Electronic Supplementary Information for:

Red-light excitable fluorescent Platinum(II) bis(aryleneethynylene) bis(trialkylphosphine) complexes showing long-lived triplet excited state as triplet photosensitizers for triplet-triplet annihilation upconversion

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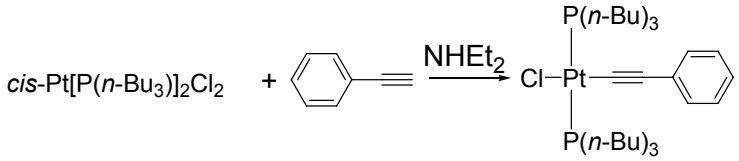
1.0 General.

All the chemicals used in synthesis are analytical pure and were used as received. Solvents were dried and distilled before used for synthesis. All samples in flash photolysis and upconversion experiments were deaerated with argon for ca. 15 min before measurement and the gas flow is kept during the measurement.

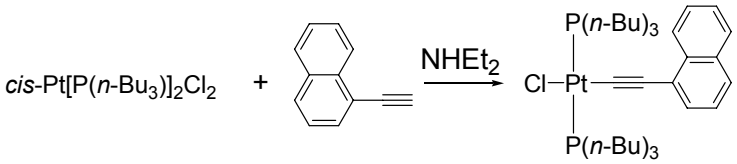
Diode pumped solid state (DPSS) laser 589 nm and 635 nm were used for the upconversions and the diameter of the 589 nm laser spot is ca. 3 mm, for 635 nm laser, it is ca. 6 mm. In order to repress the scattered laser, a black box was put behind the fluorescent cuvette to trap the laser beam after it passing through the cuvette. The luminescent photographs were obtained using Samsung NV 5 digital camera. The exposure time is the default value of the camera.

2.0 Synthesis and molecular structure characterization data



1

Synthesis of compound 1: Under Ar atmosphere, phenylacetylene (13.8 mg, 0.135 mmol) was added to the solution of *cis*-Pt[P(*n*-Bu)$_3$]$_2$Cl$_2$ (100 mg, 0.149 mmol) in diethylamine (NHEt$_2$) (6 ml), the flask was vacuumed and back-filled with Argon for several times. Then the mixture was heated to 45 °C and was allowed to stirred for 6 h. After completely consuming of the starting material, the solvents were evaporated under reduced pressure, and the crude product was further purified using column chromatography (silica gel, CH_2Cl_2:hexane = 2:3, v/v) to give **1** as light yellow solid (75.2 mg, 0.1 mmol), yield: 75.7 %. ^{1}H NMR (400 MHz, $CDCl_3$): 7.25–7.18 (m, 4H), 7.14–7.11 (m, 1H), 2.03–1.99 (m, 12H), 1.57–1.54 (m, 12H), 1.49–1.40 (m, 12H), 0.92 (t, 18H, *J* = 7.3 Hz).

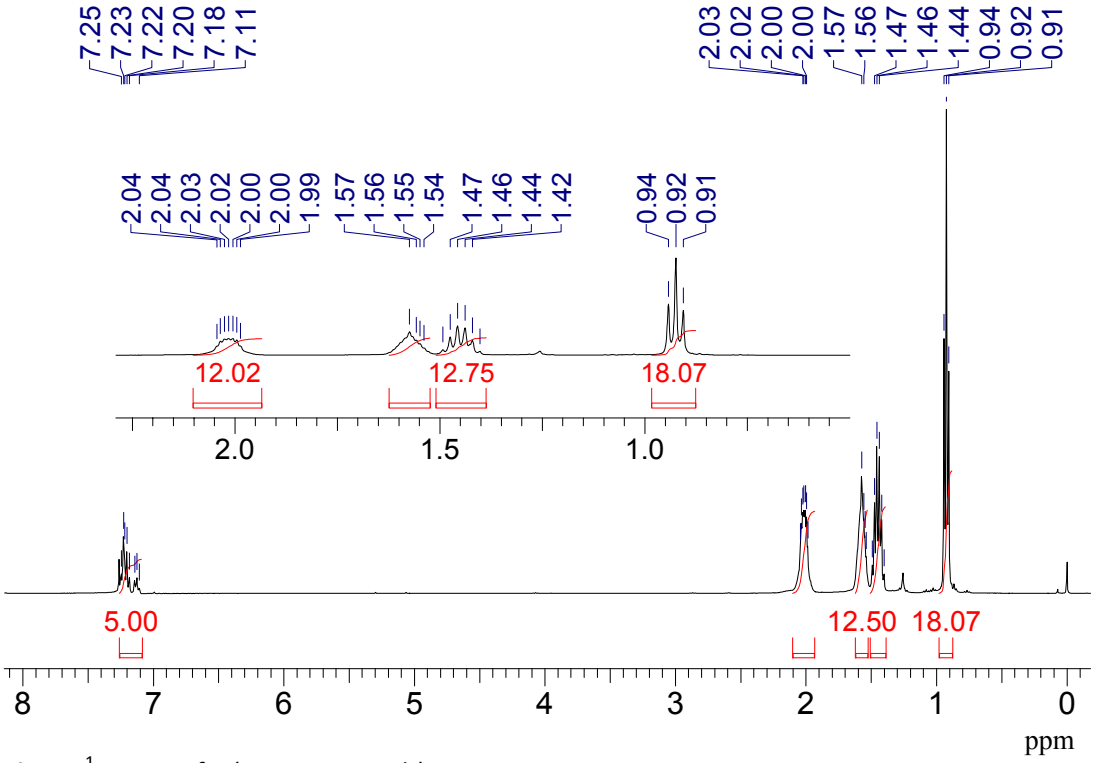


2

Synthesis of compound 2:

Compound 2 was prepared by a similar procedure as that used for compounds **1** except that 1-ethynylnaphthalene (12.3 mg, 0.081 mmol) was used instead of phenylacetylene**.** Compound 2 was obtained as light yellow solid (35.5 mg, 0.045 mmol), yield: 55.6%. ^{1}H NMR (400 MHz, $CDCl_3$): 8.47–8.45 (m, 1H), 7.80–7.78 (m, 1H), 7.64 (d, 1H, *J* = 8.2 Hz), 7.45–7.41 (m, 3H), 7.34 (t, 1H, *J* = 7.8 Hz), 2.04–2.00 (m, 12H), 1.62–1.59 (m, 12H) 1.47–1.38 (m, 12H), 0.91 (t, 18H, *J* = 7.2 Hz).

3.0 NMR and HRMS spectra



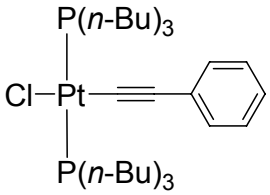
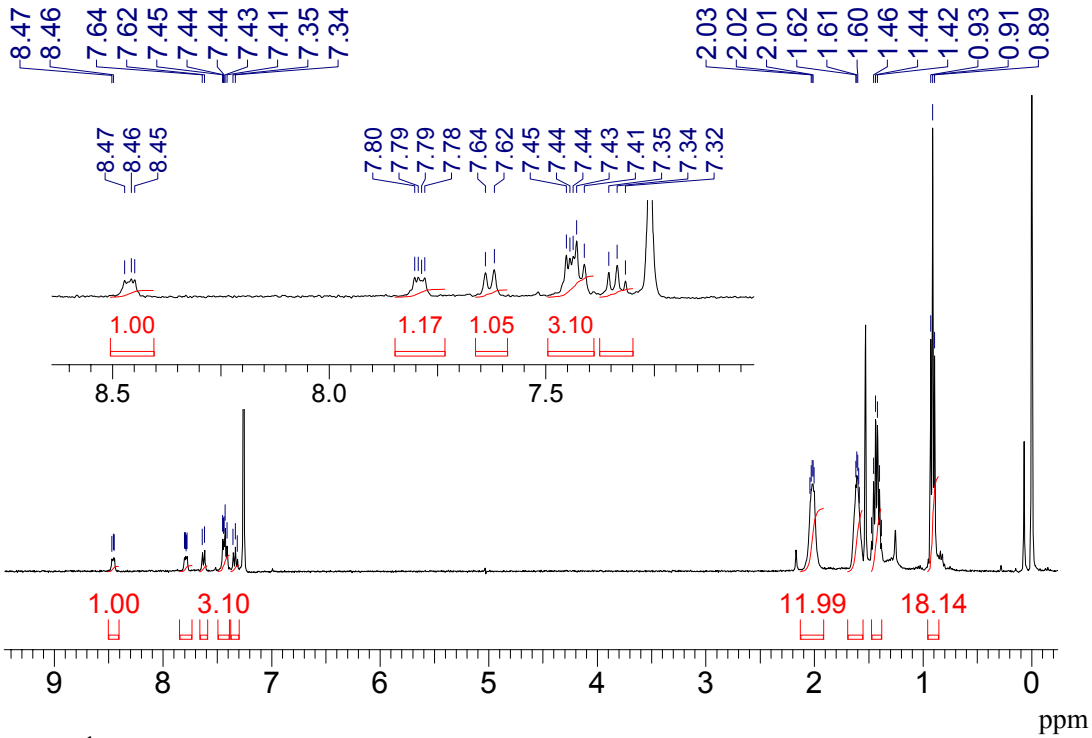


Fig. S1 ^{1}H NMR of **1** (400 MHz, $CDCl_3$).



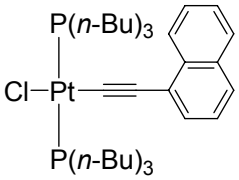


Fig. S2 ^{1}H NMR of **2** (400 MHz, $CDCl_3$).

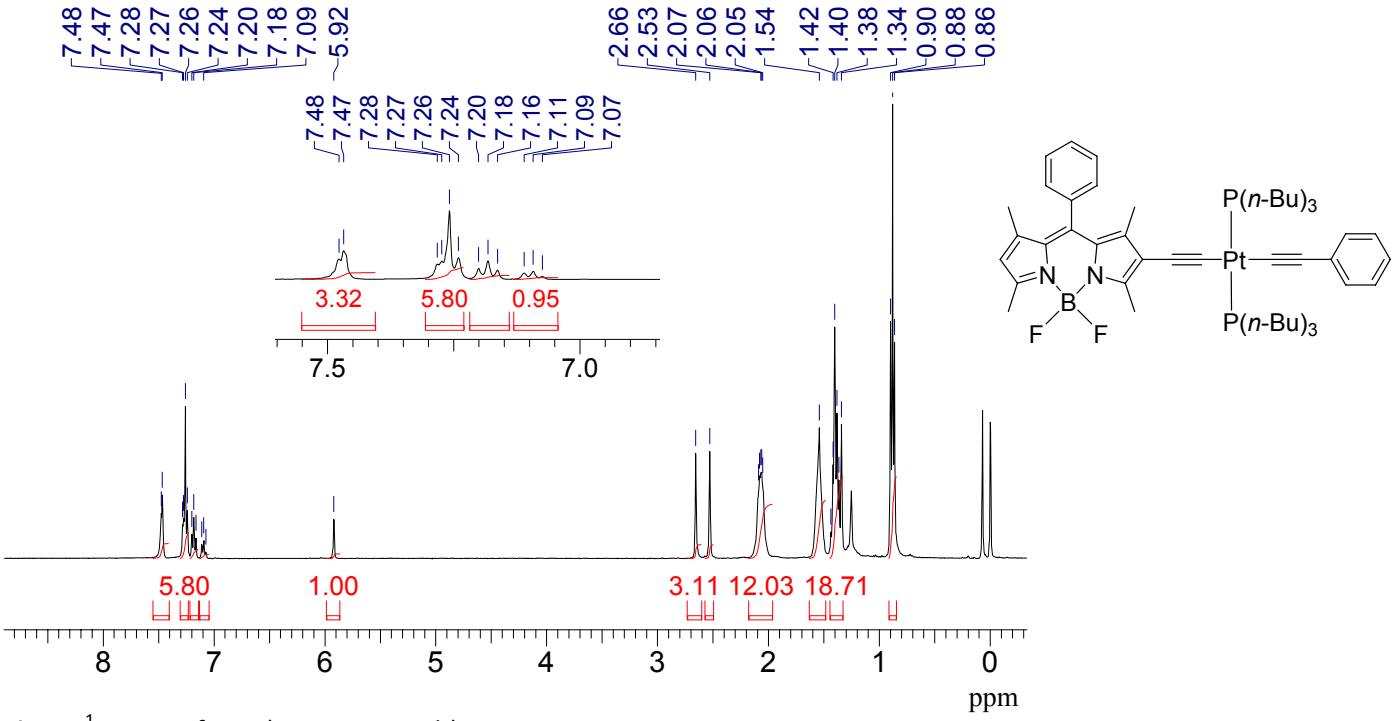


Fig. S3 ^{1}H NMR of **Pt-1** (400 MHz, $CDCl_3$).

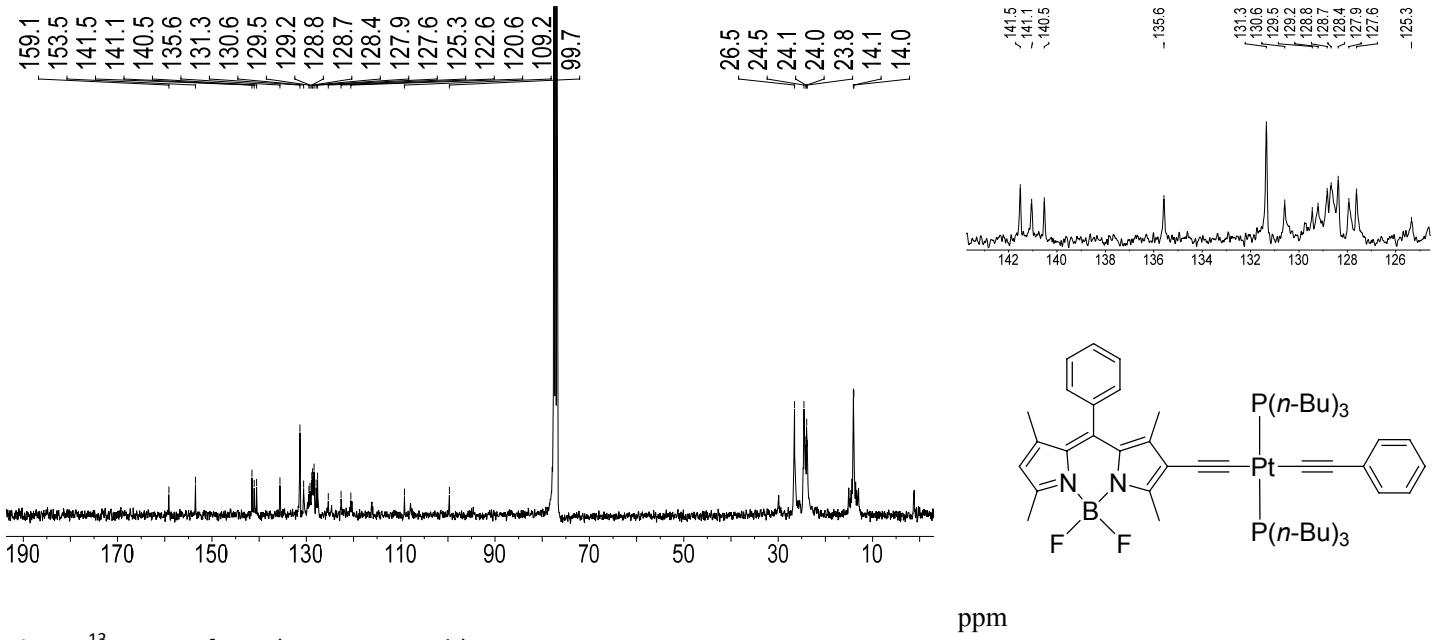


Fig. S4 ^{13}C NMR of **Pt-1** (100 MHz, $CDCl_3$).

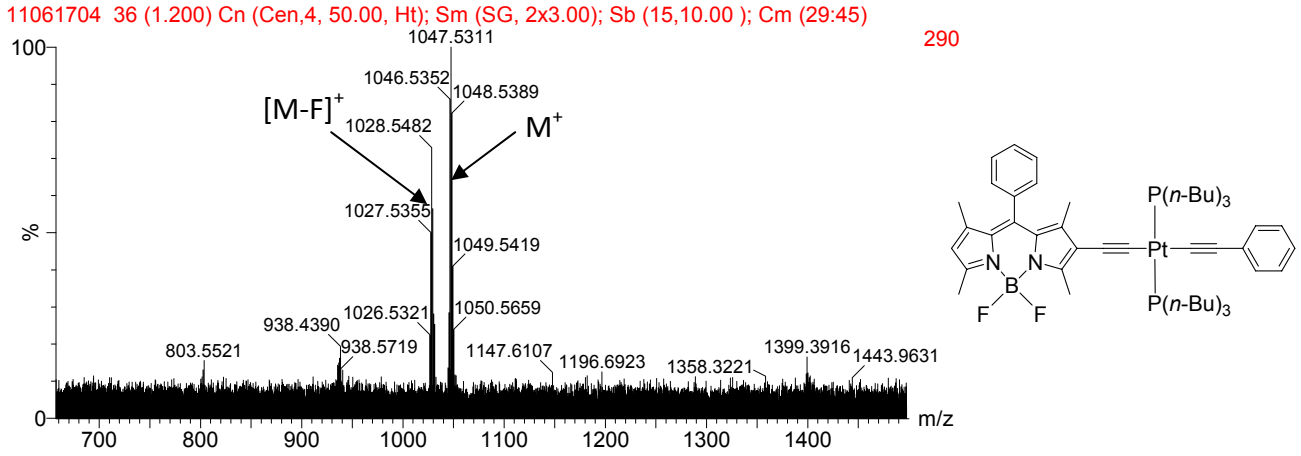


Fig. S5 MALDI-HRMS of **Pt-1.**

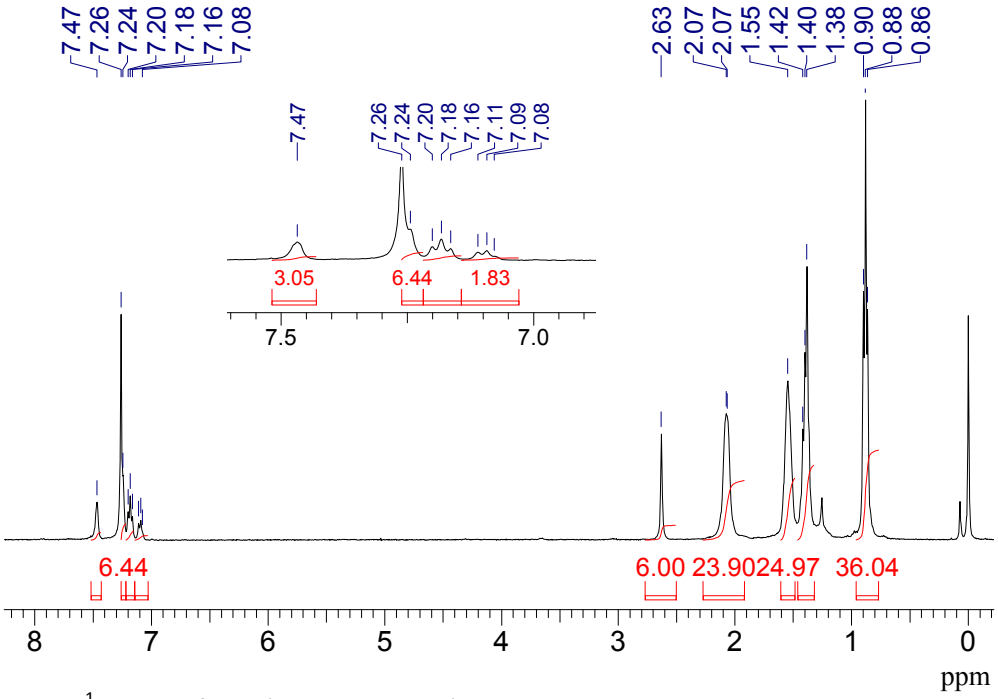
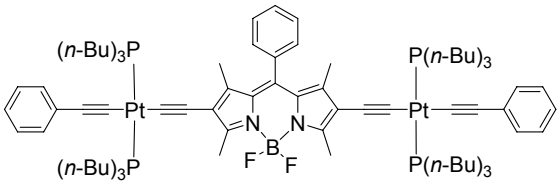
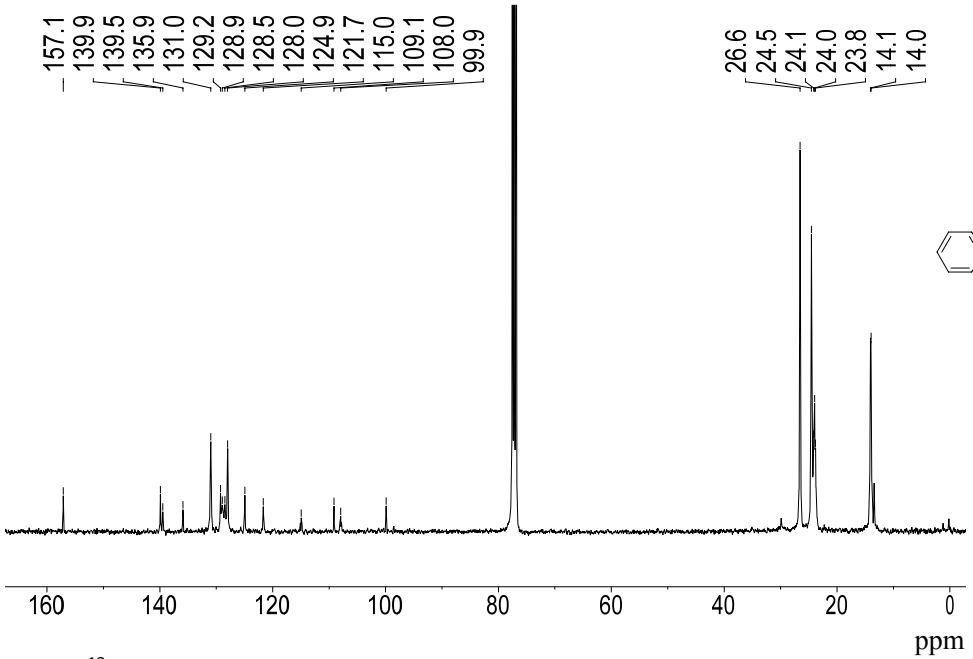


Fig. S6 ^{1}H NMR of **Pt-2** (400 MHz, $CDCl_3$).





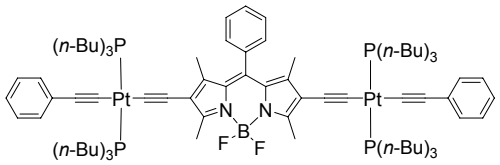


Fig. S7 ^{13}C NMR of **Pt-2** (100 MHz, $CDCl_3$).

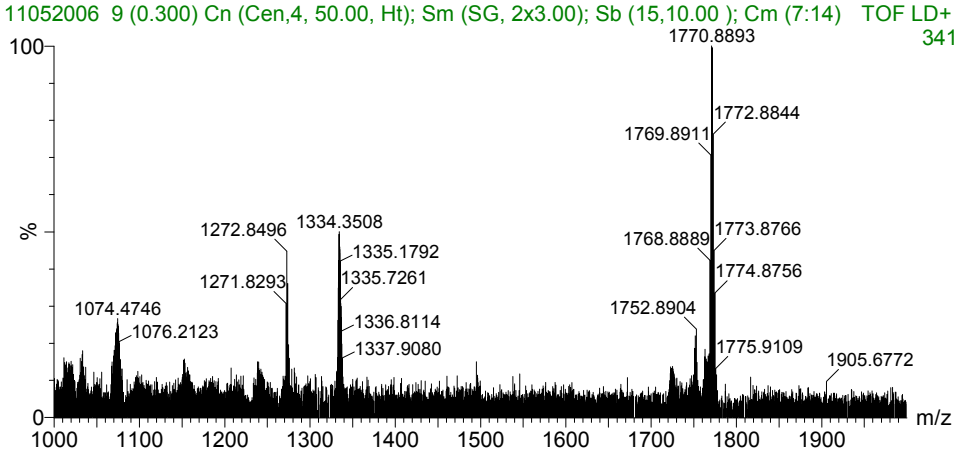
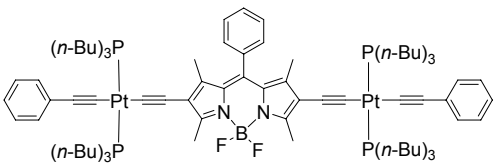


Fig. S8 MALDI-HRMS of **Pt-2.**



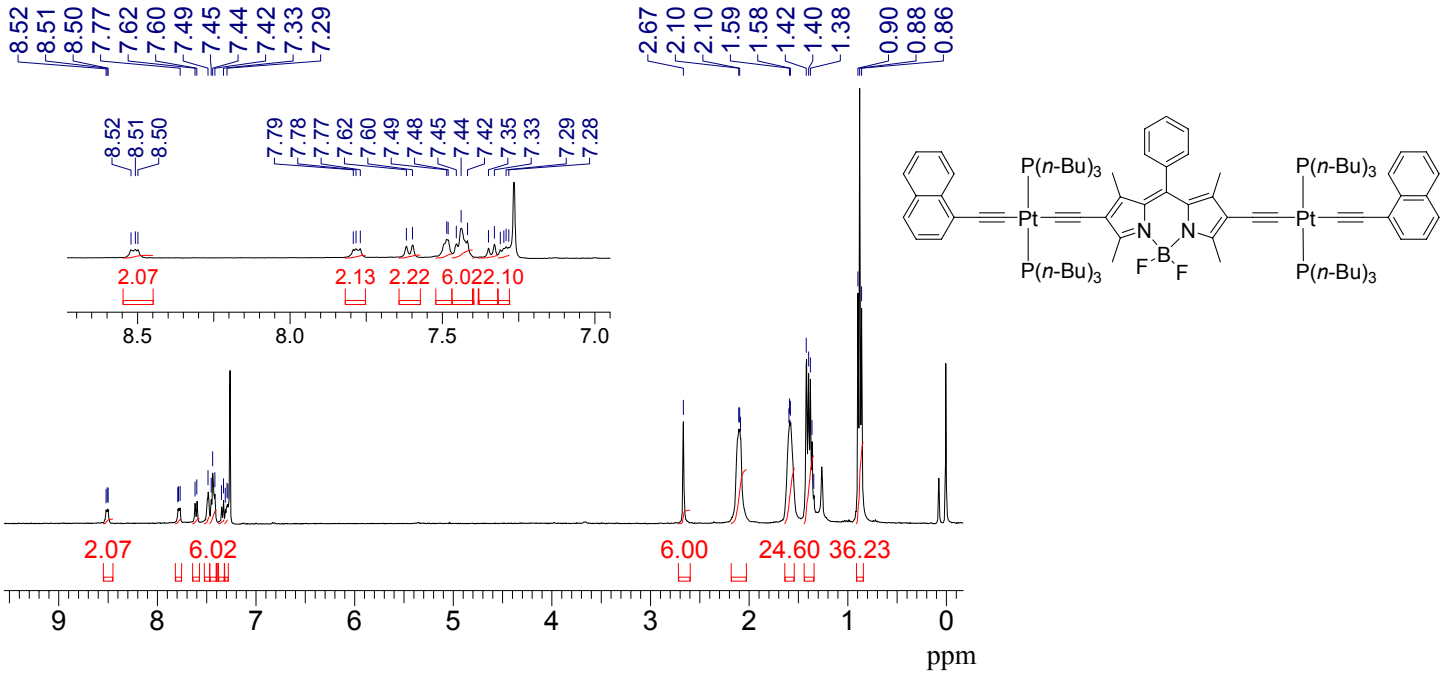


Fig. S9 ^{1}H NMR of **Pt-3** (400 MHz, $CDCl_3$).

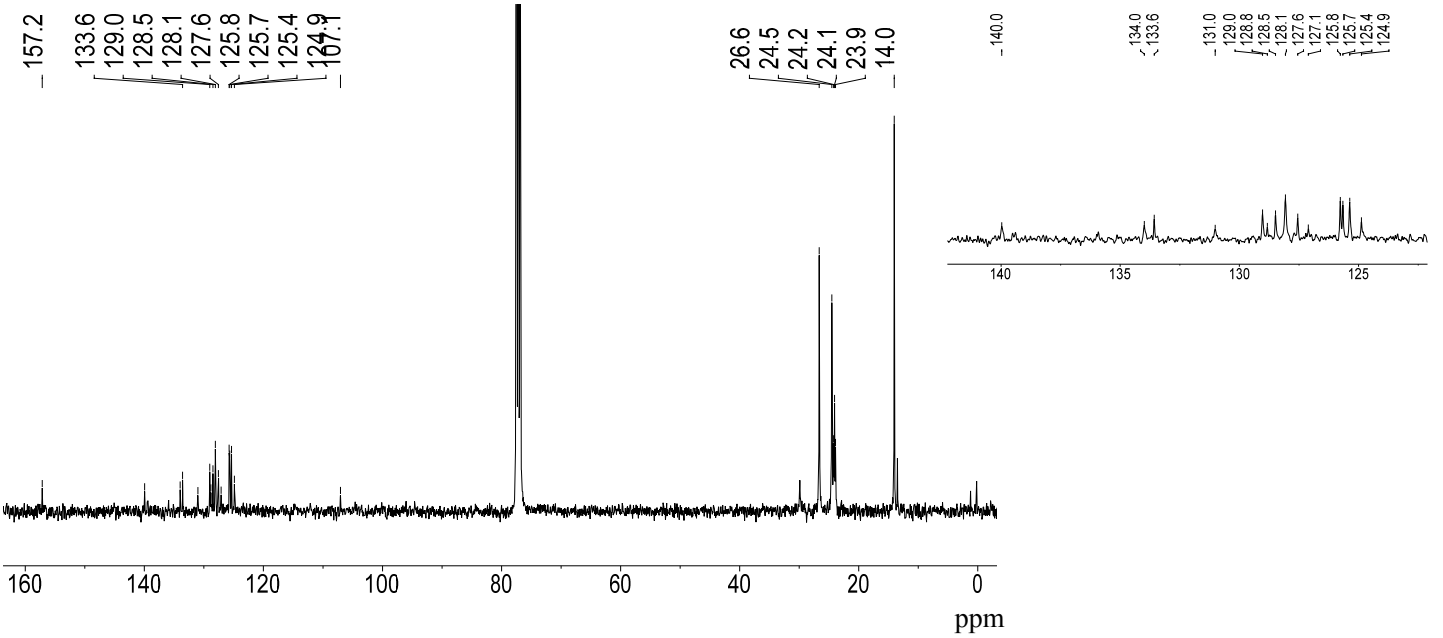


Fig. S10 ^{13}C NMR of **Pt-3** (100 MHz, $CDCl_3$).

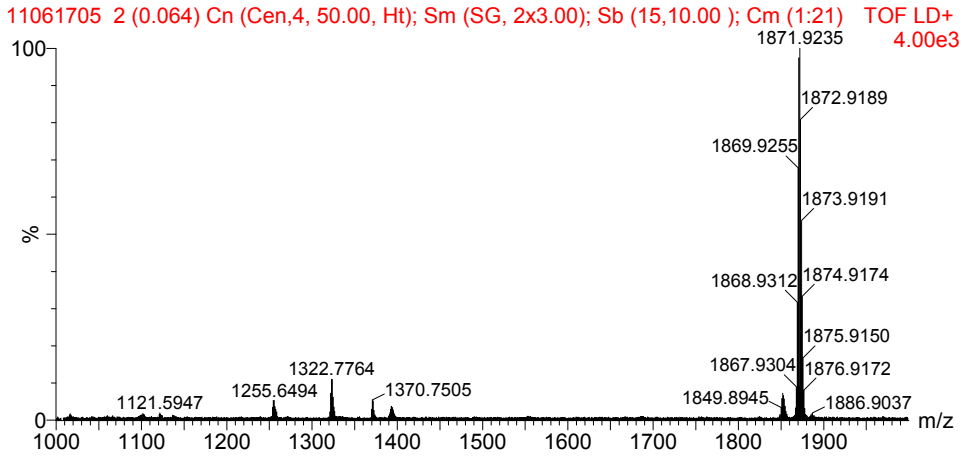
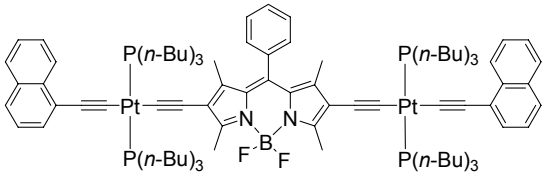


Fig. S11 MALDI-HRMS of **Pt-3.**



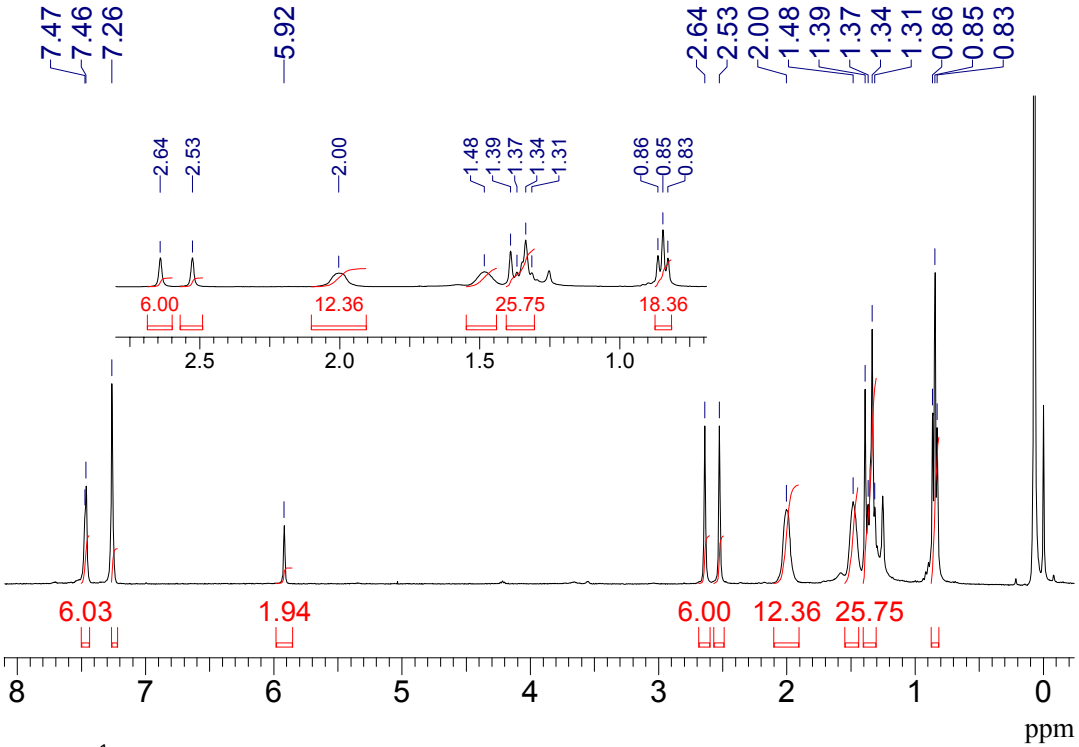
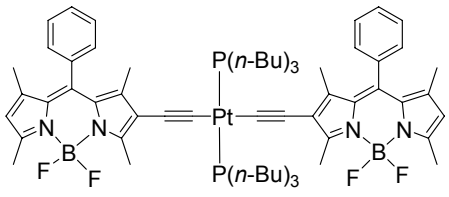


Fig. S12 ^{1}H NMR of **Pt-4** (400 MHz, $CDCl_3$).



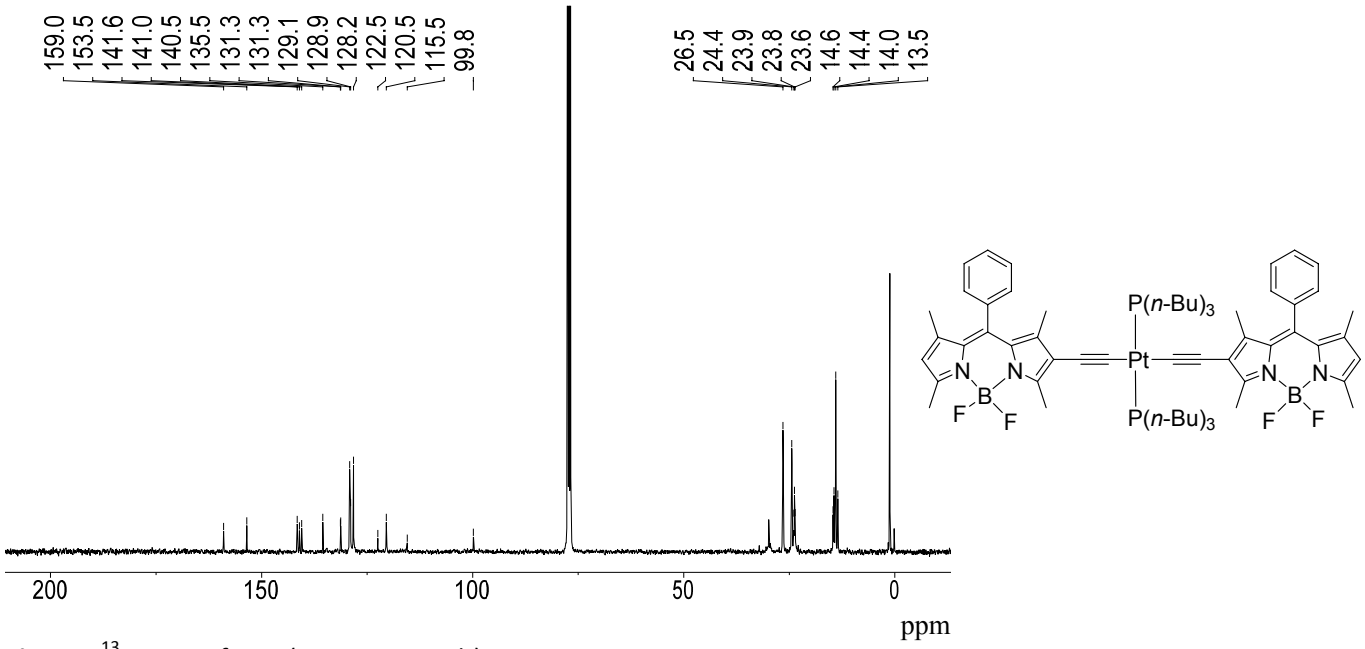


Fig. S13 ^{13}C NMR of **Pt-4** (100 MHz, $CDCl_3$).

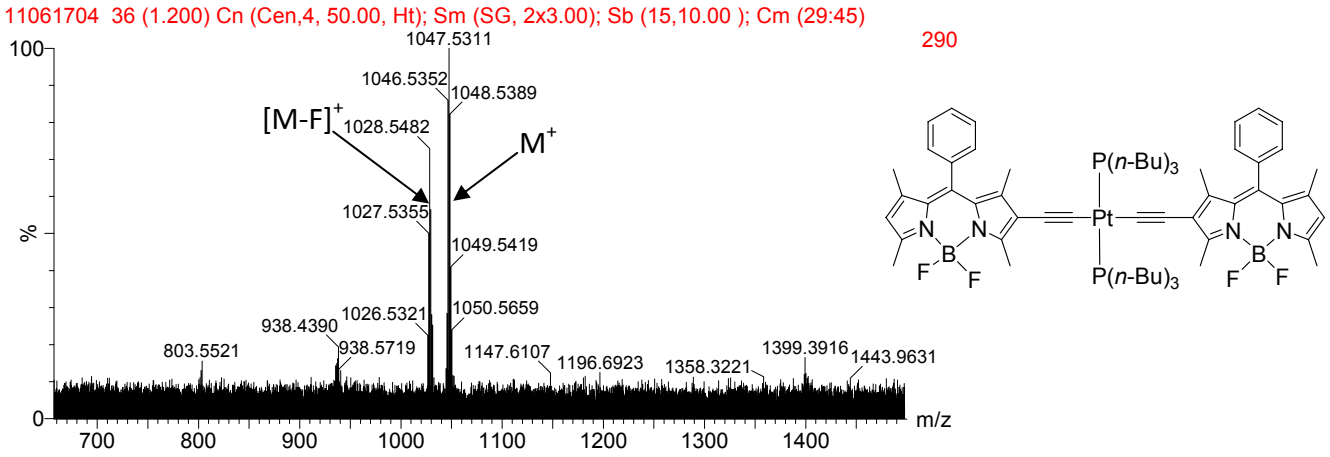


Fig. S14 MALDI-HRMS of **Pt-4.**

4.0 UV-vis and emission spectra

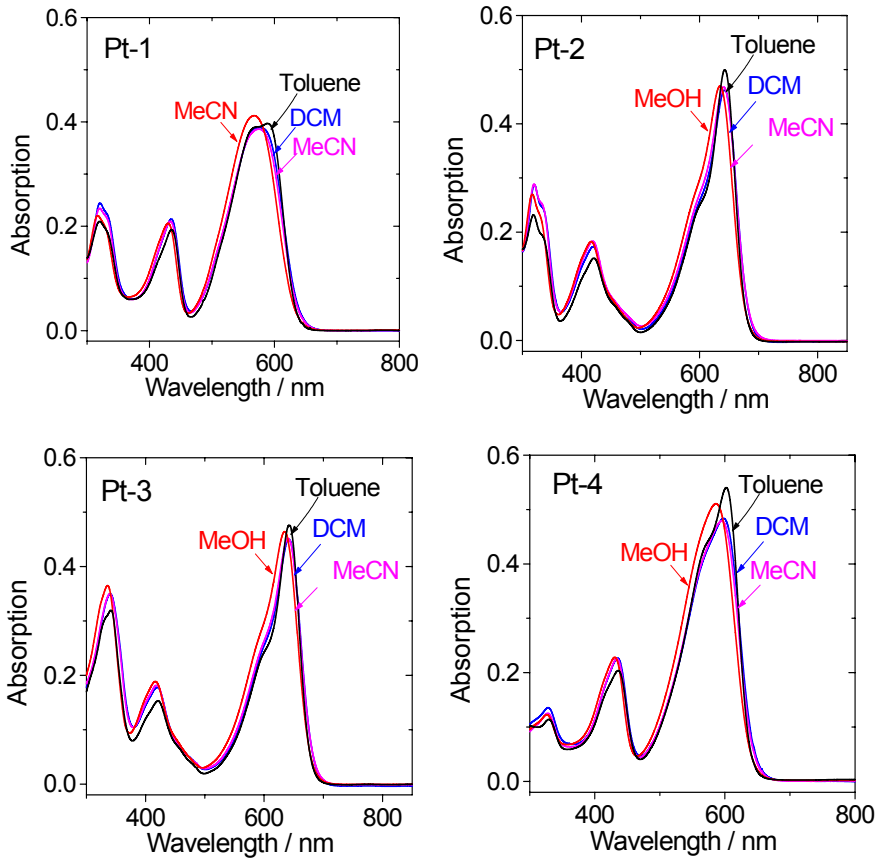


Fig. S15 Absorption spectra of the complex **Pt-1**-**Pt-4** in different solvents (1.0×10^{-5} M; 20 °C).

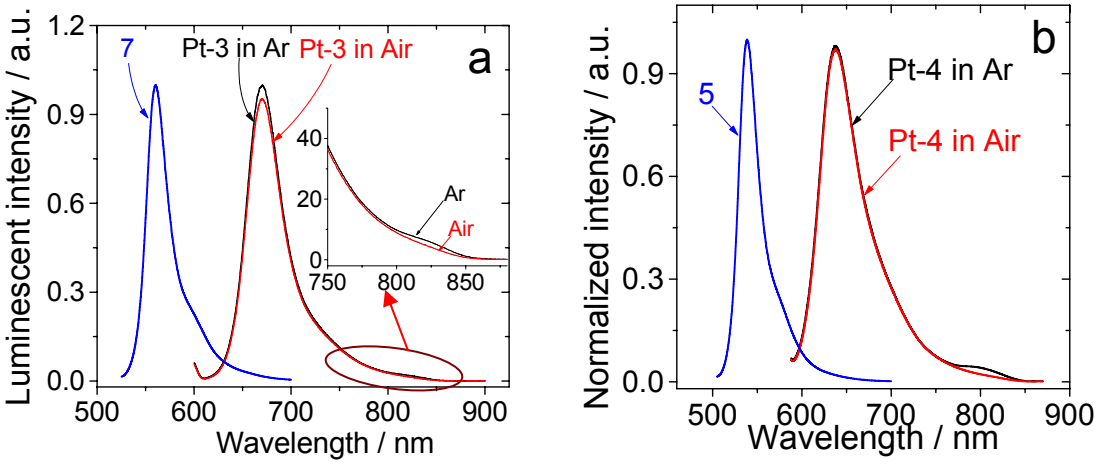


Fig. S16 Emission spectra of the complexes at different atmosphere of N_2 and air and the fluorescence of the ligands. (a) **Pt-3** and **7**: λex = 560 nm (**Pt-1**), λex = 520 nm (**7**) . (b) **Pt-4** and **5**: λex = 580 nm (**Pt-4**), λex = 500nm (**5**). In toluene (1.0×10^{-5} M; 20 °C).

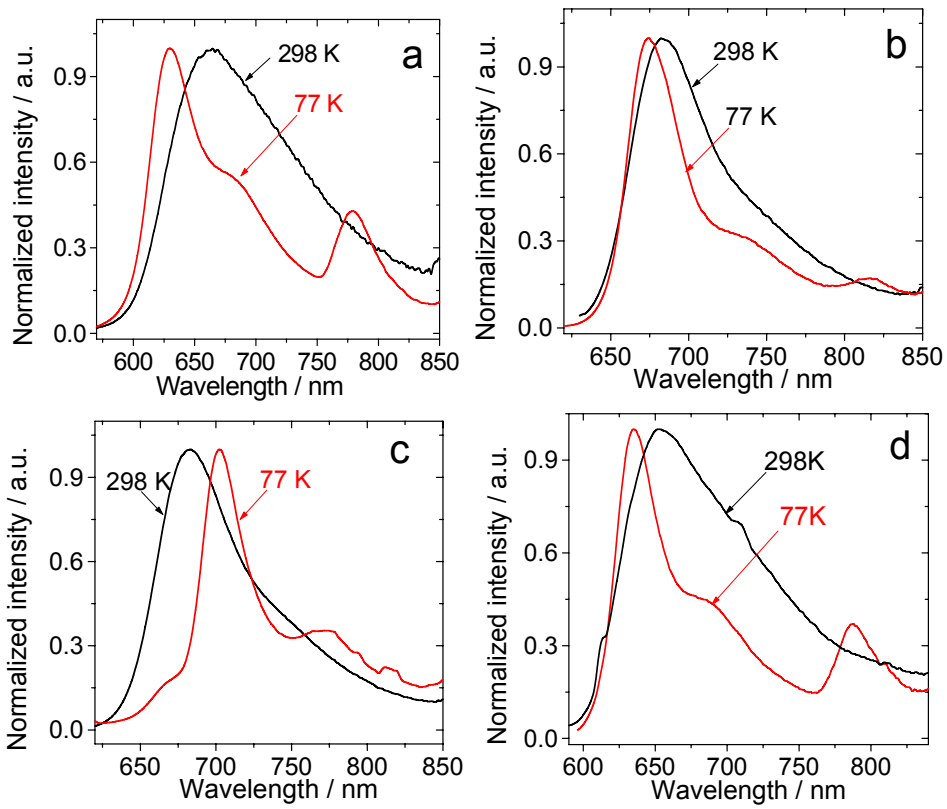


Fig. S17 Emission spectra of **Pt-1, Pt-2, Pt-3** and **Pt-4** in ethanol-methanol (4:1, V/V) glass at 77 K and solution at 298 K. (a) **Pt-1**, λex = 550 nm, (b) **Pt-2**, λex = 610 nm, (c) **Pt-3**, λex = 610 nm, (d) **Pt-4**, λex = 580 nm.

5.0 Transient difference absorption details

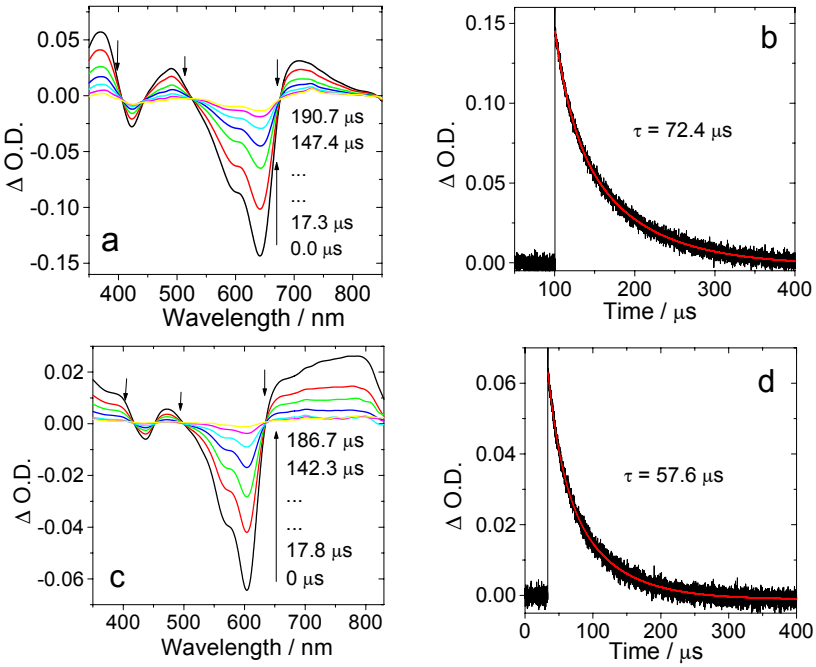


Fig. S18 (a，b): Transient absorption difference spectra of **Pt-3** and **Pt-4** after pulsed excitation (λ_{ex} = 532 nm). Decay traces of (c) **Pt-3** at 640 nm and **(d) Pt-4** at 600 nm. c = 1.0 × 10^{-5} M in deaerated toluene. 20 °C.

6.0 Upconversion details

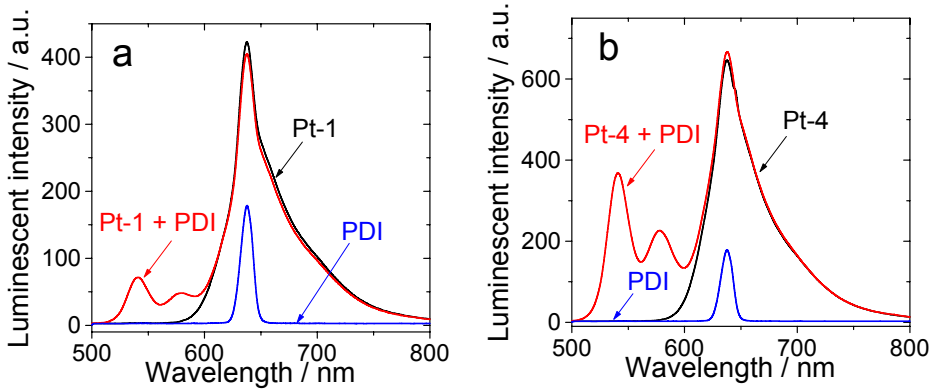


Fig. S19 Upconversions with sensitizers **Pt-1** (a) and **Pt-4** (b) using PDI as the acceptor. Excited with 635 nm laser (10 mW, power density is 70 mW cm^{-2}). C $_{[Sensitizers]}$ = 1×10^{-5} M. c [Perylene] = 1.1×10^{-4} M. In deaerated toluene. 20 °C.

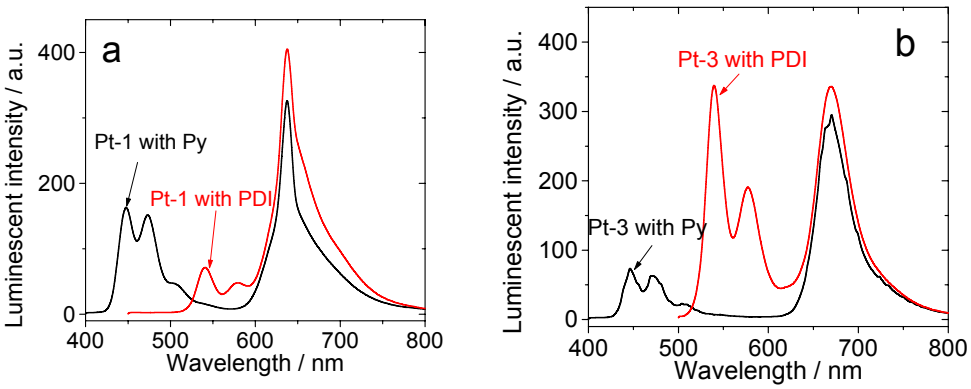


Fig. S20 Upconversions with sensitizers **Pt-1** (a) and **Pt-3** (b) using Perylene (Py) and PDI as the acceptor. Excited with 635 nm laser (10 mW, power density is 70 mW cm^{-2}). C [Sensitizers] = 1.0×10^{-5} M. *c* [Perylene] = 1.1×10^{-4} M. In deaerated toluene. 20 °C.

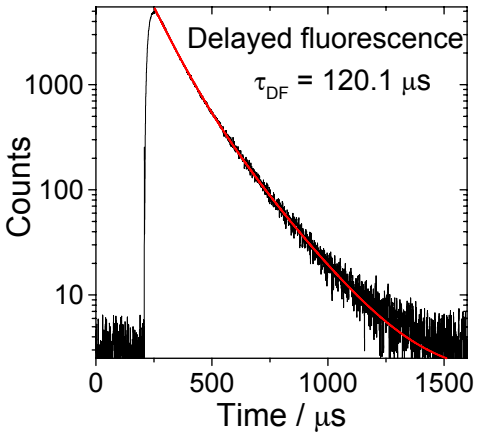


Fig. S21 Delayed fluorescence observed in the TTA upconversion with complex **Pt-3** as triplet photosensitizer and perylene as the triplet acceptor.

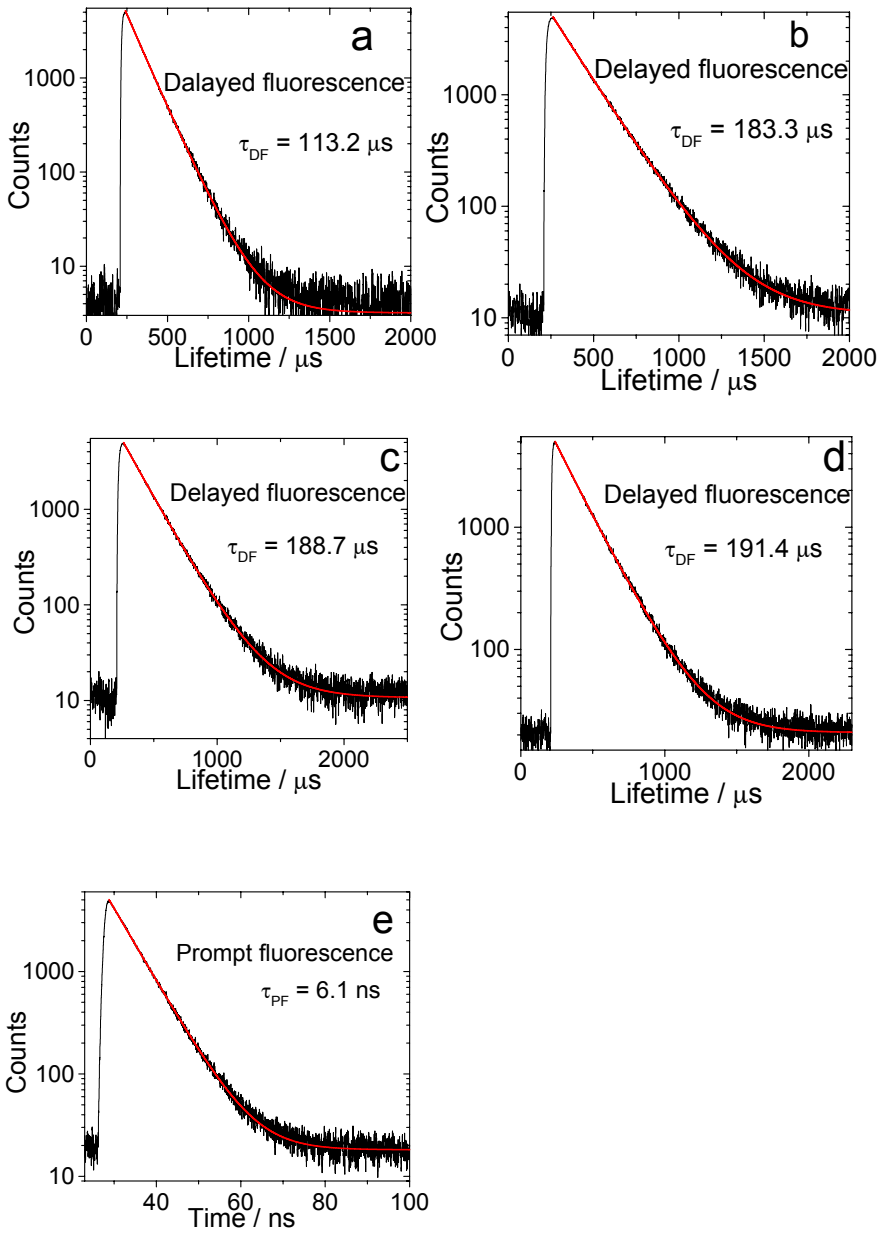


Fig. S22 (a) Delayed fluorescence observed in the TTA upconversion with complex **Pt-1** as triplet photosensitizer and PDI as the triplet acceptor. (b) **Pt-2**; (c) **Pt-3;** (d) **Pt-4**. Excited at 635 nm (nanosecond pulsed OPO laser synchronized with spectrofluorometer) and monitored at 560 nm. Under this circumstance the complexes are selectively excited and the emission is due to the upconverted emission of PDI. (e) The prompt fluorescence decay of PDI determined in a different experiment (excited with picosecond 405 nm laser, the decay of the emission was monitored at 480 nm). In deaerated toluene. c[Sensitizers] = 1.0×10^{-5}M; c [perylene] = 4.1×10^{-5} M; 20 °C.

7.0 The coordinates of the triplet optimized geometries of complexes

Complex Pt-1 (DFT//B3LYP/6-31G(d) / LanL2DZ)

Symbolic Z-matrix:

Charge = 0 Multiplicity = 3

C	-0.41196667	-0.30983162	-0.03563610
C	0.82172832	-0.24419283	-0.02915193
C	9.51199693	1.55644984	0.35495904
C	8.12230482	1.45307762	0.35107385
C	7.48914593	0.23030601	0.04008269
C	8.30370466	-0.88162949	-0.26484277
C	9.69288919	-0.77162599	-0.25874397
C	10.30516901	0.44636716	0.05053741
H	9.97810657	2.50818796	0.59701903
H	7.50897801	2.31767842	0.58818493
H	7.83142683	-1.82991378	-0.50493712
H	10.30048188	-1.64110479	-0.49645724
H	11.38852465	0.52946709	0.05447766
C	6.06405043	0.12160477	0.03467600
C	4.83969280	0.02868090	0.03516076
Pt	2.82728977	-0.11500522	0.00562139
P	2.72683423	-0.43193573	2.34013355
C	1.69587228	0.83440039	3.18795742
H	1.61934055	0.62250397	4.25980626
H	0.69874182	0.83742091	2.74009762
H	2.14432004	1.82233416	3.04655024
C	1.95958654	-2.03500825	2.81567197
H	2.57354609	-2.85946906	2.44112419
H	0.96808296	-2.10302941	2.36051460
H	1.87120502	-2.11643794	3.90434171
C	4.31947532	-0.40210985	3.25617707
H	4.98090662	-1.17907498	2.86498584
H	4.80771059	0.56380294	3.10443093
H	4.14919100	-0.56499019	4.32566314
P	2.97084500	0.20302903	-2.32554011
C	4.02542568	-1.05592682	-3.15315642
H	4.12621902	-0.83933022	-4.22204057
H	3.57806365	-2.04629118	-3.02611861
H	5.00990024	-1.05332341	-2.67871833
C	1.39524103	0.16365988	-3.27246405
H	0.72024270	0.93507135	-2.89305373
H	0.91213027	-0.80736542	-3.13514655
H	1.58265453	0.33113873	-4.33836425
C	3.73534510	1.81230322	-2.78149351
H	3.10451038	2.63136229	-2.42343831
H	4.71283713	1.88522739	-2.29808067
H	3.85154458	1.89399732	-3.86753610

C	-7.59274942	-2.13694304	-0.15193004
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C	-6.46818659	-0.19258411	-0.02880598
C	-5.33875724	0.65995918	0.02439568
C	-4.03218388	0.08226960	-0.01392961
C	-2.74044250	0.67781712	0.02343875
C	-2.56137383	-1.61243402	-0.12469991
N	-6.33873269	-1.57055510	-0.12187542
N	-3.87918360	-1.31290966	-0.10518789
B	-5.01934458	-2.36089207	-0.17860889
F	-4.92503405	-3.24834136	0.90469647
F	-4.92647422	-3.08799500	-1.37560571
C	-8.56465413	1.44862893	0.09796508
H	-8.28149435	1.99311916	1.00618753
H	-8.31662500	2.10302174	-0.74587948
H	-9.65113922	1.31281213	0.11098099
C	-2.03350303	-2.99925058	-0.21896272
H	-0.94116051	-2.98631382	-0.22643077
H	-2.38789080	-3.60479531	0.62353923
H	-2.40046401	-3.48939497	-1.12835862
C	-2.35673933	2.12517930	0.11562336
H	-2.71422509	2.59517317	1.03901956
H	-1.26528821	2.20869959	0.09517210
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H	-7.33336292	-4.12572216	0.59916032
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H	-7.33216254	-4.01194167	-1.15343332
C	-5.50121629	2.14309147	0.11564589
C	-5.60863578	2.92683269	-1.04441389
C	-5.54752089	2.78741048	1.36228699
C	-5.75819609	4.31326053	-0.96248636
C	-5.69659388	4.17362767	1.44802070
H	-5.46655137	2.19272846	2.26849375
H	-5.83965028	4.90253158	-1.87219929
H	-5.73110020	4.65398947	2.42246597
C	-5.80226386	4.94053637	0.28504263
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H	-5.57325478	2.44090878	-2.01604144
C	-1.81274081	-0.38288102	-0.04367576
C	-8.54868621	-1.11029171	-0.07707768
H	-9.62128272	-1.26002477	-0.07953963

Complex Pt-2 (DFT//B3LYP/6-31G(d) / LanL2DZ)

Symbolic Z-matrix:

Charge = 0 Multiplicity = 3

C	-4.79403041	-0.04082734	-0.01509620

C	-6.02502017	-0.11063186	-0.05132200
C	-10.04923873	-0.32877709	-0.19187269
Pt	-8.03501677	-0.21761971	-0.12419842
P	-7.91689625	0.78982033	-2.25050362
C	-7.09083416	2.43378527	-2.22616567
H	-6.99457523	2.83910856	-3.23916343
H	-6.10033040	2.32402918	-1.77707812
H	-7.67660613	3.12682308	-1.61487999
C	-6.92785524	-0.19715620	-3.44735833
H	-7.40683955	-1.16865681	-3.60164153
H	-5.93182872	-0.36219483	-3.02863004
H	-6.84395366	0.32123568	-4.40856742
C	-9.50631314	1.09458674	-3.12110222
H	-10.03774357	0.14820570	-3.24872047
H	-10.13318487	1.75368031	-2.51522797
H	-9.32782007	1.55244595	-4.09980712
P	-8.17639906	-1.22788303	1.99900187
C	-9.00604310	-2.86927676	1.96125719
H	-9.11691325	-3.27579759	2.97227317
H	-8.41418052	-3.56299696	1.35668927
H	-9.98937175	-2.75296623	1.49856263
C	-6.59574926	-1.53832803	2.88443390
H	-6.06227086	-0.59377994	3.01807605
H	-5.96558245	-2.20023146	2.28485539
H	-6.78354824	-1.99589083	3.86154466
C	-9.17472713	-0.23994180	3.18675537
H	-8.69231164	0.72830273	3.35056450
H	-10.16329924	-0.06904643	2.75310947
H	-9.27376207	-0.76142532	4.14485636
C	2.52571412	-0.95653242	-0.47925656
C	2.57695868	1.08335110	0.57388559
C	3.39150811	0.05974123	0.04515394
C	1.22709310	0.67776117	0.35792216
C	-0.00598115	1.31214234	0.67822627
C	-1.23130119	0.66440116	0.35519006
C	-2.58602925	1.06842949	0.54309145
C	-2.51113702	-0.99104325	-0.46956888
N	1.24169578	-0.57388021	-0.28352661
N	-1.23140142	-0.59669010	-0.26745704
B	0.00992907	-1.41096704	-0.69082298
F	0.00255923	-1.62537874	-2.07813189
F	0.02657135	-2.65422485	-0.03700566
C	3.10755345	2.32243155	1.23235235
H	2.85498989	3.23474468	0.67881118
H	2.71827477	2.45508843	2.24778318
H	4.19880924	2.25659363	1.29384272
C	-2.87959240	-2.28099848	-1.11356031
H	-3.96606821	-2.39610274	-1.12584981
H	-2.49840817	-2.32568358	-2.14114317
H	-2.42721330	-3.12351135	-0.57788926
C	-3.13212387	2.32705996	1.14974952
H	-2.76001847	3.22806608	0.64947903

H	-4.22406786	2.31914379	1.06908516
H	-2.87442314	2.42886717	2.21060193
C	2.90843463	-2.23449022	-1.13861346
H	2.50909676	-2.28013499	-2.15895579
H	3.99659193	-2.32731553	-1.17163642
H	2.48287093	-3.08955727	-0.60045130
C	-0.01386925	2.65239665	1.33963575
C	-0.11503706	2.76691537	2.73532700
C	0.08044413	3.82936377	0.57985271
C	-0.12220262	4.01928276	3.35409233
C	0.07331711	5.08367289	1.19496685
H	0.15784717	3.75536088	-0.50178010
H	-0.19992012	4.08670291	4.43623038
H	0.14580774	5.98306615	0.58877196
C	-0.02833561	5.18171470	2.58481314
H	-0.03411698	6.15674678	3.06496428
H	-0.18604338	1.86394041	3.33610167
C	-3.38836833	0.02870605	0.02759448
C	4.79760729	-0.00428718	0.01643257
C	6.02855190	-0.07806898	-0.01551822
C	10.05004811	-0.32908509	-0.17806393
Pt	8.03750268	-0.19912811	-0.09534401
P	8.12979744	-1.82826927	1.60390134
C	9.11061027	-1.27816532	3.05982112
H	9.19550586	-2.08127823	3.79976270
H	8.62496394	-0.41263227	3.52035606
H	10.10541508	-0.98088818	2.71833943
C	6.53199293	-2.38644944	2.32049810
H	5.90406084	-2.80519075	1.53001801
H	6.00652299	-1.53039721	2.75146691
H	6.70086339	-3.14234941	3.09470112
C	8.95045372	-3.38323133	1.06385580
H	8.36538715	-3.84441589	0.26253521
H	9.94251765	-3.13793431	0.67642445
H	9.03989663	-4.08792530	1.89766119
P	7.97060901	1.42594735	-1.80019607
C	9.57917762	1.97552002	-2.49827140
H	9.42143184	2.72716395	-3.27894020
H	10.10841567	1.11534099	-2.91568974
H	10.19708721	2.39671353	-1.70128012
C	7.00644024	0.87441714	-3.26706534
H	6.00452699	0.58362344	-2.94075822
H	7.49365659	0.00418064	-3.71696305
H	6.93604146	1.67443341	-4.01187204
C	7.14981541	2.98800573	-1.28021510
H	6.14662378	2.75456793	-0.91464855
H	7.72048646	3.44586395	-0.46671190
H	7.08477202	3.69209053	-2.11685047
C	11.27415140	-0.42066106	-0.21733685
C	12.69868295	-0.52315817	-0.26759674
C	13.32647831	-1.59247965	-0.94266752
C	14.71579095	-1.68934040	-0.99106028

H	12.70907806	-2.34281643	-1.42825325
C	15.51477721	-0.72577178	-0.36881539
H	15.17700972	-2.52140874	-1.51705395
H	16.59785635	-0.80377218	-0.40757239
C	-11.27461152	-0.40729845	-0.21698482
C	-12.70063059	-0.49672222	-0.25125843
C	-13.34406118	-1.69451634	-0.63075213
C	-14.73480836	-1.77902681	-0.66320849
H	-12.73783509	-2.55479423	-0.89980788
C	-15.51914186	-0.67440212	-0.31861838
H	-15.20829738	-2.71172726	-0.95886445
H	-16.60333905	-0.74279680	-0.34457493
C	14.90818757	0.33903320	0.30373275
H	15.52002485	1.09399348	0.79102969
C	13.51937374	0.44223008	0.35497223
H	13.05170398	1.27135564	0.87819546
C	-13.50661009	0.61001766	0.09313453
H	-13.02675226	1.53903053	0.38708689
C	-14.89694515	0.51878737	0.05911342
H	-15.49734823	1.38395393	0.32891039

Complex Pt-3 (DFT//B3LYP/6-31G(d) / LanL2DZ)

Symbolic Z-matrix:

Charge = 0 Multiplicity = 3

C	4.79609901	-0.19052735	0.01579367
C	6.02729045	-0.26340847	0.02682142
C	10.04799993	-0.55627428	0.11253983
Pt	8.03579598	-0.40412192	0.06951236
P	7.91236703	-0.07889260	2.39974953
C	7.15896118	1.53643512	2.85618692
H	7.05363073	1.62412487	3.94289241
H	6.17662453	1.61430126	2.38313920
H	7.79009173	2.35092389	2.48822289
C	6.85668011	-1.32644815	3.24468544
H	7.29336437	-2.32114791	3.11423976
H	5.86488309	-1.31806899	2.78550405
H	6.77173467	-1.10669183	4.31434538
C	9.49357833	-0.12101463	3.33601239
H	9.96787307	-1.09695901	3.20455599
H	10.17244173	0.63912937	2.94166537
H	9.31388106	0.05978992	4.40111280
P	8.17742551	-0.72500106	-2.26010097
C	8.93694504	-2.33673649	-2.71714579
H	9.04758801	-2.42104441	-3.80358398
H	8.30649168	-3.15401811	-2.35431706
H	9.91692071	-2.41142976	-2.23898640

C	6.60202086	-0.68225033	-3.20697618
H	6.12183770	0.29015520	-3.07023691
H	5.92453719	-1.45020474	-2.82514462
H	6.78887425	-0.85253129	-4.27257176
C	9.23594807	0.52827289	-3.09243064
H	8.79280007	1.52070541	-2.96663313
H	10.22184074	0.52341850	-2.62079525
H	9.33400657	0.30943795	-4.16116975
C	-2.51390624	-1.26379264	0.23007929
C	-2.58647146	0.99614632	-0.17089508
C	-3.38998860	-0.14482792	0.03691053
C	-1.23205508	0.55493140	-0.09847478
C	-0.00606328	1.26520864	-0.23028341
C	1.22592407	0.56315740	-0.11193990
C	2.57684083	1.01483851	-0.19032785
C	2.52324838	-1.24819472	0.19566894
N	-1.23365660	-0.82979668	0.14743851
N	1.23920776	-0.82279929	0.12572271
B	0.00678329	-1.73700650	0.29201671
F	0.02038407	-2.34866877	1.55634421
F	-0.00001436	-2.73449799	-0.69649153
C	-3.12949665	2.37283198	-0.41660953
H	-2.83817695	3.08506804	0.36450244
H	-2.78719633	2.79535326	-1.36803235
H	-4.22327488	2.32762992	-0.44189006
C	2.90473014	-2.66674966	0.43350779
H	3.99287759	-2.76577179	0.43954979
H	2.50046939	-3.02280309	1.38857055
H	2.48381207	-3.31643857	-0.34304350
C	3.10904272	2.39809534	-0.42288740
H	2.78441355	3.10730246	0.34734210
H	4.20356850	2.36724816	-0.41383885
H	2.79050254	2.81457505	-1.38545306
C	-2.88314403	-2.68375218	0.47879309
H	-2.43563452	-3.04241035	1.41298033
H	-3.96982492	-2.78408358	0.53294755
H	-2.49712101	-3.33038688	-0.31858150
C	-0.01222332	2.73528583	-0.50148281
C	0.00688069	3.22132445	-1.81843833
C	-0.03683148	3.66391152	0.55102019
C	0.00170228	4.59400034	-2.07754561
C	-0.04204258	5.03747272	0.29599111
H	-0.05124967	3.30175879	1.57572356
H	0.01639431	4.95002390	-3.10449204
H	-0.06067708	5.74058973	1.12480146
C	-0.02281132	5.50633899	-1.01981171
H	-0.02678991	6.57466504	-1.21937082
H	0.02552080	2.51325085	-2.64284647
C	3.38964189	-0.12174766	0.00308608
C	-4.79569224	-0.22301549	0.05737716
C	-6.02658040	-0.30177017	0.07277150
C	-10.04982353	-0.54765927	0.15069647
Pt	-8.03586853	-0.42337514	0.11373583
P	-8.13596452	-1.41881439	-2.01962731
C	-9.11538826	-0.42236392	-3.21609676

H	-9.19905230	-0.93731555	-4.17917578
H	-8.63038017	0.54685766	-3.36586310
H	-10.11106674	-0.25402473	-2.79790663
C	-6.53966918	-1.71852493	-2.88007852
H	-5.91737139	-2.38259817	-2.27478282
H	-6.00683971	-0.77163302	-2.99891817
H	-6.71057792	-2.17019222	-3.86296662
C	-8.96341528	-3.06164874	-2.01042920
H	-8.38215355	-3.75958686	-1.40044490
H	-9.95573364	-2.95089494	-1.56584078
H	-9.05449684	-3.46009337	-3.02663383
P	-7.95638605	0.57231955	2.24826886
C	-9.55993351	0.85606214	3.09976063
H	-9.39868098	1.32067535	4.07824038
H	-10.07789458	-0.09790693	3.22670882
H	-10.19094224	1.50233713	2.48453083
C	-6.97317102	-0.41253271	3.45169891
H	-5.97017815	-0.56554606	3.04497005
H	-7.44483856	-1.38942852	3.59395573
H	-6.90677975	0.10082705	4.41698244
C	-7.14609482	2.22419559	2.24474982
H	-6.14943488	2.12718572	1.80649467
H	-7.73137237	2.91653560	1.63223287
H	-7.06534248	2.62273928	3.26181474
C	-11.27522029	-0.63752383	0.16014475
C	-12.69874323	-0.73985033	0.17745004
C	-13.52433837	0.39938050	-0.14378620
C	-13.31755395	-1.94317258	0.50753196
C	-12.96799634	1.65850621	-0.49115476
C	-14.95113555	0.26241517	-0.11407092
C	-14.72309460	-2.06651675	0.53354537
H	-12.69848938	-2.80163020	0.75085321
C	-13.77595803	2.73376903	-0.79404074
H	-11.88649362	1.75394267	-0.51364758
C	-15.75603489	1.39143563	-0.43187067
C	-15.52765162	-0.99002059	0.23015548
H	-15.16688270	-3.02307734	0.79667241
C	-15.18549466	2.60009204	-0.76408197
H	-13.33125556	3.68972719	-1.05771812
H	-16.83778420	1.28126280	-0.40737261
H	-16.61071853	-1.08320025	0.24974880
H	-15.81431466	3.45327905	-1.00428417
C	11.27233537	-0.65833892	0.12763176
C	12.69440281	-0.77792889	0.15223074
C	13.53592772	0.37488289	-0.06170046
C	13.29623758	-2.01226551	0.38464304
C	12.99753946	1.66653842	-0.30146744
C	14.96074138	0.21844359	-0.03203101
C	14.70001332	-2.15433633	0.41244321
H	12.66506591	-2.88096954	0.54702777
C	13.82062381	2.75371897	-0.50496456
H	11.91752293	1.77857483	-0.31837109
C	15.78151091	1.36052983	-0.24571158
C	15.51959330	-1.06577787	0.20869248
H	15.13034941	-3.13519497	0.59668133

C	15.22817576	2.60022890	-0.47751055
H	13.38939590	3.73463342	-0.68666057
H	16.86165385	1.23521342	-0.22243024
H	16.60131347	-1.17351008	0.22911416
H	15.86899523	3.46297912	-0.63896997

Complex Pt-4 (DFT//B3LYP/6-31G(d) / LanL2DZ)

Symbolic Z-matrix:

Charge = 0 Multiplicity = 3

C	5.37434033	-1.60875446	0.08452771
C	5.59003631	0.65682193	-0.05765589
C	4.64728856	-0.38317543	0.01849965
C	6.87916538	0.03844407	-0.03572479
C	8.17694713	0.57306952	-0.08433141
C	9.30897712	-0.26114897	-0.04056817
C	10.71309307	0.02899569	-0.07810572
C	10.38814448	-2.21603376	0.07828513
N	6.69131693	-1.34956598	0.05301600
N	9.16198687	-1.65101896	0.05531623
B	7.81703405	-2.42186090	0.11502214
F	7.72399829	-3.14207345	1.30959532
F	7.71047490	-3.29141176	-0.97479534
C	5.22723828	2.10817575	-0.14184725
H	5.65537409	2.69015246	0.68133856
H	5.58243431	2.56924927	-1.07024620
H	4.13837766	2.20828267	-0.10424496
C	10.59776096	-3.69261109	0.17421922
H	11.66512486	-3.92669659	0.18583910
H	10.13390154	-4.09153707	1.08273795
H	10.12850515	-4.20614273	-0.67196246
C	11.41543326	1.35179015	-0.17708917
H	11.18446697	2.00618688	0.67031867
H	12.49816769	1.19310702	-0.19651253
H	11.13695177	1.90103039	-1.08276498
C	4.81535557	-2.98884096	0.17693537
H	5.12917600	-3.47090446	1.10957097
H	3.72438755	-2.95183945	0.13735885
H	5.18973563	-3.61192505	-0.64199349
C	8.36006008	2.05373481	-0.18527347
C	8.40988286	2.67732677	-1.43971418
C	8.48583392	2.83376600	0.97266951
C	8.58313475	4.05979946	-1.53371818
C	8.65811689	4.21627352	0.87675758
H	8.44743142	2.35517305	1.94739790
H	8.62103305	4.53223249	-2.51145453

H	8.75359174	4.81078181	1.78118804
C	8.70730704	4.83204996	-0.37621473
H	8.84156417	5.90761791	-0.45024753
H	8.31345274	2.07693576	-2.34015707
C	11.36086582	-1.20128528	-0.00254693
C	3.23215041	-0.27053022	0.02841012
C	2.00720192	-0.17524466	0.03225205
C	-3.24114743	0.22944043	0.08513206
C	-2.00938911	0.13470347	0.08617721
Pt	-0.00641799	-0.01932842	0.05821871
P	-0.10049216	0.29603311	-2.27749754
C	-0.85397724	1.90469166	-2.75693212
H	-0.94160124	1.98445932	-3.84578213
H	-0.23335241	2.72501207	-2.38420762
H	-1.84498773	1.98194827	-2.30211662
C	1.49214117	0.25014081	-3.19288416
H	1.96931165	-0.72153149	-3.04274876
H	2.16222400	1.01877739	-2.80024259
H	1.32378993	0.41646505	-4.26214491
C	-1.14156505	-0.96283710	-3.12401295
H	-0.70335459	-1.95472430	-2.97829722
H	-2.13992109	-0.95447311	-2.67902834
H	-1.21298179	-0.75361215	-4.19672825
P	0.12395289	-0.33643692	2.39073156
C	-1.45742196	-0.29095055	3.32774543
H	-1.27656675	-0.45234443	4.39569466
H	-2.13021472	-1.06467799	2.94896830
H	-1.93959766	0.67916442	3.18159900
C	0.88083505	-1.94602569	2.85807434
H	1.86317987	-2.02301061	2.38554164
H	0.25190944	-2.76506451	2.49665262
H	0.98617643	-2.02458553	3.94544171
C	1.17602883	0.92238990	3.22184472
H	2.16358341	0.91681574	2.75386542
H	0.73142468	1.91334451	3.08964913
H	1.26964350	0.70810505	4.29183849
C	-5.34775939	1.59095610	0.24943676
C	-5.59984684	-0.67433947	-0.07345905
C	-4.63899257	0.34636819	0.08384581
C	-6.87167752	-0.03969768	-0.00726979
C	-8.19581447	-0.56745345	-0.10675714
C	-9.29727416	0.31623822	-0.00011593
C	-10.72938628	0.06286282	-0.07256699
C	-10.35917663	2.28169342	0.26410539
N	-6.67431399	1.33852393	0.19199394
N	-9.12413011	1.67737797	0.20390704
B	-7.78024501	2.41533731	0.33645595
F	-7.67864753	3.04231600	1.58807494
F	-7.64269015	3.38171281	-0.67207185
C	-5.26293530	-2.12318139	-0.26857171
H	-5.72150966	-2.76481119	0.49166351
H	-5.59432635	-2.50338525	-1.24203340
H	-4.17699220	-2.25017650	-0.21020881
C	-10.52125955	3.74785598	0.47635407
H	-11.58062467	4.01666405	0.49471003

H	-10.05602326	4.05963166	1.41925987
H	-10.02157673	4.31511752	-0.31810845
C	-11.44413959	-1.23723591	-0.28707127
H	-11.23188146	-1.96551684	0.50423429
H	-12.52523506	-1.06411094	-0.30489536
H	-11.16298936	-1.71579197	-1.23229070
C	-4.77546062	2.94786438	0.45490262
H	-5.13966555	3.38083792	1.39395570
H	-3.68438435	2.89664194	0.47513702
H	-5.09594137	3.62697445	-0.34401408
C	-8.40689433	-2.03193369	-0.31939306
C	-8.44418519	-2.57398031	-1.61400348
C	-8.57240235	-2.89978249	0.77200793
C	-8.64295406	-3.94222330	-1.81339589
C	-8.77135728	-4.26845972	0.57640720
H	-8.54430415	-2.49355189	1.77978461
H	-8.67019145	-4.34259044	-2.82355179
H	-8.89790308	-4.92400210	1.43414042
C	-8.80747759	-4.79336074	-0.71785474
H	-8.96263236	-5.85793018	-0.87154472
H	-8.31758048	-1.91331542	-2.46775991
C	-11.34706769	1.29727289	0.09547878
H	12.43134520	-1.36276562	-0.00496659
H	-12.41407741	1.48265213	0.09660433