

Electronic Supplementary Information for:

Fluorene as π -Conjugation Linker in $N^{\wedge}N$ Pt(II) bisacetylide Complexes and Their Applications for Triplet-triplet Annihilation Based Upconversion

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Experimental Section

General

All the chemicals are analytical pure and were used as received. Solvents were dried and distilled for synthesis. NMR spectra were recorded on a 400 MHz Varian Unity Inova NMR spectrophotometer. Mass spectra were recorded with Q-TOF Micro MS spectrometer. UV-Vis absorption spectra were measured with a HP8453 UV-visible spectrophotometer. Fluorescence spectra were recorded on JASCO FP-6500 or a Sanco 970 CRT spectrofluorometer. Fluorescence lifetimes were measured on a Horiba Jobin Yvon Fluoro Max-4 (TCSPC) instrument. Emission curves were generated using the Origin 5.0 (Microcal software). The binding constants were calculated using custom-written nonlinear least-square curve-fitting programs implemented within SigmaPlot 2000 (SPSS Inc.).

All these calculations were performed in Gaussian 09W.

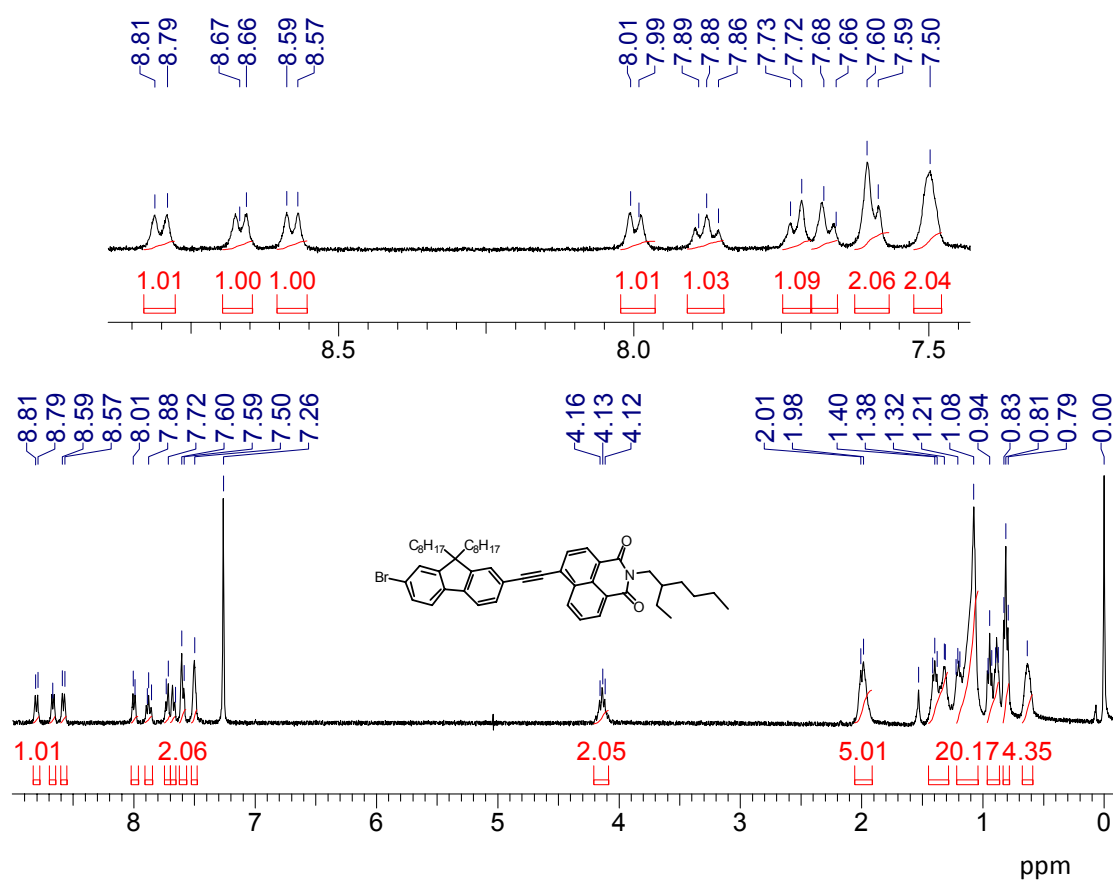


Fig. S1 1H NMR of compound a ($CDCl_3$, 400 MHz) .

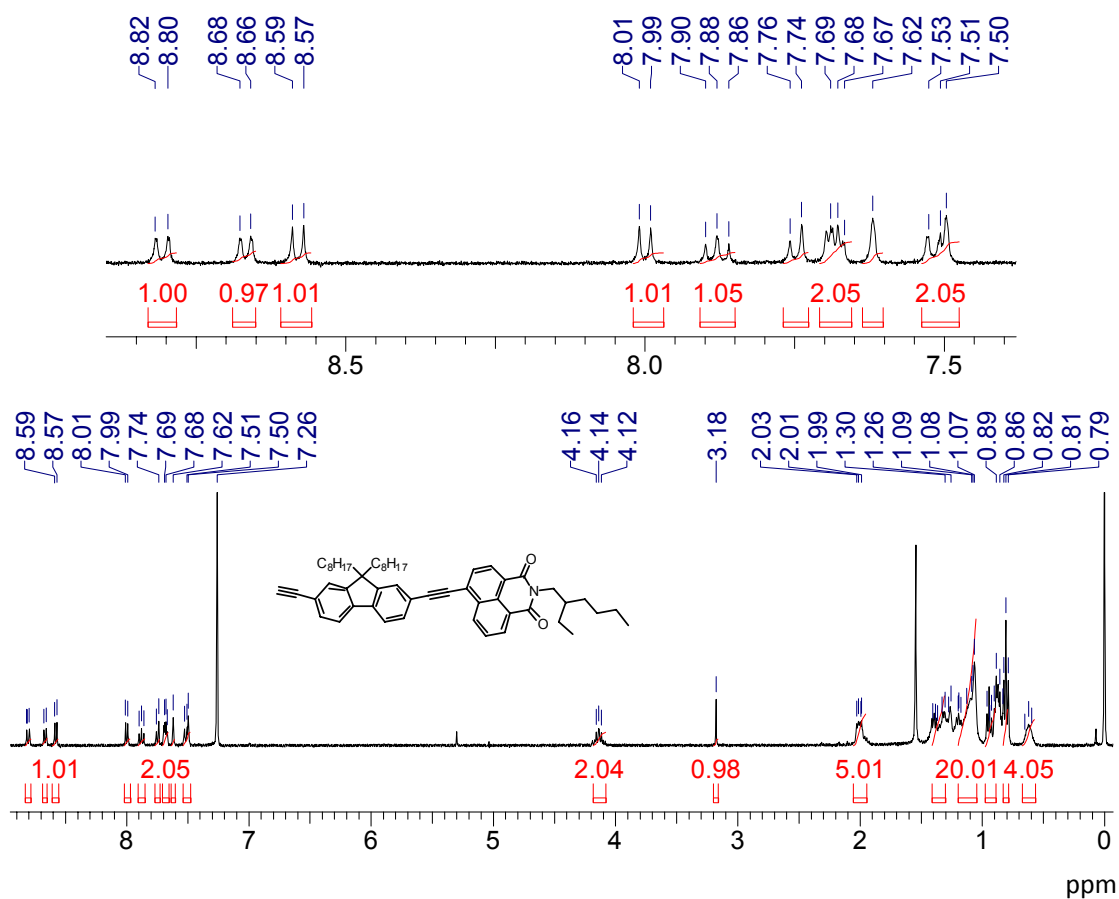


Fig. S2 ¹H NMR of compound L-1 (CDCl₃, 400 MHz).

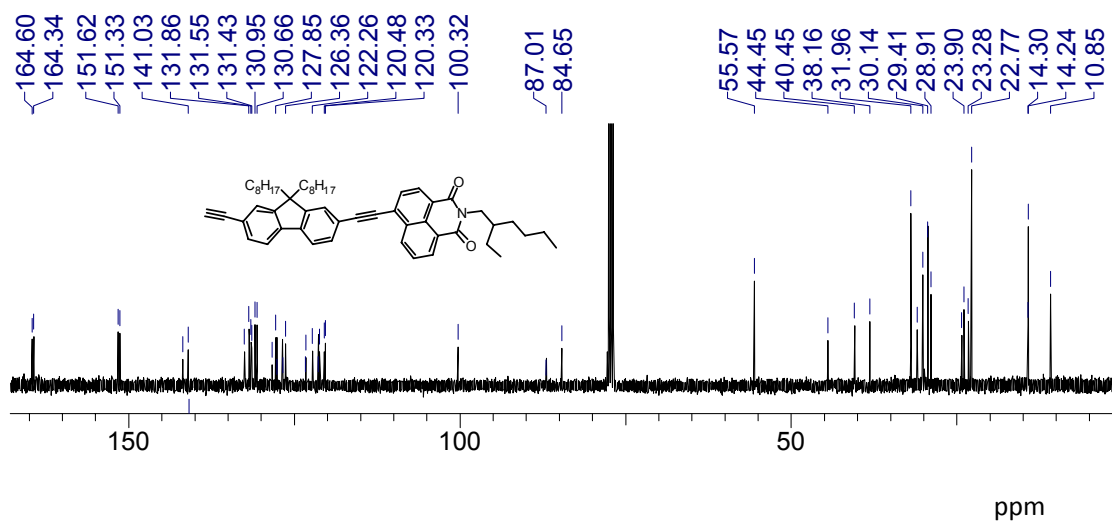


Fig. S3 ¹³C NMR of compound L-1 (CDCl₃, 100 MHz).

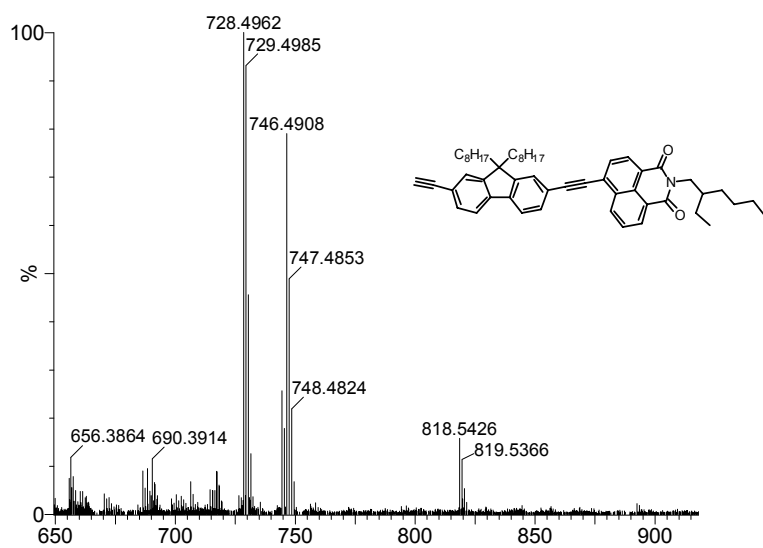


Fig. S4 HR-MALDI-MS of L-1.

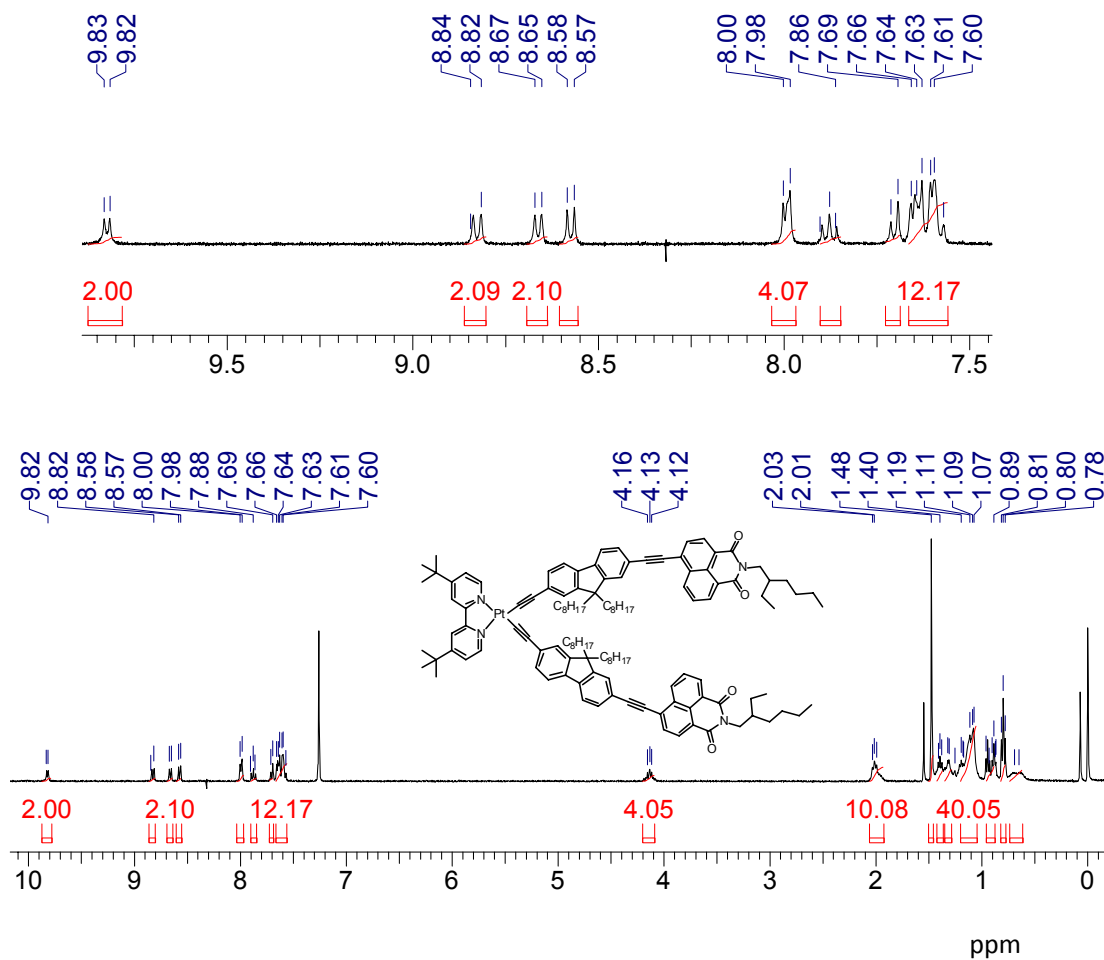


Fig. S5 ¹H NMR of compound Pt-1 (CDCl₃, 400 MHz).

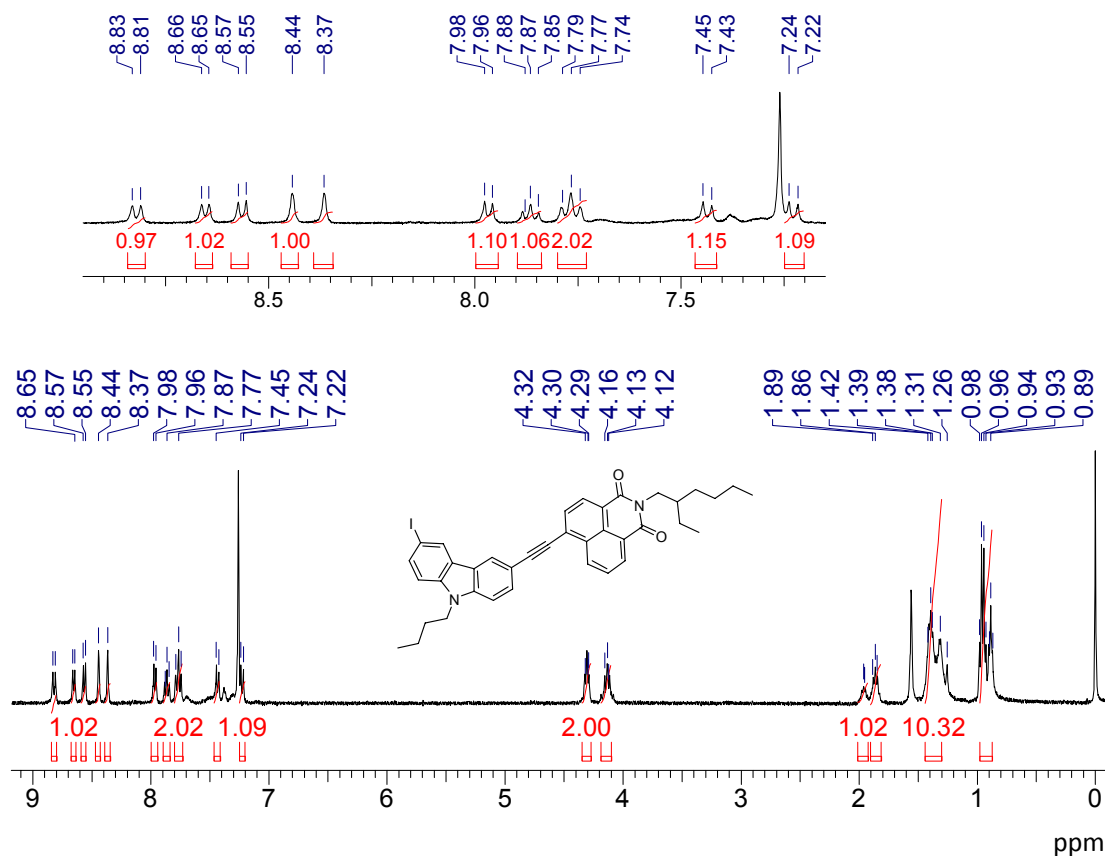


Fig. S8 ¹H NMR of compound **b** (CDCl₃, 400 MHz).

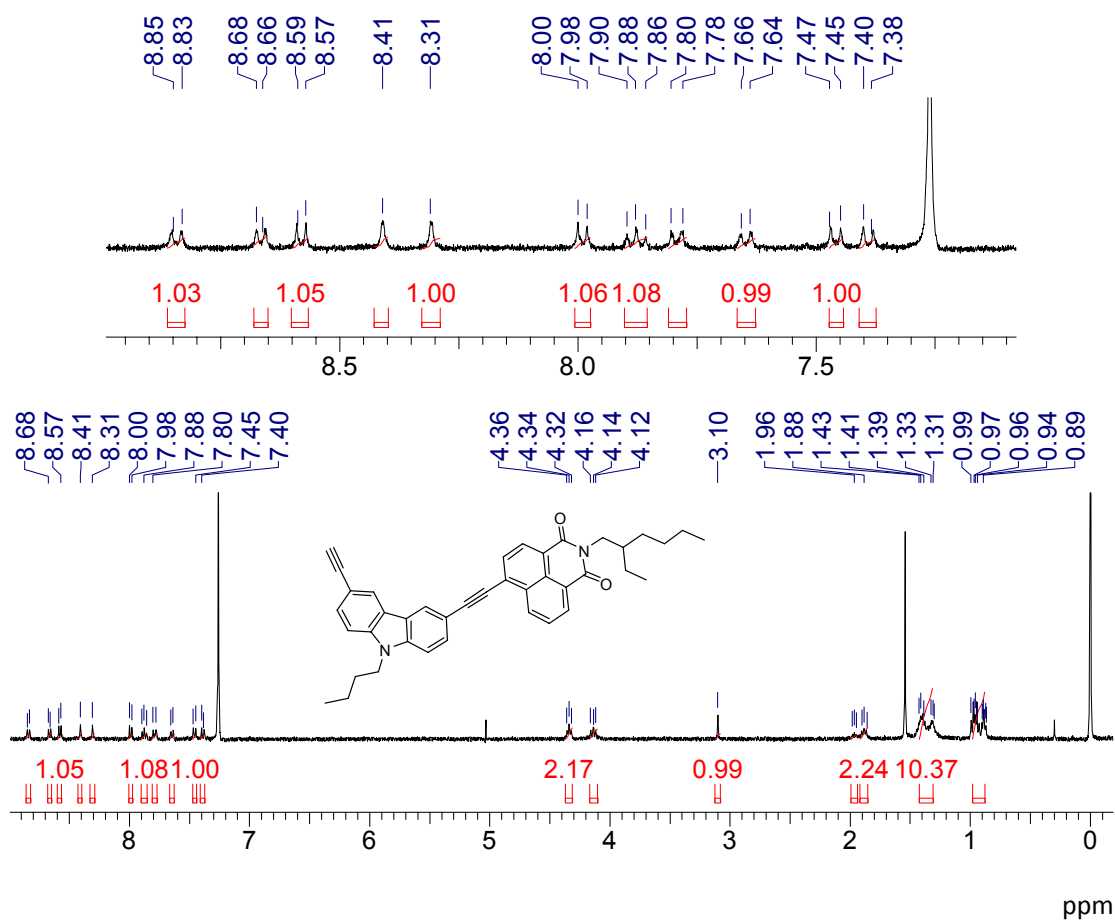


Fig. S9 ¹H NMR of compound **L-2** (CDCl₃, 400 MHz).

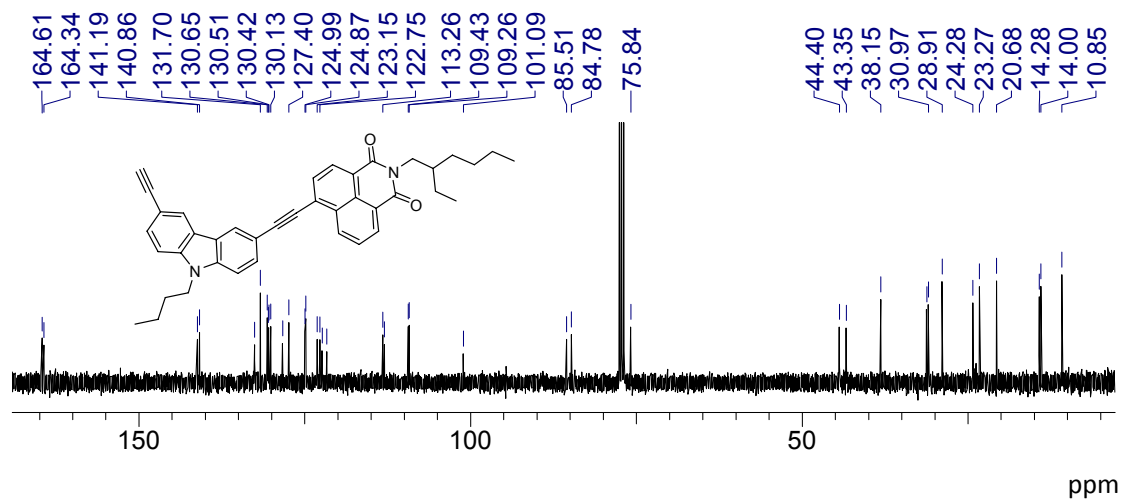


Fig. S10 ^{13}C NMR of compound L-2 (CDCl₃, 100 MHz).

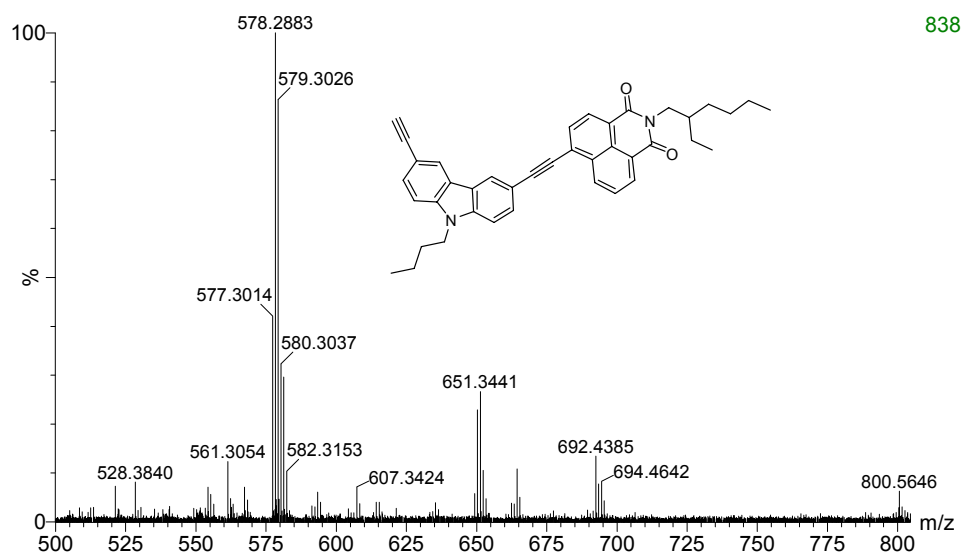


Fig. S11 HR-MALDI-MS of L-2.

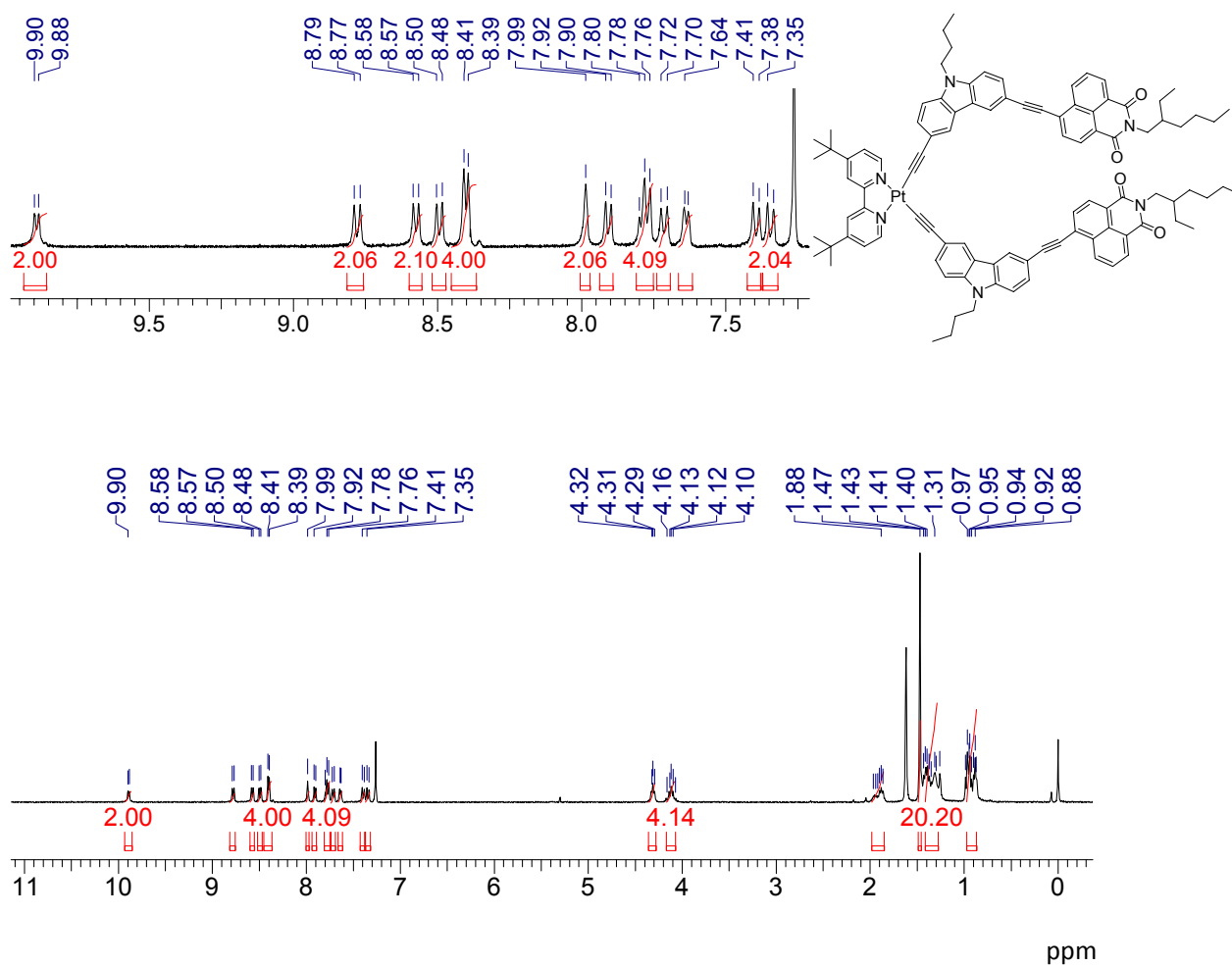


Fig. S12 ¹H NMR of compound Pt-2 (CDCl₃, 400 MHz).

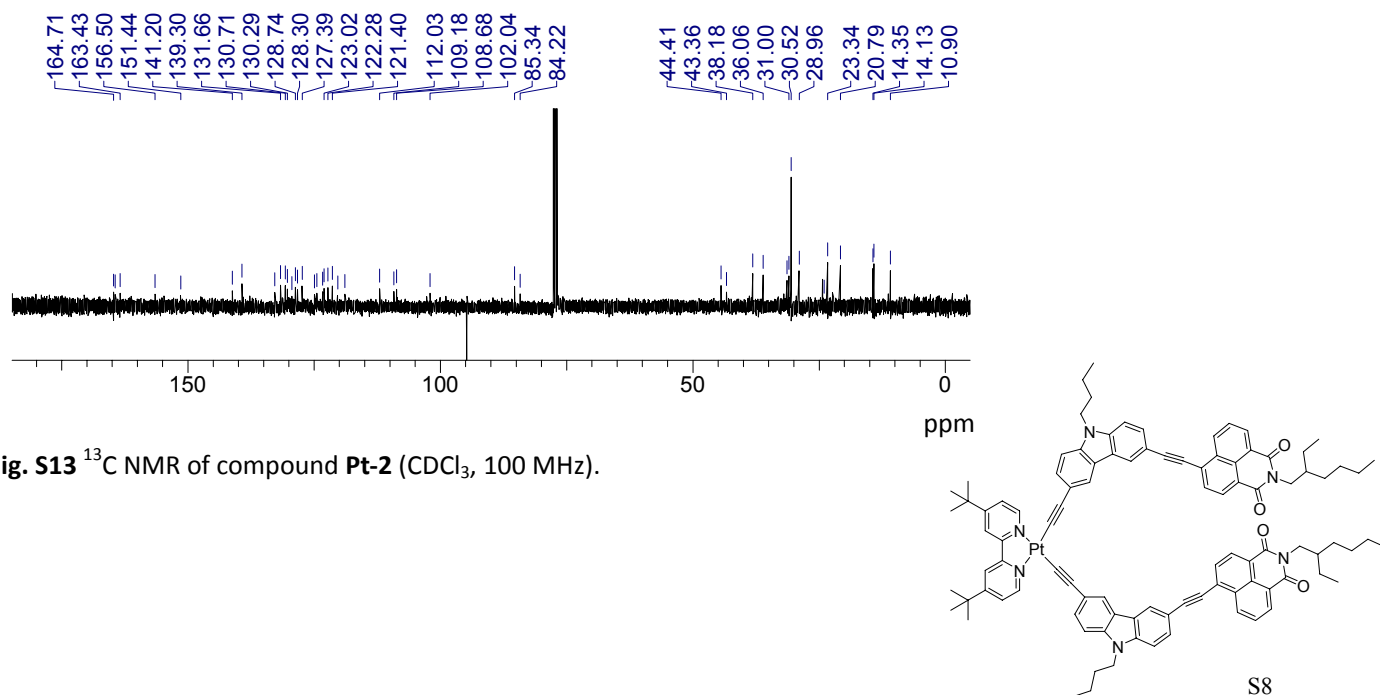


Fig. S13 ¹³C NMR of compound Pt-2 (CDCl₃, 100 MHz).

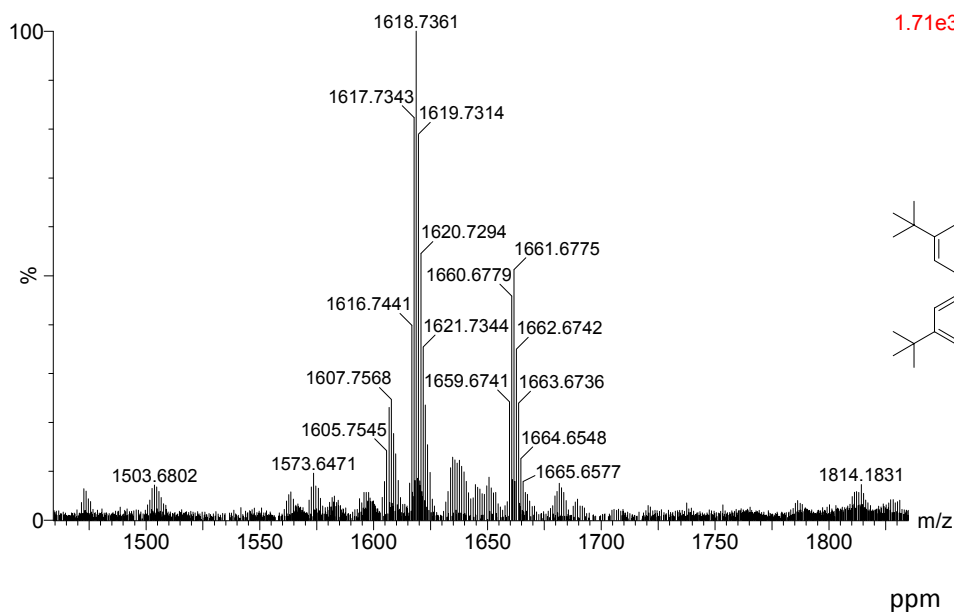


Fig. S14 HR-MALDI-MS of Pt-2.

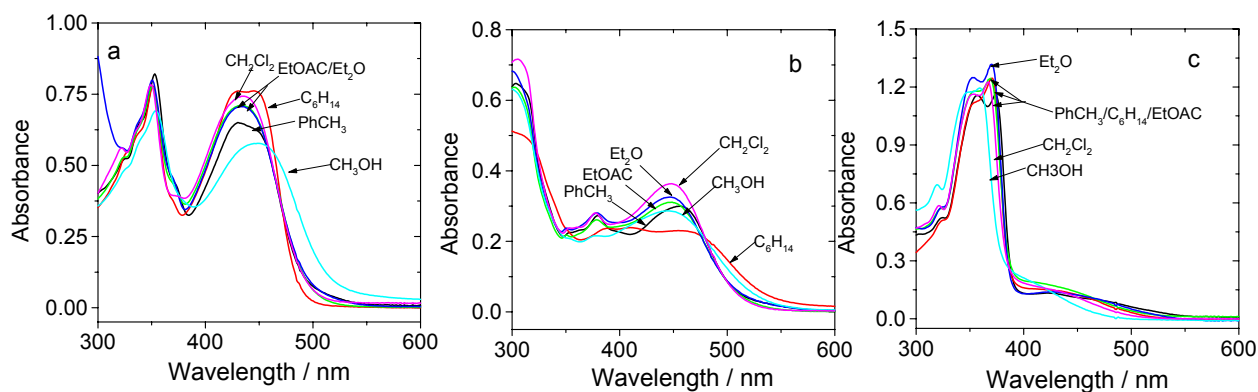


Fig. S15 UV-Vis absorption spectra of (a) Pt-1, (b) Pt-2 and (c) Pt-5 in different solutions. $c = 1.0 \times 10^{-5}$ M, 20 °C.

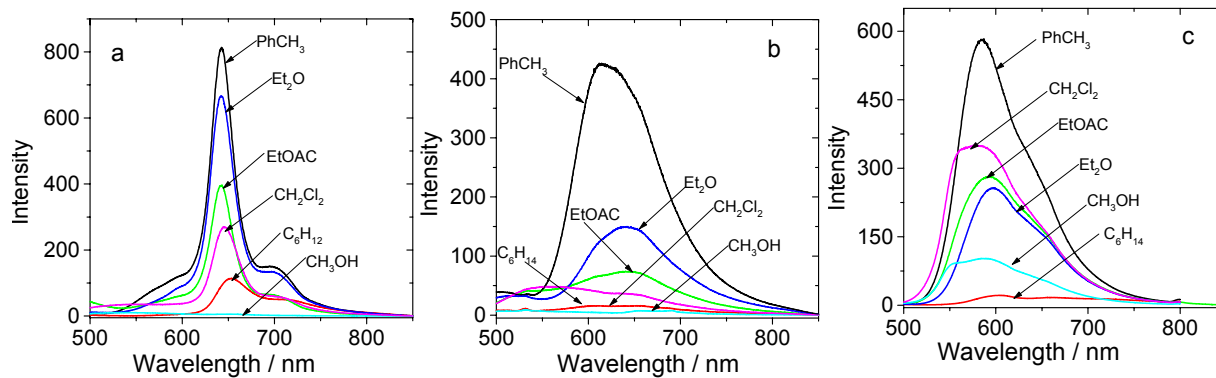


Fig. S16 Emission spectra of (a) Pt-1, (b) Pt-2 and (c) Pt-5 in different solutions. $c = 1.0 \times 10^{-5}$ M, 20 °C.

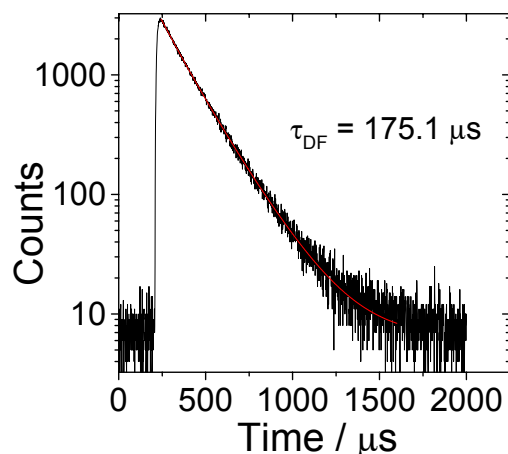


Fig. S17 Delayed fluorescence observed in the TTA upconversion with compound **Pt-2** as triplet photosensitizer and DPA as the triplet acceptor. Excited at 473 nm (nanosecond pulsed OPO laser synchronized with spectrofluorometer) and monitored at 410 nm. Under this circumstance the compound **Pt-2** is selectively excited and the emission is due to the upconverted emission of DPA. In deaerated toluene. $c[\text{Sensitizers}] = 1.0 \times 10^{-5} \text{M}$; $c[\text{DPA}] = 4.3 \times 10^{-4} \text{M}$; 20 °C.

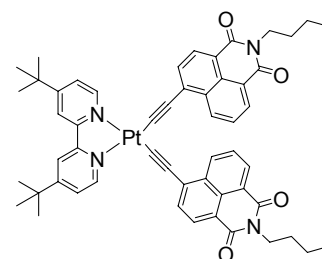
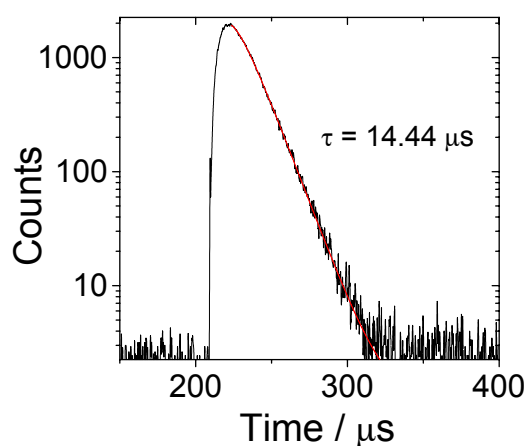
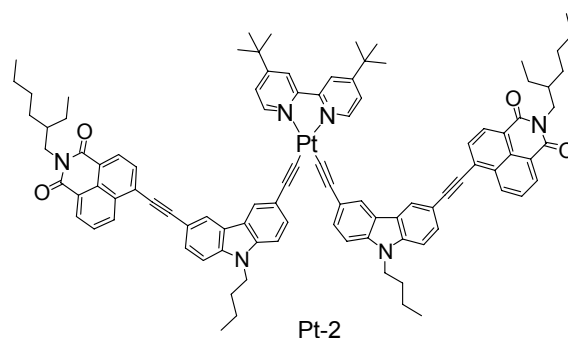


Fig. S18 Delayed fluorescence observed in the TTA upconversion with compound **Pt-3** as triplet photosensitizer and DPA as the triplet acceptor. Excited at 473 nm (nanosecond pulsed OPO laser synchronized with spectrofluorometer) and monitored at 410 nm. Under this circumstance the compound **Pt-3** is selectively excited and the emission is due to the upconverted emission of DPA. In deaerated toluene. $c[\text{Sensitizers}] = 1.0 \times 10^{-5} \text{M}$; $c[\text{DPA}] = 4.3 \times 10^{-4} \text{M}$; 20 °C.

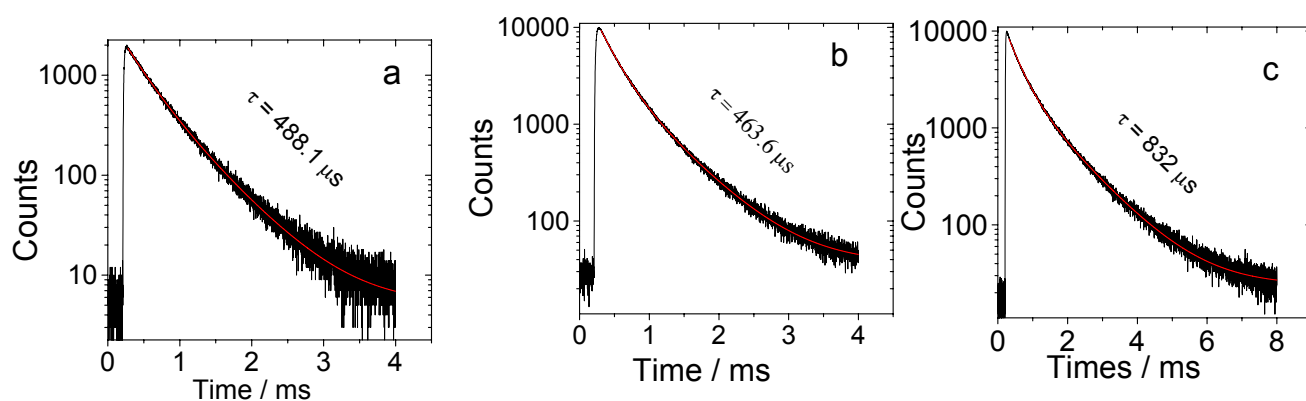


Fig. S19 Delayed fluorescence observed in the TTA upconversion with compound **Pt-1** as triplet photosensitizer and DPA as the triplet acceptor. Excited at 473 nm (nanosecond pulsed OPO laser synchronized with spectrofluorometer) and monitored at 410 nm. Under this circumstance the compound **Pt-1** is selectively excited and the emission is due to the upconverted emission of DPA. (a) $c[\text{Sensitizers}] = 1.0 \times 10^{-5} \text{ M}$; $c[\text{DPA}] = 4.3 \times 10^{-4} \text{ M}$; (b) $c[\text{Sensitizers}] = 1.0 \times 10^{-5} \text{ M}$; $c[\text{DPA}] = 2.2 \times 10^{-4} \text{ M}$; (c) $c[\text{Sensitizers}] = 5.0 \times 10^{-6} \text{ M}$; $c[\text{DPA}] = 4.3 \times 10^{-4} \text{ M}$. In deaerated toluene. 20 °C.

The integrated luminescence intensity of the upconversion experiments (Fig. 8 in the main text):

For **Pt-1** as the triplet photosensitizer,

The area of the total upconverted emission: 60631

The scattered laser peak area: 456

The peak area beyond the laser: 6993

The upconversion quantum yield is 21.3% without the above two areas are considered.

Similarly, the upconversion quantum yield with **Pt-2** as the triplet photosensitizer is 13.0% with the above correction;

Similarly, the upconversion quantum yield with **Pt-2** as the triplet photosensitizer is 15.9% with the above correction;

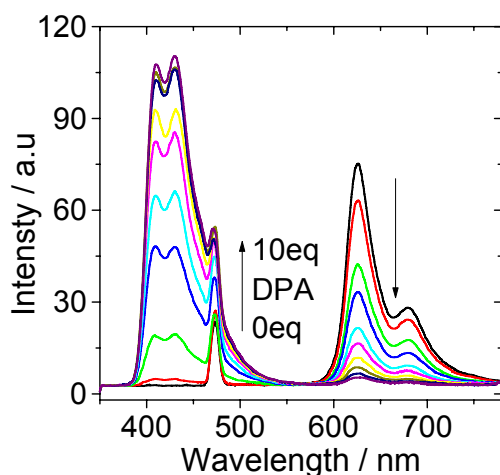


Fig. S20 The upconversion of **Pt-3** with increased DPA concentration. Excited with 473 nm laser. $c[\text{sensitizer}] = 1.0 \times 10^{-5}$ M in toluene. 25 °C.

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

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1 Ground state geometry.

C	-3.48971045	6.94745047	0.00085383
C	-2.92808307	8.23576640	0.00092148
C	-1.52384960	8.30875608	0.00098446
C	-0.73682800	7.15505490	0.00098613
C	-2.67040165	5.82123618	0.00085575
C	0.73695867	7.15502289	0.00104837
C	1.52403100	8.30868951	0.00111561
C	2.92826134	8.23563791	0.00116459
C	3.48983199	6.94729732	0.00114158
C	2.67047375	5.82111918	0.00107583
H	-4.56117963	6.80345128	0.00080120
H	-3.06307677	4.81257231	0.00080405
H	4.56129486	6.80325083	0.00117494
H	3.06310463	4.81243807	0.00105258
N	1.32261215	5.91476620	0.00103022
N	-1.32253584	5.91482383	0.00092234
Pt	0.00000293	4.27867408	0.00091451
H	1.04052207	9.27668265	0.00113013
H	-1.04029800	9.27672779	0.00103371
C	3.77056474	9.52427643	0.00124083

C	-3.77032877	9.52444254	0.00092671
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H	4.02714466	11.27752464	-1.27647193
H	3.66378255	9.79226460	-2.17852845
C	3.43372994	10.35602512	1.27033793
H	4.02710610	11.27739446	1.27914008
H	2.37606139	10.63898857	1.30418660
H	3.66369584	9.79204663	2.18103274
C	5.28698672	9.22525112	0.00125235
H	5.59091348	8.66224241	0.89101308
H	5.59094274	8.66232808	-0.88855256
H	5.84269887	10.16879284	0.00130711
C	-3.43350562	10.35621758	1.27000942
H	-2.37582562	10.63913436	1.30389158
H	-4.02683909	11.27761502	1.27875744
H	-3.66353403	9.79228032	2.18071399
C	-3.43345240	10.35625922	-1.26811469
H	-4.02678425	11.27765773	-1.27685694
H	-2.37577016	10.63917405	-1.30194299
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C	-7.59654055	-0.93196394	-0.00017809
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C	-6.64744507	-3.18369935	-0.00043860
H	-8.09165185	-4.78131857	-0.00076869
H	-9.75170470	-0.80068701	-0.00030329
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C	-2.93124328	-0.33241374	0.00021571
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C	-5.25548200	-0.97714844	-0.00002918
H	-4.94190607	2.43473969	0.00046108
H	-1.87836777	-0.59123435	0.00025057
H	-3.59994583	-2.37759042	-0.00011129
C	-2.27868112	2.04714242	0.00058063
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C	-7.15617702	0.53817847	0.00005369

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H	-7.27188179	2.30401856	-1.28899422
H	-7.31201385	0.76713133	-2.17669258
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H	-8.74862213	1.31907760	1.28867480
H	-7.31231066	0.76653817	2.17684130
H	-7.27203885	2.30366647	1.28956912
C	-12.45015407	-8.05817388	-0.00127096
C	-12.13430965	-6.70960514	-0.00114201
C	-13.15395901	-5.72223580	-0.00113225
C	-14.51943931	-6.14881865	-0.00126095
C	-14.82069060	-7.53927934	-0.00139041
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H	-11.09929002	-6.38654708	-0.00104566
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C	-15.56805509	-5.19012777	-0.00125714
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H	-18.65656673	-8.51636226	-0.00178783
H	-19.13874737	-7.03332059	0.88340093
H	-19.13866514	-7.03306320	-0.88660068
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O	-16.52867717	-9.21459730	-0.00162886
C	-11.53019709	-3.83285524	-0.00085332
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C	8.88133137	-1.44922716	-0.00009389
C	7.59647117	-0.93203836	0.00001852
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C	6.64737680	-3.18377413	-0.00028721
H	8.09158460	-4.78139257	-0.00056196
H	9.75163500	-0.80075974	-0.00002081
H	5.79288297	-3.85296475	-0.00036185
C	5.62840754	0.38847620	0.00027119
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C	3.28647274	1.04212072	0.00045208

C	2.93117358	-0.33248971	0.00025816
C	3.90079728	-1.33417761	0.00007480
C	5.25541271	-0.97722383	0.00008175
H	4.94183579	2.43466405	0.00060193
H	1.87829818	-0.59131063	0.00025872
H	3.59987671	-2.37766632	-0.00006878
C	2.27861150	2.04706648	0.00064482
C	1.37957946	2.88907744	0.00079180
C	7.15610701	0.53810387	0.00024022
C	7.65311177	1.27590730	1.27032076
H	8.74851116	1.31899852	1.28891405
H	7.27192978	2.30358991	1.28976150
H	7.31216974	0.76646034	2.17703292
C	7.65302504	1.27625499	-1.26967316
H	8.74842348	1.31934364	-1.28833323
H	7.31201507	0.76705939	-2.17650085
H	7.27184861	2.30394563	-1.28880244
C	12.45012152	-8.05823616	-0.00077438
C	12.13426578	-6.70966996	-0.00069294
C	13.15390705	-5.72229247	-0.00067696
C	14.51939099	-6.14886463	-0.00074854
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C	13.79706124	-8.47673287	-0.00084224
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H	14.05782074	-9.52877523	-0.00090455
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C	13.93261143	-3.39679883	-0.00057522
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H	13.71415515	-2.33532696	-0.00050662
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C	16.97513242	-5.62506330	-0.00081243
N	17.22181787	-7.00898108	-0.00088374
C	18.63538757	-7.42911987	-0.00094154
H	18.65653789	-8.51637512	-0.00101234
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H	19.13868572	-7.03326053	0.88407481
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O	16.52865510	-9.21462630	-0.00096248
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C	10.38730849	-3.39657090	-0.00041383

.....

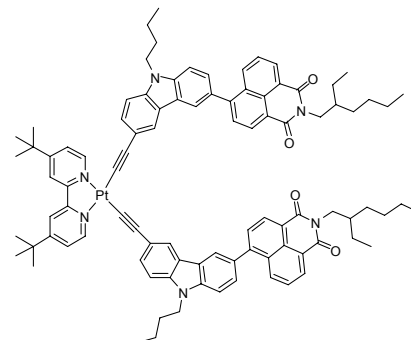
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Number of Imaginary frequencies: 0

complex pt-2 (DFT//B3LYP/6-31G(d)/ LanL2DZ)

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1 Ground state geometry.



C	3.48900200	-3.05121400	0.06270800
C	2.92798600	-4.33994500	0.05207900
C	1.52413500	-4.41347000	0.02803700
C	0.73662600	-3.25997700	0.01441700
C	2.66955600	-1.92533600	0.04935900
C	-0.73663800	-3.25997000	-0.01221500
C	-1.52416300	-4.41345500	-0.02570400
C	-2.92801300	-4.33991400	-0.04976800
C	-3.48901000	-3.05117600	-0.06055700
C	-2.66954800	-1.92530700	-0.04733400
H	4.56028200	-2.90689100	0.08126700
H	3.06155100	-0.91640000	0.05715300
H	-4.56028800	-2.90683800	-0.07914300
H	-3.06153200	-0.91636700	-0.05525600
N	-1.32168300	-2.01926300	-0.02328100
N	1.32168900	-2.01927600	0.02532800
Pt	0.00001100	-0.38434500	0.00091400
H	-1.04091800	-5.38160000	-0.01742800
H	1.04087700	-5.38160900	0.01987100
C	-3.77090100	-5.62818000	-0.06419200
C	3.77085500	-5.62822400	0.06660400
C	-3.41902000	-6.45543100	-1.33217000
H	-2.36104400	-6.73851400	-1.35378800
H	-4.01283200	-7.37636900	-1.35194100
H	-3.63729700	-5.88767600	-2.24340400
C	-3.45028900	-6.46516500	1.20558800
H	-4.04402500	-7.38637500	1.20333800
H	-2.39324200	-6.74875000	1.25169700
H	-3.69152500	-5.90471400	2.11555700
C	-5.28711500	-5.32849500	-0.08130400
H	-5.60075600	-4.76664700	0.80583000
H	-5.58057900	-4.76399900	-0.97363000
H	-5.84341500	-6.27166000	-0.08915400
C	3.41897200	-6.45538600	1.33463500

H	2.36099800	-6.73847000	1.35628300
H	4.01278000	-7.37632600	1.35446200
H	3.63726000	-5.88757400	2.24583100
C	3.45022200	-6.46528300	-1.20312200
H	4.04393600	-7.38650800	-1.20082200
H	2.39316700	-6.74884000	-1.24920500
H	3.69146400	-5.90489400	-2.11312800
C	5.28707400	-5.32856100	0.08369600
H	5.60073000	-4.76679800	-0.80348700
H	5.58054000	-4.76399000	0.97597300
H	5.84335800	-6.27173400	0.09162800
C	15.46817500	2.15788200	-0.01312400
C	14.11318900	1.87048700	-0.00210900
C	13.65207500	0.52839700	-0.01303100
C	14.61821500	-0.52639000	-0.03591200
C	16.00483300	-0.20821000	-0.04680400
C	16.41898500	1.11660900	-0.03548000
H	15.80374100	3.18913500	-0.00460200
H	13.38114000	2.67008300	0.01493200
C	12.24847400	0.18853500	-0.00210900
C	14.19602800	-1.88282400	-0.04777600
H	17.48221400	1.32696500	-0.04425600
C	12.83912100	-2.18384300	-0.03734500
C	11.87726500	-1.16328800	-0.01486800
H	12.54107400	-3.22607100	-0.04681700
H	10.82350900	-1.41637200	-0.00675700
C	17.01913600	-1.28299700	-0.07028000
C	15.18633600	-2.97156700	-0.07102900
N	16.54425600	-2.60695900	-0.08091800
C	17.52505800	-3.70775200	-0.10437800
H	18.51814000	-3.26463700	-0.10954300
H	17.39001900	-4.34207900	0.77464600
H	17.37131000	-4.32092900	-0.99525200
O	14.86819700	-4.18229500	-0.08203100
O	18.24697400	-1.04268500	-0.08039100
C	3.25409900	2.88857700	0.07263500
C	2.84904200	4.25443200	0.10143800
C	3.76704900	5.30174900	0.12609800
C	5.12847100	4.98107400	0.12648700
C	5.56927900	3.62939900	0.09212600
C	4.63335500	2.59256400	0.06726000
H	1.78660800	4.47011600	0.10087200
H	3.42362200	6.33057000	0.13881500
H	4.95358200	1.55627500	0.04180600
C	7.40100400	5.04584600	0.12520000
C	8.74819400	5.43259600	0.12197000

C	9.71785000	4.43575200	0.09646700
C	9.37061000	3.05585200	0.06907800
C	8.00803300	2.68261500	0.06571700
C	7.02343700	3.66702600	0.09128400
H	9.04009500	6.47678300	0.13326800
H	10.76748000	4.70827400	0.09389300
H	7.74395400	1.63091500	0.04129900
N	6.24970900	5.82622700	0.15805300
C	6.20217600	7.27980200	0.17733400
H	6.11147200	7.70139100	-0.83171600
H	5.34856400	7.61173400	0.77450600
H	7.10984200	7.67164700	0.64209100
C	10.38806900	2.06314100	0.04302700
C	11.25559600	1.20054000	0.02163100
C	2.27006800	1.85675300	0.04791200
C	1.37787700	1.00850200	0.02837100
C	-15.46817300	2.15790500	0.01055000
C	-14.11318700	1.87050200	-0.00013600
C	-13.65208300	0.52840700	0.01074600
C	-14.61824000	-0.52637400	0.03323000
C	-16.00485900	-0.20818500	0.04379100
C	-16.41899800	1.11663700	0.03252600
H	-15.80372900	3.18916200	0.00206100
H	-13.38113000	2.67009700	-0.01689000
C	-12.24847800	0.18853100	0.00016800
C	-14.19606900	-1.88281200	0.04504200
H	-17.48222700	1.32700100	0.04105700
C	-12.83916100	-2.18384200	0.03494900
C	-11.87728800	-1.16329600	0.01286100
H	-12.54112700	-3.22607400	0.04437600
H	-10.82353400	-1.41639300	0.00500700
C	-17.01917700	-1.28296700	0.06685800
C	-15.18639000	-2.97155200	0.06788200
N	-16.54431000	-2.60693500	0.07741800
C	-17.52512900	-3.70772300	0.10044800
H	-18.51821300	-3.26460600	0.10486700
H	-17.38947000	-4.34222400	-0.77835000
H	-17.37201000	-4.32072400	0.99155800
O	-14.86826300	-4.18228300	0.07881800
O	-18.24701500	-1.04264700	0.07670800
C	-3.25405500	2.88858800	-0.07117500
C	-2.84899600	4.25445300	-0.09950300
C	-3.76700000	5.30177000	-0.12424500
C	-5.12842000	4.98108900	-0.12519800
C	-5.56923200	3.62940200	-0.09131600
C	-4.63331000	2.59256700	-0.06636800

H	-1.78656300	4.47014300	-0.09850200
H	-3.42357100	6.33059500	-0.13660000
H	-4.95353900	1.55626900	-0.04129400
C	-7.40095400	5.04584500	-0.12467900
C	-8.74814200	5.43259600	-0.12181400
C	-9.71780500	4.43574200	-0.09685900
C	-9.37056900	3.05583700	-0.06966800
C	-8.00799400	2.68260000	-0.06594900
C	-7.02339200	3.66701700	-0.09096300
H	-9.04003600	6.47678600	-0.13297600
H	-10.76743600	4.70826200	-0.09457600
H	-7.74392700	1.63089300	-0.04169500
N	-6.24965500	5.82624100	-0.15695700
C	-6.20215300	7.27982100	-0.17587800
H	-6.11210900	7.70119000	0.83332300
H	-5.34816600	7.61190700	-0.77242400
H	-7.10952900	7.67174800	-0.64113700
C	-10.38804900	2.06313300	-0.04414900
C	-11.25559300	1.20053900	-0.02316000
C	-2.27002100	1.85676900	-0.04634500
C	-1.37784100	1.00851100	-0.02670800

SCF Done: E(RB+HF-LYP) = -3754.94977082 a.u.

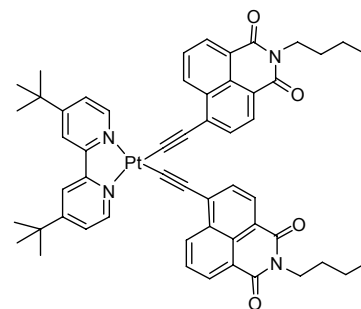
Number of Imaginary frequencies: 0

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

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1 Ground state geometry.

C	-4.46613800	3.40968300	0.11963000
C	-5.72242900	2.79322900	0.15860300
C	-5.72557800	1.39034900	0.12741000
C	-4.53826300	0.66343000	0.05781800
C	-3.30994400	2.63999700	0.05023000
C	-4.47593500	-0.81642800	0.02050800
C	-5.59752400	-1.64207200	0.07098100
C	-5.47841400	-3.03964400	0.03514800
C	-4.17667500	-3.54701300	-0.05586100
C	-3.08915000	-2.68124200	-0.10312700
H	-4.36368700	4.48734200	0.14059700
H	-2.32013200	3.08246700	0.01648800
H	-3.98604500	-4.61228300	-0.08919600
H	-2.06757600	-3.03940900	-0.17188200



N	-3.22652600	-1.34799300	-0.06567900
N	-3.33694000	1.30033800	0.01784000
Pt	-1.63203600	0.04902400	-0.11254600
C	-0.19139400	-1.25983800	-0.24312400
C	0.67258600	-2.12530400	-0.33587100
C	-0.30650700	1.47928200	-0.13666300
C	0.49627900	2.40608400	-0.14811800
H	-6.58025700	-1.19272500	0.14143900
H	-6.66901300	0.85925600	0.15597900
C	-6.73032400	-3.92646300	0.09512200
C	-7.04388300	3.57229200	0.22955900
C	-7.49662300	-3.63613800	1.40854900
H	-7.82257500	-2.59247500	1.47383400
H	-8.39139300	-4.26627100	1.46506800
H	-6.87487400	-3.85022500	2.28486800
C	-7.63804800	-3.60415700	-1.11684000
H	-8.53905000	-4.22723100	-1.08496400
H	-7.95952500	-2.55703700	-1.12356500
H	-7.12098700	-3.80355000	-2.06200500
C	-6.37967300	-5.42605700	0.05702100
H	-5.86211800	-5.70280000	-0.86840400
H	-5.75274400	-5.72188300	0.90574700
H	-7.29998900	-6.01733600	0.10715300
C	-7.90593600	3.22268100	-1.00785900
H	-8.13905000	2.15367800	-1.05886300
H	-8.85600900	3.76738900	-0.96656700
H	-7.39550000	3.50079400	-1.93658300
C	-7.80154400	3.17177000	1.51877200
H	-8.74741100	3.72156900	1.58106000
H	-8.03798700	2.10249400	1.54225200
H	-7.21296200	3.40639100	2.41257600
C	-6.81598800	5.09549700	0.25009800
H	-6.23279400	5.41123200	1.12248800
H	-6.30352200	5.44471300	-0.65334800
H	-7.78214700	5.60858400	0.29798800
C	1.68041900	-3.11951400	-0.44517000
C	2.86777600	-3.05946900	0.37092600
C	1.54402400	-4.17481400	-1.35215600
C	3.08836800	-2.02652700	1.31558900
C	3.86144100	-4.07460500	0.22621300
C	2.52833400	-5.16390700	-1.48055900
H	0.65529200	-4.21604500	-1.97388700
C	4.24189800	-1.99438900	2.07758000
H	2.32746900	-1.26035700	1.42936600
C	5.03597400	-4.02296500	1.02101100
C	3.67823100	-5.12706200	-0.70615200

H	2.40997300	-5.97609600	-2.19045200
C	5.22145000	-2.99609000	1.93111100
H	4.39426800	-1.19373900	2.79542100
H	6.13141100	-2.98528300	2.52219500
C	1.47347700	3.43515100	-0.15930300
C	2.87814000	3.10611000	-0.16720200
C	1.10215200	4.78298700	-0.15886900
C	3.34403600	1.76795500	-0.17193300
C	3.83811100	4.16276700	-0.16783400
C	2.05728500	5.80808900	-0.16356100
H	0.04608500	5.03421200	-0.15468500
C	4.69757900	1.48707500	-0.17137400
H	2.61267000	0.96563900	-0.18001800
C	5.22256800	3.85080900	-0.16922100
C	3.41292800	5.51567500	-0.16662800
H	1.75420600	6.85009400	-0.16351600
C	5.64263900	2.53122800	-0.16951200
H	5.03409600	0.45457900	-0.16999500
H	6.70839600	2.32692200	-0.16971300
C	6.07756300	-5.06883200	0.88390200
C	4.69668300	-6.18741900	-0.86656000
N	5.84136000	-6.08317000	-0.05453900
O	4.56688000	-7.11403400	-1.65850500
O	7.10870600	-5.07505800	1.54554400
C	6.88371500	-7.10642500	-0.17793000
H	7.83227000	-6.63745400	-0.45110200
H	7.01889700	-7.61712300	0.77906300
H	6.56704900	-7.80890200	-0.94556100
C	4.39419400	6.62208200	-0.16843100
C	6.23224400	4.93530600	-0.16939300
O	7.43945100	4.72574300	-0.16856000
O	4.06007100	7.80189500	-0.16791500
N	5.75170900	6.25312400	-0.17051100
C	6.76525600	7.31168600	-0.17252100
H	7.40101700	7.21510400	-1.05630400
H	6.24446300	8.26657300	-0.17673100
H	7.39826500	7.22185000	0.71403000

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SCF Done: E(RB+HF-LYP) = -2492.34147236 a.u.

Number of Imaginary frequencies: 0