

Electronic Supplementary Information for:

Effect of the regioisomeric naphthalimide acetylides ligands on the photophysical properties of $N^{\wedge}N$ Pt(II) bisacetylide complexes

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Table of Contents

1.0 NMR and HRMS spectra.....	S2
2.0 Absorption spectra.....	S15
3.0 Emission spectra.....	S16
4.0 TTA upconversion details.....	S17
5.0 Photosensitizing of $^1\text{O}_2$	S18
6.0 DFT calculations.....	S19
7.0 The coordinates of the optimized ground state geometries of complexes.....	S23
8.0 The coordinates of the optimized triplet state geometries of complexes.....	S31

1.0 NMR and HRMS spectra

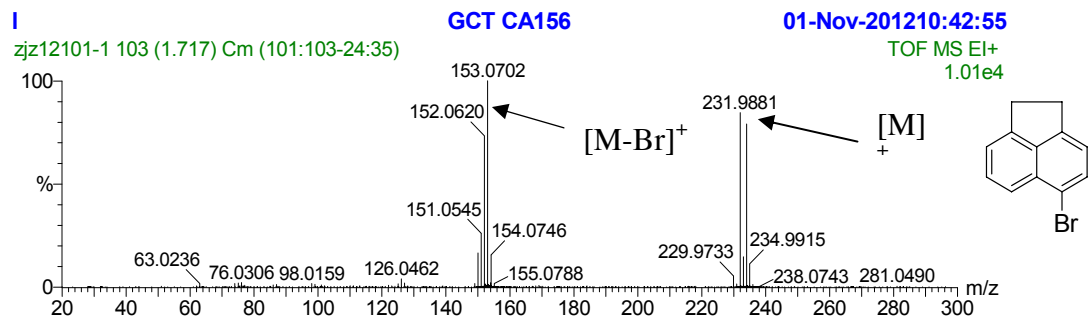


Figure S1. EI-HRMS of **1**.

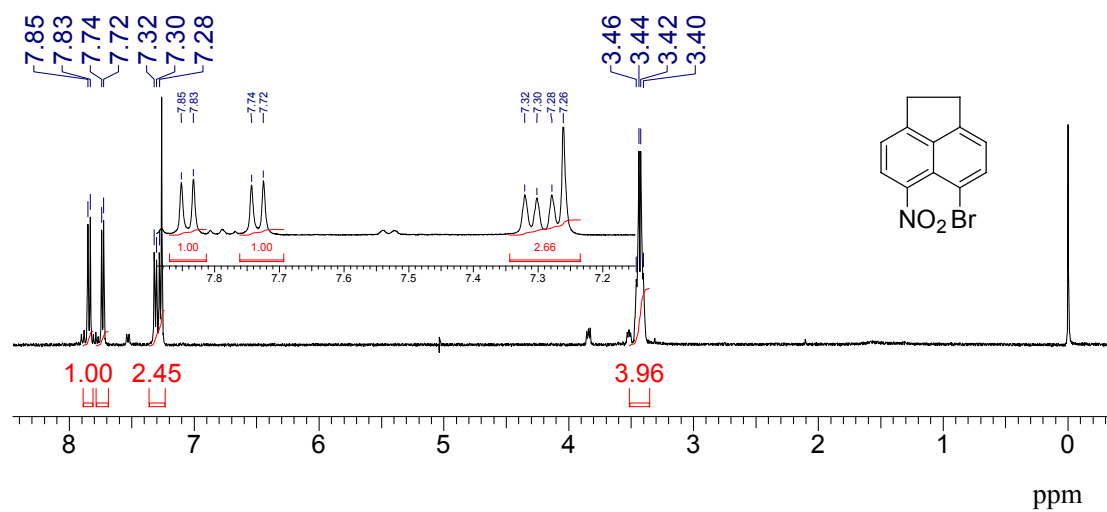


Figure S2. ¹H NMR of **2** (400 MHz, CDCl₃).

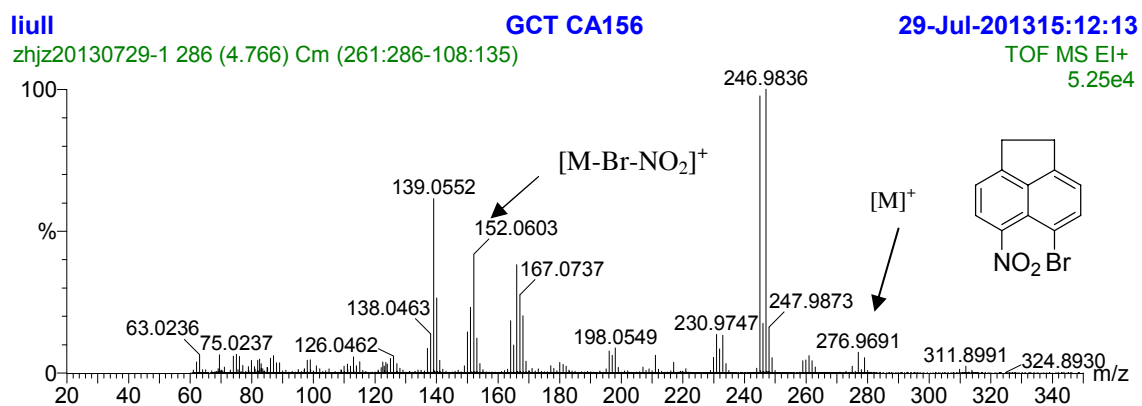


Figure S3. EI-HRMS of **2**.

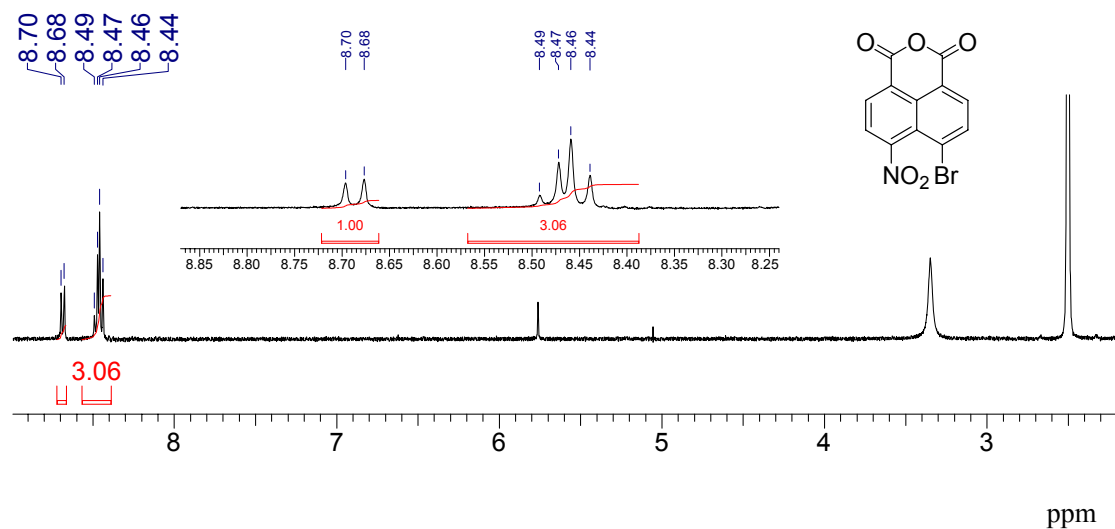


Figure S4. ¹H NMR of **3** (400 MHz, DMSO).

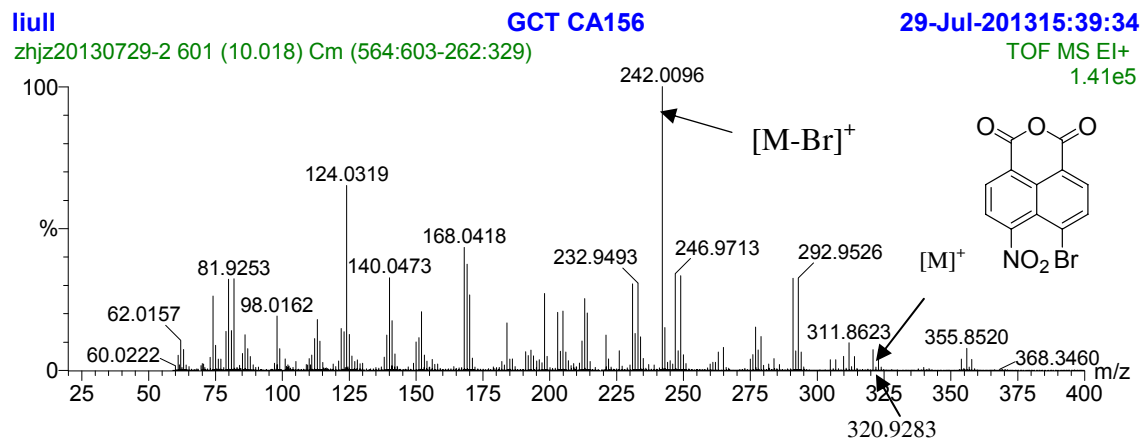


Figure S5. EI-MS of 3.

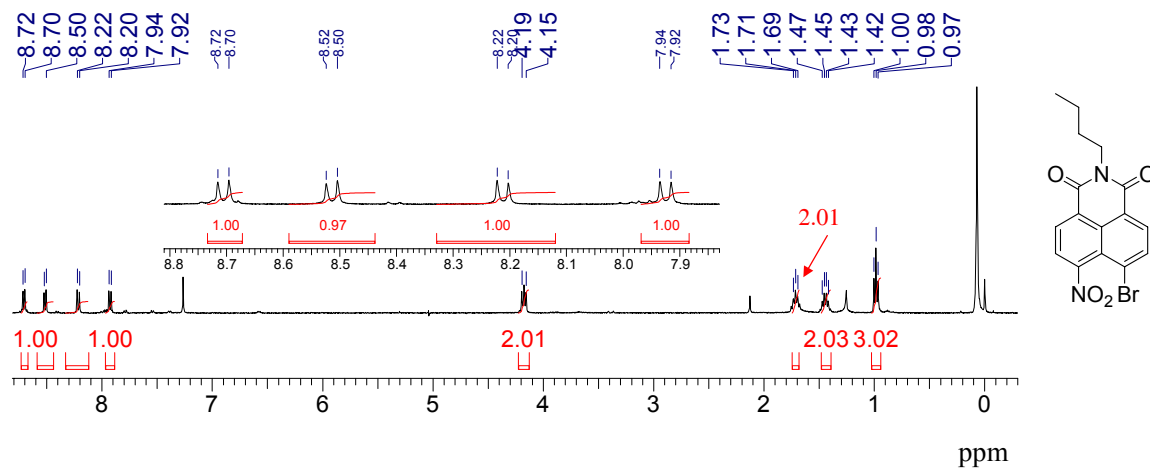


Figure S6. ^1H NMR of 4 (400 MHz, CDCl_3).

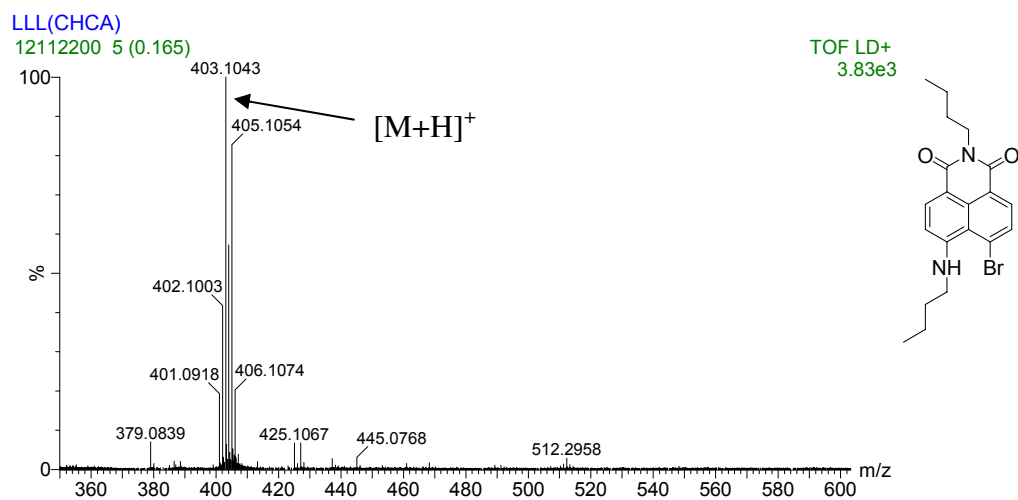


Figure S9. MALDI-HRMS of 5.

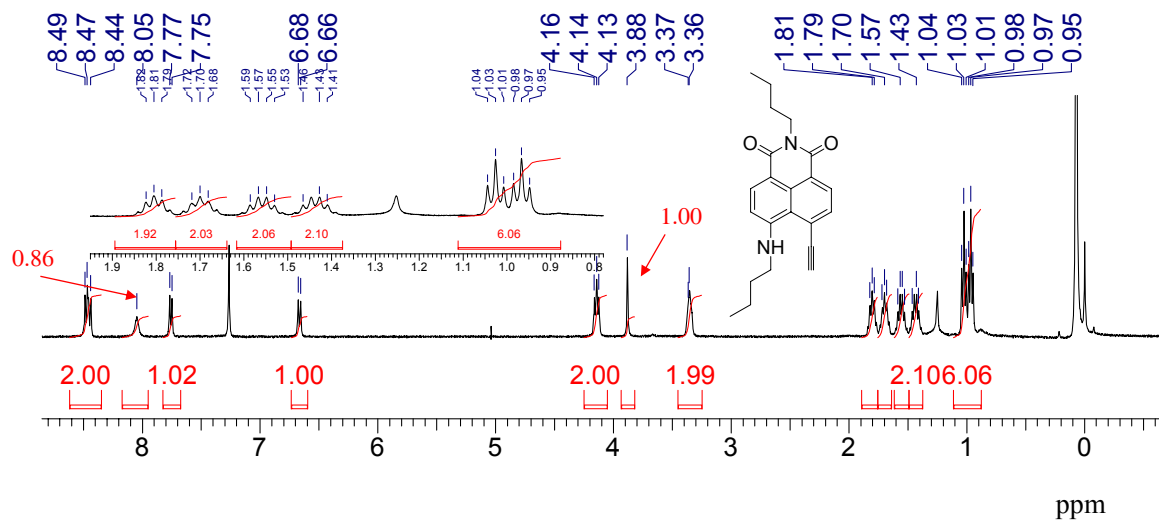


Figure S10. ¹H NMR of L-1 (400 MHz, CDCl₃).

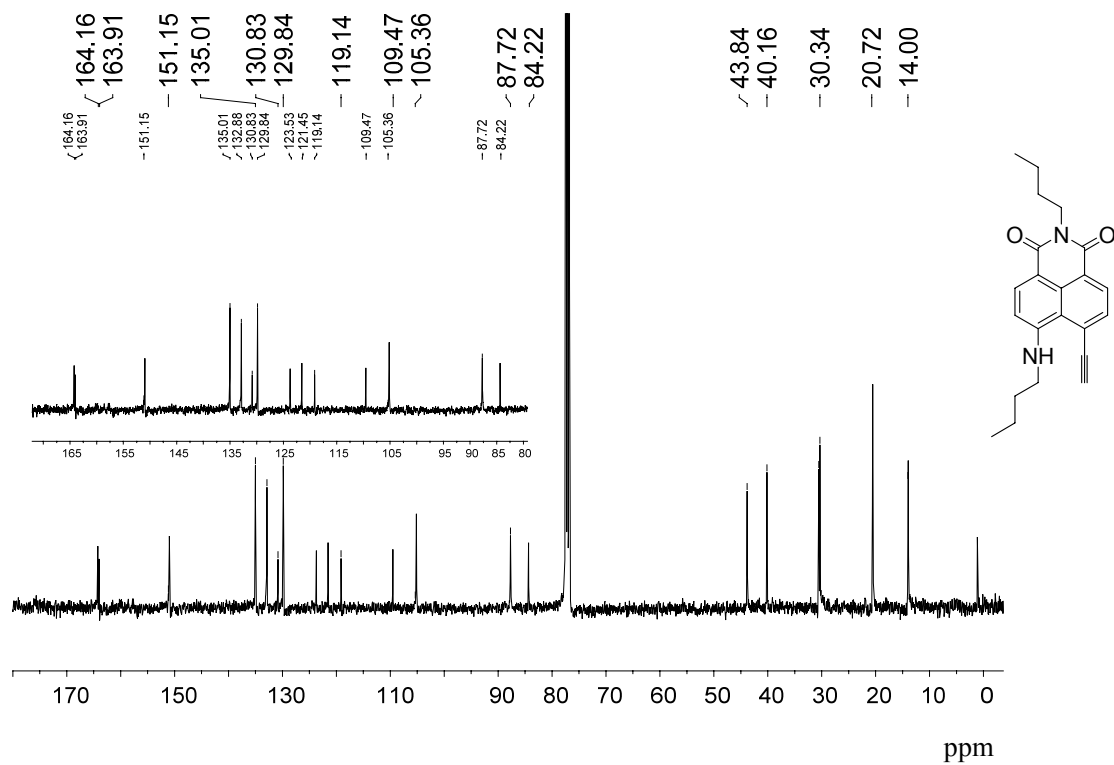


Figure S11. ¹³C NMR of L-1 (100 MHz, CDCl₃).

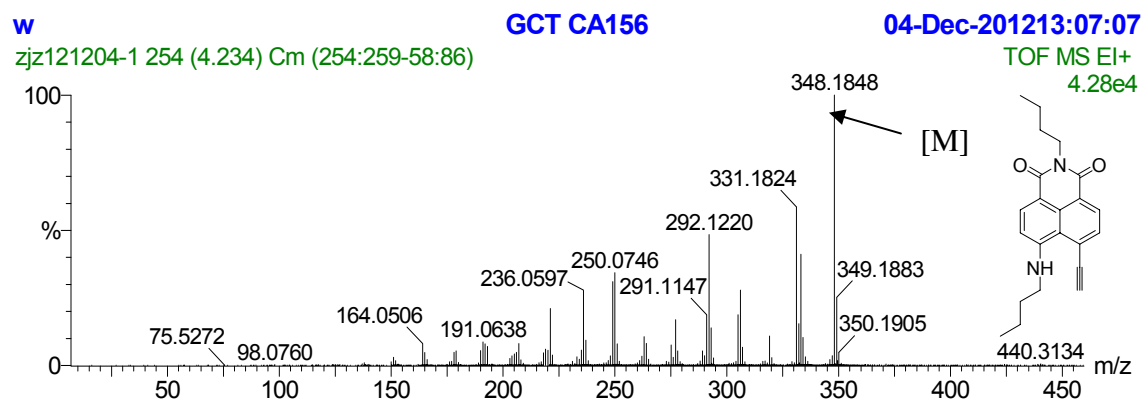


Figure S12. EI-HRMS of L-1.

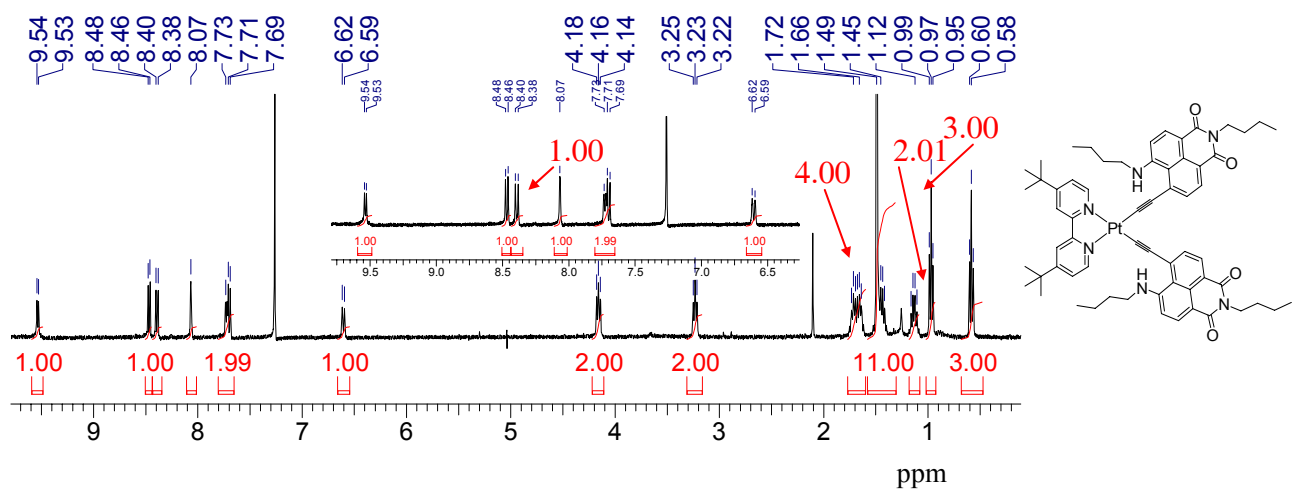


Figure S13. ¹H NMR of Pt-1 (400 MHz, CDCl₃).

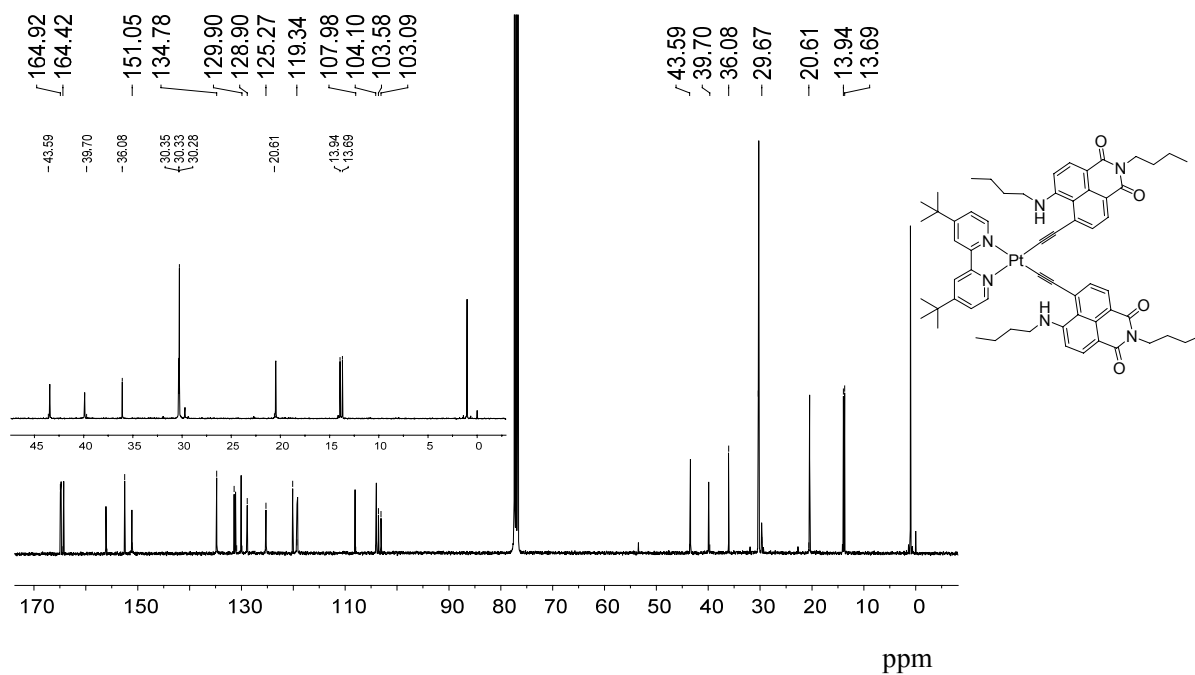


Figure S14. ¹³C NMR of Pt-1 (100 MHz, CDCl₃).

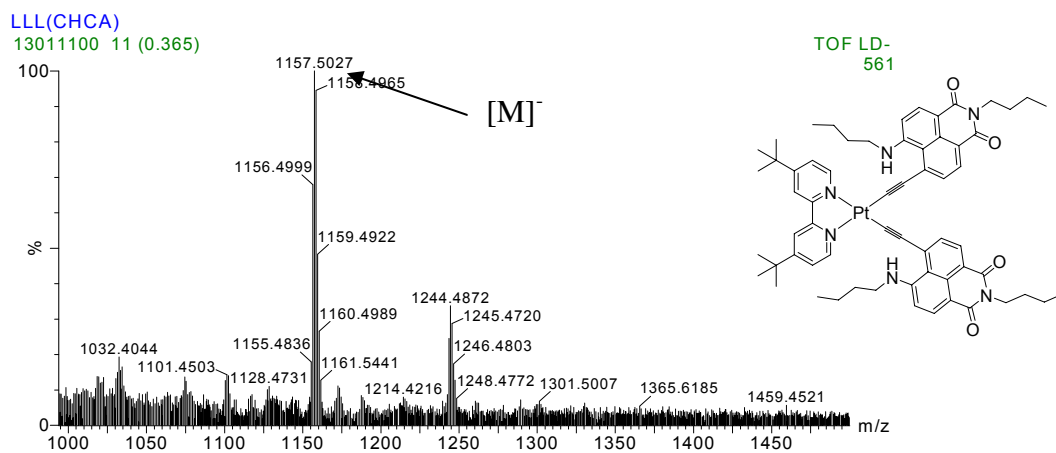


Figure S15. MALDI-HRMS of Pt-1.

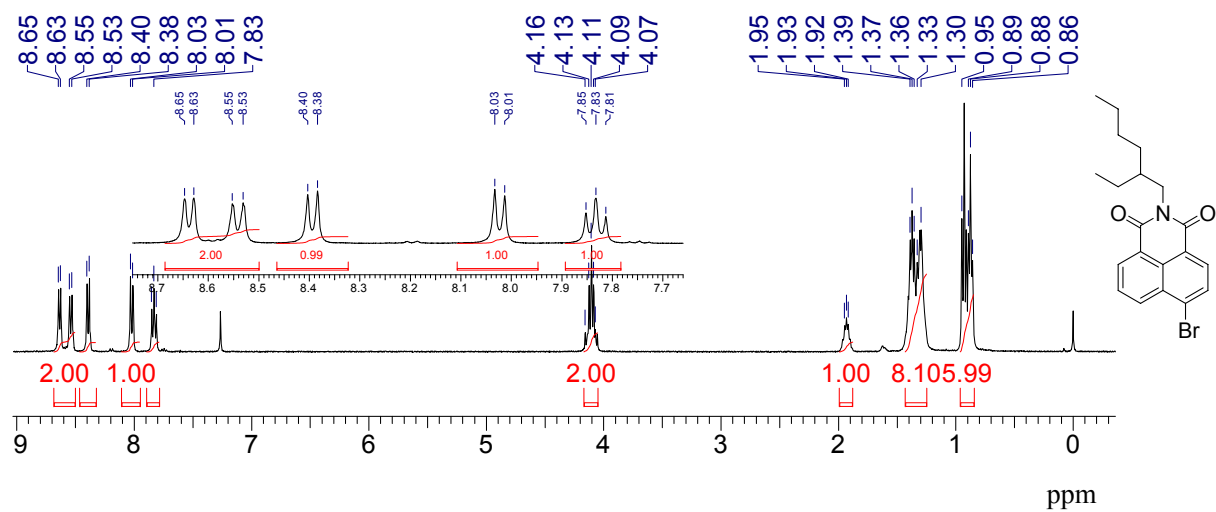
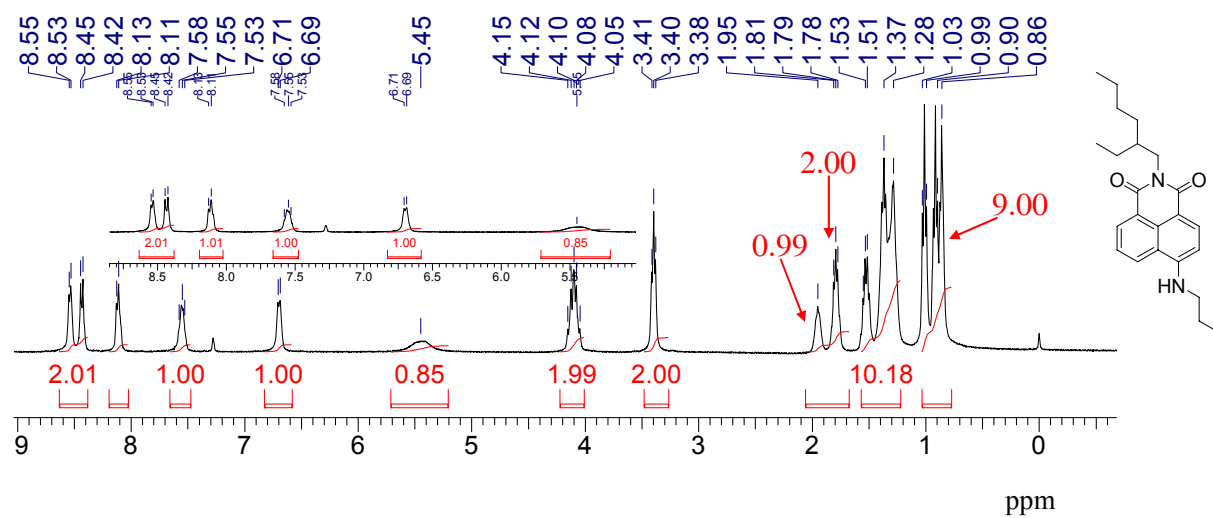
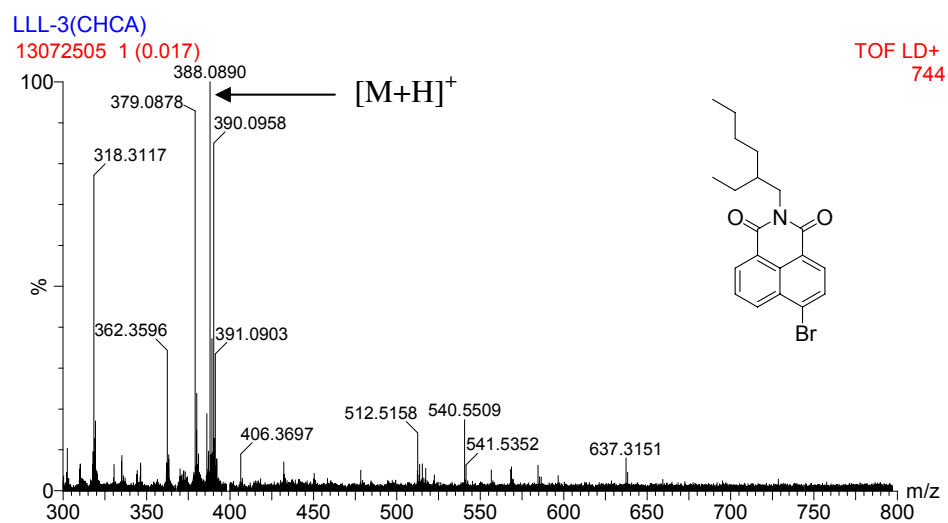


Figure S16. ¹H NMR of 6 (400 MHz, CDCl₃).



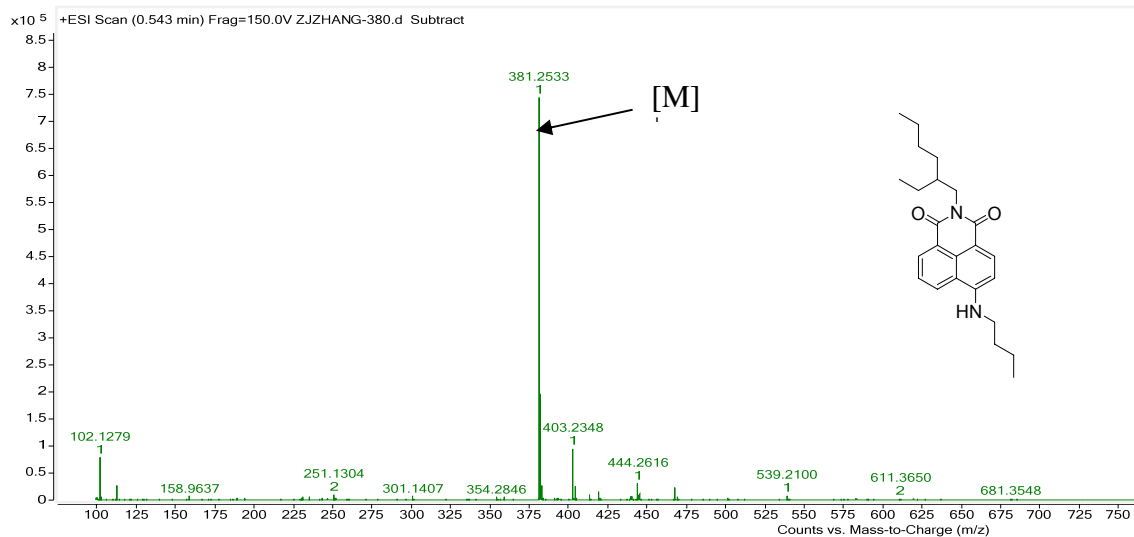


Figure S19. ESI-HRMS of **7**.

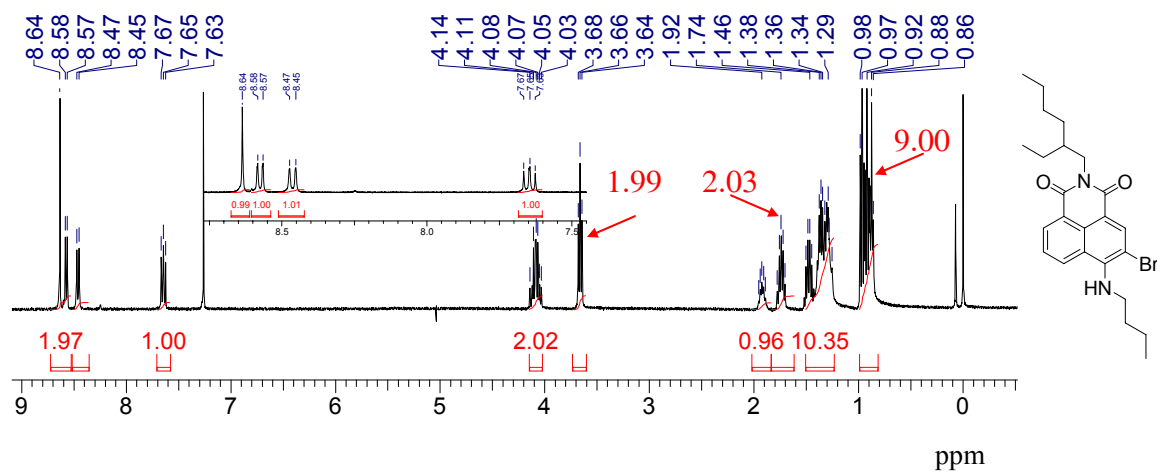


Figure S20. ^1H NMR of **8** (400 MHz, CDCl_3).

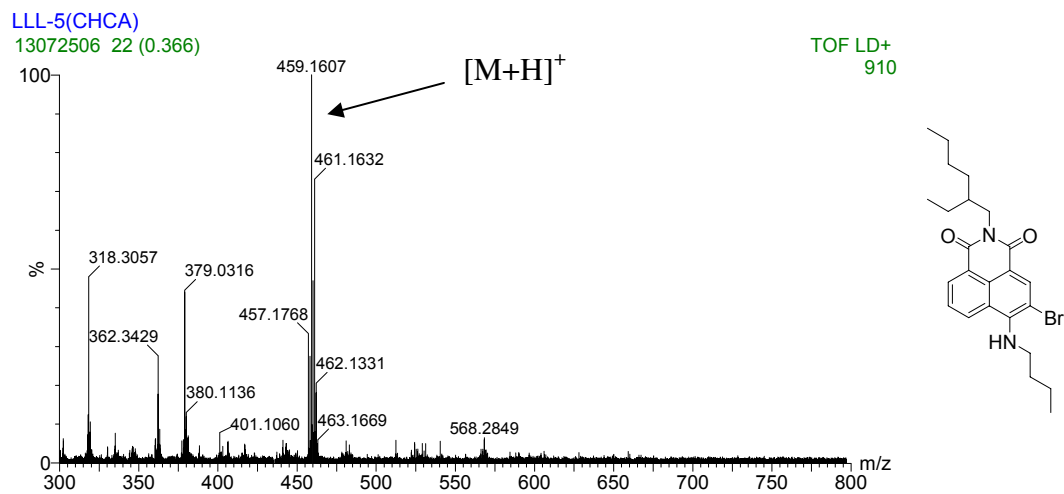


Figure S21. MALDI-HRMS of **8**.

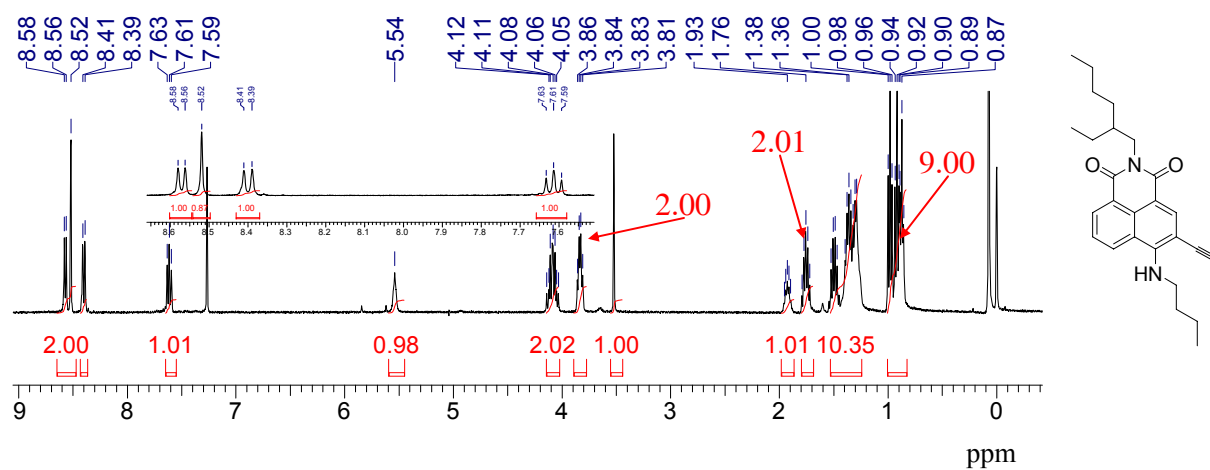


Figure S22. ^1H NMR of **L-2** (400 MHz, CDCl_3).

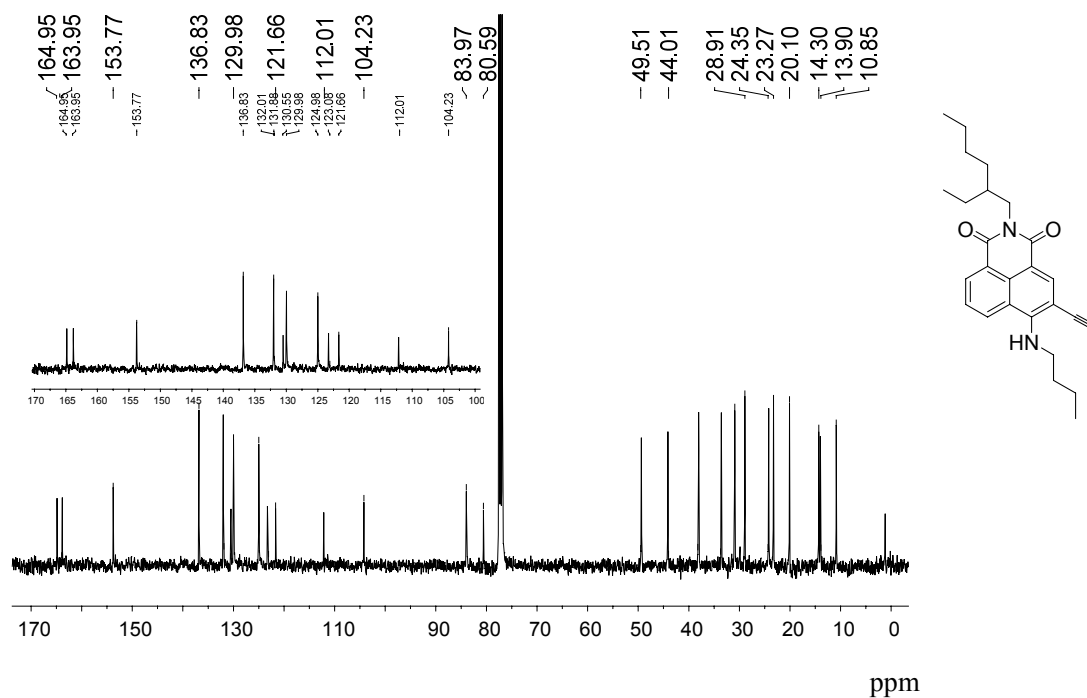


Figure S23. ¹³C NMR of L-2 (100 MHz, CDCl₃).

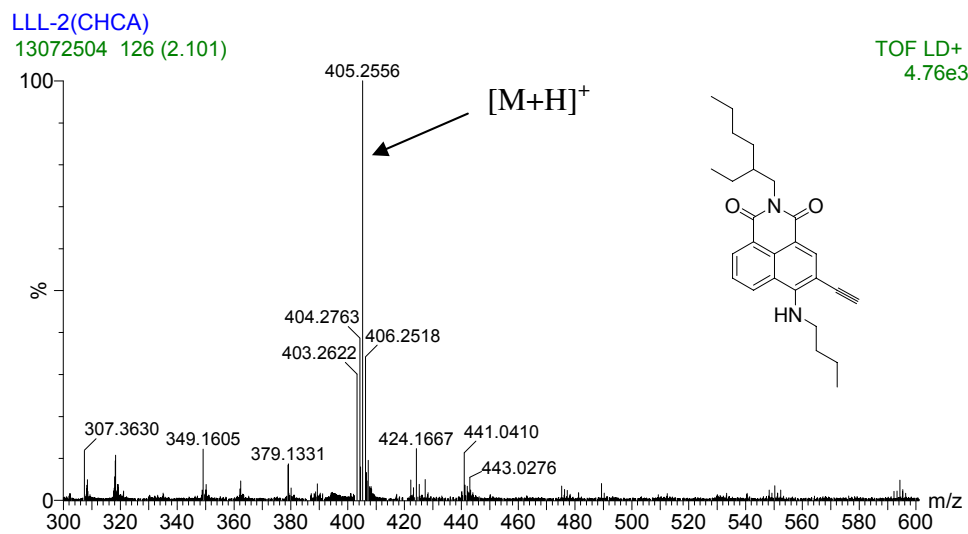


Figure S24. MALDI-HRMS of L-2.

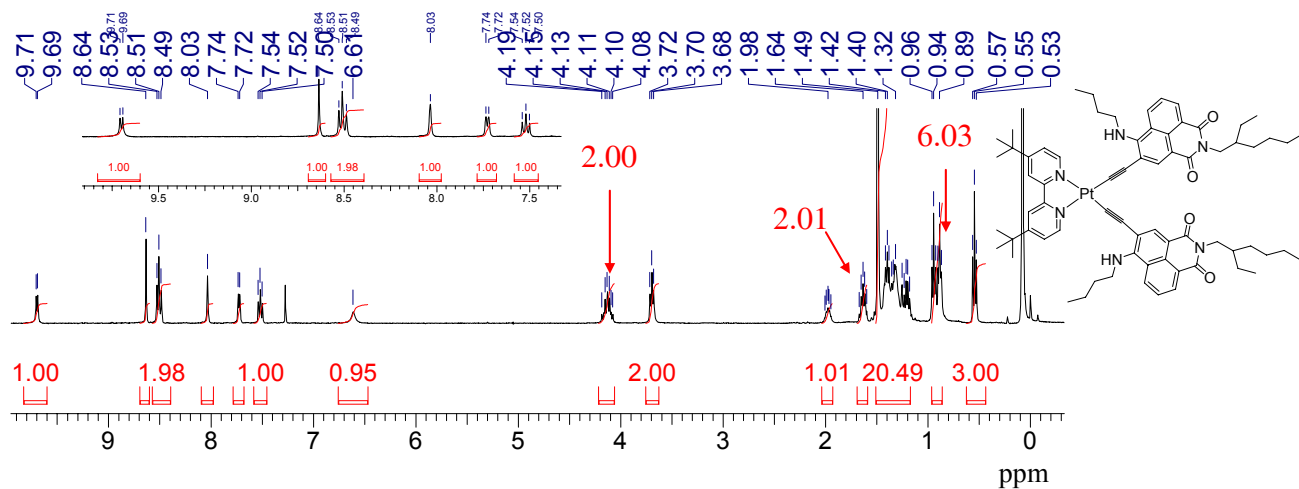


Figure S25. ¹H NMR of Pt-2 (400 MHz, CDCl₃).

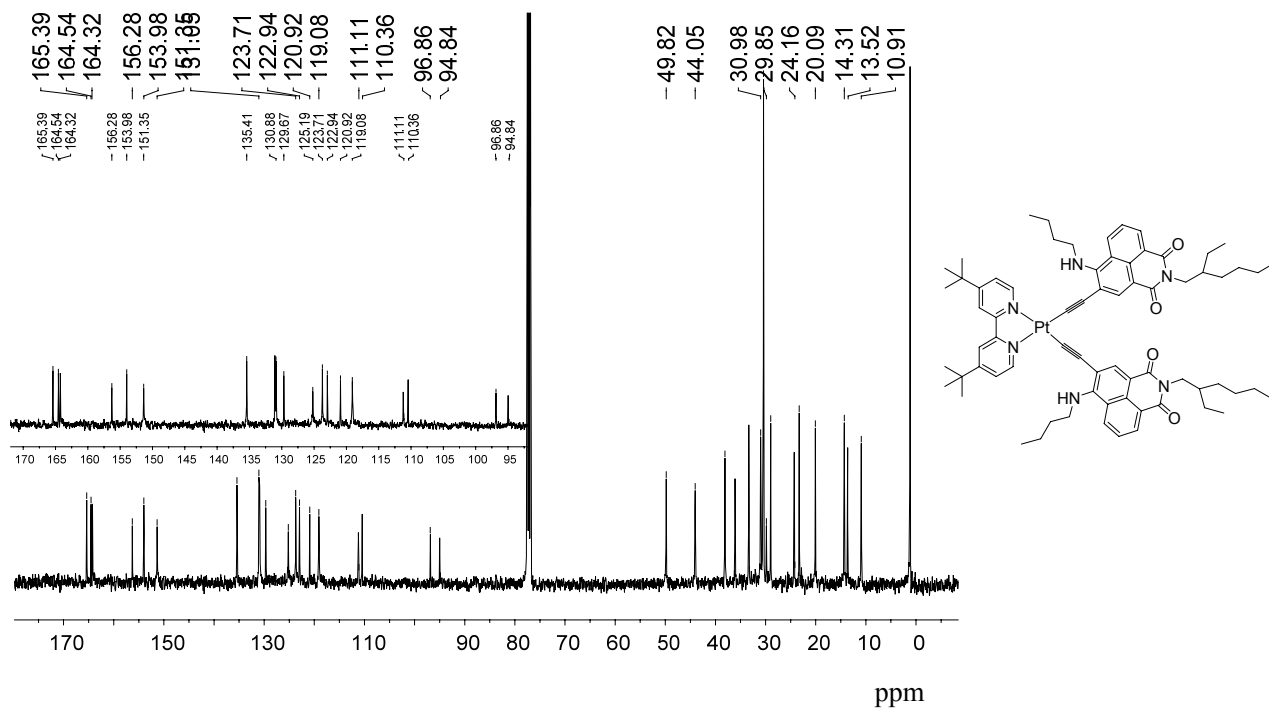


Figure S26. ¹³C NMR of Pt-2 (100 MHz, CDCl₃).

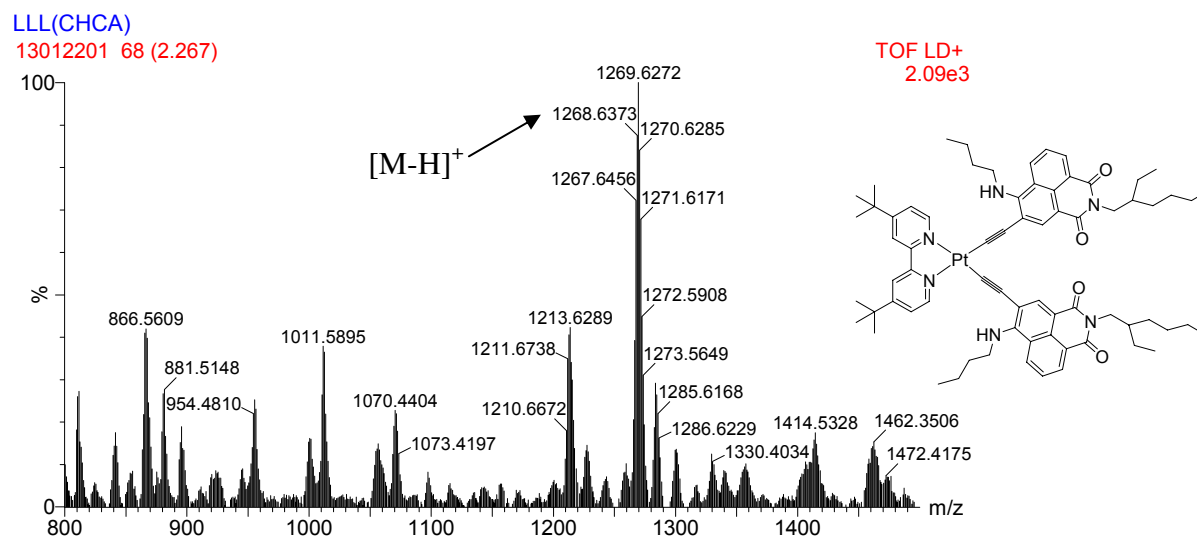


Figure S27. MALDI-HRMS of **Pt-2**.

2.0 Absorption spectra

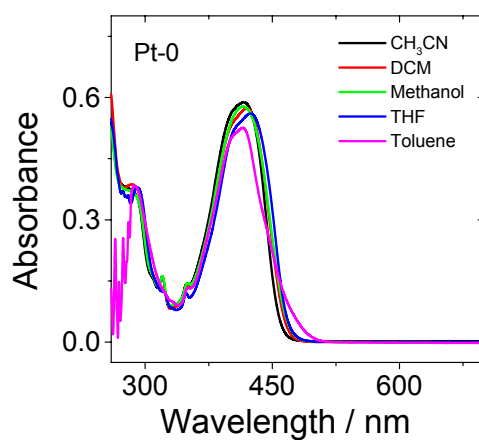


Figure S28. UV-Vis absorption of **Pt-0** in CH₃CN, DCM, Methanol, THF and toluene. $c = 1.0 \times 10^{-5}$ M, 20 °C.

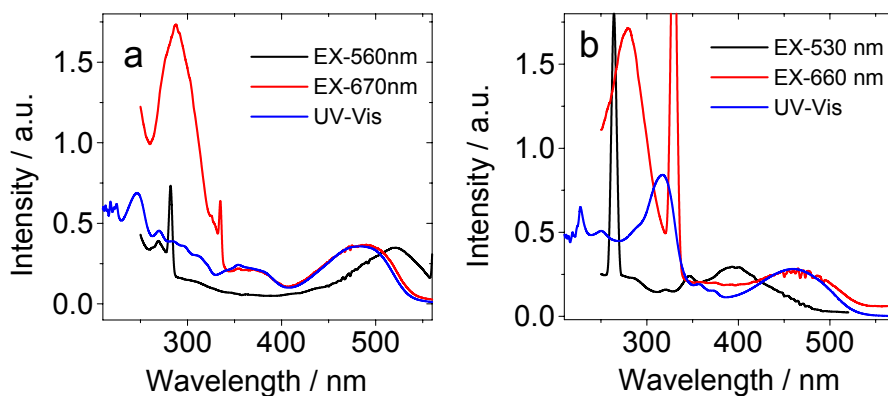


Figure S29. The excitation spectra (a) **Pt-1** ($\lambda_{em} = 560$ nm, 670 nm), (b) **Pt-2** ($\lambda_{em} = 530$ nm, 660 nm). In deaerated CH_2Cl_2 . $c = 1.0 \times 10^{-5}$ M, 20 °C.

3.0 Emission spectra

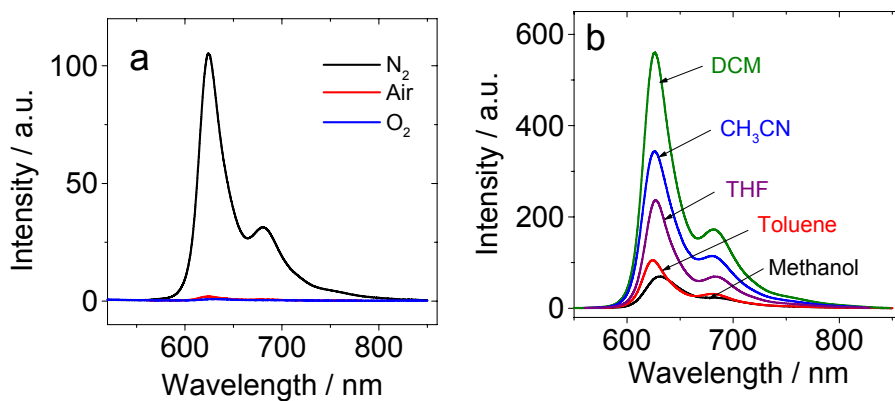


Figure S30. The emission spectra of (a) **Pt-0** ($\lambda_{ex} = 420$ nm) under different atmosphere and (b) in different solvent. $c = 1.0 \times 10^{-5}$ M, 20 °C. In Toluene. $c = 1.0 \times 10^{-5}$ M, 20 °C.

4.0 TTA upconversion details

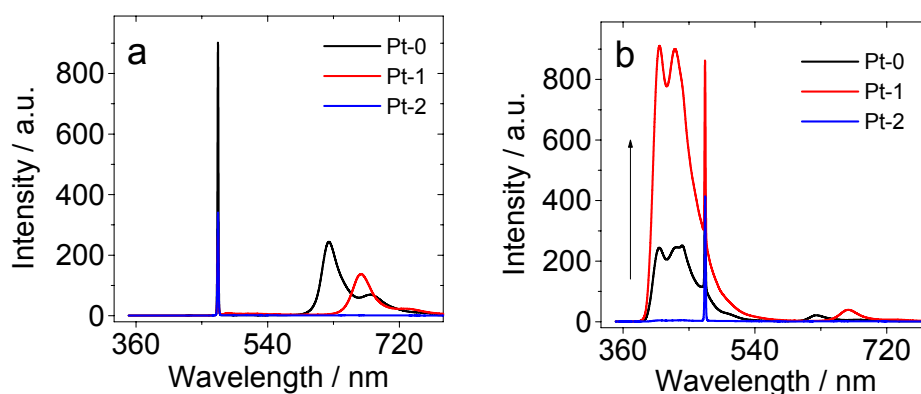


Figure S31. Emission and upconversion of the complexes with 473 nm (5 mW) laser excitation. (a) Emission of the complexes alone. (b) The up-converted DPA fluorescence and the residual fluorescence and phosphorescence of the complexes. c [DPA] = 3.0×10^{-5} M; c [sensitizers] = 0.5×10^{-5} M. In deaerated toluene. The asterisks in (a) and (b) indicate the scattered 473 nm excitation laser (5 mW). 20°C.

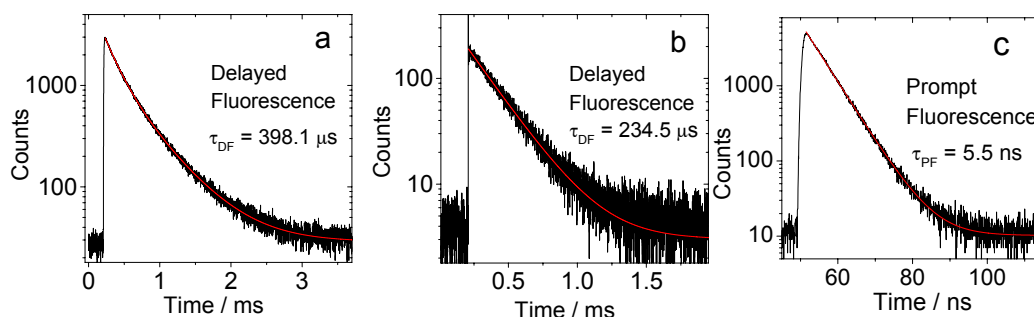


Figure S32. Delayed fluorescence observed in the TTA upconversion with (a) **Pt-1** and (b) **Pt-2** as triplet photosensitizer and DPA as the triplet acceptor. Excited at 532 nm and monitored at 410 nm. (c) The prompt fluorescence decay of DPA determined in a different experiment (excited with picosecond 405 nm laser, the decay of the emission was monitored at 410 nm). c [DPA] = 1.4×10^{-4} M; c [sensitizers] = 1.0×10^{-5} M. In deaerated toluene. 20°C.

5.0 Photosensitizing of $^1\text{O}_2$

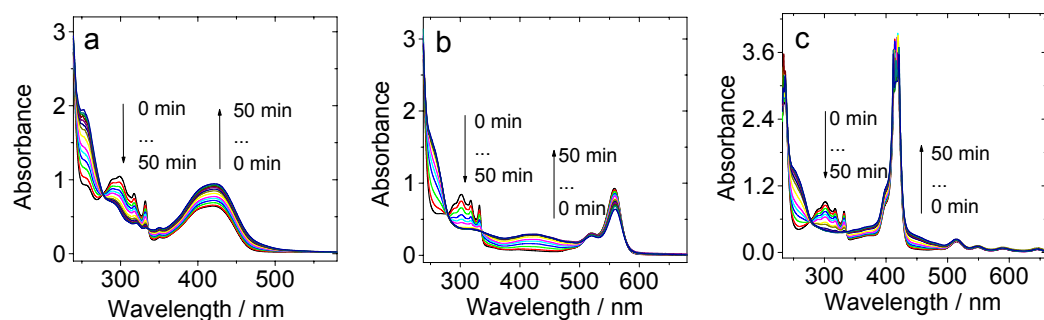


Figure S33. Photosensitizing of $^1\text{O}_2$ with the complexes as photosensitizers. Irradiation time-dependent decrease of absorbance at 301 nm of DHN (1.0×10^{-4} M) with different $^1\text{O}_2$ sensitizers (a) **Pt-0**, (b) **RM**, (c) **TPP**. c [sensitizers] = 1.0×10^{-5} M. In $\text{CH}_2\text{Cl}_2/\text{MeOH}$ (9:1, v/v), 12 mW/cm 2 , 20 °C.

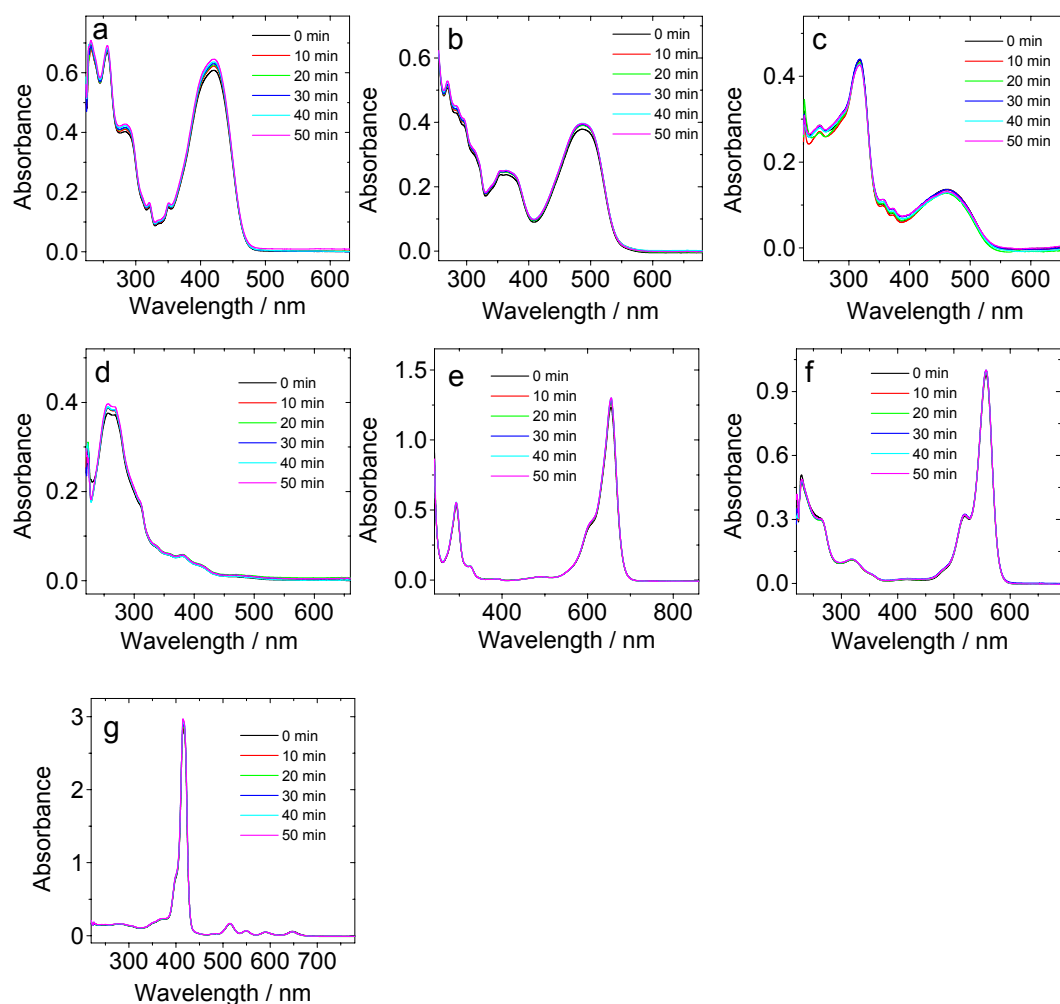


Figure S34. UV-vis absorption spectra of the sensitizers (a) **Pt-0**, (b) **Pt-1**, (c) **Pt-2**, (d) **Ir(ppy) $_2$ bpy**, (e) **MB**, (f) **RM**, (g) **TPP** in $\text{CH}_2\text{Cl}_2/\text{MeOH}$ (9 : 1 v/v) before and after the irradiation. c [sensitizers] = 1.0×10^{-5} M. 12 mW/cm 2 , 20 °C.

6.0 DFT calculations

Table 1. Electronic Excitation Energies (eV) and corresponding Oscillator Strengths (f), main configurations and CI coefficients of the Low-lying Electronically Excited States of complex **Pt-1**, Calculated by TDDFT//CAM-B3LYP/6-31G/LanL2DZ, based on the DFT//CAM-B3LYP/6-31G/LanL2DZ Optimized Ground State Geometries.

		TDDFT// CAM-B3LYP/6-31G				
Electronic transition		Energy (eV) ^a	f ^b	Composition ^c	CI ^d	character
Singlet	S ₀ →S ₁	2.34 eV 531 nm	0.0145	H→L	0.6948	LLCT
	S ₀ →S ₂	2.46 eV 504 nm	0.1308	H-2 →L	0.1308	MLCT
				H-1 →L	0.6844	MLCT
	S ₀ →S ₃	2.71 eV 458 nm	0.0049	H→L+1	0.6961	LLCT
	S ₀ →S ₄	2.78 eV 446 nm	0.4868	H-2 →L	0.4868	MLCT
				H →L+2	0.5290	ILCT
Triplet	T ₁ → S ₀	1.86 eV 665 nm	0.0000 ^e	H-1→L	0.2648	MLCT
				H-1→L+1	0.5789	ILCT
	T ₂ → S ₀	1.86 eV 665 nm	0.0000	H-1→L+1	0.1388	ILCT
				H →L+2	0.6452	ILCT
	T ₃ → S ₀	2.91 eV 425 nm	0.0000	H-2 →L+2	0.3706	MLCT

^a Only the selected low-lying excited states are presented. ^b oscillator strength. ^c H stands for HOMO and L stands for LUMO. Only the main configurations are presented. ^d The CI coefficients are in absolute values. ^e No spin-orbital coupling effect was considered, thus the f values are zero.

Table 2. Electronic Excitation Energies (eV) and corresponding Oscillator Strengths (f), main configurations and CI coefficients of the Low-lying Electronically Excited States of complex **Pt-2**, Calculated by TDDFT//CAM-B3LYP/6-31G/LanL2DZ, based on the DFT//CAM-B3LYP/6-31G/LanL2DZ Optimized Ground State Geometries.

	Electronic transition	TDDFT//B3LYP/6-31G				
		Energy (eV) ^a	f ^b	Composition ^c	CI ^d	character
Singlet	S ₀ →S ₁	2.26 eV 550 nm	0.0028	H-1→L	0.5689	LLCT
	S ₀ →S ₂	2.43 eV 509 nm	0.0028	H-1→L	0.6976	LLCT
	S ₀ →S ₃	2.63 eV 471 nm	0.0031	H →L+1	0.7050	LLCT
	S ₀ →S ₄	2.68 eV 463 nm	0.1365	H→L+2	0.6984	MLCT
Triplet	T ₁ → S ₀	1.96 eV 632 nm	0.0000 ^e	H→L+2	0.6025	MLCT
	T ₂ → S ₀	1.99 eV 622 nm	0.0000	H-1→L+1	0.6132	MLCT
	T ₃ → S ₀	2.95 eV 420 nm	0.0000	H-2→L	0.2199	MLCT
				H→L	0.3483	MLCT

^a Only the selected low-lying excited states are presented. ^b oscillator strength. ^c H stands for HOMO and L stands for LUMO. Only the main configurations are presented. ^d The CI coefficients are in absolute values. ^e No spin-orbital coupling effect was considered, thus the f values are zero.

Table 3. Electronic Excitation Energies (eV) and corresponding Oscillator Strengths (f), main configurations and CI coefficients of the Low-lying Electronically Excited States of complex **L-1**, Calculated by TDDFT//B3LYP/6-31G/LanL2DZ, based on the DFT//B3LYP/6-31G/LanL2DZ Optimized Ground State Geometries.

	Electronic transition	TDDFT//B3LYP/6-31G				
		Energy (eV) ^a	f ^b	Composition ^c	CI ^d	character
Singlet	S ₀ →S ₁	2.87 eV 432 nm	0.2795	H-1 →L	0.1117	ILCT
				H→L	0.6931	ILCT
	S ₀ →S ₂	3.68 eV 337 nm	0.0003	H-2 →L	0.6877	ILCT
	S ₀ →S ₃	3.75 eV 331 nm	0.1678	H-1→L	0.6830	ILCT
	S ₀ →S ₄	3.93 eV 316 nm	0.0122	H-3→L	0.5722	ILCT
				H→L+1	0.1809	
Triplet	T ₁ → S ₀	1.91 eV 650 nm	0.0000 ^e	H-1 →L	0.6789	ILCT
	T ₂ → S ₀	2.91 eV 423 nm	0.0000	H-1→L	0.6087	ILCT
				H →L	0.1304	
				H →L+1	0.2389	
	T ₃ → S ₀	3.41 eV 363 nm	0.0000	H-4 →L	0.1026	ILCT
				H-3 →L	0.6351	ILCT

^a Only the selected low-lying excited states are presented. ^b oscillator strength. ^c H stands for HOMO and L stands for LUMO. Only the main configurations are presented. ^d The CI coefficients are in absolute values. ^e No spin-orbital coupling effect was considered, thus the f values are zero.

Table 4. Electronic Excitation Energies (eV) and corresponding Oscillator Strengths (f), main configurations and CI coefficients of the Low-lying Electronically Excited States of complex **L-2**, Calculated by TDDFT//B3LYP/6-31G/LanL2DZ, based on the DFT//B3LYP/6-31G/LanL2DZ Optimized Ground State Geometries.

	Electronic transition	TDDFT//B3LYP/6-31G				
		Energy (eV) ^a	f ^b	Composition ^c	CI ^d	character
Singlet	S ₀ →S ₁	3.01 eV 411 nm	0.2430	H →L	0.6990	ILCT
	S ₀ →S ₂	3.76 eV 330 nm	0.0091	H-1 →L	0.4922	ILCT
	S ₀ →S ₃	3.83 eV 324 nm	0.0005	H-2→L	0.6872	ILCT
	S ₀ →S ₄	4.17 eV 300 nm	0.2288	H-1→L	0.4311	ILCT
				H→L+1	0.4107	ILCT
Triplet	T ₁ → S ₀	2.05 eV 606 nm	0.0000 ^e	H→L	0.6820	ILCT
	T ₂ → S ₀	3.22 eV 385 nm	0.0000	H-1→L	0.1045	ILCT
				H →L+1	0.5474	
	T ₃ → S ₀	3.32 eV 374 nm	0.0000	H-1→L+1	0.1190	ILCT

^a Only the selected low-lying excited states are presented. ^b oscillator strength. ^c H stands for HOMO and L stands for LUMO. Only the main configurations are presented. ^d The CI coefficients are in absolute values. ^e No spin-orbital coupling effect was considered, thus the f values are zero.

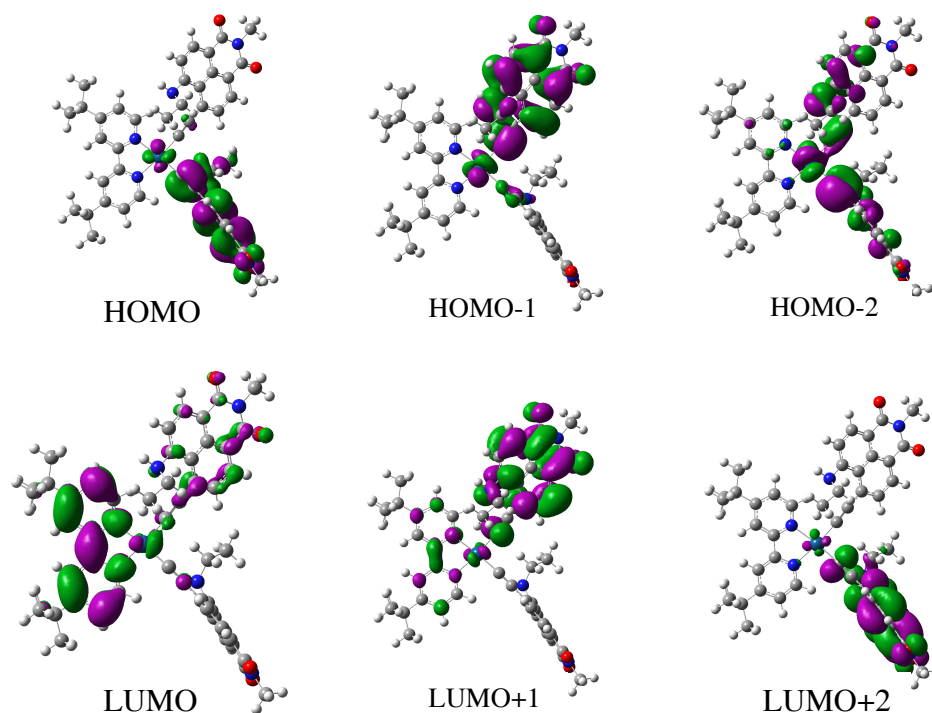


Figure S35. Electron density maps of the frontier molecular orbitals of complex **Pt-1** based on the optimized ground-state geometry. The solvent toluene was considered in the calculations (PCM model). Calculated at the CAM-B3LYP/6-31G/LANL2DZ level with Gaussian 09W.

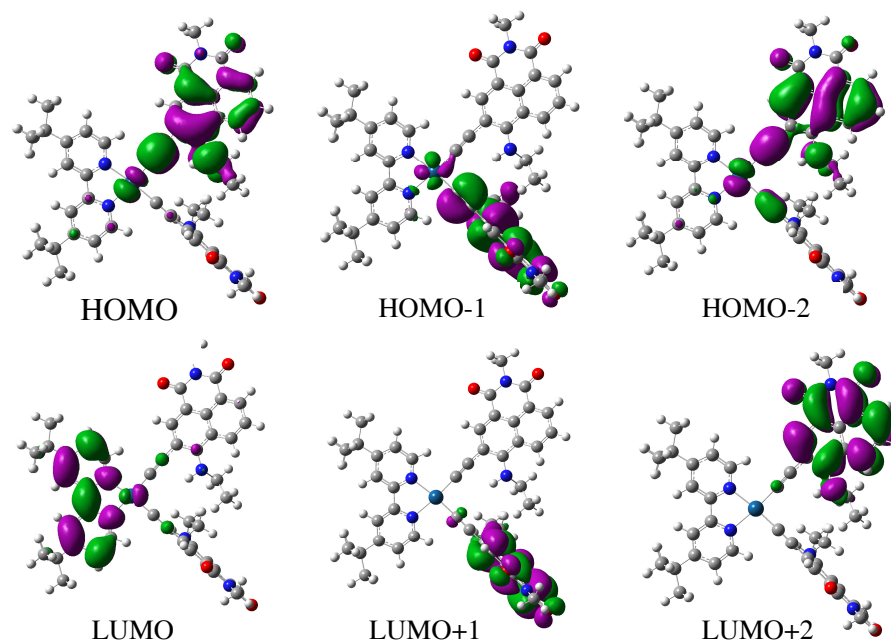


Figure S36. Electron density maps of the frontier molecular orbitals of complex **Pt-2** based on the optimized ground-state geometry. The solvent toluene was considered in the calculations (PCM model). Calculated at the CAM-B3LYP/6-31G/LANL2DZ level with Gaussian 09W.

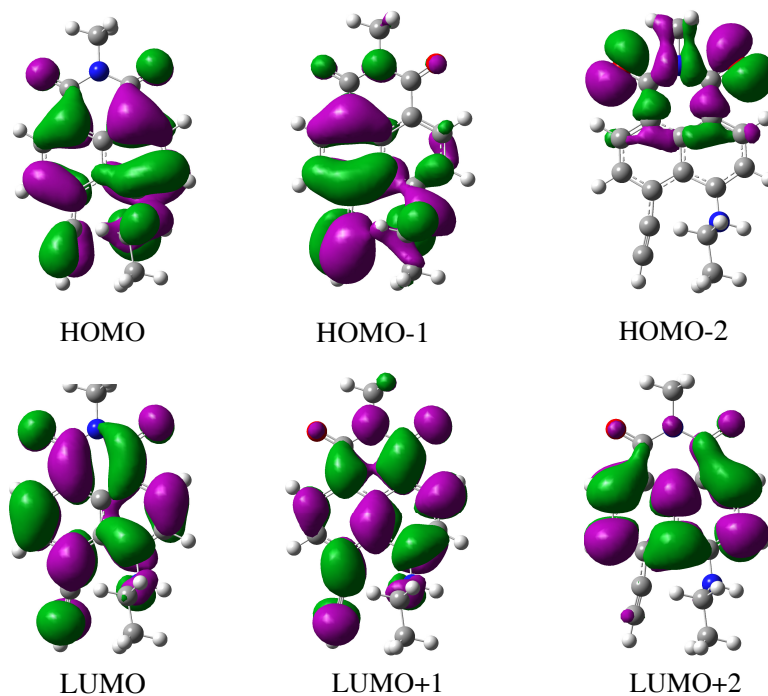


Figure S37. Electron density maps of the frontier molecular orbitals of complex **L-1** based on the optimized ground-state geometry. The solvent toluene was considered in the calculations (PCM model). Calculated at the B3LYP/6-31G/LANL2DZ level with Gaussian 09W.

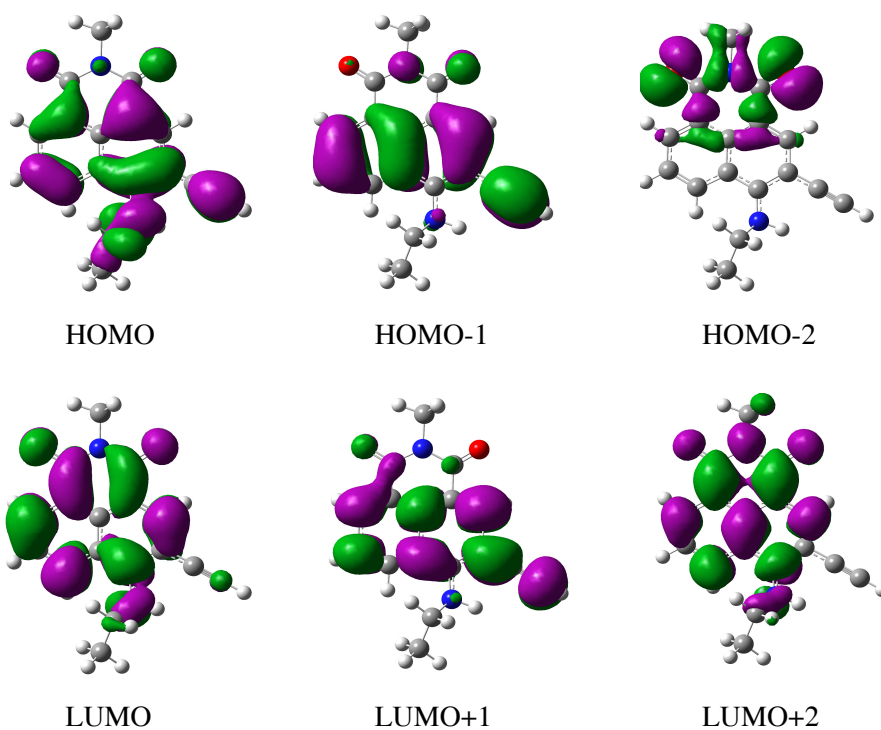


Figure. S38 Electron density maps of the frontier molecular orbitals of complex **L-2** based on the optimized ground-state geometry. The solvent toluene was considered in the calculations (PCM model). Calculated at the B3LYP/6-31G/LANL2DZ level with Gaussian 09W.

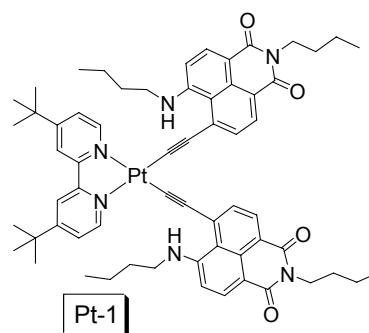
7.0 The coordinates of the optimized ground state geometries of complexes

Complex Pt-1 (DFT//B3LYP/GENECP/LanL2DZ)

Symbolic Z-matrix :

Charge = 0 Multiplicity = 1

C	-2.66495426	7.06476056	3.36979339
C	-3.16315679	8.16121495	2.65843438
C	-3.63348088	7.89863654	1.36266105
C	-3.60040259	6.61253407	0.82622639
C	-2.65150966	5.79753970	2.79350413
C	-4.08245582	6.27560869	-0.53433411
C	-4.61921777	7.20979321	-1.41870037
C	-5.06078361	6.83498154	-2.69686783
C	-4.93022542	5.48138853	-3.02427312
C	-4.38801797	4.58365498	-2.10873109
H	-2.27862397	7.16066346	4.37661210
H	-2.26758031	4.93813485	3.33469444
H	-5.24080872	5.09013408	-3.98478877
H	-4.28113447	3.53050046	-2.35019518
N	-3.97253474	4.96683830	-0.89130036
N	-3.10731932	5.57168202	1.55140561
Pt	-3.13404199	3.68768903	0.57789385
H	-4.69533006	8.24498227	-1.10925420
H	-4.03100654	8.70902579	0.76398901
C	-5.64847494	7.88404348	-3.65246445
C	-3.21079530	9.58758754	3.22611843
C	-6.89433826	8.52832505	-2.99806007
H	-6.65125093	9.02665397	-2.05336979
H	-7.32414263	9.28084219	-3.66954149
H	-7.66450215	7.77653795	-2.79275400
C	-4.58593952	8.97549669	-3.92678598
H	-4.99263909	9.73258736	-4.60745814
H	-4.27528963	9.48677844	-3.00920634
H	-3.69132006	8.54623984	-4.39141932
C	-6.07060094	7.26630317	-4.99910584
H	-5.22253221	6.81428000	-5.52531880
H	-6.84364645	6.50016871	-4.87306864
H	-6.48257399	8.04803440	-5.64658390



C	-2.37036685	10.52337504	2.32417793
H	-2.74883893	10.55303895	1.29668516
H	-2.39633204	11.54642622	2.71736456
H	-1.32419900	10.19983348	2.28754114
C	-4.67897175	10.07673502	3.25265603
H	-4.72800923	11.09530371	3.65516821
H	-5.12497698	10.09337737	2.25232271
H	-5.29780399	9.43104285	3.88559929
C	-2.64831665	9.65803877	4.65855997
H	-3.22000277	9.03299686	5.35350180
H	-1.59872404	9.34665057	4.70143968
H	-2.70189020	10.69013831	5.02181491
C	-2.36308053	2.51156105	1.92876076
C	-2.21553594	0.51936378	4.80443368
C	0.00246500	0.48611743	3.75863868
C	-3.57309404	0.92179780	4.86792337
C	-1.70652485	-0.32801363	5.83424939
C	0.48239212	-0.34660521	4.78067845
H	0.66774468	0.79867625	2.96073095
C	-4.38702544	0.50417535	5.90252178
C	-2.56136165	-0.74436106	6.88684094
C	-0.35381272	-0.75188841	5.80775999
H	1.51330071	-0.68288460	4.78140535
C	-3.88189740	-0.33305850	6.91790725
H	-5.42471288	0.82126046	5.93750725
H	-4.51393178	-0.66594435	7.73415087
C	-2.04674289	-1.62444740	7.96513586
C	0.18809573	-1.63274412	6.87569722
N	-0.70154029	-2.01022952	7.89038047
O	-2.74495970	-2.01197311	8.89316632
O	1.35275179	-2.01185858	6.87338806
C	-0.21265171	-2.87762907	8.97009467
H	0.83870383	-3.08114536	8.78281040
H	-0.34032759	-2.37587487	9.93188526
H	-0.78530185	-3.80781776	8.98492116
C	-1.32279654	0.92457234	3.75153053
C	-1.88816827	1.78706620	2.76089478
C	-3.15848632	1.96432263	-0.31261766
C	-2.21106539	-0.78434588	-2.48948005
C	-4.28431351	-1.19742448	-1.24636743

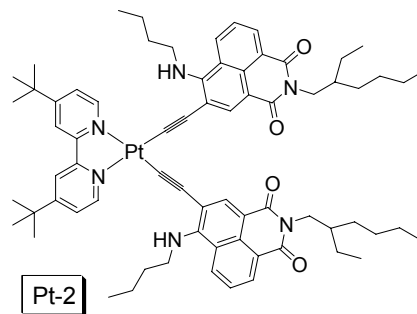
C	-1.07546119	-0.00441743	-2.82274088
C	-2.39376008	-2.03843507	-3.14640018
C	-4.44478510	-2.42647152	-1.90364558
H	-5.01873864	-0.87720199	-0.51491403
C	-0.16462587	-0.44649749	-3.76201239
C	-1.44492079	-2.47188756	-4.10757813
C	-3.51731984	-2.84787373	-2.84205799
H	-5.29643114	-3.06192072	-1.68740446
C	-0.34721376	-1.68561055	-4.40883771
H	0.70010052	0.16248611	-4.00685811
H	0.36306749	-2.04071328	-5.14771299
C	-1.62146527	-3.77264482	-4.79965250
C	-3.71924191	-4.15485217	-3.52109874
N	-2.75124648	-4.53008851	-4.46222153
O	-0.82991326	-4.19106681	-5.63469254
O	-4.68166036	-4.87101775	-3.27408786
C	-2.90801203	-5.81164691	-5.16237112
H	-3.82515380	-6.27465735	-4.80696280
H	-2.95862676	-5.63887024	-6.23972243
H	-2.04962320	-6.45429886	-4.95364615
C	-3.19163988	-0.37305967	-1.52040833
C	-3.17362164	0.89725680	-0.86400035
N	-0.68508359	1.32529534	-2.33246618
H	-0.63814615	1.96337989	-3.10100049
C	0.63154764	1.24140604	-1.68412616
H	0.75725410	2.07334300	-1.02308246
H	0.69744112	0.33016897	-1.12716561
C	1.73511433	1.26765484	-2.75792854
H	2.52521423	1.91617039	-2.44159052
H	2.11972611	0.27909049	-2.89833619
H	1.32716618	1.62594147	-3.67994210
N	-4.32012248	1.81581998	3.97150110
H	-4.57373040	2.64741634	4.46559677
C	-5.53537449	1.13507217	3.50177250
H	-5.26612581	0.22426561	3.00898802
H	-6.16670251	0.91540371	4.33727875
C	-6.28737163	2.04894691	2.51641303
H	-6.00685776	3.06698228	2.68908606
H	-6.03601917	1.77499409	1.51308268
H	-7.34172928	1.93982900	2.66243778

Complex Pt-2 (DFT//B3LYP/GENECP/LanL2DZ)

Symbolic Z-matrix :

Charge = 0 Multiplicity = 1

C	-0.30707600	-5.48655000	-0.04372900
C	0.88385400	-6.20703700	-0.08192600
C	2.06443300	-5.45807700	-0.11758000
C	2.03362500	-4.07313400	-0.11355500
C	-0.28091900	-4.10092600	-0.04275700
C	3.24850400	-3.22323900	-0.14862300
C	4.53814900	-3.72753900	-0.18389700
C	5.64652700	-2.87504000	-0.21493900
C	5.37890000	-1.50861800	-0.20859800
C	4.06886200	-1.05756600	-0.17303800
H	-1.26830100	-5.98156600	-0.01485900
H	-1.18848500	-3.50950000	-0.01462800
H	6.17331600	-0.77483400	-0.23063100
H	3.82567700	-0.00162500	-0.16784300
N	3.02555400	-1.88906900	-0.14332600
N	0.85758600	-3.40573400	-0.07628600
Pt	1.00623600	-1.30492600	-0.08636100
H	4.68853200	-4.79874600	-0.18698000
H	3.01857300	-5.96687800	-0.14933600
C	7.06035500	-3.45393600	-0.25452700
C	0.94144400	-7.73435000	-0.08708200
C	7.28264800	-4.32690500	0.99434200
H	6.57818100	-5.16242500	1.04390100
H	8.29351300	-4.74616900	0.97709700
H	7.17491000	-3.73815700	1.91063900
C	7.21527200	-4.31499000	-1.52170900
H	8.22465900	-4.73626300	-1.56133300
H	6.50669000	-5.14827700	-1.54238200
H	7.06112800	-3.71693700	-2.42521300
C	8.12932400	-2.35559200	-0.27747200
H	8.03859700	-1.71612400	-1.16100100
H	8.08356900	-1.72279000	0.61435900
H	9.12114800	-2.81587600	-0.30444000



C	1.64104500	-8.20619500	-1.37516100
H	2.66408000	-7.82624700	-1.44977600
H	1.69081200	-9.29945300	-1.39027400
H	1.09255200	-7.87874800	-2.26377900
C	1.74017200	-8.21242700	1.13955700
H	1.78961300	-9.30575000	1.14585600
H	2.76661800	-7.83421000	1.13469500
H	1.26433100	-7.88851700	2.07038600
C	-0.45641800	-8.36121300	-0.03365500
H	-0.99598800	-8.07813400	0.87560900
H	-1.06388300	-8.07848900	-0.89908500
H	-0.36491300	-9.45107500	-0.03726800
C	-5.54415700	-0.23712400	1.47034500
C	-7.59112300	-0.08014000	2.77360900
C	-4.12237300	-0.37930300	1.36932200
C	-6.31719800	-0.15721300	0.28464100
C	-8.34242600	0.06673500	1.59538100
H	-8.09423200	-0.08725300	3.73458100
C	-3.53550300	-0.55947100	0.10871700
C	-5.69390100	-0.28737000	-0.97726500
C	-7.71796900	0.01479400	0.36972300
H	-9.41821800	0.19589800	1.62813300
C	-4.33985600	-0.51222900	-1.04922800
H	-3.87825600	-0.62815000	-2.02321800
C	-6.48786200	-0.20950500	-2.21313000
C	-8.53625600	0.12099600	-0.85973900
N	-7.86175800	0.00624400	-2.07478000
O	-6.00570200	-0.32179600	-3.32960000
O	-9.74408200	0.29688700	-0.82335000
C	-8.62823700	0.09533400	-3.31407200
H	-9.66688600	0.27310400	-3.05008000
H	-8.24590500	0.91219700	-3.92848900
H	-8.53326300	-0.83420300	-3.87834600
C	-6.22639800	-0.23349500	2.71155300
H	-5.65996100	-0.39163300	3.62151900
N	-3.33055200	-0.40396200	2.51438900
H	-2.39177800	-0.70316000	2.25814100
C	-3.23718200	0.80178700	3.35237500
H	-2.66847800	1.58615200	2.83106300
H	-4.23874800	1.20053600	3.51749100

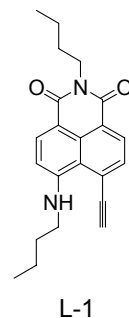
C	-2.12318800	-0.76472700	0.00868800
C	-0.91791300	-0.94584000	-0.02722000
C	2.71454071	5.06516754	-1.62284780
C	3.71136063	6.91627138	-2.84731588
C	2.34588857	3.68358195	-1.50173739
C	2.45645534	5.94702218	-0.54220988
C	3.38432196	7.79691440	-1.80367640
H	4.23475425	7.28796085	-3.72162991
C	1.86679539	3.20683979	-0.26849416
C	1.91553418	5.45116887	0.66578385
C	2.78011613	7.31810599	-0.66270175
H	3.62363303	8.85250273	-1.86377657
C	1.66213095	4.10548564	0.79480636
H	1.26385445	3.73762548	1.73356277
C	1.64560087	6.35543888	1.79036146
C	2.49280664	8.25587994	0.44577327
N	1.93695605	7.70965663	1.60222318
O	1.18447383	5.98312639	2.85970943
O	2.72932857	9.45152705	0.36476372
C	1.64568108	8.59462622	2.72561252
H	1.89888400	9.60730539	2.42477849
H	0.58806069	8.52695135	2.98592985
H	2.23454755	8.29932766	3.59617026
C	3.38830622	5.58258276	-2.75564116
H	3.68678474	4.90462387	-3.54616476
N	2.51845275	2.80328513	-2.55451198
H	2.36952183	1.84849550	-2.23581197
C	1.85777252	3.01448459	-3.84966490
H	0.83708872	2.60738377	-3.81226225
H	1.75588608	4.08526631	-4.02770760
C	1.55988200	1.81863000	-0.13188900
C	1.32958700	0.62183300	-0.11125300
C	-2.57496300	0.47437800	4.68080100
H	-1.56963800	0.06766100	4.52767100
H	-2.48122200	1.37494200	5.29460000
H	-3.15933300	-0.26688000	5.23386900
C	2.63602353	2.35589441	-4.97804626
H	2.74126296	1.28024836	-4.80440590
H	2.11686141	2.49262705	-5.93167206
H	3.63940518	2.78427513	-5.06241804

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

Symbolic Z-matrix :

Charge = 0 Multiplicity = 1

C	0.56847653	-1.46092076	-0.00331259
C	0.03907081	0.26078600	-1.66757703
C	0.43787587	-2.06191665	1.27367429
C	1.44859233	-2.06178383	-0.95306039
C	0.90918016	-0.34579286	-2.58588751
H	-0.50111842	1.15862571	-1.94869309
C	1.14565004	-3.20379412	1.59376536
C	2.16506294	-3.23453505	-0.60182748
C	1.60807910	-1.49076416	-2.24096651
H	1.04736416	0.07339322	-3.57636472
C	2.01370583	-3.79538639	0.65375460
H	1.03526183	-3.65219588	2.57626854
H	2.57342631	-4.69222578	0.89650174
C	3.08444941	-3.87031237	-1.57785007
C	2.52324307	-2.10641389	-3.23771712
N	3.20575668	-3.26187502	-2.83446249
O	3.72296620	-4.88337441	-1.32304612
O	2.67657911	-1.63128536	-4.35615253
C	4.12408627	-3.90555901	-3.78289198
H	4.12031966	-3.31998399	-4.69882346
H	5.12868859	-3.94203569	-3.35564128
H	3.79377272	-4.92775933	-3.98138248
C	-0.14294026	-0.27178920	-0.39013935
N	-0.35503859	-1.62233043	2.43080462
H	-0.94857324	-2.36897703	2.73119681
C	-1.05972063	0.33463074	0.68845632
C	-1.89072568	0.84831280	1.62015442
H	-2.47107572	1.26943583	2.41435164
C	0.54732741	-1.24226100	3.52724560
H	0.90666753	-2.12403623	4.01535125
H	1.37494413	-0.69041698	3.13301376
C	-0.21566753	-0.36923889	4.54078944



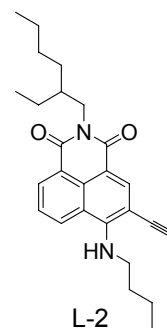
H	0.17265612	-0.54094054	5.52294182
H	-0.09484550	0.66265030	4.28484659
H	-1.25494587	-0.62284641	4.51879514

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

Symbolic Z-matrix :

Charge = 0 Multiplicity = 1

C	-5.67750602	2.52320576	1.39577379
C	-8.11396037	2.72668558	1.20444449
C	-4.35395792	2.98562648	1.18760175
C	-5.86712401	1.27749851	2.06653427
C	-8.27788259	1.50018256	1.86561180
H	-8.98544198	3.28086680	0.87225516
C	-3.27040677	2.24862966	1.62353669
C	-4.73903497	0.53803998	2.50546060
C	-7.17509875	0.77949374	2.29323888
H	-9.26855007	1.09944287	2.04957514
C	-3.46055970	1.01902704	2.28613896
H	-2.61542795	0.43363623	2.63197712
C	-4.91981467	-0.75902696	3.20334342
C	-7.38499281	-0.51744979	2.98889933
N	-6.23423614	-1.20449424	3.39787191
O	-3.97877171	-1.43281800	3.60255160
O	-8.50522852	-0.96716542	3.19622671
C	-6.38933558	-2.49231993	4.08680295
H	-7.45282617	-2.70761698	4.15371863
H	-5.87465816	-3.27487989	3.52483623
H	-5.94777128	-2.43345100	5.08427697
C	-6.84201426	3.24840903	0.96243390
H	-6.85434470	4.24094249	0.34196683
N	-4.09591567	4.25199646	0.48715815
H	-3.10977864	4.41006080	0.43666640
C	-1.84078965	2.76968965	1.38627863
C	-0.59684370	3.14928896	1.22942570
H	0.41860799	3.47979374	1.16216164
C	-4.65119830	4.18209454	-0.87213392



H	-3.85226759	4.17522650	-1.58386600
H	-5.22894586	3.28746880	-0.97582836
C	-5.55126108	5.40634094	-1.12254903
H	-5.53434088	5.65457185	-2.16321954
H	-6.55390872	5.17840923	-0.82650028
H	-5.19090167	6.23665416	-0.55191688

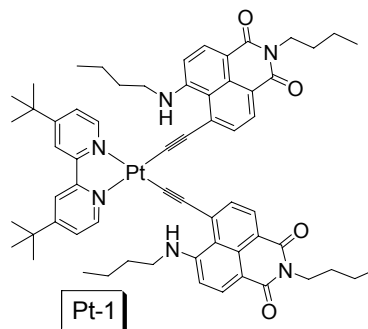
8.0 The coordinates of the triplet optimized geometries of complexes

Complex Pt-1 (DFT//B3LYP/GENECP/LanL2DZ)

Symbolic Z-matrix:

Charge = 0 Multiplicity = 3

C	-3.55444600	3.58738300	-0.12187300
C	-3.01788800	4.87084100	-0.07101300
C	-1.62293600	4.96129000	-0.02074500
C	-0.83287700	3.82378100	-0.01088800
C	-2.71956800	2.47978000	-0.11115600
C	0.64958800	3.85409900	0.03301300
C	1.39219300	5.02255900	0.07992300
C	2.78995900	4.98833000	0.11987600
C	3.37917500	3.72713400	0.11890300
C	2.59098900	2.58679000	0.07362500
H	-4.62239900	3.42212300	-0.17093500
H	-3.10788000	1.46868400	-0.17425900
H	4.45348800	3.60426700	0.15304500
H	3.02418500	1.59176000	0.09357500
N	1.25782300	2.64564000	0.02506800
N	-1.39042800	2.59160500	-0.04769300
Pt	-0.03139900	0.98243600	-0.02348400
H	0.88107500	5.97600100	0.08697800
H	-1.15150600	5.93440900	0.00912000
C	3.58952300	6.29015600	0.16550300
C	-3.86937800	6.13997900	-0.07440900
C	3.26405600	7.12441100	-1.08717900
H	2.20170600	7.37814800	-1.14719000
H	3.82870300	8.06178800	-1.06482600
H	3.53567700	6.58581200	-2.00034600
C	3.19572600	7.07898300	1.42797100



H	3.76206100	8.01452300	1.47150500
H	2.13203200	7.33398200	1.43798400
H	3.41515400	6.50644600	2.33456400
C	5.10051700	6.03453500	0.20140700
H	5.39765900	5.46747900	1.08922000
H	5.44386600	5.49368800	-0.68597400
H	5.62927900	6.99154300	0.22951700
C	-3.58027700	6.94306100	1.20726900
H	-2.53000200	7.24063600	1.27776500
H	-4.18506600	7.85524700	1.21712700
H	-3.82808200	6.36149600	2.10063500
C	-3.50526600	6.98684100	-1.30786900
H	-4.10841400	7.90007700	-1.32145700
H	-2.45254900	7.28413600	-1.30589000
H	-3.69998600	6.43730200	-2.23412700
C	-5.36891300	5.82537300	-0.12410100
H	-5.64167800	5.27926500	-1.03260900
H	-5.69181200	5.23959500	0.74221400
H	-5.93554000	6.76089400	-0.11965100
C	-1.38864600	-0.42171600	-0.01623900
C	-4.65230400	-2.14684000	-0.30418600
C	-2.92232400	-3.33641700	0.94290700
C	-5.15312900	-1.11352300	-1.17088000
C	-5.58387500	-3.12973200	0.14987200
C	-3.82822700	-4.33312500	1.29797500
H	-1.89717300	-3.39150900	1.28988500
C	-6.51836600	-1.01507500	-1.39780400
C	-6.96375200	-3.01431300	-0.14805900
C	-5.15136200	-4.22633800	0.93266000
H	-3.51582800	-5.18365400	1.89293500
C	-7.42024600	-1.94419400	-0.88140200
H	-6.88348600	-0.21977600	-2.04134700
H	-8.48179900	-1.86465600	-1.08687200
C	-7.93277300	-4.01786000	0.32101000
C	-6.09386900	-5.26761400	1.38760800
N	-7.43544200	-5.09602300	1.04751400
O	-9.13226700	-3.94187800	0.09535600
O	-5.73118800	-6.23760300	2.03637800
C	-8.40797000	-6.09241600	1.48369900
H	-7.86823300	-6.87245600	2.01325700

H	-9.14779300	-5.62966000	2.13967300
H	-8.92671700	-6.50751900	0.61789400
C	-3.29817600	-2.23393500	0.17958200
C	-2.30466200	-1.22528900	0.01143100
C	1.38086900	-0.36723100	-0.03890100
C	4.69719400	-2.00216600	0.21522500
C	2.93276000	-3.31555800	-0.84604800
C	5.22105800	-0.88757400	0.96059900
C	5.62319600	-3.01074800	-0.19220100
C	3.83712200	-4.32939200	-1.15200300
H	1.89444000	-3.41210000	-1.14079700
C	6.59526600	-0.74981500	1.10716400
C	7.01330500	-2.85199200	0.02730900
C	5.17306500	-4.17700600	-0.85525900
H	3.51237600	-5.23225300	-1.65634700
C	7.48558600	-1.71198300	0.63591200
H	6.97715300	0.10729900	1.65414600
H	8.55423300	-1.60075200	0.78127800
C	7.97540700	-3.88147200	-0.39479700
C	6.11010500	-5.24389900	-1.25879100
N	7.46257400	-5.02687500	-0.99775400
O	9.18291600	-3.77180400	-0.23388800
O	5.73362300	-6.27229500	-1.80132600
C	8.42993800	-6.04641000	-1.38951700
H	7.87870400	-6.87805000	-1.81934400
H	9.12950600	-5.63626100	-2.12045500
H	8.99654000	-6.37447000	-0.51640600
C	3.32433400	-2.14669600	-0.19725800
C	2.31930900	-1.14448700	-0.06275400
N	4.39231000	0.08644000	1.52319100
H	4.95825800	0.86804900	1.84040800
C	3.46383400	-0.29994000	2.59954500
H	2.64521000	0.42570400	2.61505500
H	3.01666000	-1.25832900	2.34140100
C	4.14426400	-0.38008400	3.96208200
H	3.42162200	-0.66223500	4.73416500
H	4.94690800	-1.12424600	3.95860600
H	4.57728400	0.58539100	4.24839200
N	-4.30724000	-0.19014700	-1.79893200
H	-4.87377500	0.54131200	-2.21953400

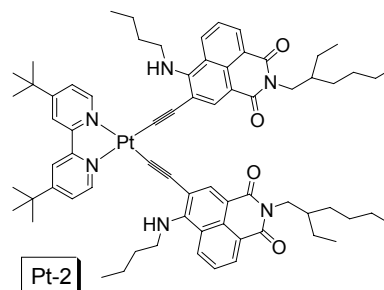
C	-3.39225600	-0.71083800	-2.83037200
H	-2.73885100	-1.45325300	-2.37493300
H	-3.96445600	-1.21175200	-3.62597200
C	-2.55629000	0.41492300	-3.41264200
H	-3.18941200	1.20474000	-3.83431900
H	-1.91598000	0.85244500	-2.64238400
H	-1.91946500	0.03539900	-4.21690600

Complex Pt-2 (DFT//B3LYP/GENECP/LanL2DZ)

Symbolic Z-matrix:

Charge = 0 Multiplicity = 3

C	-0.30707600	-5.48655000	-0.04372900
C	0.88385400	-6.20703700	-0.08192600
C	2.06443300	-5.45807700	-0.11758000
C	2.03362500	-4.07313400	-0.11355500
C	-0.28091900	-4.10092600	-0.04275700
C	3.24850400	-3.22323900	-0.14862300
C	4.53814900	-3.72753900	-0.18389700
C	5.64652700	-2.87504000	-0.21493900
C	5.37890000	-1.50861800	-0.20859800
C	4.06886200	-1.05756600	-0.17303800
H	-1.26830100	-5.98156600	-0.01485900
H	-1.18848500	-3.50950000	-0.01462800
H	6.17331600	-0.77483400	-0.23063100
H	3.82567700	-0.00162500	-0.16784300
N	3.02555400	-1.88906900	-0.14332600
N	0.85758600	-3.40573400	-0.07628600
Pt	1.00623600	-1.30492600	-0.08636100
H	4.68853200	-4.79874600	-0.18698000
H	3.01857300	-5.96687800	-0.14933600
C	7.06035500	-3.45393600	-0.25452700
C	0.94144400	-7.73435000	-0.08708200
C	7.28264800	-4.32690500	0.99434200
H	6.57818100	-5.16242500	1.04390100
H	8.29351300	-4.74616900	0.97709700
H	7.17491000	-3.73815700	1.91063900
C	7.21527200	-4.31499000	-1.52170900
H	8.22465900	-4.73626300	-1.56133300



H	6.50669000	-5.14827700	-1.54238200
H	7.06112800	-3.71693700	-2.42521300
C	8.12932400	-2.35559200	-0.27747200
H	8.03859700	-1.71612400	-1.16100100
H	8.08356900	-1.72279000	0.61435900
H	9.12114800	-2.81587600	-0.30444000
C	1.64104500	-8.20619500	-1.37516100
H	2.66408000	-7.82624700	-1.44977600
H	1.69081200	-9.29945300	-1.39027400
H	1.09255200	-7.87874800	-2.26377900
C	1.74017200	-8.21242700	1.13955700
H	1.78961300	-9.30575000	1.14585600
H	2.76661800	-7.83421000	1.13469500
H	1.26433100	-7.88851700	2.07038600
C	-0.45641800	-8.36121300	-0.03365500
H	-0.99598800	-8.07813400	0.87560900
H	-1.06388300	-8.07848900	-0.89908500
H	-0.36491300	-9.45107500	-0.03726800
C	-5.54415700	-0.23712400	1.47034500
C	-7.59112300	-0.08014000	2.77360900
C	-4.12237300	-0.37930300	1.36932200
C	-6.31719800	-0.15721300	0.28464100
C	-8.34242600	0.06673500	1.59538100
H	-8.09423200	-0.08725300	3.73458100
C	-3.53550300	-0.55947100	0.10871700
C	-5.69390100	-0.28737000	-0.97726500
C	-7.71796900	0.01479400	0.36972300
H	-9.41821800	0.19589800	1.62813300
C	-4.33985600	-0.51222900	-1.04922800
H	-3.87825600	-0.62815000	-2.02321800
C	-6.48786200	-0.20950500	-2.21313000
C	-8.53625600	0.12099600	-0.85973900
N	-7.86175800	0.00624400	-2.07478000
O	-6.00570200	-0.32179600	-3.32960000
O	-9.74408200	0.29688700	-0.82335000
C	-8.62823700	0.09533400	-3.31407200
H	-9.66688600	0.27310400	-3.05008000
H	-8.24590500	0.91219700	-3.92848900
H	-8.53326300	-0.83420300	-3.87834600
C	-6.22639800	-0.23349500	2.71155300

H	-5.65996100	-0.39163300	3.62151900
N	-3.33055200	-0.40396200	2.51438900
H	-2.39177800	-0.70316000	2.25814100
C	-3.23718200	0.80178700	3.35237500
H	-2.66847800	1.58615200	2.83106300
H	-4.23874800	1.20053600	3.51749100
C	-2.12318800	-0.76472700	0.00868800
C	-0.91791300	-0.94584000	-0.02722000
C	2.71454071	5.06516754	-1.62284780
C	3.71136063	6.91627138	-2.84731588
C	2.34588857	3.68358195	-1.50173739
C	2.45645534	5.94702218	-0.54220988
C	3.38432196	7.79691440	-1.80367640
H	4.23475425	7.28796085	-3.72162991
C	1.86679539	3.20683979	-0.26849416
C	1.91553418	5.45116887	0.66578385
C	2.78011613	7.31810599	-0.66270175
H	3.62363303	8.85250273	-1.86377657
C	1.66213095	4.10548564	0.79480636
H	1.26385445	3.73762548	1.73356277
C	1.64560087	6.35543888	1.79036146
C	2.49280664	8.25587994	0.44577327
N	1.93695605	7.70965663	1.60222318
O	1.18447383	5.98312639	2.85970943
O	2.72932857	9.45152705	0.36476372
C	1.64568108	8.59462622	2.72561252
H	1.89888400	9.60730539	2.42477849
H	0.58806069	8.52695135	2.98592985
H	2.23454755	8.29932766	3.59617026
C	3.38830622	5.58258276	-2.75564116
H	3.68678474	4.90462387	-3.54616476
N	2.51845275	2.80328513	-2.55451198
H	2.36952183	1.84849550	-2.23581197
C	1.85777252	3.01448459	-3.84966490
H	0.83708872	2.60738377	-3.81226225
H	1.75588608	4.08526631	-4.02770760
C	1.55988200	1.81863000	-0.13188900
C	1.32958700	0.62183300	-0.11125300
C	-2.57496300	0.47437800	4.68080100
H	-1.56963800	0.06766100	4.52767100

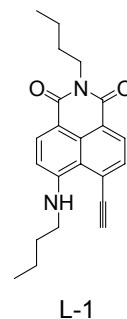
H	-2.48122200	1.37494200	5.29460000
H	-3.15933300	-0.26688000	5.23386900
C	2.63602353	2.35589441	-4.97804626
H	2.74126296	1.28024836	-4.80440590
H	2.11686141	2.49262705	-5.93167206
H	3.63940518	2.78427513	-5.06241804

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

Symbolic Z-matrix:

Charge = 0 Multiplicity = 3

C	-1.00832969	-0.03008376	-0.18622358
C	-0.63581637	2.39208006	-0.04080089
C	-1.81952477	-1.21796767	-0.30258985
C	0.41346466	-0.20209447	-0.06703059
C	0.73017639	2.19592140	0.17715893
H	-1.03591614	3.39919713	-0.08474948
C	-1.19140592	-2.45223999	-0.47802453
C	1.00111617	-1.48861357	-0.18812633
C	1.26041700	0.91862569	0.13985757
H	1.39450657	3.03766388	0.33842307
C	0.19709779	-2.58905697	-0.43454398
H	-1.81014294	-3.33835731	-0.59495174
H	0.66162445	-3.56332221	-0.54402610
C	2.45798562	-1.67833585	-0.06960615
C	2.72650859	0.75816368	0.30300151
N	3.23444947	-0.53950866	0.18653696
O	3.00396680	-2.77257925	-0.18049351
O	3.46473613	1.71315448	0.52524191
C	4.67947342	-0.74967642	0.32295666
H	5.13857687	0.21623609	0.51856406
H	4.87716444	-1.44035086	1.14607367
H	5.07949844	-1.18343611	-0.59659527
C	-1.50904274	1.31862190	-0.24092299
N	-3.21688958	-1.16726615	-0.27109944
H	-3.52037116	-0.19642522	-0.24181748
C	-2.88939009	1.67140378	-0.36750326
C	-4.05851772	1.97020325	-0.47471432
H	-5.09786894	2.18827951	-0.58068709



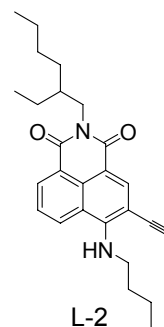
C	-3.97686131	-1.86647996	-1.33082861
H	-3.71216174	-1.46193513	-2.32114792
H	-3.69756538	-2.92086781	-1.32693190
C	-5.47447138	-1.72341321	-1.08801685
H	-6.03641934	-2.22738770	-1.88139230
H	-5.75375437	-2.16402298	-0.12616264
H	-5.77758556	-0.66880478	-1.08398101

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

Symbolic Z-matrix:

Charge = 0 Multiplicity = 3

C	0.85673900	-0.71512300	-0.14304500
C	0.16893600	-3.05133200	-0.33377600
C	1.86509200	0.31632300	-0.10643400
C	-0.52134100	-0.34236600	-0.06047300
C	-1.17723100	-2.68393100	-0.17146000
H	0.42989700	-4.09453700	-0.48255500
C	1.44918800	1.67147800	-0.14341300
C	-0.89693700	1.02532300	-0.03153900
C	-1.52217500	-1.34722200	-0.05245700
H	-1.96561800	-3.42888600	-0.16620200
C	0.07915200	2.00044400	-0.10653000
H	-0.21941700	3.04306600	-0.10476800
C	-2.31286400	1.41839900	0.05267500
C	-2.95697800	-0.98485400	0.06150900
N	-3.25881100	0.38181100	0.11073800
O	-2.69017800	2.58653900	0.07682200
O	-3.84250700	-1.83323400	0.10748200
C	-4.66378200	0.79042800	0.21346400
H	-5.27021500	-0.11099300	0.25399800
H	-4.80967200	1.39018800	1.11491000
H	-4.93830800	1.39652100	-0.65320300
C	1.16162700	-2.08850500	-0.32419000
H	2.18717200	-2.38954200	-0.49922900
N	3.21183900	0.02510100	-0.10664300
H	3.76840600	0.86631500	-0.22998600
C	2.42649000	2.71250000	-0.16555300
C	3.27470300	3.57803800	-0.19026700



H	4.00350500	4.35769700	-0.20537000
C	3.86692500	-0.91756700	0.82091300
H	4.30706400	-0.34436800	1.64883400
H	3.10822800	-1.56458200	1.26338000
C	4.95161300	-1.74044700	0.12913600
H	5.44762000	-2.39750200	0.85201400
H	4.53305200	-2.35854700	-0.67255000
H	5.71363600	-1.08917400	-0.31371300