254	1011.94	1.0651
195	812.06	13.8757	225	926.83	30.2769	255	1019.93	88.0534
196	813.46	5.4259	226	927.98	1.8427	256	1022.48	82.06
197	813.97	17.4462	227	928.31	1.3797	257	1024.52	0.2223
198	824.11	24.4307	228	932.96	8.076	258	1026.22	56.5795
199	833.15	24.0363	229	938.7	1.3943	259	1026.89	67.6797
200	834.61	70.0809	230	938.77	21.2022	260	1026.99	2.7526
201	837.86	80.72	231	949.49	9.6322	261	1034.66	4.5133
202	842.57	81.5555	232	956.56	5.1255	262	1036.79	0.798
203	844.97	5.9274	233	968.69	0.2708	263	1036.99	4.7186
204	847.16	27.2173	234	971.04	0.4237	264	1037.49	6.0105
205	849.74	3.7001	235	972.61	1.2693	265	1038.19	2.703
206	851.13	14.5473	236	972.9	0.0829	266	1052.16	1.0842
207	852.24	5.6456	237	979.77	0.1292	267	1053.31	0.5767
208	852.36	15.127	238	980.85	4.2961	268	1053.85	2.6346
209	853.98	41.4152	239	981.36	18.048	269	1054.51	3.717
210	855.95	2.7031	240	983.35	4.3797	270	1055.88	0.3745

#	Frequency	Infrared	#	Frequency	Infrared	#	Frequency	Infrared
271	1057.41	1.9994	301	1175.13	0.3879	331	1305.66	29.9129
272	1067.54	0.4993	302	1178.52	0.5948	332	1308.02	17.8068
273	1073.36	3.9735	303	1186.65	1.4581	333	1319.66	9.9155
274	1075.16	5.1078	304	1187.1	0.146	334	1320.58	19.6919
275	1079.06	1.5044	305	1205.6	0.2155	335	1332.61	0.2633
276	1079.54	9.3144	306	1205.79	0.9271	336	1333.38	1.2619
277	1086.01	1.3695	307	1206.91	1.5886	337	1341.46	1.8806
278	1086.96	21.0097	308	1209.47	0.2604	338	1342.4	11.4734
279	1089.62	0.9368	309	1221.62	2.9781	339	1343.27	0.7628
280	1090.73	7.7234	310	1223.42	0.9341	340	1343.9	8.2793
281	1098.97	3.6185	311	1224.53	0.6628	341	1348.18	3.7575
282	1100.74	8.1651	312	1229.79	13.3757	342	1350.11	2.2398
283	1104.63	2.3162	313	1231.13	25.2882	343	1352.71	1.3931
284	1105.82	5.6525	314	1231.43	160.337	344	1353.77	1.5613
285	1123.9	0.439	315	1231.92	8.6561	345	1360.47	3.9123
286	1124.74	3.3581	316	1232.43	179.1216	346	1360.74	26.8355
287	1127.87	0.3391	317	1233.52	107.1474	347	1361.72	35.2094
288	1129.33	0.631	318	1234.02	147.284	348	1362.65	8.4848
289	1133.95	0.8602	319	1238.77	7.6492	349	1365.35	32.0749
290	1135.96	3.0684	320	1240.89	4.9489	350	1366.51	13.5148
291	1137.1	0.1112	321	1254.12	3.7049	351	1376.47	11.065
292	1137.74	9.3627	322	1254.81	2.4456	352	1377.91	12.7518
293	1161.51	5.1446	323	1271.37	28.2315	353	1378.3	7.3591
294	1163.39	7.4763	324	1272.54	119.2	354	1378.94	4.04
295	1164.04	6.6244	325	1274.53	33.1644	355	1379.76	7.9846
296	1165.5	0.958	326	1279.59	56.1303	356	1380.37	18.8669
297	1165.86	8.8301	327	1280.45	47.4308	357	1381.15	8.0162
298	1167.02	0.4239	328	1281.8	86.4969	358	1383.09	52.3089
299	1167.15	3.7426	329	1288.58	268.2673	359	1421.56	28.8125
300	1167.22	0.5761	330	1290.98	283.7076	360	1423.45	106.1974

#	Frequency	Infrared	#	Frequency	Infrared	#	Frequency	Infrared
361	1427.82	67.3893	391	1533.26	23.3398	421	1650.86	125.6989
362	1430.32	79.5186	392	1535.56	15.951	422	1653	23.7121
363	1438.12	21.694	393	1538.24	6.8292	423	1662.28	5.0794
364	1441.02	93.8654	394	1541.62	9.4694	424	1667.13	10.291
365	1461.28	2.4556	395	1545.5	47.6364	425	1668.69	53.0372
366	1463.08	11.3871	396	1546.08	46.837	426	1672.29	126.088
367	1482.56	81.2031	397	1550.8	8.8564	427	1676.57	34.5949
368	1483.48	184.3021	398	1557.64	28.9915	428	1677.22	41.7965
369	1484.38	34.3652	399	1587.31	18.1026	429	1678.69	114.178
370	1484.94	10.9144	400	1588.19	200.3623	430	1679.34	130.7312
371	1485.58	31.0724	401	1588.52	5.3441	431	2223.55	42.1619
372	1487.33	42.0439	402	1589.69	68.2405	432	2226.98	313.2664
373	1494.96	24.2593	403	1595.54	21.2024	433	3035.75	42.6956
374	1495.83	200.6671	404	1597.4	18.683	434	3037.66	21.8352
375	1497.48	13.7928	405	1608.7	3.3795	435	3039.76	109.8115
376	1497.9	3.6618	406	1611.86	1.5805	436	3042.47	72.8191
377	1498.41	11.7821	407	1614.31	44.0542	437	3108.01	40.0003
378	1500.37	77.9412	408	1614.51	67.1035	438	3111.21	39.3848
379	1500.9	2.3462	409	1615.15	11.9474	439	3124.34	11.7428
380	1503.57	30.0494	410	1620.48	220.8557	440	3130.61	13.0472
381	1507.26	29.4492	411	1627.59	68.4617	441	3176.36	5.9331
382	1508.32	158.406	412	1630.26	178.8845	442	3181.3	26.4918
383	1508.82	16.689	413	1635.14	65.0923	443	3181.59	25.9832
384	1508.96	10.3275	414	1638.21	39.767	444	3183.03	5.8391
385	1510.66	21.0183	415	1640.46	1.5833	445	3184.36	27.1697
386	1512.22	98.0198	416	1642.36	195.2337	446	3184.44	26.94
387	1518.41	20.4506	417	1644.36	7.8604	447	3192.53	4.9629
388	1519.16	44.7959	418	1647.29	2.8761	448	3193.47	21.9903
389	1532.48	10.6388	419	1647.78	21.9781	449	3206.26	11.8294
390	1532.71	11.5527	420	1650.18	1.229	450	3208.54	9.0034

#	Frequency	Infrared	#	Frequency	Infrared
451	3210.74	18.9935	481	3249.88	8.2119
452	3211.92	11.0263	482	3250.13	1.0112
453	3213.23	37.2465	483	3252.27	12.9073
454	3215.07	15.371	484	3253.26	0.9826
455	3216.34	48.373	485	3253.62	10.9564
456	3217.64	18.9167	486	3256.76	0.2574
457	3218.23	6.6354	487	3259.11	4.462
458	3221.63	8.6644	488	3263.55	2.9042
459	3222.05	4.1575	489	3312.3	2.8349
460	3227.54	8.2201	490	3314.7	1.6886
461	3230.06	13.6051	491	3322.99	1.7037
462	3230.23	6.5096	492	3326.63	3.4376
463	3230.79	4.5374			
464	3232.95	2.9199			
465	3235.68	5.2194			
466	3236.42	12.3781			
467	3236.65	2.861			
468	3237.84	5.1478			
469	3238.7	4.5421			
470	3240.04	10.9226			
471	3240.31	7.5968			
472	3240.42	0.9088			
473	3242.77	5.6815			
474	3243.96	5.4325			
475	3245.1	12.775			
476	3245.11	4.5202			
477	3246.61	0.717			
478	3246.66	2.9268			
479	3248.72	16.1246			
480	3249.87	3.322			

Table S3. Cartesian coordinate of the calculated structure of complex **1** in the monomeric state.
Standard orientation: E = –2333.15332599 Hartree,
Imaginary frequency = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	7.559528	-3.361958	-0.109078
2	6	0	6.220309	-2.957427	-0.099724
3	7	0	5.924956	-1.634742	-0.001764
4	6	0	6.867503	-0.648436	0.090592
5	6	0	8.220327	-1.027011	0.083474
6	6	0	8.555725	-2.380053	-0.016244
7	6	0	6.282489	0.693805	0.186065
8	6	0	5.033149	-3.835034	-0.187104
9	6	0	4.846393	0.766055	0.168162
10	6	0	4.256640	2.035388	0.259630
11	6	0	5.040953	3.191329	0.364287
12	6	0	6.440836	3.108508	0.380161
13	6	0	7.059298	1.861134	0.291233
14	6	0	5.093281	-5.229332	-0.293284
15	6	0	3.910050	-5.969160	-0.368895
16	6	0	2.680200	-5.303436	-0.337236
17	6	0	2.670682	-3.912116	-0.230812
18	7	0	3.813929	-3.197225	-0.157882
19	78	0	3.993584	-1.045817	0.011608
20	6	0	2.099415	-0.511011	0.020015
21	6	0	0.892878	-0.252891	0.018376
22	6	0	-0.503733	0.025784	0.014756
23	6	0	-0.982100	1.352830	0.001647
24	6	0	-2.359681	1.627836	-0.003838
25	6	0	-3.281798	0.569321	0.004435
26	6	0	-2.826507	-0.759463	0.018027
27	6	0	-1.448492	-1.024025	0.023054
28	6	0	-3.785630	-1.859294	0.025775
29	6	0	-2.833599	3.007904	-0.019165
30	6	0	-5.153927	-1.925050	0.037947
31	6	0	-5.482779	-3.320009	0.039922
32	7	0	-4.386330	-4.087153	0.029350
33	8	0	-3.277970	-3.149005	0.020242
34	6	0	-2.211089	4.227871	-0.038313

35	6	0	-3.258800	5.206347	-0.046201
36	7	0	-4.468916	4.635850	-0.032972
37	8	0	-4.204979	3.208380	-0.015288
38	6	0	-6.815387	-3.936962	0.052255
39	6	0	-3.135648	6.669332	-0.066091
40	6	0	-7.983694	-3.148460	0.050325
41	6	0	-9.244035	-3.735982	0.061935
42	6	0	-9.364719	-5.133662	0.075736
43	6	0	-8.214858	-5.936752	0.077806
44	6	0	-6.954966	-5.335996	0.066171
45	6	0	-1.879375	7.293079	-0.087222
46	6	0	-1.759716	8.686658	-0.106305
47	6	0	-2.916020	9.476472	-0.104361
48	6	0	-4.182729	8.868410	-0.083434
49	6	0	-4.289439	7.484850	-0.064590
50	8	0	-10.663981	-5.623573	0.086612
51	8	0	-2.918127	10.864856	-0.122036
52	6	0	-10.872390	-7.060660	0.101163
53	6	0	-1.648085	11.568194	-0.144456
54	1	0	7.827597	-4.407762	-0.185973
55	1	0	8.996125	-0.275506	0.154833
56	1	0	9.599172	-2.675209	-0.021932
57	1	0	3.175800	2.112595	0.249005
58	1	0	4.559880	4.162945	0.434401
59	1	0	7.041859	4.008356	0.461543
60	1	0	8.144239	1.801455	0.304422
61	1	0	6.052004	-5.732365	-0.316452
62	1	0	3.949412	-7.049497	-0.451052
63	1	0	1.756452	-3.332979	-0.200693
64	1	0	-0.261395	2.162182	-0.004534
65	1	0	-4.340852	0.793944	-0.001129
66	1	0	-1.102373	-2.049500	0.034435
67	1	0	-5.841288	-1.097019	0.046642
68	1	0	-1.151127	4.413395	-0.046185
69	1	0	-7.910467	-2.066556	0.039018
70	1	0	-10.147009	-3.137320	0.060438
71	1	0	-8.287166	-7.017233	0.088605
72	1	0	-6.063576	-5.952704	0.068097
73	1	0	-0.974557	6.694798	-0.089507
74	1	0	-0.774166	9.134955	-0.122495
75	1	0	-5.060917	9.503037	-0.082372

76	1	0	-5.265386	7.014143	-0.048340
77	1	0	-11.953788	-7.191044	0.107577
78	1	0	-10.439129	-7.516141	0.999308
79	1	0	-10.447711	-7.533020	-0.792356
80	1	0	-1.908459	12.625784	-0.155273
81	1	0	-1.071870	11.319450	-1.043418
82	1	0	-1.052986	11.342433	0.748251
83	1	0	1.744383	-5.845868	-0.393217

Table S4. Cartesian coordinate of the calculated structure of complex **1** in the dimeric state.

Standard orientation: E = –4666.83172235 Hartree,
Imaginary frequency = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.722489	-3.943176	-0.033966
2	6	0	-5.561113	-3.235567	-0.360050
3	7	0	-5.668135	-2.077081	-1.059440
4	6	0	-6.852989	-1.544973	-1.489839
5	6	0	-8.032130	-2.238660	-1.179305
6	6	0	-7.957878	-3.430847	-0.452734
7	6	0	-6.676459	-0.299706	-2.238055
8	6	0	-4.172266	-3.606744	-0.021318
9	6	0	-5.320722	0.143098	-2.424266
10	6	0	-5.111125	1.319970	-3.155852
11	6	0	-6.188270	2.046727	-3.671419
12	6	0	-7.509348	1.616799	-3.468130
13	6	0	-7.751630	0.444571	-2.753918
14	6	0	-3.809664	-4.767709	0.666960
15	6	0	-2.460069	-5.016898	0.935260
16	6	0	-1.489226	-4.097268	0.523536
17	6	0	-1.902963	-2.950450	-0.158648
18	7	0	-3.203218	-2.722893	-0.433400
19	78	0	-3.998865	-1.059415	-1.528474
20	6	0	-2.306494	-0.176701	-1.964181
21	6	0	-1.145962	0.218923	-2.078602
22	6	0	0.241083	0.520248	-2.091024
23	6	0	0.723545	1.841950	-2.033017
24	6	0	2.102968	2.100543	-1.995381
25	6	0	3.022447	1.042336	-2.019050
26	6	0	2.556000	-0.280310	-2.061081
27	6	0	1.179885	-0.534413	-2.105455
28	6	0	3.497118	-1.387454	-1.993290
29	6	0	2.588973	3.465185	-1.869473
30	6	0	4.813659	-1.484656	-1.627959
31	6	0	5.141935	-2.876098	-1.720321
32	7	0	4.098526	-3.612371	-2.118796
33	8	0	3.021208	-2.652034	-2.300127
34	6	0	2.045759	4.619378	-1.371530
35	6	0	3.083400	5.603765	-1.444434
36	7	0	4.207161	5.104565	-1.969661
37	8	0	3.896054	3.714380	-2.251050
38	6	0	6.416222	-3.523364	-1.402487
39	6	0	3.047269	6.989932	-0.975224

40	6	0	7.376224	-2.869689	-0.605881
41	6	0	8.568817	-3.500870	-0.268160
42	6	0	8.826940	-4.799619	-0.729068
43	6	0	7.889188	-5.459194	-1.535266
44	6	0	6.691697	-4.823506	-1.857926
45	6	0	1.988290	7.450688	-0.181200
46	6	0	1.978193	8.752938	0.325808
47	6	0	3.045972	9.607614	0.032300
48	6	0	4.106139	9.168838	-0.773782
49	6	0	4.105420	7.873369	-1.270387
50	8	0	10.029226	-5.353991	-0.317291
51	8	0	3.160187	10.907866	0.522449
52	6	0	10.379332	-6.688495	-0.784534
53	6	0	2.062616	11.450456	1.302357
54	1	0	-6.670595	-4.867545	0.525905
55	1	0	-8.989679	-1.851689	-1.501650
56	1	0	-8.867987	-3.970044	-0.214408
57	1	0	-4.097679	1.674022	-3.295064
58	1	0	-6.001850	2.961782	-4.225078
59	1	0	-8.338374	2.190019	-3.870058
60	1	0	-8.774137	0.109721	-2.601768
61	1	0	-4.569916	-5.468326	0.988203
62	1	0	-2.167708	-5.920548	1.457694
63	1	0	-1.215979	-2.189568	-0.503615
64	1	0	0.012319	2.659659	-2.023748
65	1	0	4.081674	1.257925	-1.973781
66	1	0	0.826521	-1.556804	-2.132096
67	1	0	5.455988	-0.678912	-1.315328
68	1	0	1.050735	4.746553	-0.981891
69	1	0	7.185064	-1.865628	-0.241794
70	1	0	9.312344	-3.012887	0.350055
71	1	0	8.068857	-6.466491	-1.885959
72	1	0	5.951866	-5.334812	-2.461602
73	1	0	1.167737	6.786663	0.066932
74	1	0	1.151310	9.077445	0.944301
75	1	0	4.926461	9.846785	-0.972378
76	1	0	4.932664	7.518896	-1.871542
77	1	0	11.372306	-6.875154	-0.377456
78	1	0	10.418038	-6.719435	-1.879817
79	1	0	9.674601	-7.437054	-0.409333
80	1	0	2.356692	12.471967	1.538600
81	1	0	1.914607	10.882658	2.228537
82	1	0	1.132537	11.454992	0.723024
83	1	0	-0.434258	-4.263105	0.712162
84	6	0	-8.118790	-0.832682	1.958806
85	6	0	-6.724520	-0.785870	2.011694
86	7	0	-6.071991	0.245706	1.415649

87	6	0	-6.691626	1.263844	0.749752
88	6	0	-8.093720	1.234580	0.671315
89	6	0	-8.794890	0.190558	1.277669
90	6	0	-5.751774	2.235479	0.191064
91	6	0	-5.829429	-1.759877	2.665652
92	6	0	-4.356373	1.960493	0.397119
93	6	0	-3.421885	2.826380	-0.183196
94	6	0	-3.840700	3.939623	-0.920709
95	6	0	-5.205173	4.214150	-1.094870
96	6	0	-6.158956	3.360023	-0.543237
97	6	0	-6.266133	-2.900680	3.346630
98	6	0	-5.330869	-3.751052	3.940638
99	6	0	-3.967262	-3.450029	3.844566
100	6	0	-3.577931	-2.306624	3.150126
101	7	0	-4.483945	-1.487516	2.576308
102	78	0	-4.061207	0.293967	1.463273
103	6	0	-2.103898	0.295433	1.528979
104	6	0	-0.878228	0.175199	1.544590
105	6	0	0.519055	-0.064110	1.483834
106	6	0	1.451333	0.985204	1.369516
107	6	0	2.825643	0.717504	1.275070
108	6	0	3.285135	-0.606285	1.282612
109	6	0	2.368341	-1.664189	1.373900
110	6	0	1.001215	-1.389441	1.491965
111	6	0	2.840633	-3.036817	1.303648
112	6	0	3.774075	1.812738	1.138908
113	6	0	4.085019	-3.601655	1.295087
114	6	0	3.882259	-5.005752	1.112621
115	7	0	2.586726	-5.324314	1.041513
116	8	0	1.892731	-4.042671	1.164069
117	6	0	3.705465	3.156356	1.379936
118	6	0	4.990594	3.690884	1.034388
119	7	0	5.825873	2.740106	0.603217
120	8	0	5.040994	1.507282	0.661432
121	6	0	4.917098	-6.031920	0.973336
122	6	0	5.430389	5.084488	1.125578
123	6	0	6.196392	-5.838026	1.527304
124	6	0	7.190944	-6.794749	1.370571
125	6	0	6.920219	-7.963911	0.648279
126	6	0	5.652284	-8.180749	0.096010
127	6	0	4.659230	-7.213272	0.261768
128	6	0	4.738326	6.006611	1.923310
129	6	0	5.158403	7.335358	2.025468
130	6	0	6.287582	7.752469	1.312945
131	6	0	6.986839	6.843002	0.503394
132	6	0	6.561923	5.525905	0.409642
133	8	0	7.994807	-8.840796	0.498776

134	8	0	6.784705	9.047270	1.321661
135	6	0	7.769728	-10.098154	-0.192009
136	6	0	6.140938	10.038718	2.169228
137	1	0	-8.668660	-1.641849	2.420420
138	1	0	-8.620257	2.011398	0.133699
139	1	0	-9.877218	0.167390	1.219451
140	1	0	-2.367671	2.606126	-0.071237
141	1	0	-3.101104	4.596960	-1.369124
142	1	0	-5.519430	5.078622	-1.669909
143	1	0	-7.213565	3.556497	-0.708220
144	1	0	-7.324310	-3.119158	3.412079
145	1	0	-5.662462	-4.634280	4.474509
146	1	0	-2.543644	-2.013992	3.022100
147	1	0	1.088115	2.003932	1.317118
148	1	0	4.343652	-0.799388	1.179353
149	1	0	0.295465	-2.203149	1.578756
150	1	0	5.033655	-3.097958	1.345866
151	1	0	2.856034	3.707423	1.742494
152	1	0	6.416019	-4.928988	2.074459
153	1	0	8.185294	-6.644352	1.771820
154	1	0	5.432808	-9.076026	-0.471310
155	1	0	3.680877	-7.356302	-0.180975
156	1	0	3.864140	5.689815	2.481466
157	1	0	4.592536	8.029030	2.632777
158	1	0	7.847538	7.200036	-0.048689
159	1	0	7.081574	4.826209	-0.232362
160	1	0	8.725111	-10.619497	-0.156275
161	1	0	7.475607	-9.930801	-1.234624
162	1	0	7.001649	-10.692750	0.314709
163	1	0	6.756991	10.932030	2.073844
164	1	0	6.127233	9.709073	3.214801
165	1	0	5.125562	10.255496	1.825282
166	1	0	-3.217549	-4.090295	4.291918

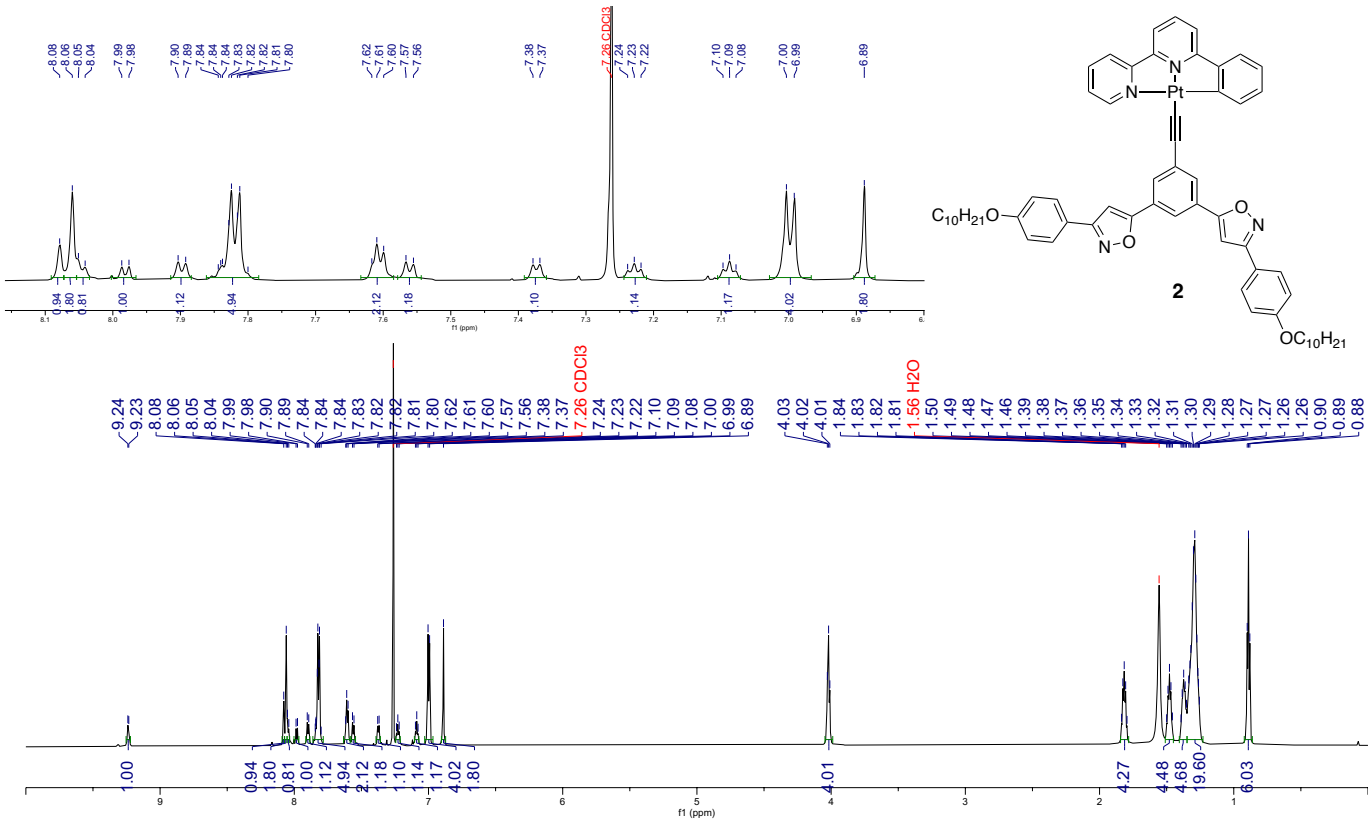


Figure S8. ^{1}H NMR spectra of complex **2** ($CDCl_3$).

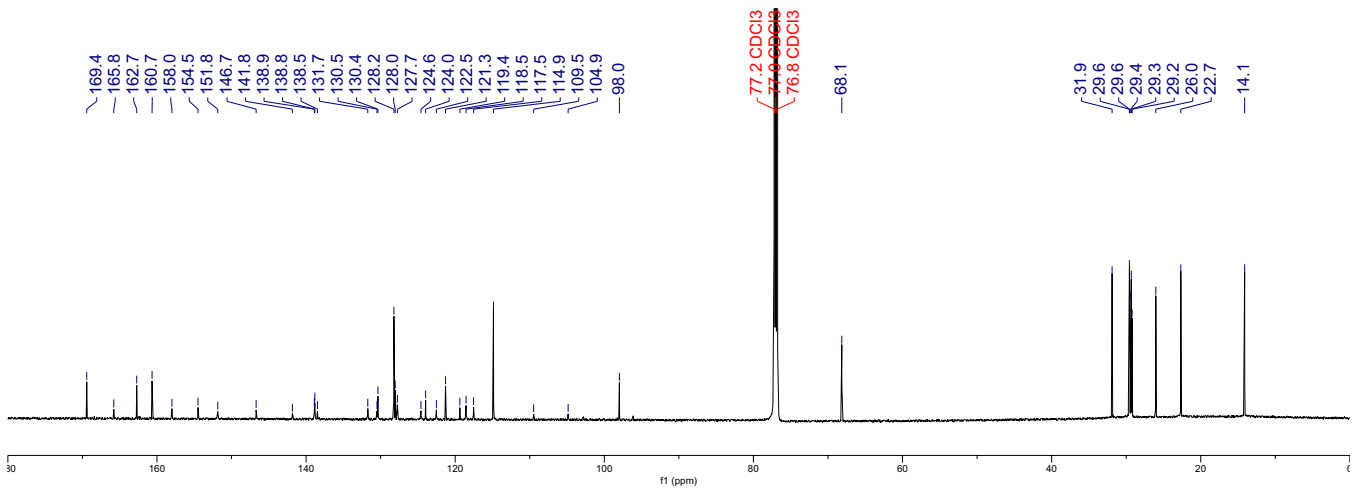


Figure S9. ^{13}C NMR spectra of complex **2** ($CDCl_3$).