

Electronic Supplementary Information for:

Visible light-harvesting *trans* bis(alkylphosphine) Platinum(II)-alkynyl complexes showing long-lived triplet excited states as triplet photosensitizers for triplet-triplet annihilation upconversion

Lianlian Liu,^a Dandan Huang,^a Sylvia M. Draper,^b Xiuyu Yi,^a Wanhua Wu^a and Jianzhang Zhao^{*a}

^a State Key Laboratory of Fine Chemicals, School of Chemical Engineering, Dalian University of Technology,
E-208 West Campus, 2 Ling Gong Road, Dalian 116024, P. R. China.

^b School of Chemistry, University of Dublin, Trinity College, Dublin 2, Ireland.

Phone/Fax: +86 411 8498 6236 (J. Z.)

E-mail: zhaojzh@dlut.edu.cn (J. Z.)

web: <http://finechem.dlut.edu.cn/photochem> (J. Z.)

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General Experimental conditions:

Nanosecond time-resolved transient difference absorption spectra

Nanosecond time-resolved transient absorption spectra were measured on LP 920 laser flash photolysis spectrometer (Edinburgh Instruments, UK) and recorded on a Tektronix TDS 3012B oscilloscope. The lifetime values (by monitoring the decay trace of the transients) were obtained with the LP900 software. All samples in flash photolysis experiments were deaerated with N₂ for ca. 15 min before measurement.

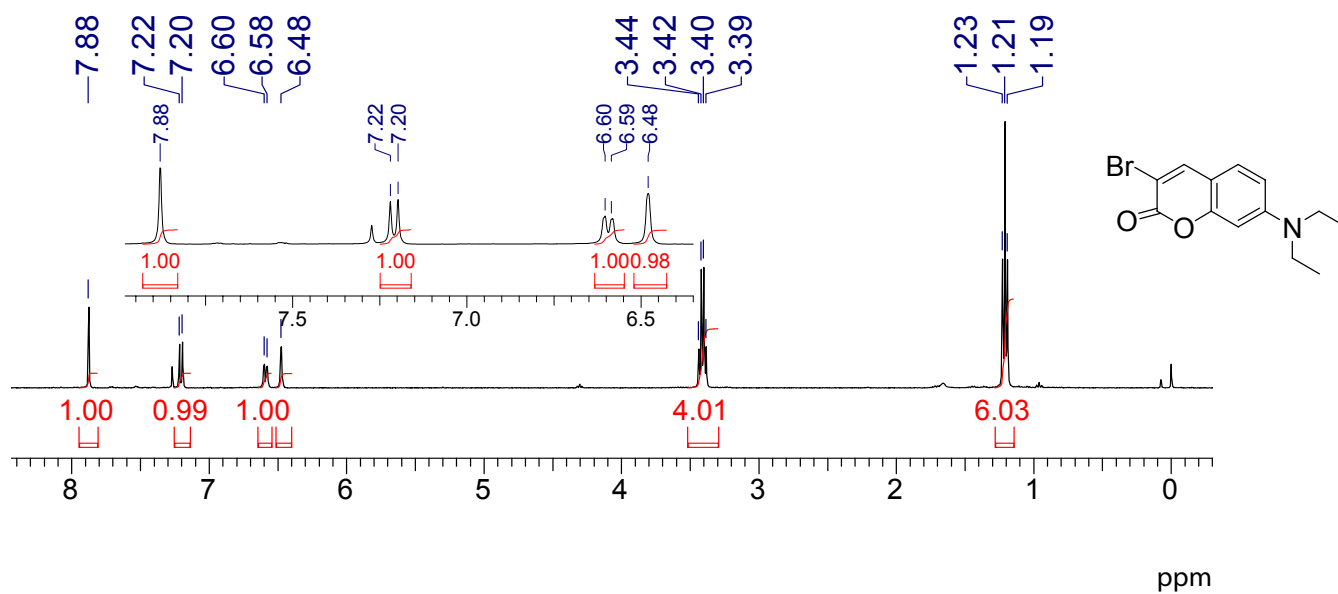
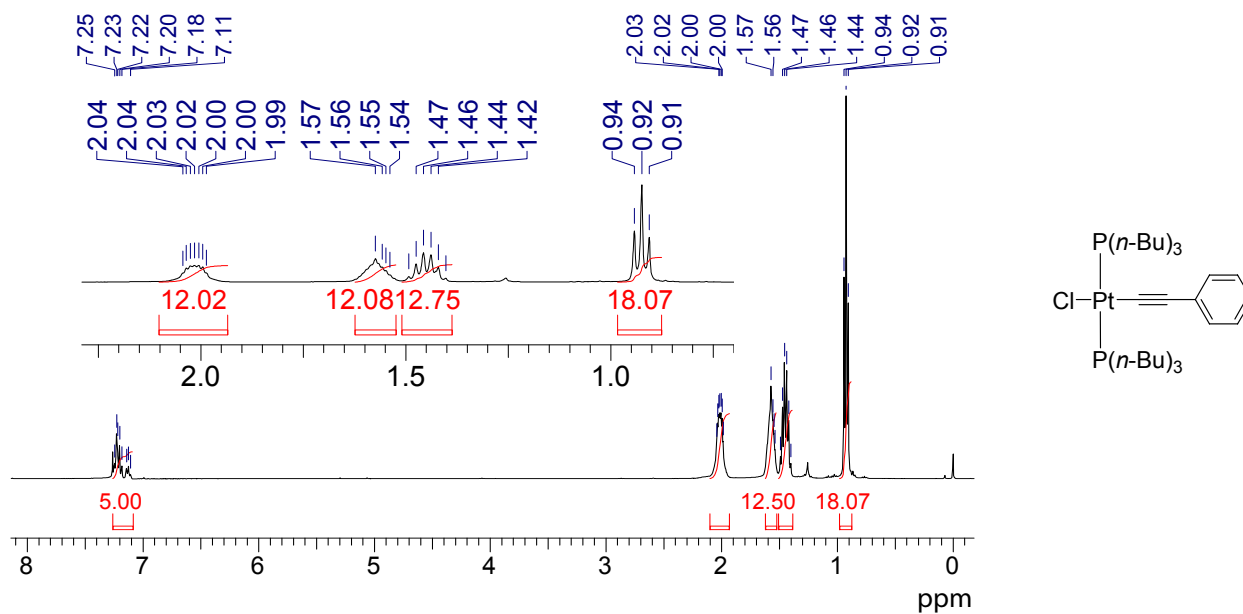
Delayed fluorescence

The delayed fluorescence feature of the upconversion was measured with a nanosecond pulsed laser (Opolette™ 355II+UV nanosecond pulsed laser, typical pulse length: 7 ns. Pulse repetition: 20 Hz. Peak OPO energy: 4 mJ. The wavelength is tunable in the range of 210 – 355 nm and 410 – 2200 nm. OPOTEK, USA), which is synchronized to FLS 920 spectrofluorometer (Edinburgh Instruments, UK). The pulsed laser is sufficient to sensitize the TTA upconversion. The decay kinetics of the upconverted fluorescence (delayed fluorescence) was monitored with an FLS920 spectrofluorometer (synchronized to the OPO nanosecond pulse laser). The prompt fluorescence lifetime of the triplet acceptor DPA was measured with EPL picosecond pulsed laser (405 nm) which was synchronized to the FLS 920 spectrofluorometer.

Time-resolved emission spectra

The nanosecond and the microsecond time-resolved emission spectra of the triplet photosensitizers alone and the TTA upconversion were recorded with picosecond EPL-470 nm pulsed laser (470 ±10 nm, pulse width: 88.2 ps, maximum average power: 5 mW; and 445 ±10 nm, pulse width: 94.1 ps, maximum average power: 5 mW; Edinburgh Instrument Ltd., UK). OPO nanosecond pulsed laser was also used for the measurement of the time-resolve emission spectra). All the pulsed laser was synchronized to FLS 920 spectrofluorometer.

1.0 NMR and HRMS spectra



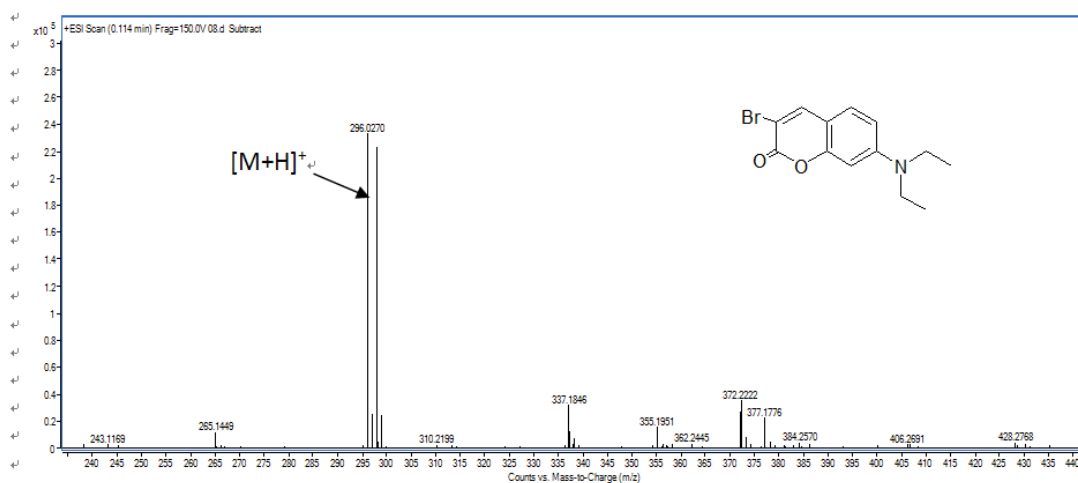


Fig. S3 ESI -HRMS of **2**.

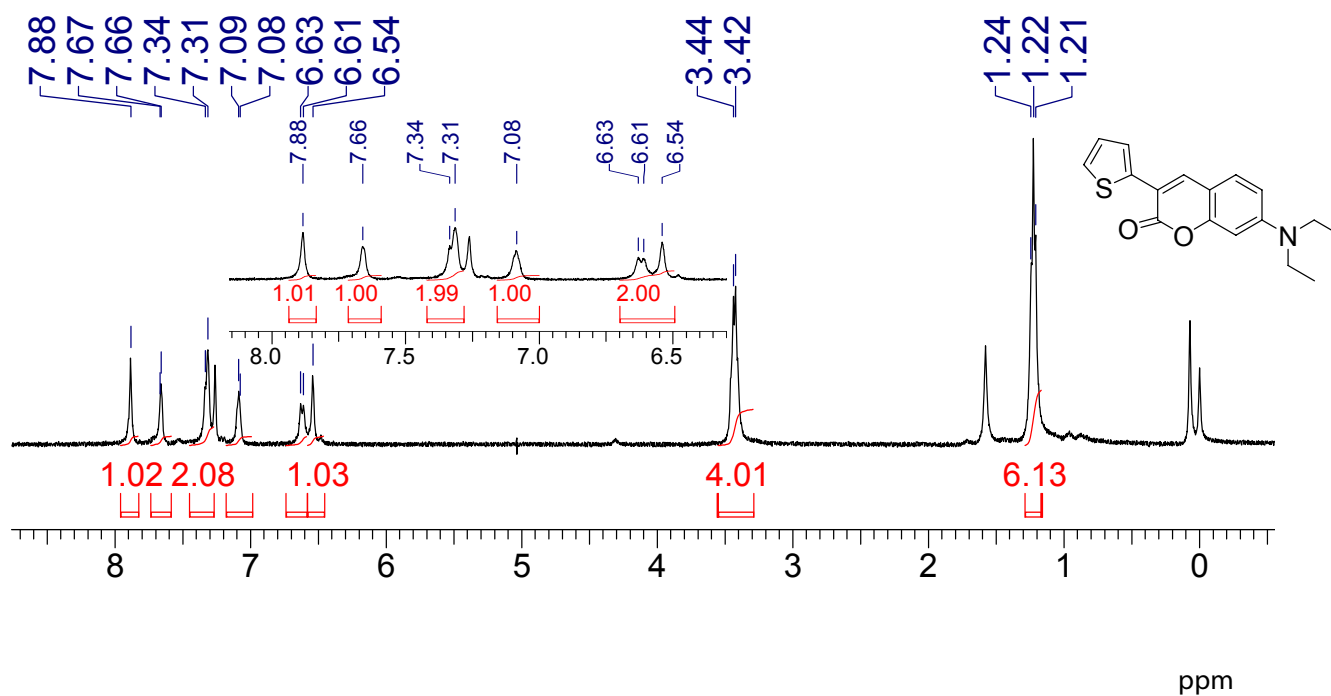


Fig. S4 ¹H NMR of **3** (400 MHz, CDCl₃).

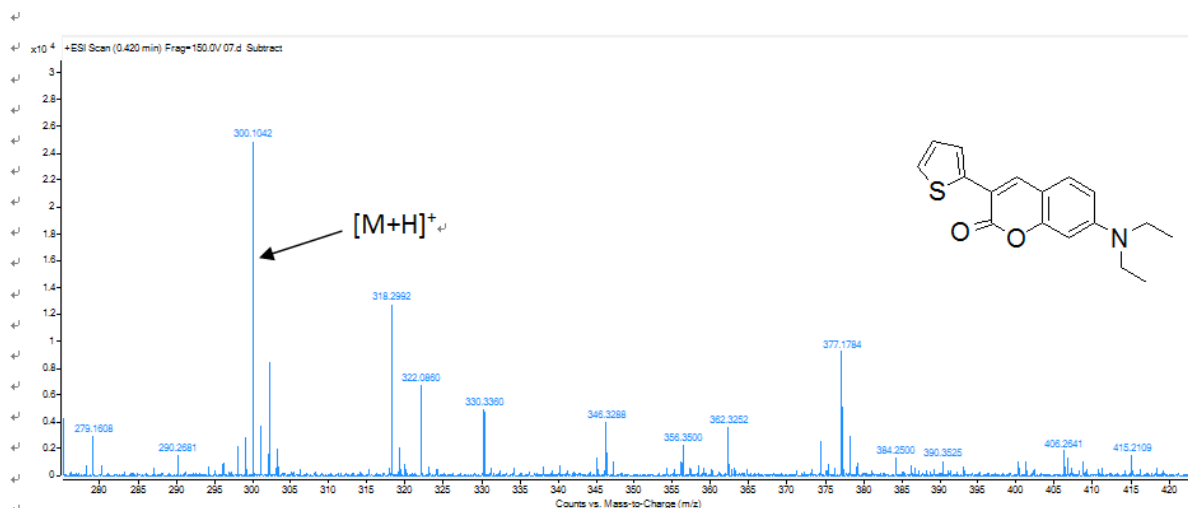


Fig. S5 ESI -HRMS of **3**.

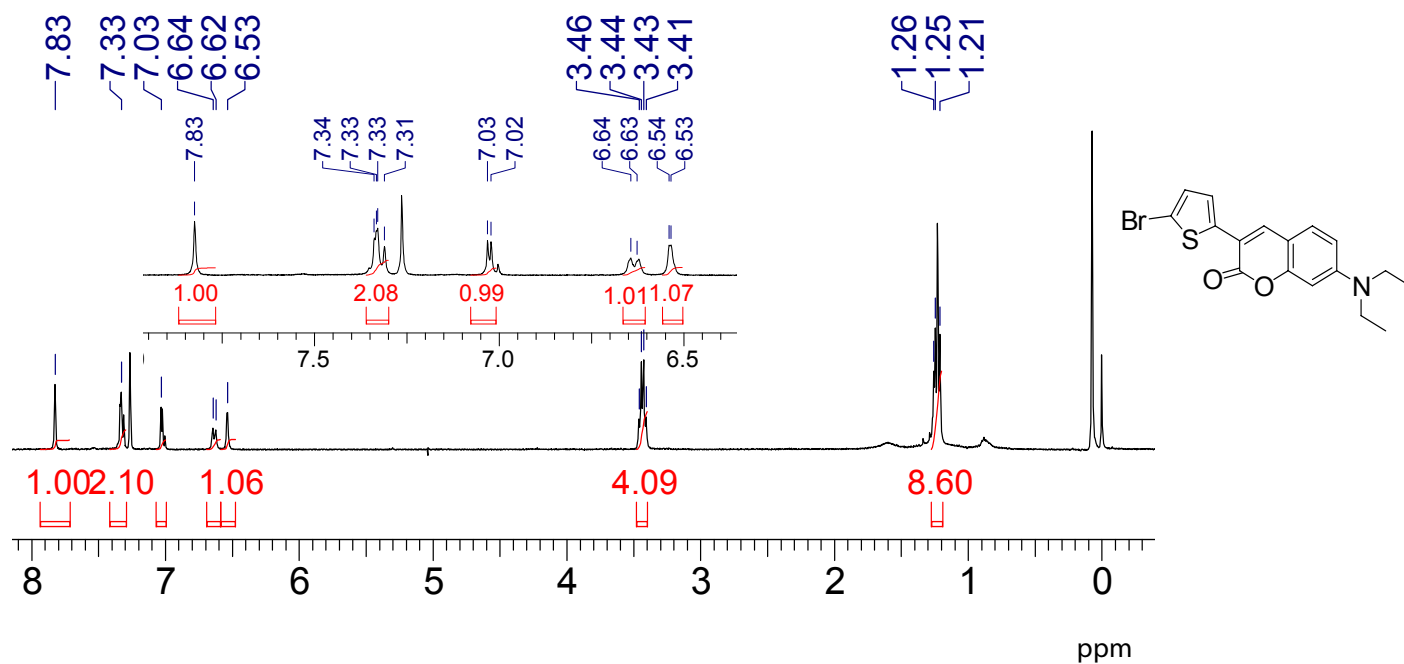


Fig. S6 ¹H NMR of **4** (400 MHz, CDCl₃).

LLL

10:16:58

12101614 13 (0.347) AM (Top,4, Ar,5000.0,475.28,1.00,LS 10); Sm (Mn, 2x1.00); Sb (1,40.00); Cm (360)

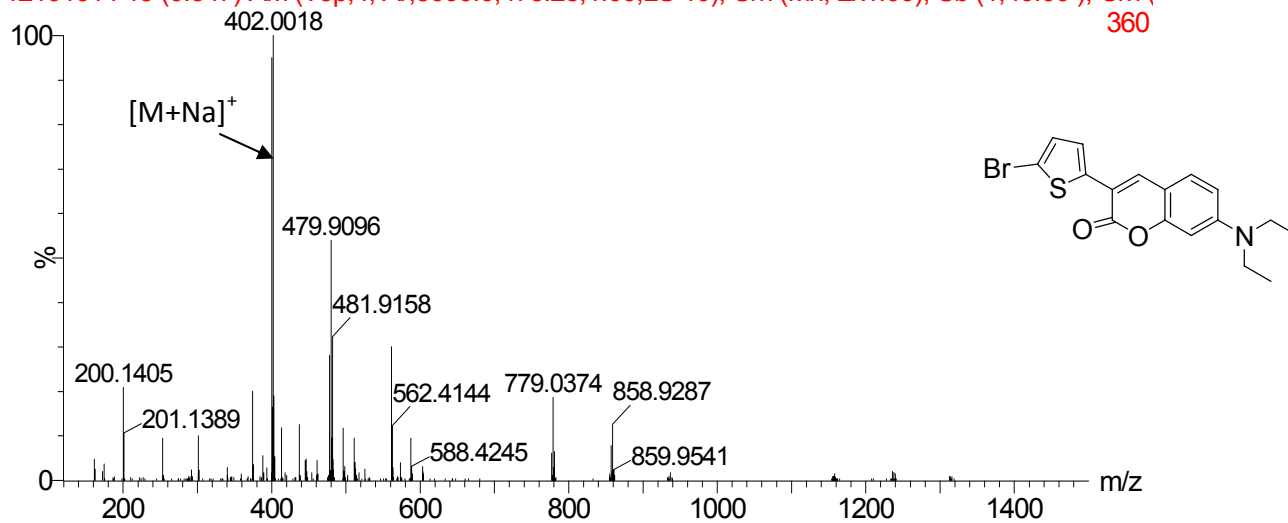


Fig. S7 ESI -HRMS of 4.

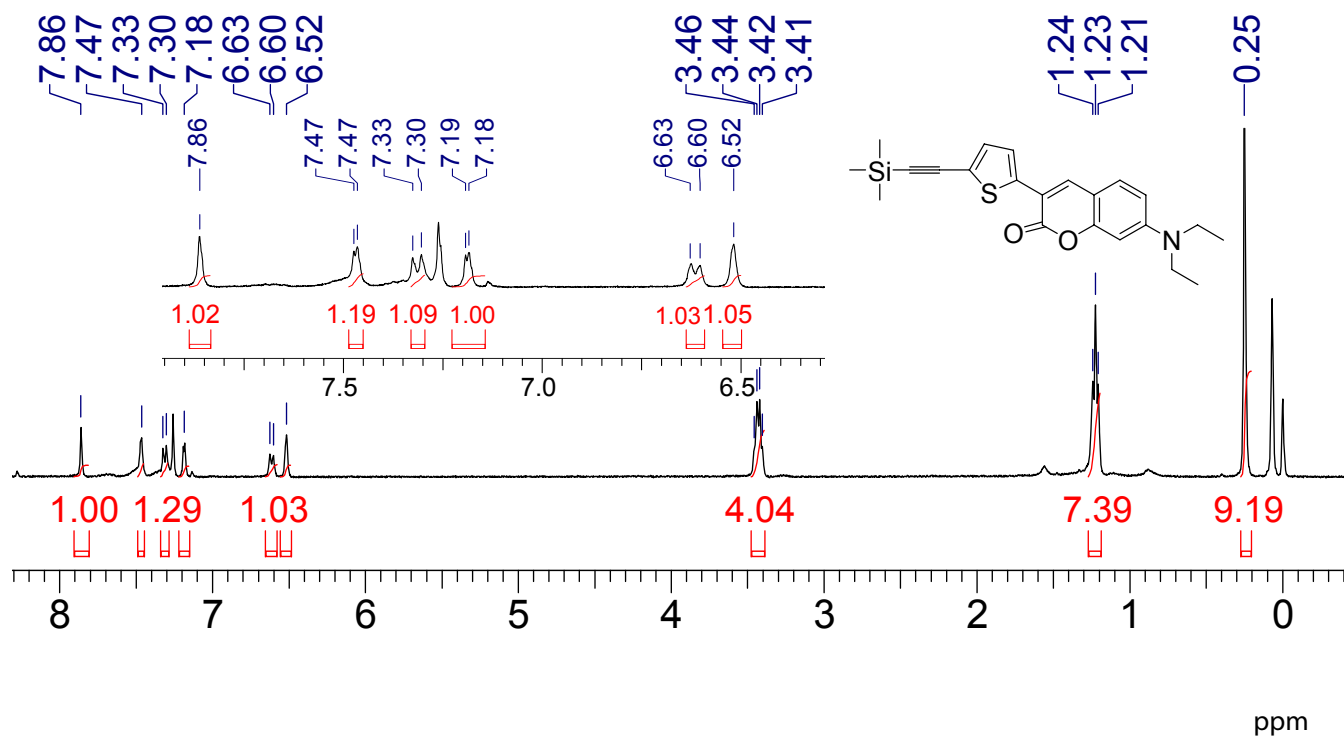


Fig. S8 ^1H NMR of 5 (400 MHz, CDCl_3).

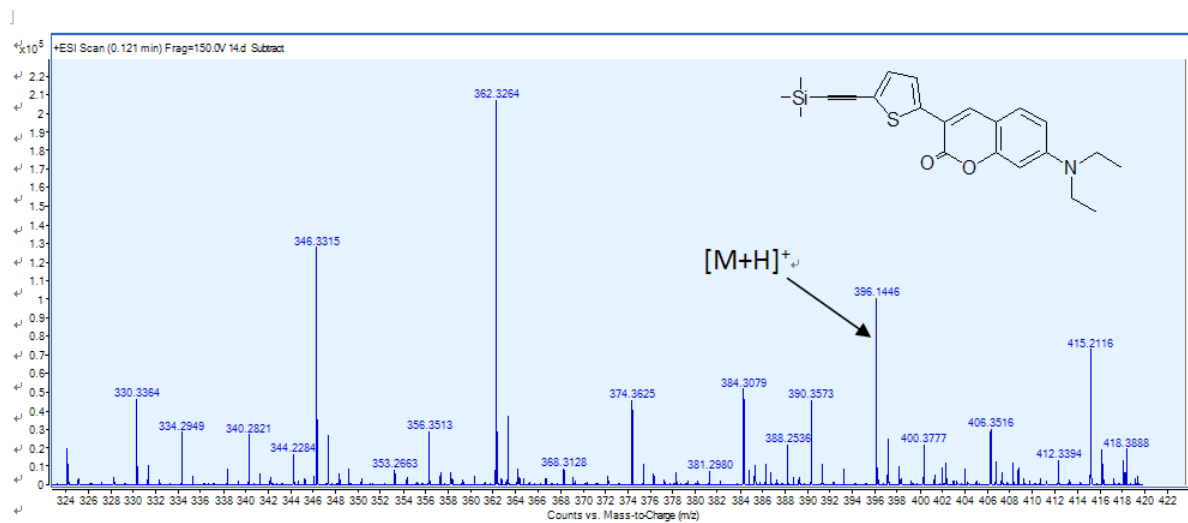


Fig. S9 ESI -HRMS of **5**.

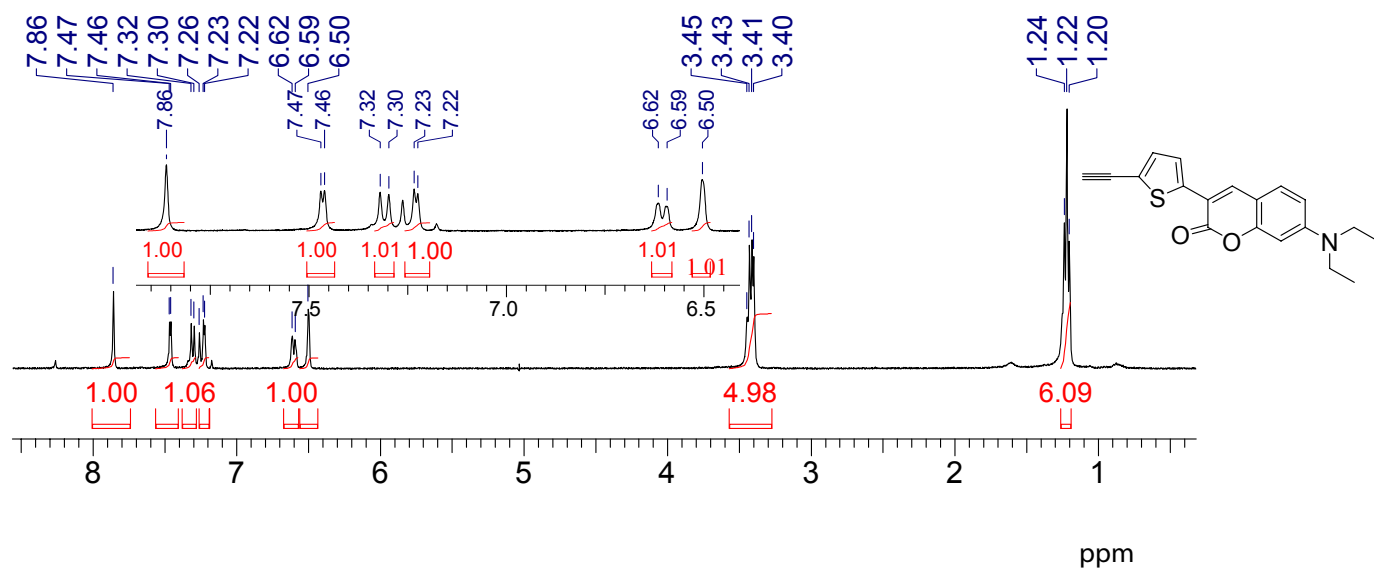


Fig. S10 ¹H NMR of **L-1** (400 MHz, CDCl₃).

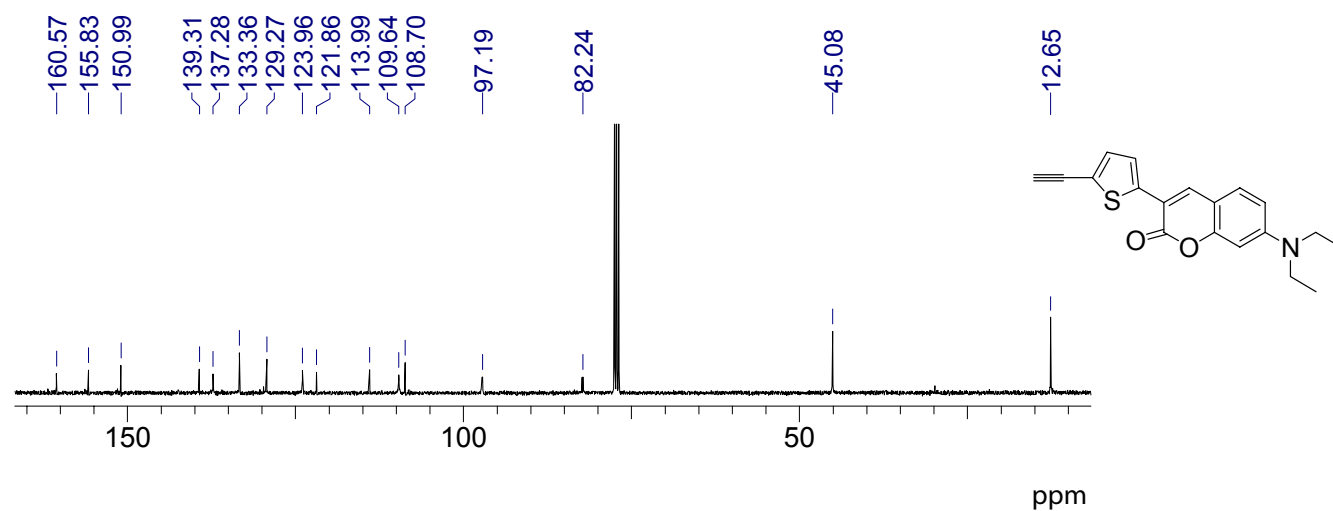


Fig. S11 ^{13}C NMR of L-1 (100 MHz, CDCl_3).

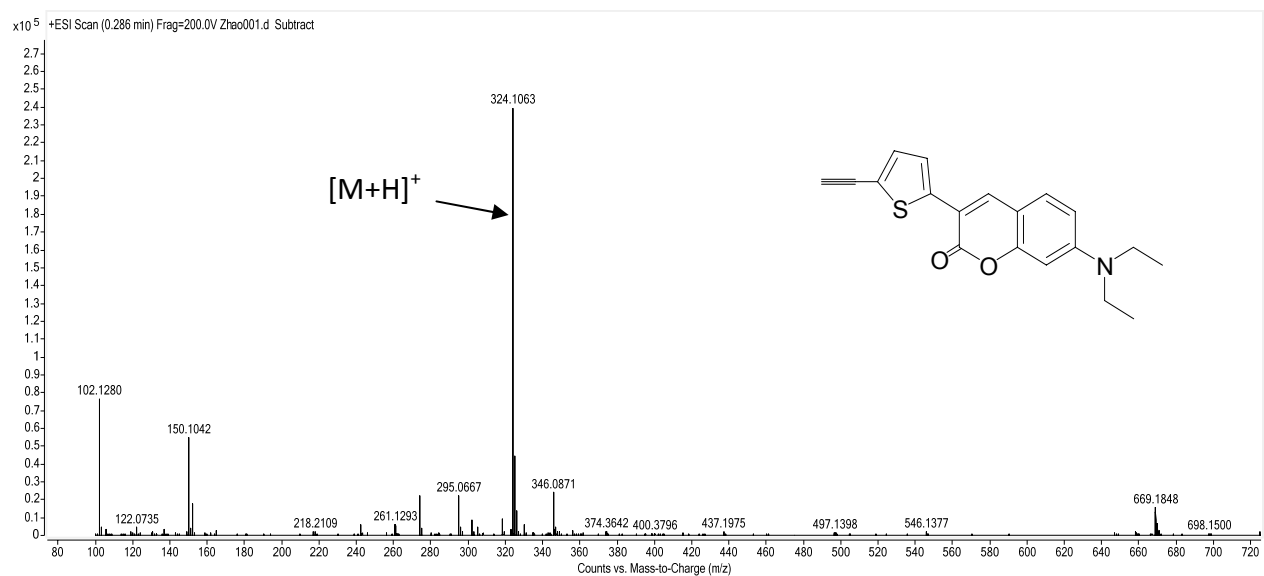


Fig. S12 ESI -HRMS of L-1.

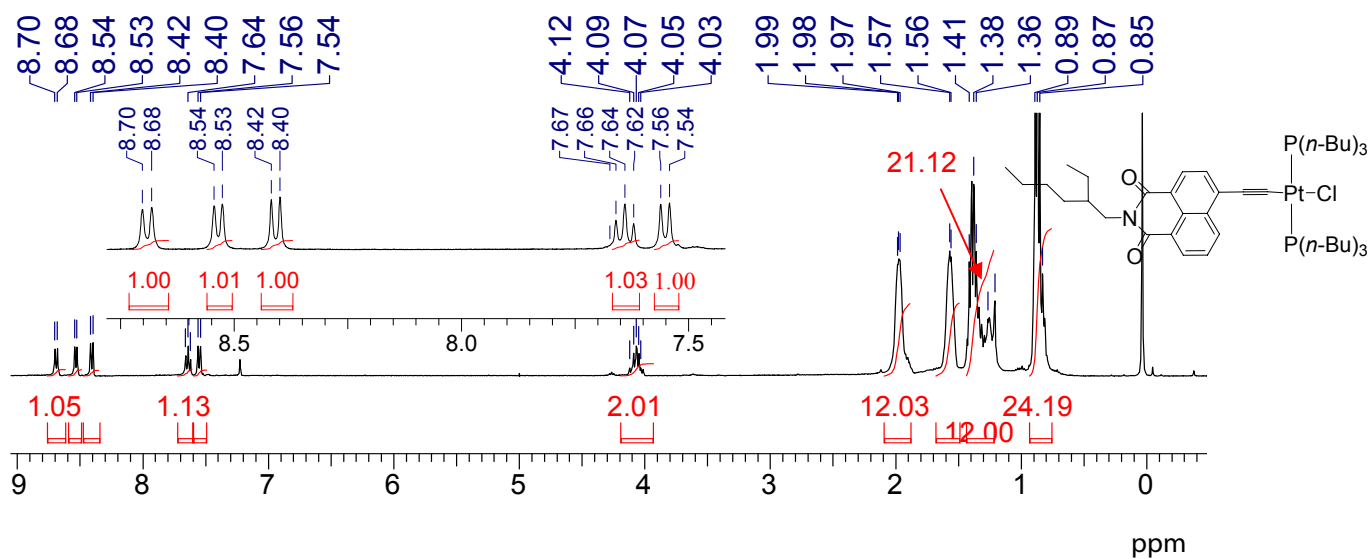


Fig. S13 ¹H NMR of **Pt-0** (400 MHz, CDCl₃).

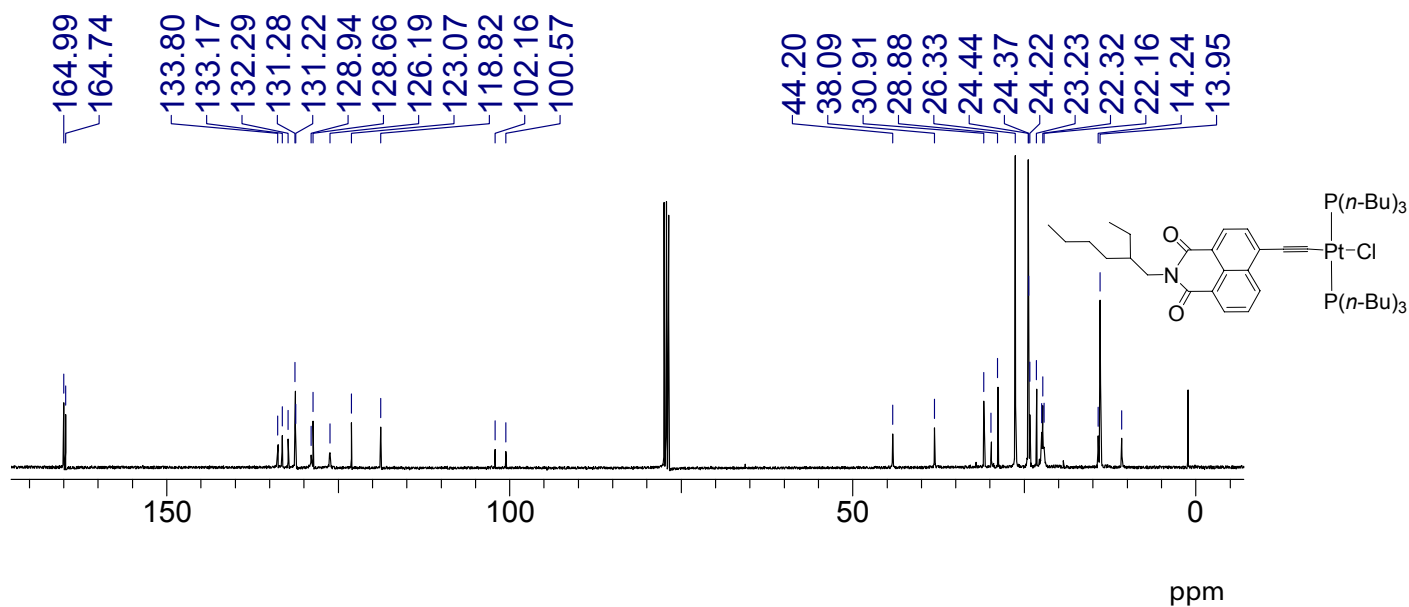


Fig. S14 ¹³C NMR of **Pt-0** (100 MHz, CDCl₃).

LLL-1(CHCA)

12101701 14 (0.466) Cn (Cen,4, 50.00, Ht); Sm (SG, 2x3.00); Sb (15,10.00); Cm (14:20)

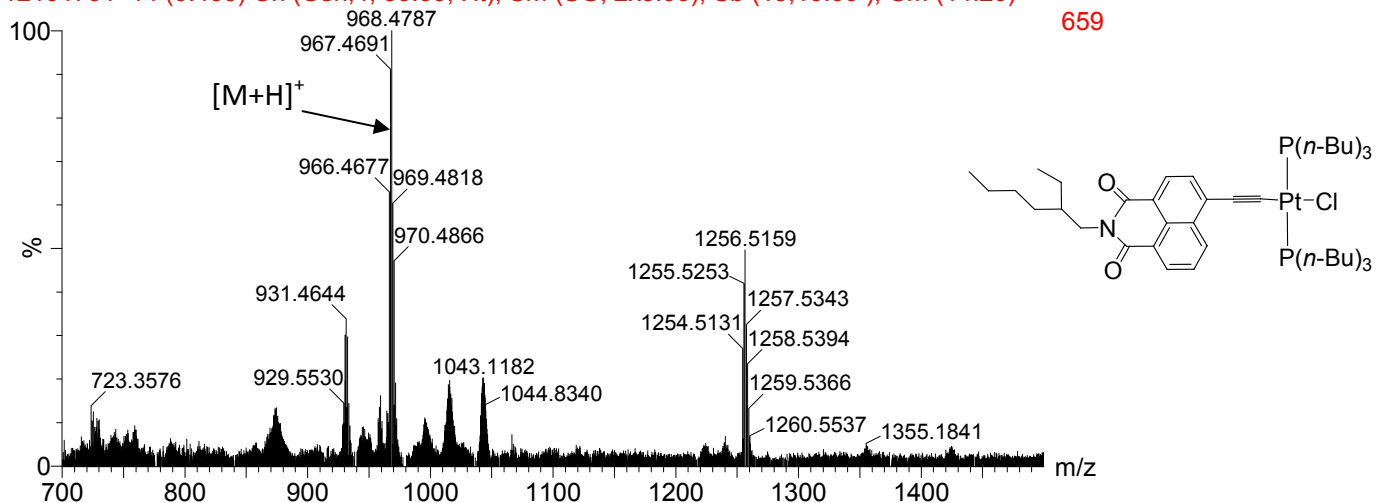


Fig. S15 MALDI-HRMS of Pt-0.

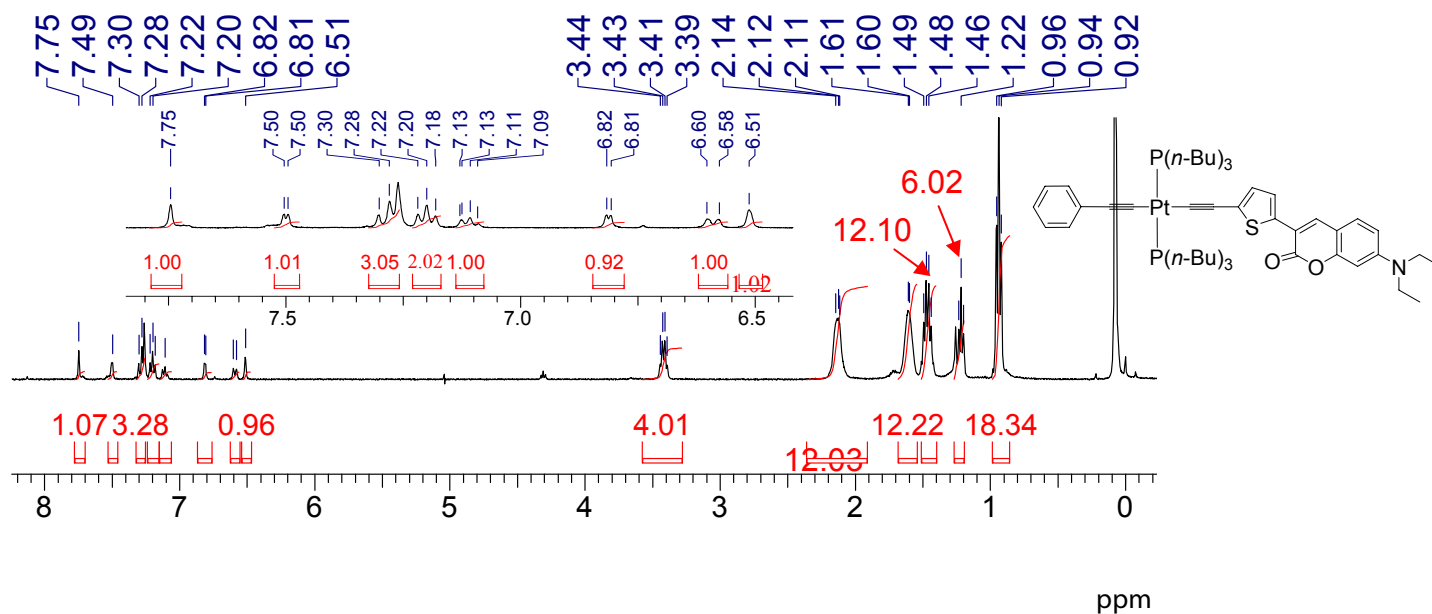


Fig. S16 ¹H NMR of Pt-1 (400 MHz, CDCl₃).

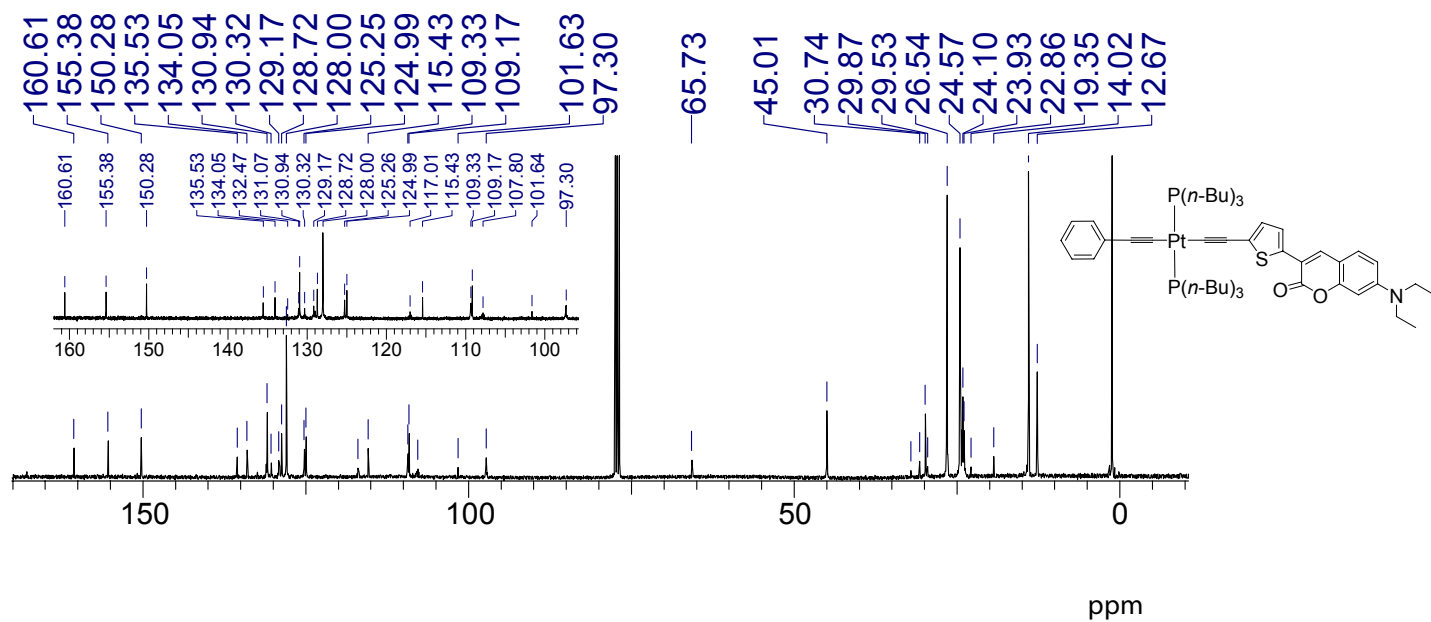


Fig. S17 ¹³C NMR of **Pt-1** (100 MHz, CDCl₃).

LLL(DTH)

12053100 15 (0.499) Cn (Cen,4, 50.00, Ht); Sm (SG, 2x3.00); Sb (15,10.00); Cm (1:25)

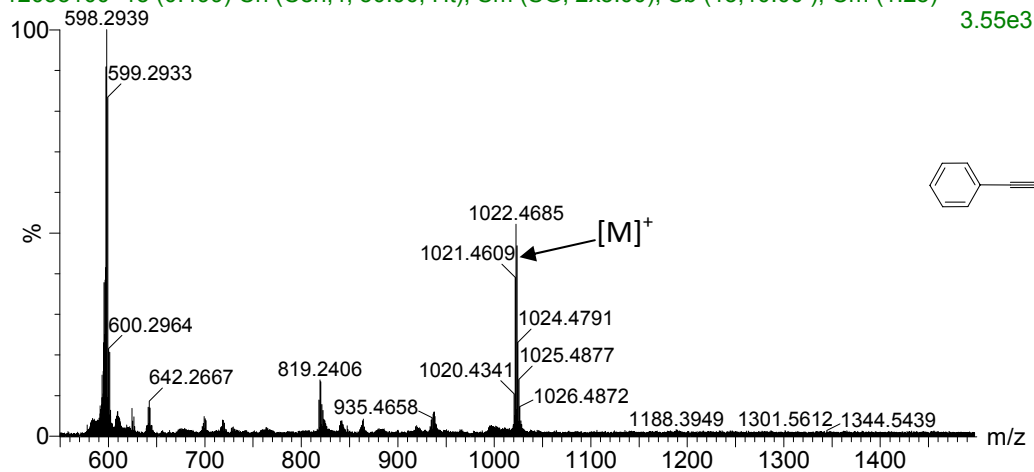


Fig. S18 MALDI-HRMS of **Pt-1**.

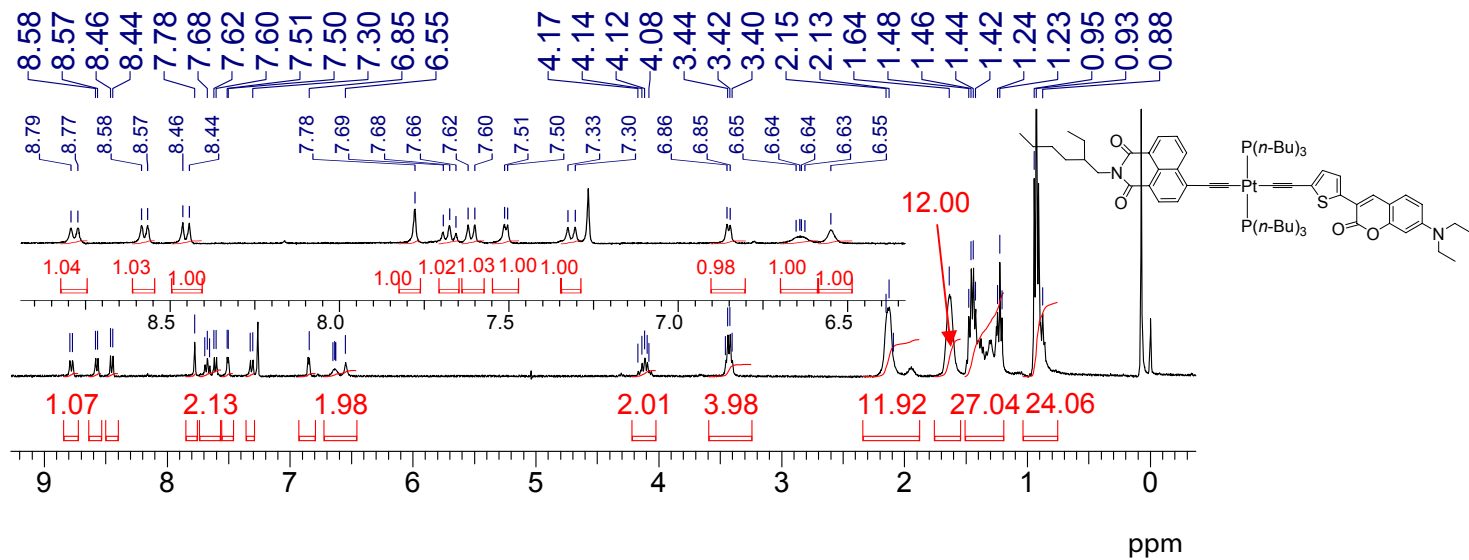


Fig. S19 ^1H NMR of **Pt-2** (400 MHz, CDCl_3).

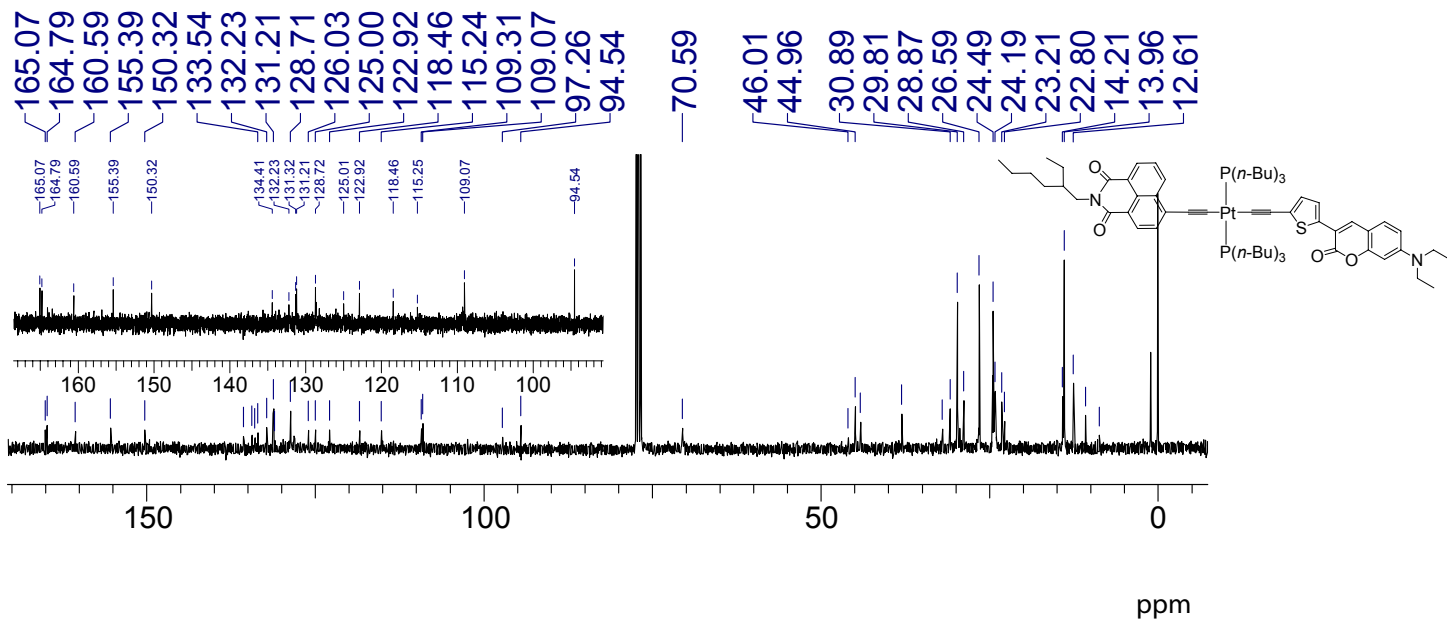


Fig. S20 ^{13}C NMR of **Pt-2** (100 MHz, CDCl_3).

LLL-4(CHCA)

12101705 13 (0.432) Cn (Cen,4, 50.00, Ht); Sm (SG, 2x3.00); Sb (15,10.00); Cm (13:18)

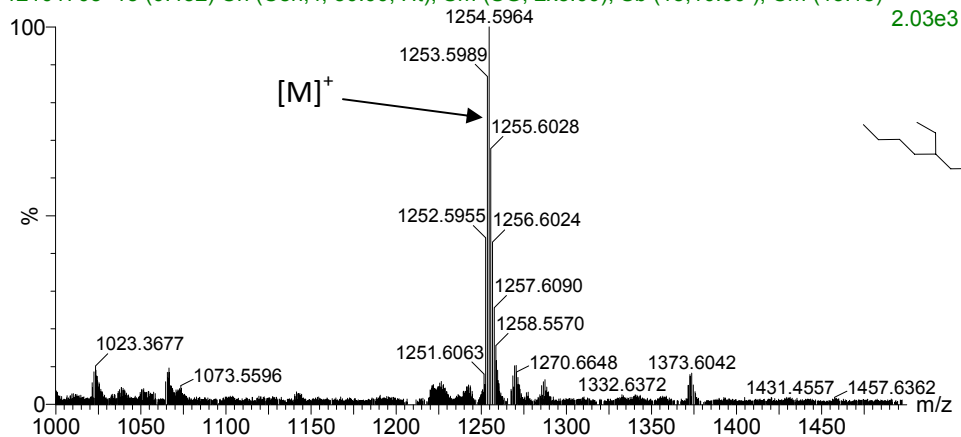


Fig. S21 MALDI-HRMS of Pt-2.

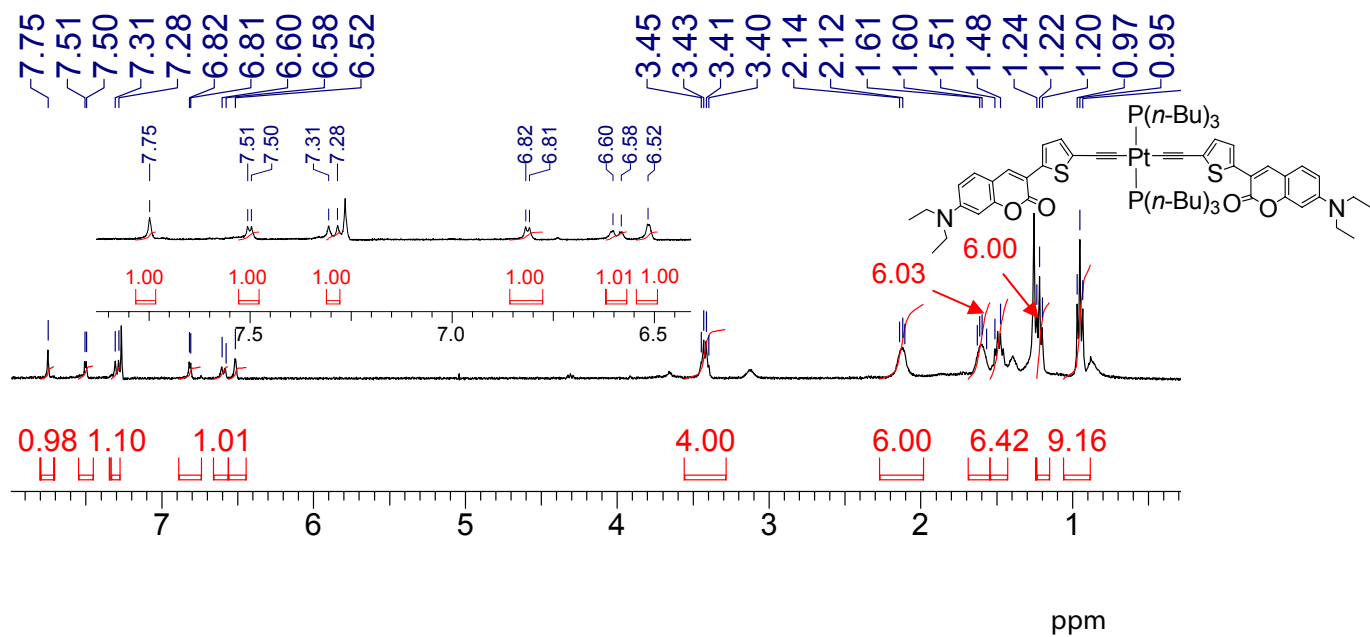


Fig. S22 ^1H NMR of Pt-3 (400 MHz, CDCl_3).

LLL-3(CHCA)

12101704 33 (1.099) Cn (Cen,4, 50.00, Ht); Sm (SG, 2x3.00); Sb (15,10.00); Cm (25:33)

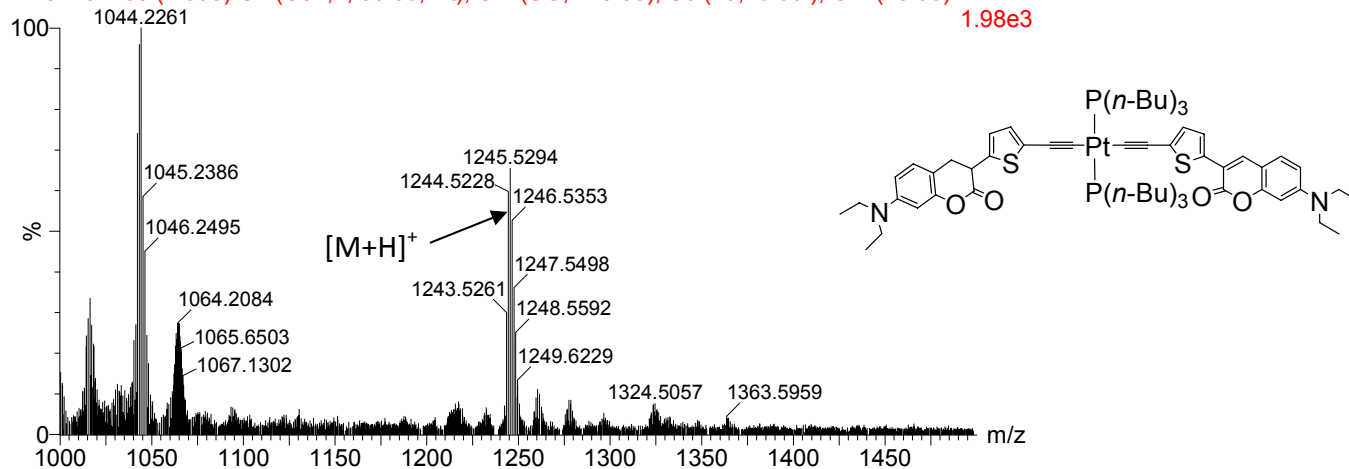


Fig. S23 MALDI-HRMS of Pt-3.

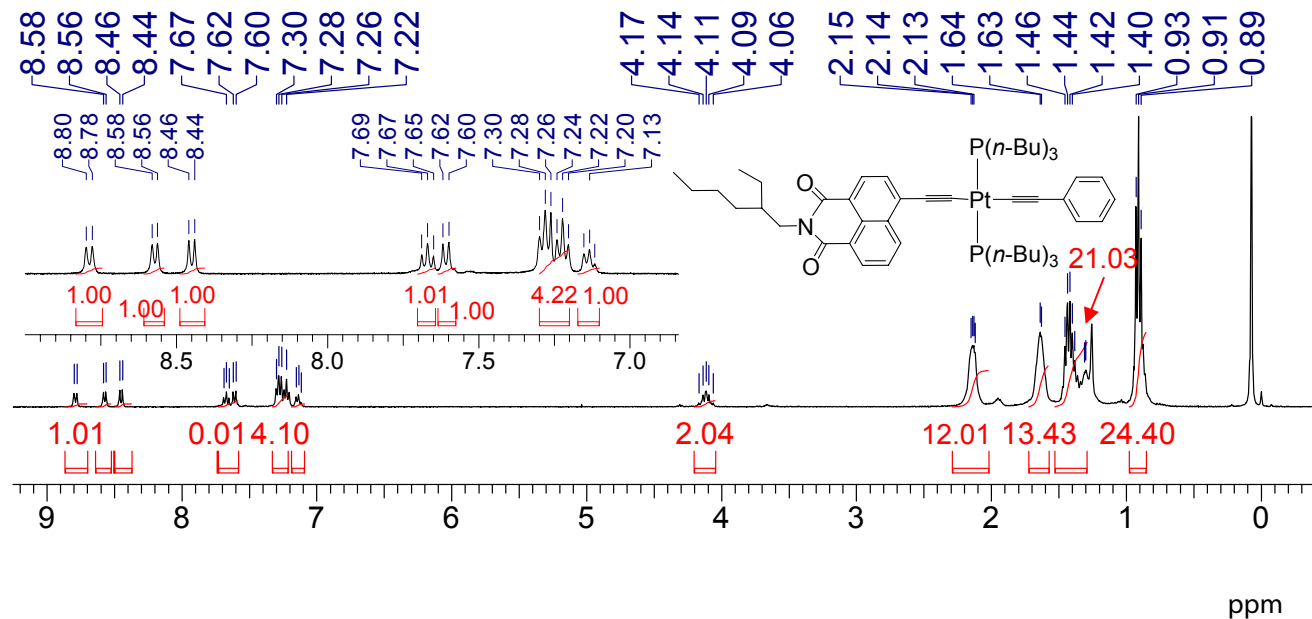


Fig. S24 ^1H NMR of Pt-4 (400 MHz, CDCl_3).

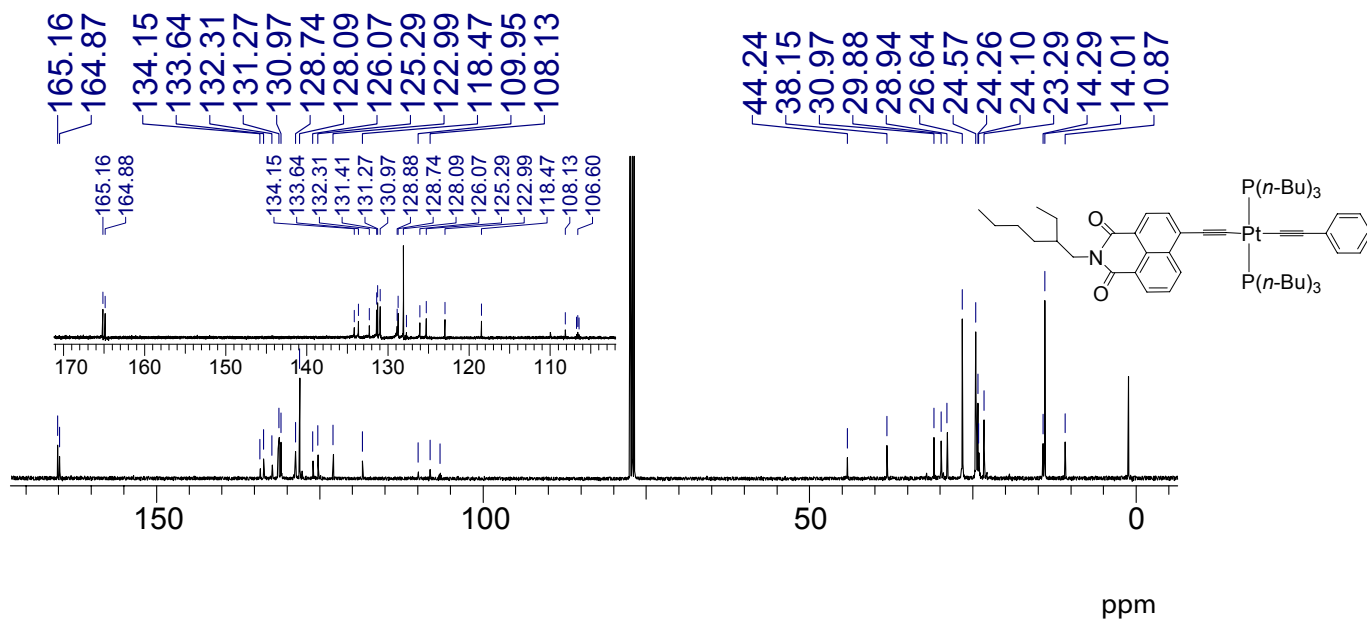


Fig. S25 ¹³C NMR of **Pt-4** (100 MHz, CDCl₃).

LLL-2(CHCA)

12101703 98 (3.266) Cn (Cen,4, 50.00, Ht); Sm (SG, 2x3.00); Sb (15,10.00); Cm (96:98)

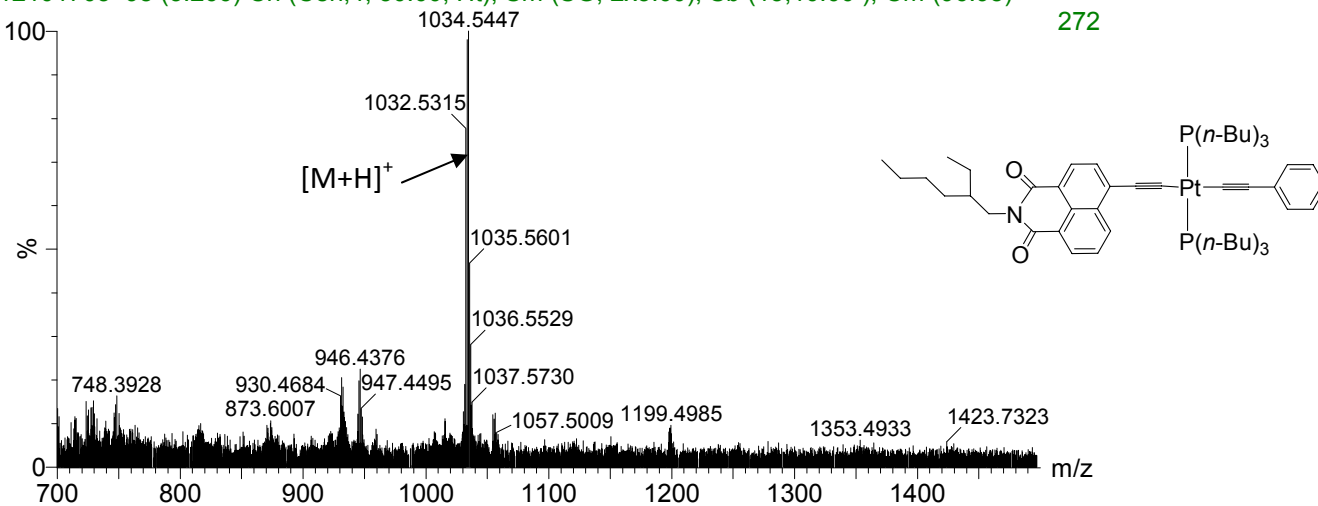


Fig. S26 MALDI-HRMS of **Pt-4**.

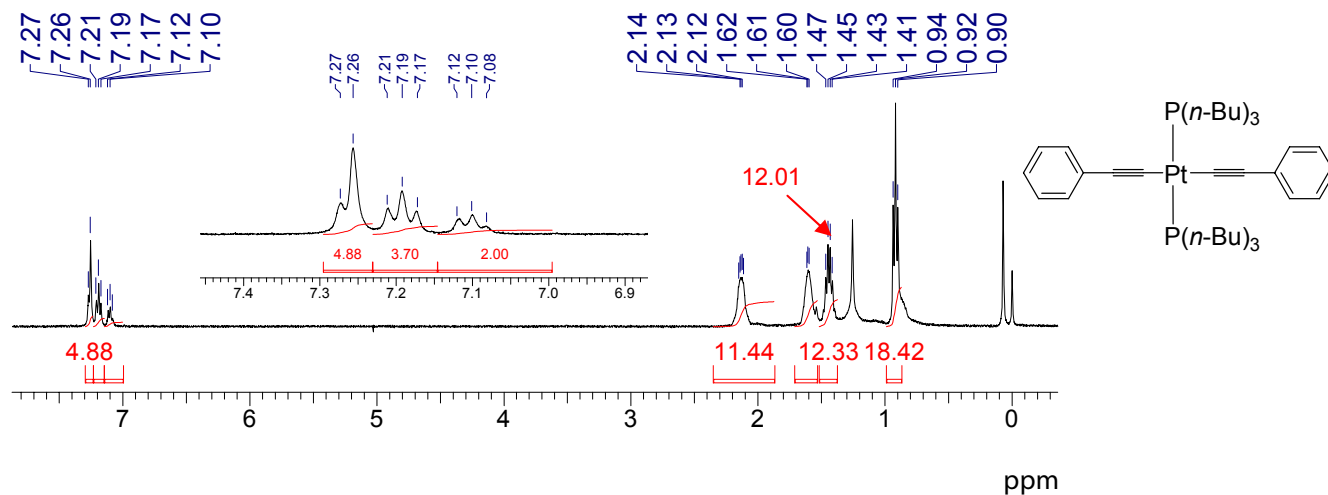


Fig. S27 ¹H NMR of **Pt-5** (400 MHz, CDCl₃).

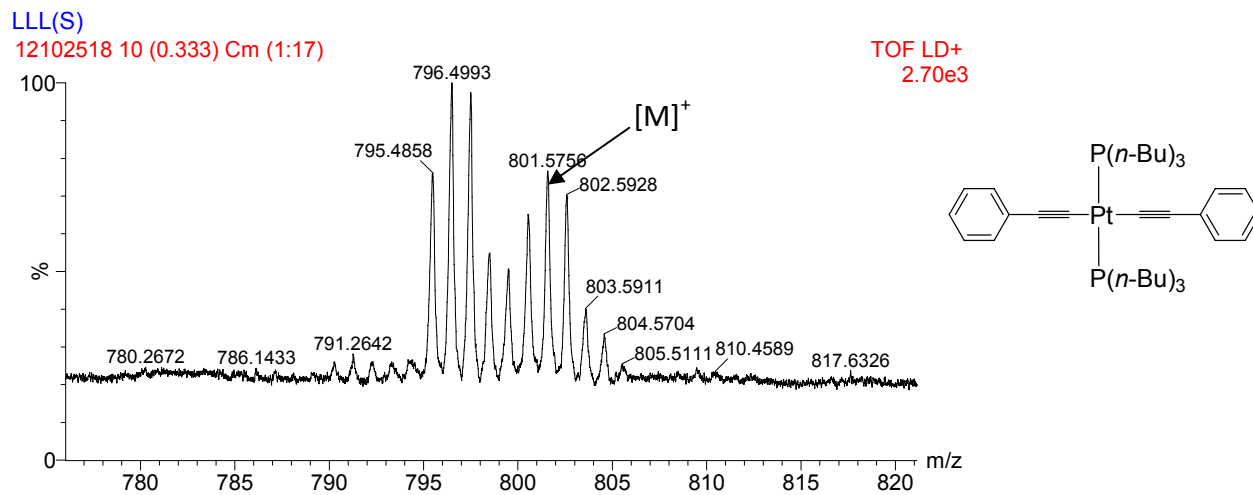


Fig. S28 MALDI-HRMS of **Pt-5**.

2.0 Emission spectra

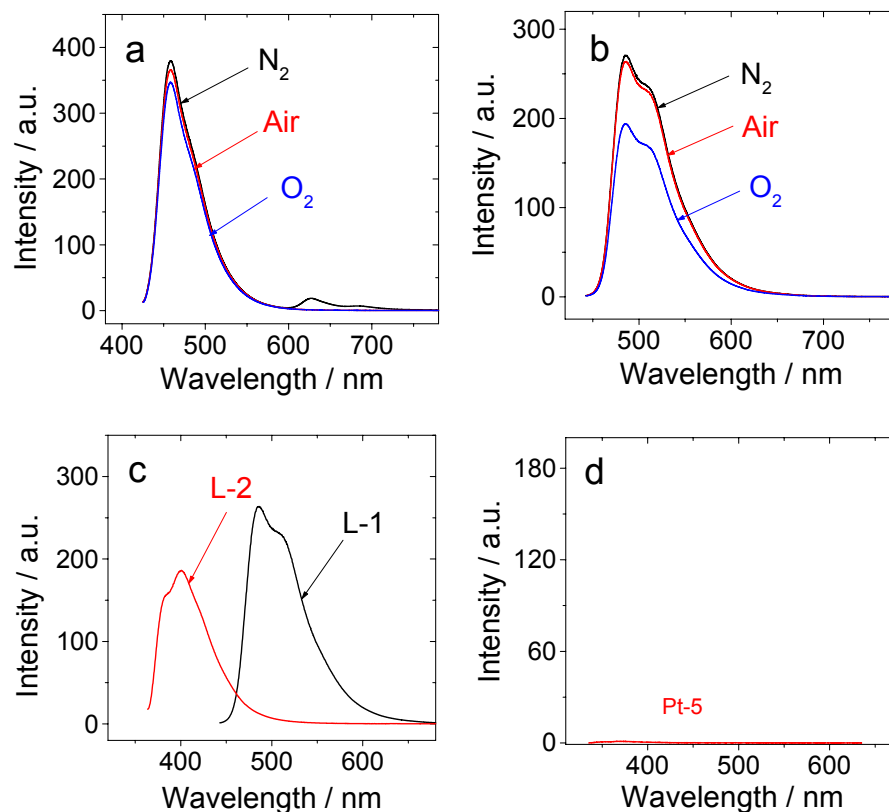


Fig. S29 The emission spectra of (a) **Pt-0** ($\lambda_{\text{ex}} = 420$ nm) and (b) **L-1** ($\lambda_{\text{ex}} = 436$ nm) under different atmosphere, (c) **L-1** ($\lambda_{\text{ex}} = 436$ nm) and **L-2** ($\lambda_{\text{ex}} = 350$ nm) under Air, (d) **Pt-5** ($\lambda_{\text{ex}} = 325$ nm) under N_2 . $c = 1.0 \times 10^{-5}$ M in toluene, 25 °C.

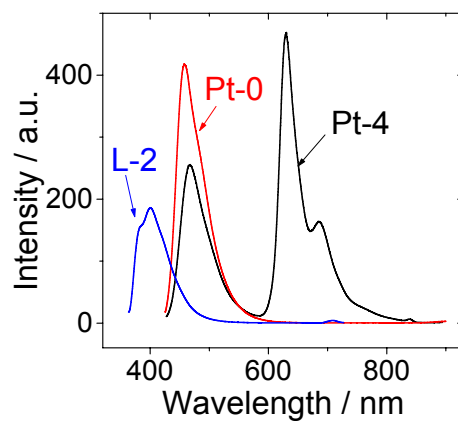


Fig. S30 The emission spectra of **Pt-4** (under N_2 , $\lambda_{\text{ex}} = 420$ nm), **Pt-0** (under Air, $\lambda_{\text{ex}} = 420$ nm) and **L-2** (under Air, $\lambda_{\text{ex}} = 350$ nm). $c = 1.0 \times 10^{-5}$ M in toluene, 25 °C.

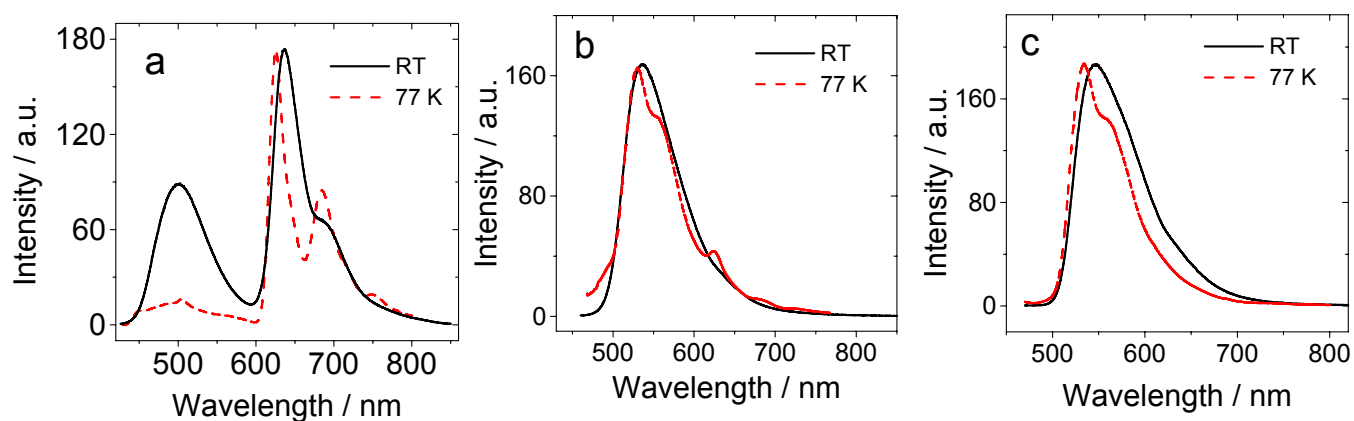


Fig. S31 Photoluminescence spectra of (a) **Pt-0** ($\lambda_{\text{ex}} = 420$ nm), (b) **Pt-2** ($\lambda_{\text{ex}} = 450$ nm), (c) **Pt-3** ($\lambda_{\text{ex}} = 459$ nm) at RT and 77 K. $c = 6.0 \times 10^{-5}$ M in deaerated ethanol-methanol (4:1, v/v).

3.0 Transient absorption details

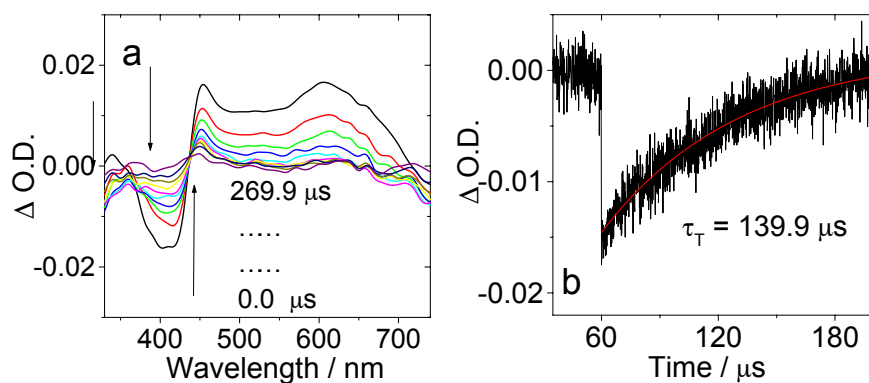


Fig. S32 Nanosecond time-resolved transient absorption difference spectra of (a) **Pt-0** after pulsed excitation ($\lambda_{\text{ex}} = 355$ nm). Decay traces of (b) **Pt-0** at 400 nm. $c = 1.0 \times 10^{-5}$ M in deaerated toluene, 25 °C.

4.0 TTA upconversion details

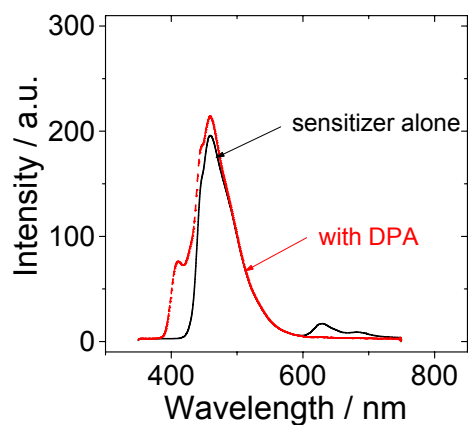


Fig. S33 Emission and upconversion of **Pt-0** with 445 nm (5 mW) laser excitation. c [DPA] = 6.0×10^{-5} M, c [sensitizers] = 1.0×10^{-5} M in deaerated toluene, 25°C.

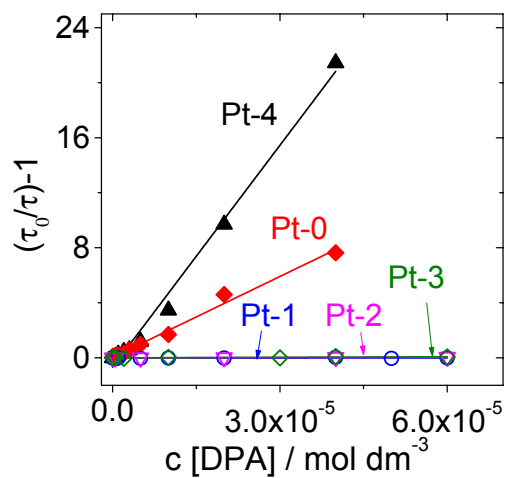


Fig. 34 Stern-Volmer plots for lifetime quenching of **Pt-0**, **Pt-1**, **Pt-2**, **Pt-3** and **Pt-4** with increasing the concentration of DPA after pulsed excitation ($\lambda_{\text{ex}} = 355$ nm). c [sensitizers] = 1.0×10^{-5} M in deaerated toluene, 25 °C.

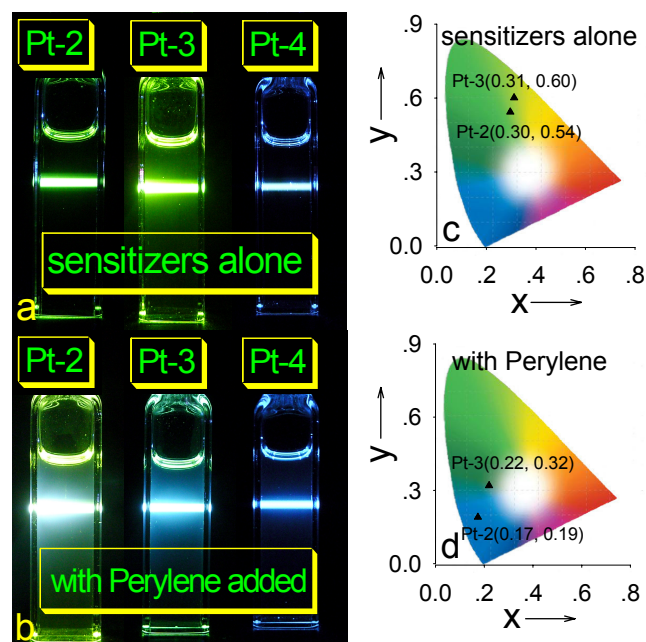


Fig. S35 Photographs of the emission of (a) sensitizers alone and (b) the upconversion. CIE diagram of the emission of (c) sensitizers alone and (d) in the presence of perylene (Py). $\lambda_{\text{ex}} = 473 \text{ nm}$ (laser power: 5 mW). **Pt-4** cannot be excited by 473 nm laser. In deaerated toluene, $c [\text{sensitizers}] = 1.0 \times 10^{-5} \text{ M}$, $c [\text{Py}] = 6.0 \times 10^{-5} \text{ M}$, 25°C .

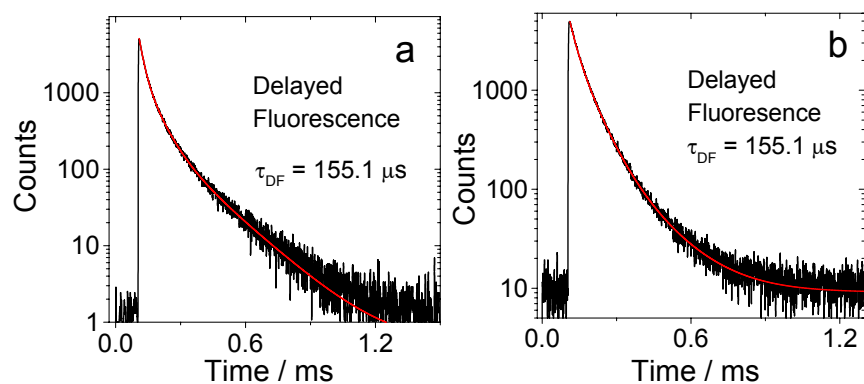


Fig. S36 Delayed fluorescence observed in the TTA upconversion with (a)**Pt-2**, (b)**Pt-3** as triplet photosensitizers and perylene (Py) as the triplet acceptor. Excited at 473 nm (nanosecond pulsed OPO laser synchronized with spectrofluorometer) and monitored at 445 nm. $c [\text{sensitizers}] = 1.0 \times 10^{-5} \text{ M}$, $c [\text{Py}] = 4.0 \times 10^{-5} \text{ M}$, in toluene, 25°C .

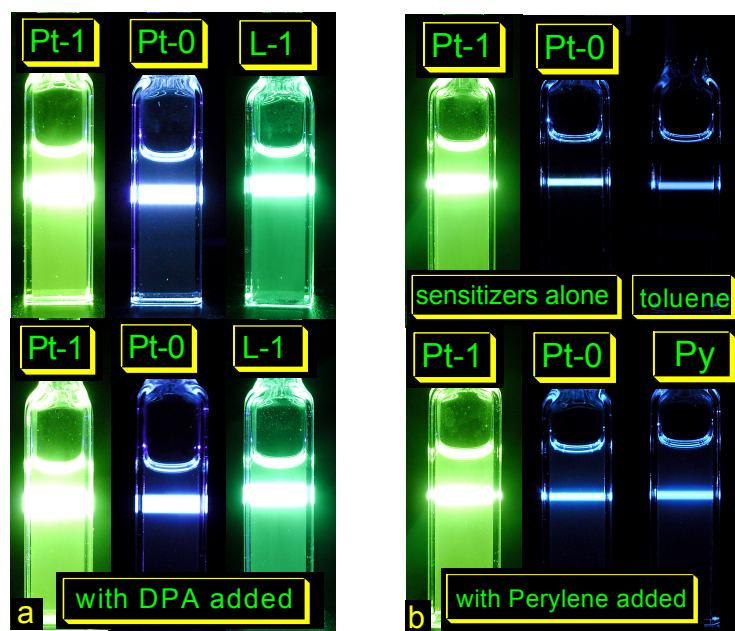


Fig. S37 (a) Photographs of the emission of triplet photosensitizers alone and the TTA upconversion in the presence of DPA ($\lambda_{\text{ex}} = 445$ nm, laser power: 5 mW) and (b) in the presence of perylene (Py) ($\lambda_{\text{ex}} = 473$ nm, laser power: 5 mW). In deaerated toluene, c [sensitizers] = 1.0×10^{-5} M, c [DPA] = 6.0×10^{-5} M, c [Py] = 4.0×10^{-5} M, 25 °C.

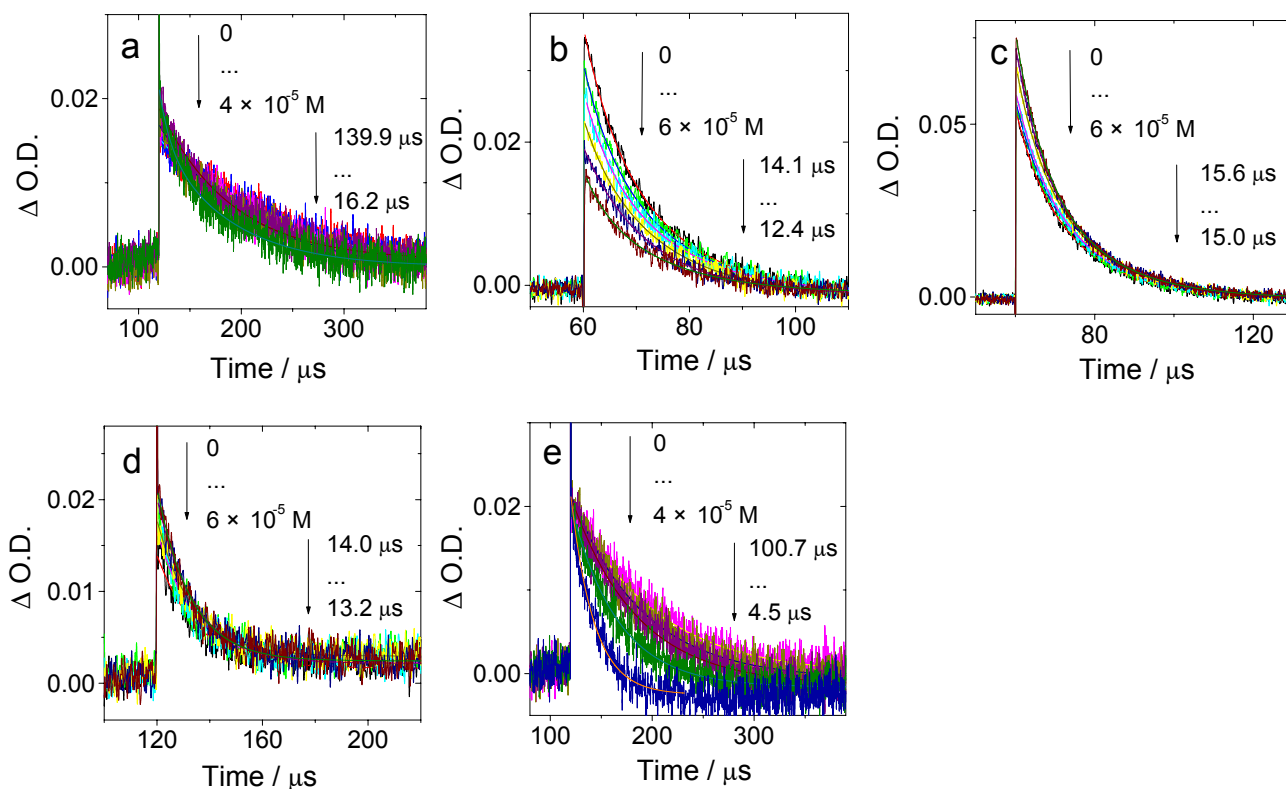


Fig. S38 Quenching of the lifetime of the triplet photosensitizers with increasing the concentration of DPA, (a) **Pt-0**, c [DPA] = 0 - 4.0×10^{-5} M, τ_T = 139.9 μs - 16.2 μs . (b) **Pt-1**, c [DPA] = 0 - 6.0×10^{-5} M, τ_T = 14.1 μs - 12.4 μs . (c) **Pt-2**, c [DPA] = 0 - 6.0×10^{-5} M, τ_T = 15.6 μs - 15.0 μs . (d) **Pt-3**, c [DPA] = 0 - 6.0×10^{-5} M, τ_T = 14.0 μs - 13.2 μs . (e) **Pt-4**, c [DPA] = 0 - 4.0×10^{-5} M, τ_T = 100.7 μs - 4.5 μs . c [sensitizers] = 1.0×10^{-5} M, in deaerated toluene. 25 °C.

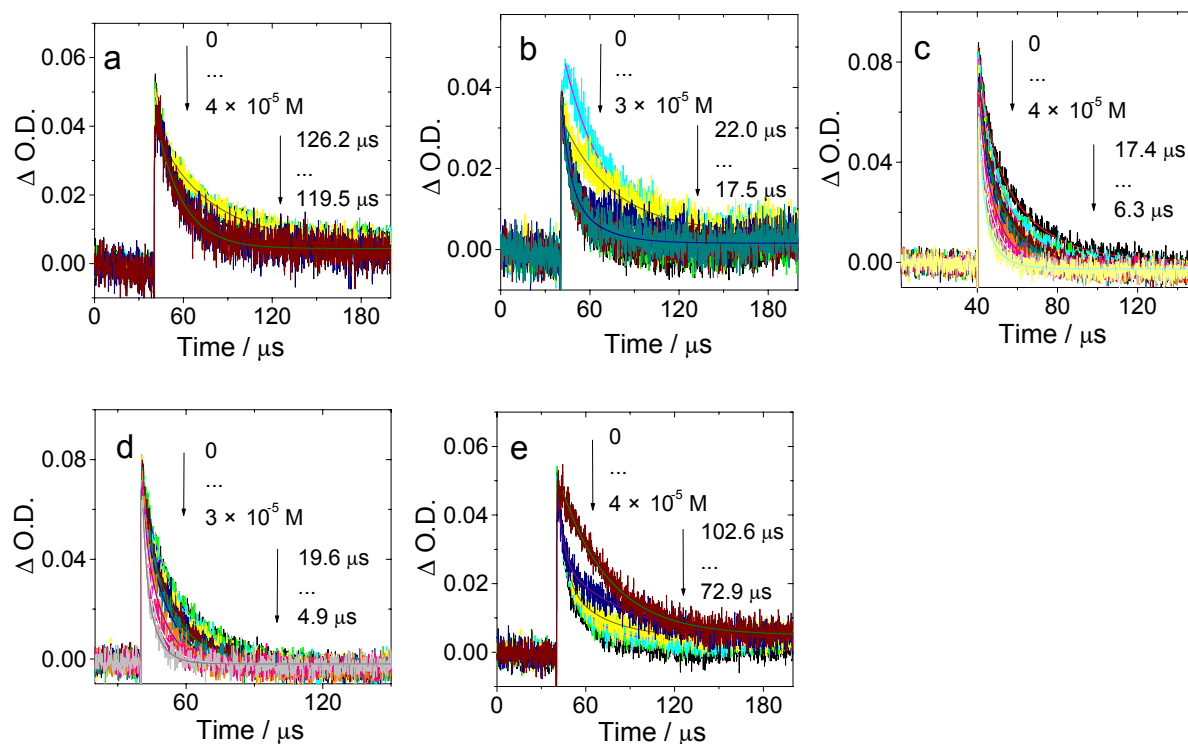


Fig. S39 Quenching of the lifetime of the triplet photosensitizers with increasing the concentration of perylene (Py). (a) **Pt-0**, $c[\text{Py}] = 0 - 4.0 \times 10^{-5} \text{ M}$, $\tau_T = 126.2 \mu\text{s} - 119.5 \mu\text{s}$. (b) **Pt-1**, $c[\text{Py}] = 0 - 3.0 \times 10^{-5} \text{ M}$, $\tau_T = 22.0 \mu\text{s} - 17.5 \mu\text{s}$. (c) **Pt-2**, $c[\text{Py}] = 0 - 4.0 \times 10^{-5} \text{ M}$, $\tau_T = 17.4 \mu\text{s} - 6.3 \mu\text{s}$. (d) **Pt-3**, $c[\text{Py}] = 0 - 3.0 \times 10^{-5} \text{ M}$, $\tau_T = 19.6 \mu\text{s} - 4.9 \mu\text{s}$. (e) **Pt-4**, $c[\text{Py}] = 0 - 4.0 \times 10^{-5} \text{ M}$, $\tau_T = 102.6 \mu\text{s} - 72.9 \mu\text{s}$. $c[\text{sensitizers}] = 1.0 \times 10^{-5} \text{ M}$, in deaerated toluene. 25 °C.

Table S1. Quenching of the lifetime of the triplet photosensitizers with increasing the concentration of DPA and perylene (Py).^a

$c[\text{DPA}]^b$	0	0.01	0.05	0.1	0.2	0.3	0.5	1.0	2.0	3.0	4.0	5.0	6.0
$\tau_{\text{Pt-0}}/\mu\text{s}^d$	139.9	126.2	119.0	116.7	105.0	88.8	70.6	52.0	25.0	—	16.2	—	—
$\tau_{\text{Pt-1}}/\mu\text{s}^d$	14.1	13.7	13.4	13.5	—	—	13.9	13.6	13.8	—	13.0	14.0	12.4
$\tau_{\text{Pt-2}}/\mu\text{s}^d$	15.6	—	15.7	—	—	—	15.8	—	15.2	—	15.2	—	15.0
$\tau_{\text{Pt-3}}/\mu\text{s}^d$	14.0	—	13.9	—	14.6	—	—	13.6	—	14.1	12.8	—	13.2
$\tau_{\text{Pt-4}}/\mu\text{s}^d$	100.7	100.6	98.3	81.0	70.0	64.5	46.0	22.7	9.4	—	4.5	—	—
$c[\text{Py}]^c$	0	0.01	0.05	0.1	0.2	0.3	0.5	1.0	2.0	3.0	4.0	5.0	6.0
$\tau_{\text{Pt-0}}/\mu\text{s}^d$	126.2	123.2	—	—	—	126.9	125.2	—	—	123.9	119.5	—	—
$\tau_{\text{Pt-1}}/\mu\text{s}^d$	22.0	22.7	17.5	17.5	—	19.0	—	19.1	—	17.5	—	—	—
$\tau_{\text{Pt-2}}/\mu\text{s}^d$	17.4	17.0	16.4	15.4	14.1	13.4	11.9	10.6	9.2	7.2	6.3	—	—
$\tau_{\text{Pt-3}}/\mu\text{s}^d$	19.6	16.8	16.3	15.0	—	13.1	—	8.7	—	4.9	—	—	—
$\tau_{\text{Pt-4}}/\mu\text{s}^d$	102.6	101.3	94.1	97.5	—	—	101.7	—	84.8	—	72.9	—	—

^a In deaerated toluene, pulsed excitation ($\lambda_{\text{ex}} = 355 \text{ nm}$), 25 °C. ^b $c[\text{DPA}] : 10^{-5} \text{ M}$. ^c $c[\text{Py}] : 10^{-5} \text{ M}$. ^d The lifetime of the triplet excited states of the triplet photosensitizers **Pt-0**, **Pt-1**, **Pt-2**, **Pt-3** and **Pt-4**.

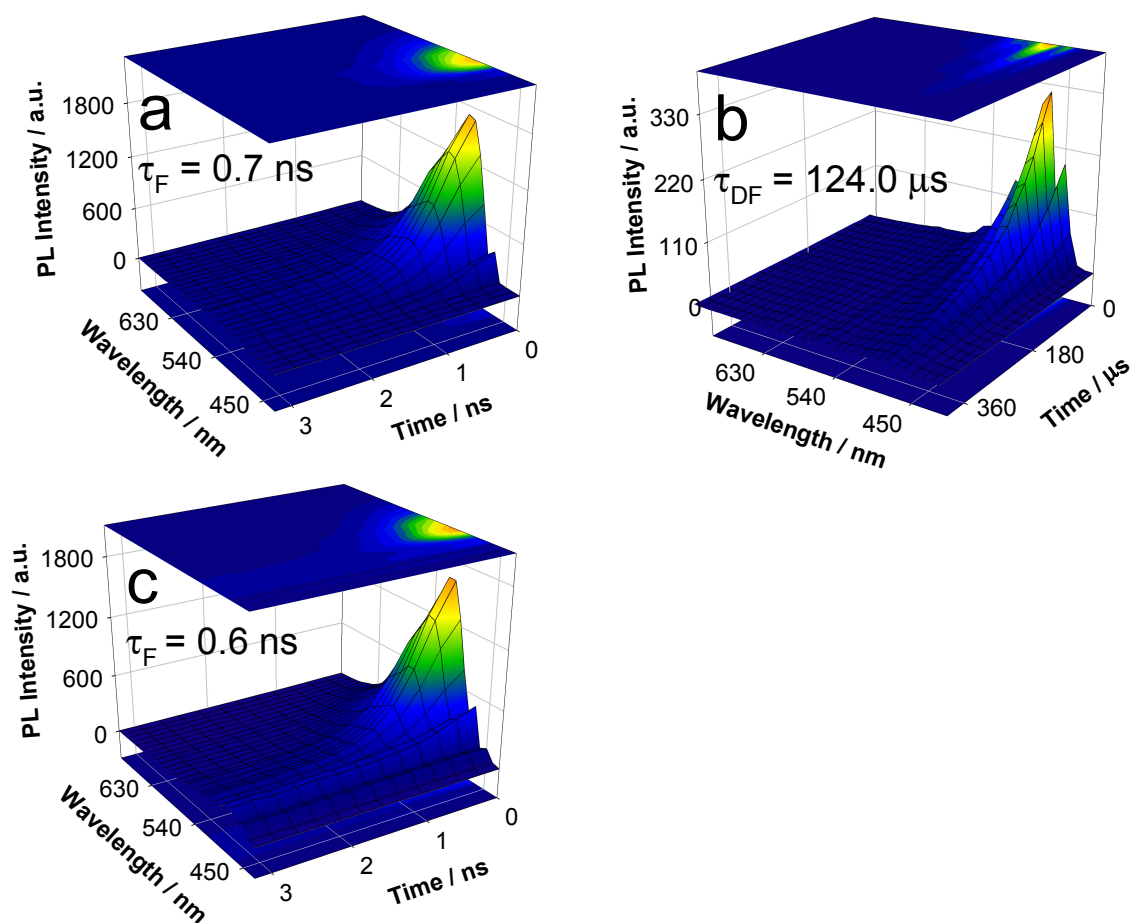


Fig. S40 Time-resolved emission spectra (TRES) of **Pt-2** alone and the TTA upconversion. With perylene (Py) as triplet acceptor. (a) **Pt-2** alone, the fluorescence region was measured (430 nm – 700 nm, $\tau = 0.7$ ns). (b) TRES of **Pt-2** in the presence of perylene. Upconverted emission in the range of 430 nm – 530 nm was observed ($\tau = 124.0$ μs). (c) TRES of **Pt-2** in the presence of perylene. The fluorescence of **Pt-2** in the range of 460 nm – 620 nm was observed ($\tau = 0.6$ ns). c [Py] = 4.0×10^{-5} M; c [sensitizers] = 1.0×10^{-5} M. In deaerated toluene. Excited with nanosecond pulsed OPO laser synchronized with spectrofluorometer ($\lambda_{ex} = 473$ nm), pico-second pulsed laser ($\lambda_{ex} = 473$ nm). 25°C.

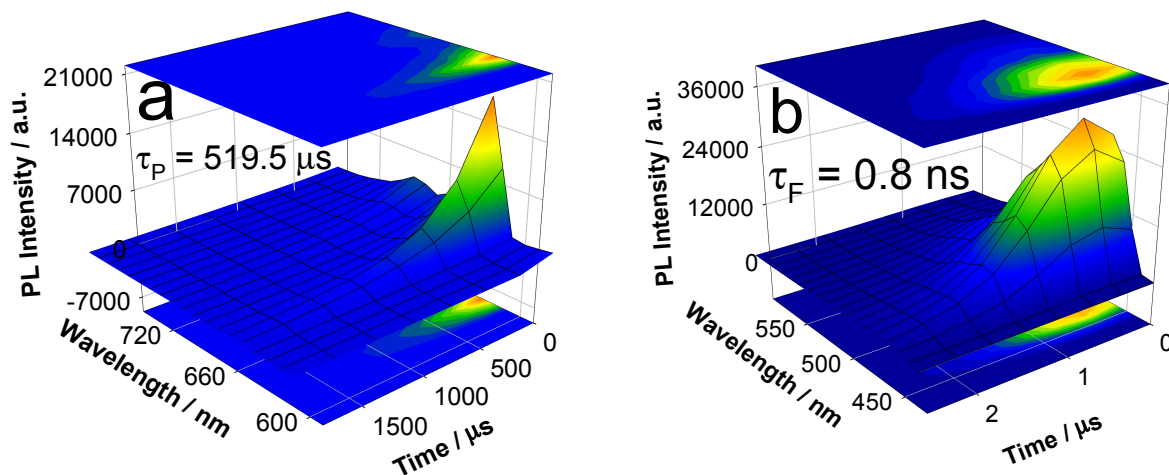


Fig. S41 Time-resolved emission spectra (TRES) of **Pt-4** alone at 77 K. (a) The phosphorescence region was measured (590 nm – 750 nm, $\tau = 519.5 \mu s$) excited with OPO nanosecond laser (420 nm) and (b) the fluorescence region was measured (430 nm – 590 nm, $\tau = 0.8 ns$) excited with pico-second pulsed laser (405 nm). c [sensitizers] = $1.0 \times 10^{-5} M$ in deaerated ethanol-methanol (4:1, v/v).

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

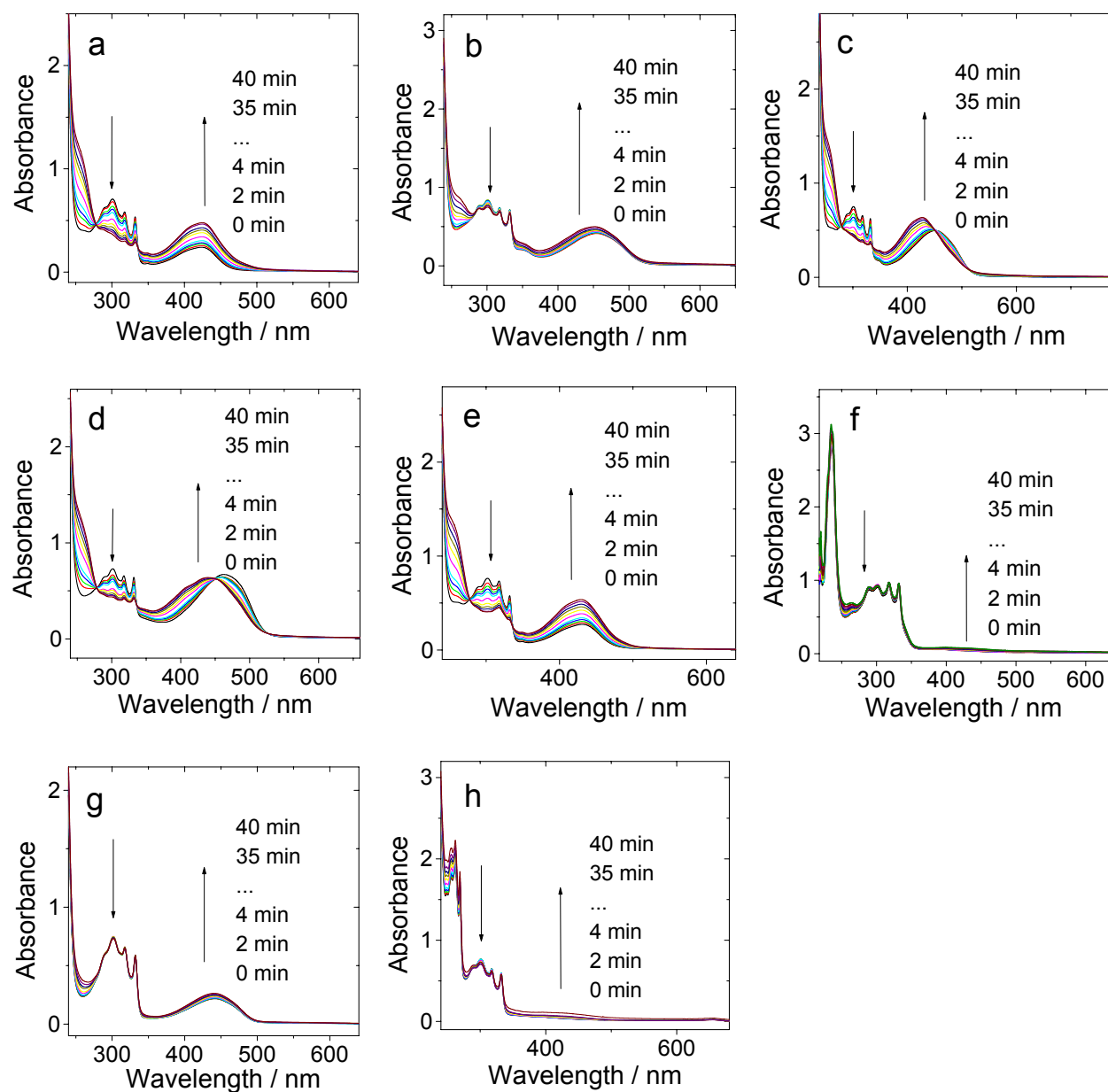


Fig. S42 Photosensitizing of $^1\text{O}_2$ with the complexes as photosensitizers. Irradiation time-dependent decrease of absorbance at 301 nm of DHN (1.0×10^{-4} M) with different $^1\text{O}_2$ sensitizers (a) **Pt-0**, (b) **Pt-1**, (c) **Pt-2**, (d) **Pt-3**, (e) **Pt-4**, (f) **Pt-5**, (g) **L-1**, (h) **Ir(ppy)₃**. $c[\text{sensitizers}] = 1.0 \times 10^{-5}$ M. In $\text{CH}_2\text{Cl}_2/\text{MeOH}$ (9:1, v/v). 20 mW/cm². 20 °C.

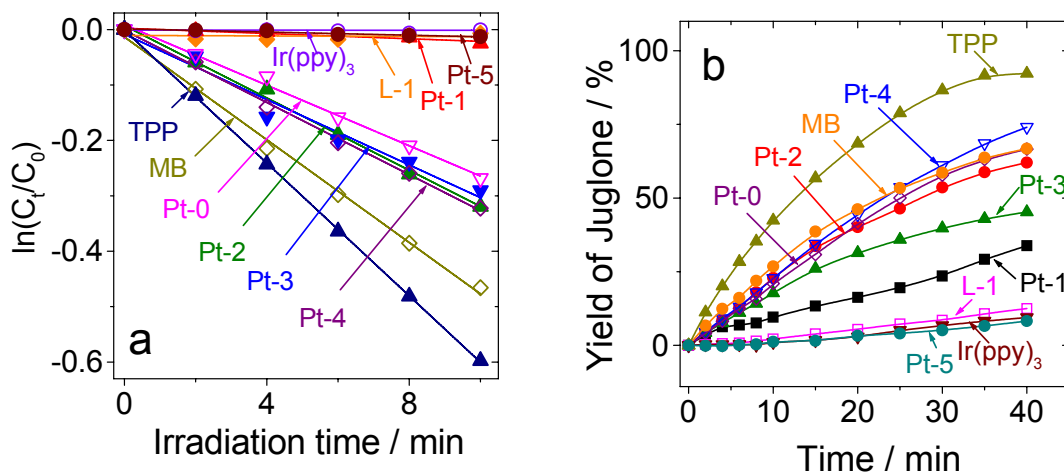


Fig. S43 Photosensitizing of $^1\text{O}_2$ with the complexes as photosensitizers. Irradiation time-dependent decrease of absorbance at 301 nm of DHN (1×10^{-4} M) with different $^1\text{O}_2$ sensitizers. (a) Plots of $\ln(C_t/C_0)$ vs. irradiation time. (b) Plots of chemical yield as a function of irradiation time for the photooxidation of DHN. c [sensitizers] = 1.0×10^{-5} M, In $\text{CH}_2\text{Cl}_2/\text{MeOH}$ (9:1, v/v), 20 °C.

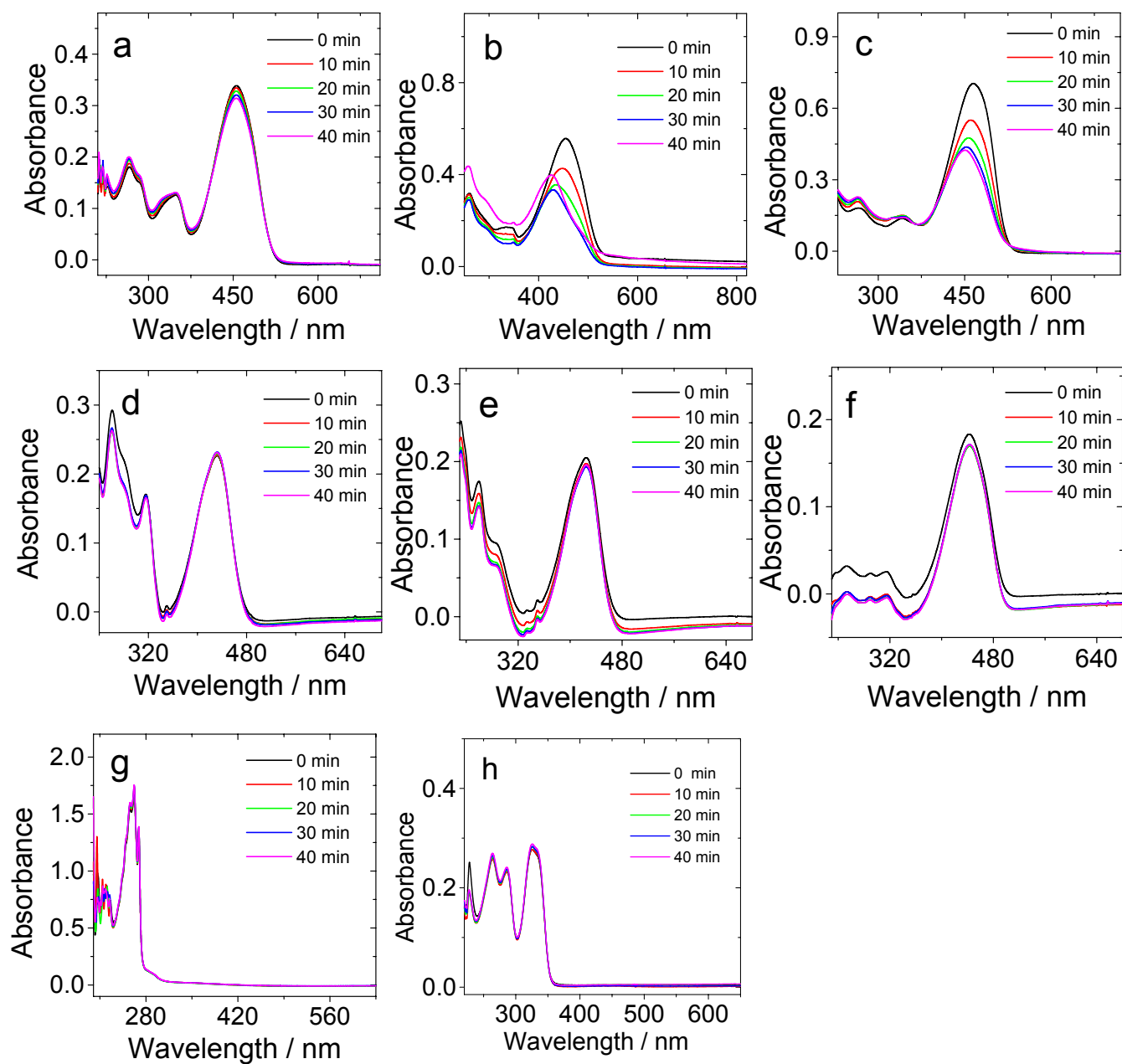


Fig. S44 UV-Vis absorption spectra of the sensitizers (a) **Pt-1**, (b) **Pt-2**, (c) **Pt-3**, (d) **Pt-4**, (e) **Pt-0**, (f) **L-1**, (g) **Ir(ppy)₃**, (h) **Pt-5** in CH₂Cl₂/MeOH (9 : 1 v/v) before and after the irradiation. c [sensitizers] = 1.0×10⁻⁵ M. 20 mW/cm², 20 °C.

6.0 DFT calculations

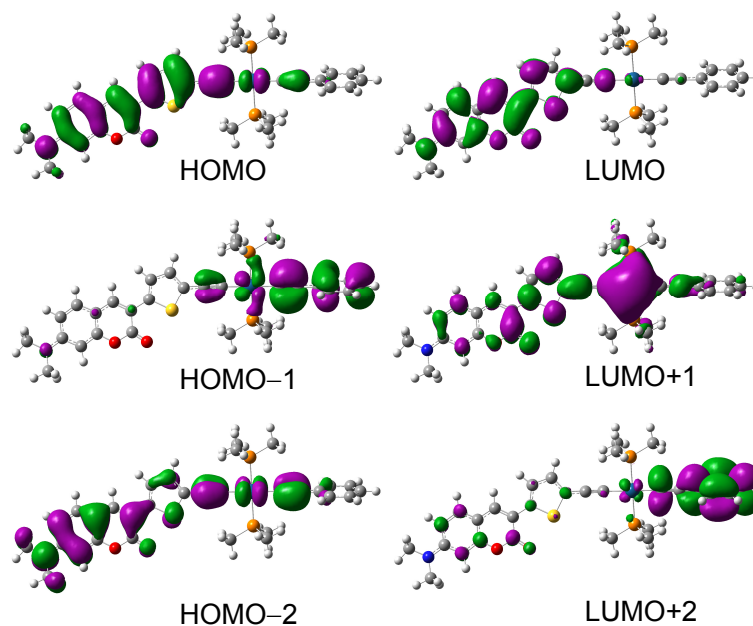


Fig. S45 Electron density maps of the frontier molecular orbitals of complex **Pt-1** based on the optimized ground-state geometry. The solvent toluene was considered in the calculations (PCM model). Calculated at the B3LYP/6-31G/LANL2DZ level with Gaussian 09W.

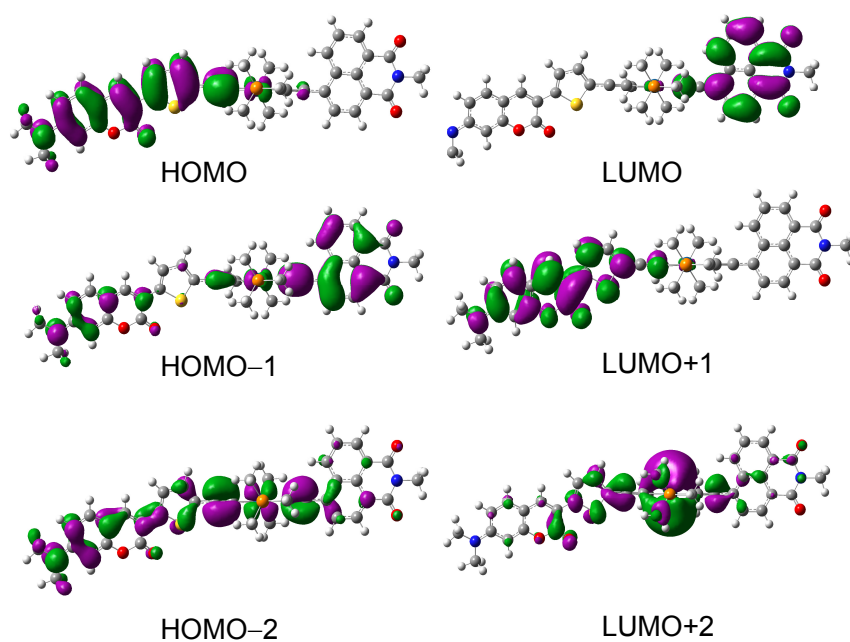


Fig. S46 Electron density maps of the frontier molecular orbitals of complex **Pt-2** based on the optimized ground-state geometry. The solvent toluene was considered in the calculations (PCM model). Calculated at the B3LYP/6-31G/LANL2DZ level with Gaussian 09W.

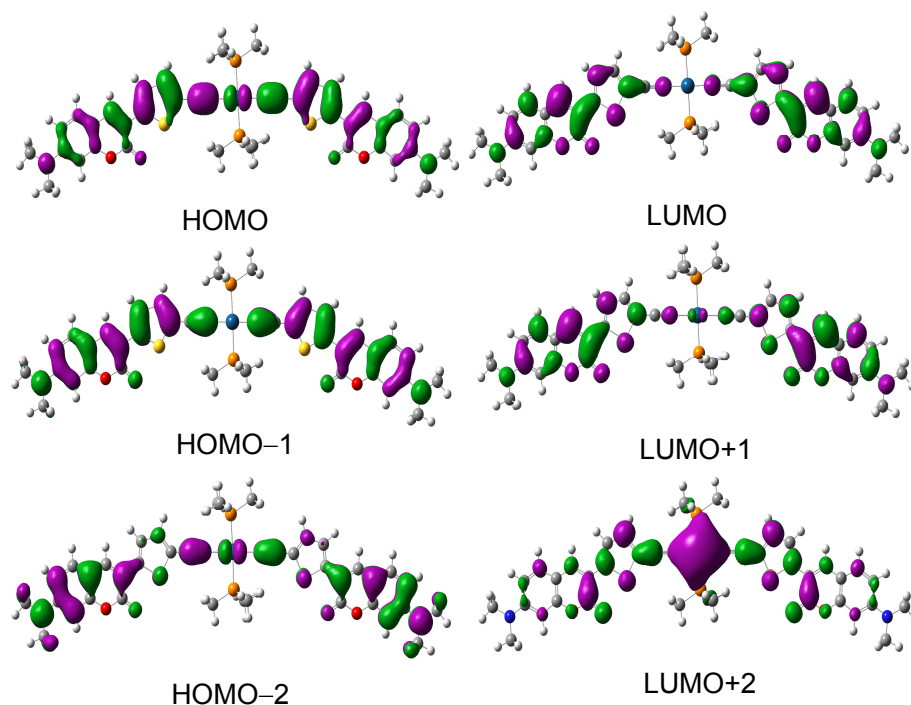


Fig. S47 Electron density maps of the frontier molecular orbitals of complex **Pt-3** based on the optimized ground-state geometry. Toluene was used as the solvent in the calculations (PCM model). Calculated at the B3LYP/6-31G/LANL2DZ level with Gaussian 09W.

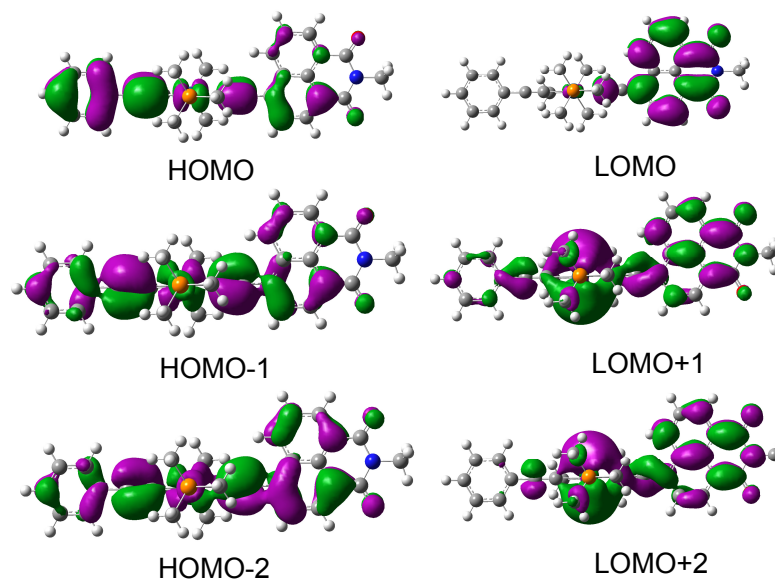


Fig. S48 Electron density maps of the frontier molecular orbitals of complex **Pt-4** based on the optimized ground-state geometry. Toluene was used as the solvent in the calculations (PCM model). Calculated at the B3LYP/6-31G/LANL2DZ level with Gaussian 09W.

Table S2. 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//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	<i>f</i> ^b	Composition ^c	CI ^d	character
Singlet	S ₀ →S ₁	2.52 eV / 491 nm	1.4682	H → L	0.7041	ILCT
	S ₀ →S ₂	3.24 eV / 382 nm	0.0086	H-1 → L	0.6843	MLCT
				H-1 → L+1	0.1006	MLCT
				H-2 → L	0.6015	MLCT
	S ₀ →S ₄	3.49 eV / 355 nm	0.1106	H-2 → L	0.6015	MLCT
Triplet	T ₁ →S ₀	1.65 eV / 753 nm	0.0000 ^e	H → L	0.5941	MLCT
				H-3 → L	0.6744	ILCT
				H-2 → L	0.1380	MLCT
	T ₂ →S ₀	2.62 eV / 474 nm	0.0000	H → L+1	0.4342	MLCT
				H-3 → L	0.4540	MLCT
				H-2 → L	0.1499	MLCT
	T ₃ →S ₀	3.06 eV / 406 nm	0.0000	H-2 → L	0.4365	MLCT
				H → L	0.1034	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 S3. 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//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	<i>f</i> ^b	Composition ^c	CI ^d	character
Singlet	S ₀ →S ₁	2.27 eV / 546 nm	0.1441	H → L	0.7026	ILCT
	S ₀ →S ₂	2.63 eV / 471 nm	1.5293	H → L+1	0.6988	ILCT
	S ₀ →S ₃	2.93 eV / 423 nm	0.0563	H-3 → L	0.3160	MLCT
				H-2 → L	0.5831	MLCT
				H-1 → L	0.1924	MLCT
Triplet	S ₀ →S ₄	2.98 eV / 416 nm	0.3466	H-1 → L	0.6514	MLCT
	T ₁ →S ₀	1.69 eV / 734 nm	0.0000 ^e	H → L+1	0.6758	ILCT
	T ₂ →S ₀	1.96 eV / 633 nm	0.0000	H-2 → L	0.1669	MLCT
				H-1 → L	0.5866	MLCT
				H → L	0.2251	ILCT
	T ₃ →S ₀	2.30 eV / 540 nm	0.0000	H → L	0.6596	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 S4. Electronic Excitation Energies (eV) and corresponding Oscillator Strengths (f), main configurations and CI coefficients of the Low-lying Electronically Excited States of complex **Pt-3**, Calculated by TDDFT//B3LYP/6-31G/LanL2DZ, based on the DFT//B3LYP/6-31G/LanL2DZ Optimized Ground State Geometries.

	Electronic transition	Energy (eV) ^a	TDDFT//B3LYP/6-31G			
			<i>f</i> ^b	Composition ^c	CI ^d	character
Singlet	S ₀ →S ₁	2.31 eV / 538 nm	2.3105	H→L	0.6923	MLCT
	S ₀ →S ₂	2.52 eV / 492 nm	0.0784	H→L+1	0.7016	ILCT
	S ₀ →S ₃	2.78 eV / 446 nm	0.0782	H-1→L	0.6998	ILCT
	S ₀ →S ₄	2.91 eV / 427 nm	0.5855	H-1→L+1	0.5855	ILCT
Triplet				H→L	0.1274	MLCT
	T ₁ →S ₀	1.60 eV / 774 nm	0.0000 ^e	H→L	0.5753	MLCT
	T ₂ →S ₀	1.66 eV / 748 nm	0.0000	H→L+1	0.5168	MLCT
	T ₃ →S ₀	2.47 eV / 501 nm	0.0000	H-2→L	0.3085	MLCT
				H-1→L+1	0.3846	ILCT
				H→L+2	0.3789	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 S5. Electronic Excitation Energies (eV) and corresponding Oscillator Strengths (f), main configurations and CI coefficients of the Low-lying Electronically Excited States of complex **Pt-4**, Calculated by TDDFT//B3LYP/6-31G/LanL2DZ, based on the DFT//B3LYP/6-31G/LanL2DZ Optimized Ground State Geometries.

	Electronic transition	Energy (eV) ^a	TDDFT//B3LYP/6-31G			
			<i>f</i> ^b	Composition ^c	CI ^d	character
Singlet	S ₀ →S ₁	2.79 eV / 445 nm	0.3914	H-1→L	0.1726	MLCT
	S ₀ →S ₂	2.87 eV / 431 nm	0.0221	H-2→L	0.4433	MLCT
				H-1→L	0.5093	MLCT
	S ₀ →S ₃	3.10 eV / 400 nm	0.2976	H-2→L	0.6515	MLCT
Triplet	S ₀ →S ₄	3.74 eV / 332 nm	0.0001	H-8→L	0.6515	
	T ₁ →S ₀	1.96 eV / 634 nm	0.0000 ^e	H-1→L	0.3276	MLCT
				H→L	0.4238	ILCT
	T ₂ →S ₀	2.82 eV / 440 nm	0.0000	H-2→L	0.5127	MLCT
				H-1→L	0.3792	MLCT
				H→L	0.2350	ILCT
	T ₃ →S ₀	2.87 eV / 432 nm	0.0000	H→L	0.4775	ILCT

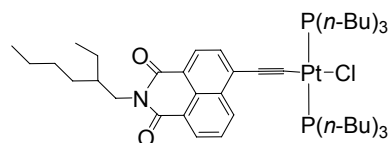
^a Only the selected low-lying excited states are presented. ^b oscillator strength. ^c H stands for HOMO and L stands for LUMO. Only the main configurations are presented. ^d The CI coefficients are in absolute values. ^e No spin-orbital coupling effect was considered, thus the *f* values are zero.

7.0 The coordinates of the optimized ground state geometries of complexes

Complex Pt-0 (DFT//B3LYP/6-31G(d) / LanL2DZ)

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1



C	-0.79180900	0.00151700	-0.29880900
Pt	-2.73516700	0.02780900	-0.03658300
P	-2.89885300	-2.31704800	-0.13927000
C	-3.97640900	-2.87766600	-1.51988700
H	-4.10647400	-3.96549000	-1.50181200
H	-3.52850500	-2.58231500	-2.47345300
H	-4.94553900	-2.38184700	-1.42154900
C	-1.33673300	-3.26068100	-0.36440200
H	-0.65804800	-3.04942200	0.46614600
H	-0.84519200	-2.94015900	-1.28661900
H	-1.53680500	-4.33668800	-0.40915600
C	-3.66027800	-3.04363700	1.36903600
H	-3.01162600	-2.85812700	2.23048600
H	-4.61890000	-2.54797500	1.54186400
H	-3.80983300	-4.12301500	1.25403800
P	-2.60192400	2.37575700	0.05464000
C	-4.18411800	3.28953800	0.23919500
H	-4.00079100	4.36912400	0.27550500
H	-4.68812500	2.96397600	1.15225600
H	-4.84126100	3.05092800	-0.60067500
C	-1.55596700	2.97611900	1.44484400
H	-0.56371000	2.52570700	1.35707500
H	-1.99844200	2.65968300	2.39414200
H	-1.46827800	4.06807000	1.43290600
C	-1.81890400	3.10471800	-1.44275700
H	-0.83784100	2.64345200	-1.58347600
H	-2.43515600	2.88137700	-2.31883100
H	-1.70877200	4.19038300	-1.34535700
C	2.74234500	-0.07609100	0.42908400
C	2.35517400	0.10376000	-1.97580800
C	2.29800100	-0.17749400	1.77067900
C	4.14764100	-0.05920500	0.17674200
C	3.73791000	0.11783400	-2.20570300
H	1.66911500	0.16685900	-2.81448000
C	3.19975600	-0.25656000	2.81521000
H	1.22836200	-0.19311300	1.95763700
C	5.05507500	-0.14116100	1.26472200
C	4.63499300	0.03931600	-1.15114800
H	4.13130600	0.19150400	-3.21437900
C	4.58548200	-0.23802200	2.56340900
H	2.84076700	-0.33393300	3.83749800
H	5.30664700	-0.29877800	3.37193600
C	6.51785700	-0.12367600	1.02082900
C	6.08771200	0.05977500	-1.42897000

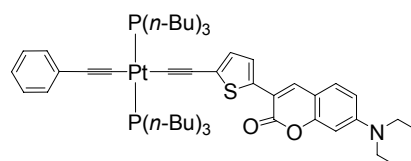
N	6.93976900	-0.02303100	-0.31144700
O	7.34447700	-0.19241800	1.92250500
O	6.54194600	0.14455900	-2.56387400
C	8.38890000	-0.00470700	-0.53261500
H	8.55793600	0.09015900	-1.60284400
H	8.83491200	0.83587400	0.00479000
H	8.83460600	-0.92770000	-0.15288500
C	1.82911900	0.01071000	-0.68386400
C	0.42333600	0.00612200	-0.47449500
Cl	-5.15823100	0.04075100	0.28185100

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

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	5.15290200	-0.20585500	0.01471400
C	1.21148900	0.65250100	-0.08775700
Pt	3.18088000	0.22783700	-0.04057100
P	3.56775900	2.52307500	0.20614800
C	2.74473800	3.23282500	1.69170800
H	2.87803300	4.31945200	1.73991700
H	3.16679000	2.77651700	2.59218500
H	1.68038200	2.98736000	1.64718800
C	5.31620200	3.07315200	0.35548200
H	5.87092500	2.76681000	-0.53507100
H	5.77742500	2.58044400	1.21523800
H	5.37562700	4.16068400	0.47448300
C	2.89668000	3.51412100	-1.19251500
H	3.41818300	3.23950400	-2.11440600
H	1.83766000	3.26901300	-1.30955400
H	3.01531100	4.58897700	-1.01513900
P	2.79655800	-2.07143400	-0.28340700
C	1.05088100	-2.63140800	-0.41729200
H	0.99979000	-3.71846000	-0.54327500
H	0.57394200	-2.13894500	-1.26853000
H	0.50271000	-2.34015300	0.48235700
C	3.61204500	-2.77366400	-1.77648700
H	4.67690400	-2.53010300	-1.73490300
H	3.18496100	-2.31382600	-2.67277400
H	3.47749100	-3.85990900	-1.82807300
C	3.48520500	-3.05846300	1.10891100
H	4.54461400	-2.81089100	1.21500000
H	2.96993300	-2.78637600	2.03507400
H	3.36747800	-4.13331100	0.93158700
C	0.00841900	0.90800900	-0.11220400
C	6.34913900	-0.47980100	0.05171500
C	-7.70183200	0.76534500	-0.12543800
C	-6.35865200	1.23749800	-0.18964500
C	-5.27638400	0.40418000	-0.04123400
C	-7.91324500	-0.60848000	0.09723300
O	-6.84806000	-1.44951800	0.24239300
C	-5.52713300	-1.02843800	0.18181500
O	-4.67772000	-1.88403000	0.31788200

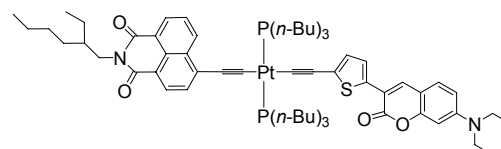


C	-10.12436400	1.03778700	-0.18810500
H	-10.97546400	1.69792400	-0.29904200
C	-9.17957900	-1.17125700	0.18005300
H	-9.24876100	-2.23654800	0.35594500
C	-10.32269800	-0.35585400	0.03467300
C	-8.85206300	1.56999300	-0.26552800
H	-8.72822100	2.63664000	-0.43643500
N	-11.59103500	-0.89206500	0.10360800
C	-12.75703900	-0.02935900	0.01195200
H	-12.78515700	0.51217900	-0.94316900
H	-13.65895900	-0.64020100	0.07502700
H	-12.79028900	0.71109300	0.82449800
C	-11.76405200	-2.30720900	0.38721600
H	-12.82881300	-2.54551500	0.38993700
H	-11.28026100	-2.93166800	-0.37575000
H	-11.34842200	-2.58499700	1.36667900
C	-3.89693900	0.87392100	-0.09692300
C	-3.46856400	2.18227100	-0.26308000
C	-2.06673700	2.33774400	-0.28579900
C	-1.37848300	1.14375000	-0.13630700
S	-2.50724500	-0.19241600	0.03884300
H	-4.15016300	3.02033800	-0.36434300
H	-1.56451600	3.29107000	-0.40827100
C	10.49949600	-1.40216300	0.18068600
C	9.70478700	-1.56794100	1.31800900
C	8.34518200	-1.26703900	1.27899800
C	7.74280000	-0.79005700	0.09508000
C	8.55926100	-0.62774100	-1.04467500
C	9.91821600	-0.93065400	-0.99934700
H	11.55987500	-1.63784500	0.21366800
H	10.14679400	-1.93376000	2.24161600
H	7.72975100	-1.39513700	2.16481400
H	8.10927400	-0.26193100	-1.96312700
H	10.52721000	-0.79812700	-1.89036700
H	-6.20412300	2.29899600	-0.36395200

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

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1



C	9.54466400	0.62290500	0.48757700
C	8.18753800	0.97189200	0.74571900
C	7.13322800	0.23023500	0.27139300
C	9.79995800	-0.52389600	-0.28806900
O	8.76206600	-1.26762000	-0.77092000
C	7.42853000	-0.95776100	-0.54391500
O	6.60547100	-1.69672200	-1.04247700
C	11.95603900	0.94532900	0.64781000
H	12.78480300	1.53407000	1.02042600
C	11.08357500	-0.94845100	-0.60248000
H	11.18786800	-1.83873600	-1.20832500
C	12.19947300	-0.22024200	-0.13567100
C	10.66766500	1.34410100	0.94456300

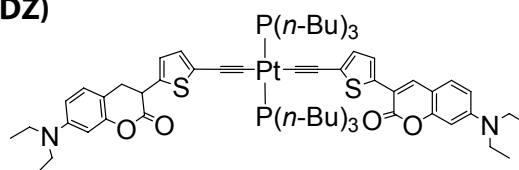
H	10.50910300	2.23712000	1.54419500
N	13.48420700	-0.62488500	-0.42789100
C	14.61980000	0.17639500	-0.00150000
H	14.65806200	0.27382100	1.09162600
H	15.54137100	-0.31003400	-0.32471800
H	14.59939800	1.18741600	-0.43355500
C	13.70219700	-1.78496300	-1.27665200
H	14.77446500	-1.95785600	-1.37998700
H	13.25500300	-2.68875900	-0.84222800
H	13.27899500	-1.64605100	-2.28211100
C	5.73968700	0.57180300	0.53492400
C	5.27398900	1.60892600	1.32765000
C	3.86788400	1.71595800	1.37835600
C	3.21763900	0.75449900	0.62201300
S	4.38307800	-0.30344900	-0.15934000
H	5.93040800	2.28212900	1.86899000
H	3.33622100	2.46635400	1.95291400
H	7.99932900	1.86322800	1.33821800
C	-3.32762400	-0.15100900	-0.27853500
C	0.63008300	0.37382800	0.27609600
Pt	-1.34729500	0.10445700	-0.00545900
P	-1.28406200	2.03954700	-1.33157400
C	-0.16632500	1.85488200	-2.78101300
H	-0.10080400	2.78766300	-3.35215800
H	-0.54230400	1.05858000	-3.43036400
H	0.82481900	1.56838300	-2.41984300
C	-2.87115400	2.62364000	-2.05604200
H	-3.58271100	2.83795000	-1.25430100
H	-3.30030100	1.83433000	-2.67872400
H	-2.71485300	3.52456300	-2.65953200
C	-0.62821100	3.50853100	-0.43875800
H	-1.30405100	3.76749200	0.38191300
H	0.34637600	3.24833800	-0.01805400
H	-0.52896900	4.36785400	-1.11111400
P	-1.35471900	-1.84598100	1.30033100
C	0.25771500	-2.40559000	1.98181300
H	0.13046200	-3.31385200	2.58119800
H	0.68876100	-1.61218400	2.59748500
H	0.95274700	-2.59995100	1.16084200
C	-2.44882300	-1.71015400	2.77451000
H	-3.45424200	-1.44200400	2.43942800
H	-2.07747700	-0.91615400	3.42935500
H	-2.48234400	-2.65289800	3.33177600
C	-1.99892400	-3.31409000	0.39725800
H	-2.99264000	-3.07747000	0.00827000
H	-1.33993200	-3.53722800	-0.44716200
H	-2.05425700	-4.18921900	1.05407300
C	1.83407400	0.55764400	0.44113100
C	-6.87844000	0.13971700	0.27264500
C	-6.42603900	-1.26754100	-1.67112000
C	-6.47049300	0.94761600	1.36246200
C	-8.27608900	-0.05649500	0.05679100
C	-7.80141700	-1.44936800	-1.86889200
H	-5.71820700	-1.73891500	-2.34549100
C	-7.39927300	1.53438000	2.20161300
H	-5.40628100	1.09488200	1.52110200

C	-9.21190000	0.55607700	0.93043200
C	-8.72760500	-0.85699000	-1.02290000
H	-8.16730300	-2.05757300	-2.68983200
C	-8.77719900	1.33902300	1.98640100
H	-7.06734300	2.15048400	3.03245100
H	-9.51982900	1.79222200	2.63494500
C	-10.66694900	0.36400900	0.71999400
C	-10.17090500	-1.06855800	-1.26128700
N	-11.05274000	-0.43588100	-0.36354800
O	-11.51784600	0.86894100	1.44317500
O	-10.59611600	-1.75336400	-2.18462300
C	-12.49484700	-0.61324900	-0.55690600
H	-12.63479500	-1.25028600	-1.42733500
H	-12.93501500	-1.07273500	0.33179300
H	-12.97118900	0.35852000	-0.70988600
C	-5.93363100	-0.48671700	-0.62037100
C	-4.53634400	-0.31197100	-0.43763000

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

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1



C	-8.36100600	-25.26818900	-17.39554000
C	-8.99674800	-24.21302500	-16.67913400
C	-8.30082500	-23.14312200	-16.17055900
C	-6.96732200	-25.20004000	-17.58125700
O	-6.26183700	-24.14458200	-17.07979200
C	-6.84460100	-23.09940100	-16.37670800
O	-6.09914000	-22.22603200	-15.98495400
C	-8.33286500	-27.37552200	-18.62198200
H	-8.88384600	-28.21883400	-19.01900500
C	-6.25047000	-26.17438200	-18.26240900
H	-5.18053300	-26.04303600	-18.35467800
C	-6.92227500	-27.29048500	-18.80627100
C	-9.01977300	-26.39104100	-17.93882600
H	-10.09610700	-26.47931600	-17.81272100
N	-6.23526500	-28.26689400	-19.49622100
C	-6.93361600	-29.43908700	-19.99684600
H	-7.72087900	-29.16596000	-20.71227800
H	-6.22234000	-30.08450000	-20.51456300
H	-7.39584800	-30.02322200	-19.18790800
C	-4.79030200	-28.17994300	-19.62702100
H	-4.43119800	-29.02576000	-20.21533900
H	-4.48867800	-27.25822900	-20.14219700
H	-4.28534600	-28.20331000	-18.65034400
C	-8.93866900	-22.05531300	-15.43875400
C	-10.29063200	-21.91913400	-15.16162600
C	-10.62134000	-20.76107200	-14.42799300
C	-9.52354900	-19.97179400	-14.12119200
S	-8.05537900	-20.69448800	-14.76405100
H	-11.03603300	-22.63989300	-15.48120500
H	-11.63044700	-20.50119400	-14.12826800
H	-10.07267600	-24.27446900	-16.53963700

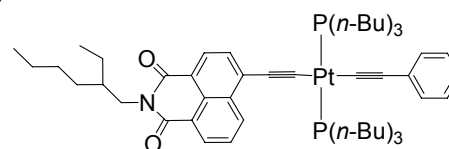
C	-9.39971700	-17.69591500	-12.79542700
Pt	-9.23657500	-15.95943500	-11.78896600
P	-6.94353000	-16.02581500	-12.28625600
C	-6.60448500	-16.10007000	-14.09297100
H	-5.53149200	-16.20189800	-14.28949800
H	-6.97449000	-15.18661200	-14.56840100
H	-7.14194300	-16.95321800	-14.51479400
C	-5.91193600	-14.62580600	-11.69058300
H	-5.98279600	-14.55593000	-10.60217400
H	-6.29056100	-13.68913300	-12.10767800
H	-4.86534300	-14.76283700	-11.98409300
C	-6.11634900	-17.52147600	-11.60538000
H	-6.17567800	-17.50191600	-10.51294900
H	-6.64524600	-18.40740500	-11.96614300
H	-5.06510100	-17.56690900	-11.91045500
P	-11.52316800	-15.89077600	-11.28940800
C	-12.56359900	-17.27988600	-11.89893800
H	-13.60977400	-17.14648300	-11.60180700
H	-12.18117900	-18.22100800	-11.49526700
H	-12.49176700	-17.33353900	-12.98836400
C	-11.86093900	-15.83718900	-9.48087200
H	-11.30921600	-14.99638400	-9.05230800
H	-11.49769500	-16.75973500	-9.01798600
H	-12.93206800	-15.72684700	-9.27757300
C	-12.35116500	-14.38440000	-11.94745700
H	-11.80942500	-13.50750000	-11.58323100
H	-12.29970900	-14.39209500	-13.04043600
H	-13.40006900	-14.33411200	-11.63428200
C	-9.46910400	-18.75804000	-13.41256300
C	-9.06205200	-14.22549300	-10.77975000
C	-8.97022700	-13.16819500	-10.15713100
C	-6.83508500	-6.67269000	-6.58985300
C	-7.63231200	-7.74731900	-7.08016300
C	-7.11369800	-8.75643500	-7.85488000
C	-5.46624600	-6.65708900	-6.91786200
O	-4.93610900	-7.65345600	-7.68563200
C	-5.67916600	-8.71669100	-8.17955700
O	-5.07999900	-9.53549500	-8.84463300
C	-6.47143600	-4.60616300	-5.34785400
H	-6.88248500	-3.81476400	-4.73376300
C	-4.60138300	-5.65935300	-6.48914400
H	-3.56309600	-5.72826600	-6.78514600
C	-5.08826100	-4.60185100	-5.69084900
C	-7.30848900	-5.61240800	-5.78894900
H	-8.36006800	-5.59256300	-5.51333100
N	-4.25149800	-3.59507300	-5.25760800
C	-4.75511900	-2.55161000	-4.38019200
H	-5.13814600	-2.95725500	-3.43264300
H	-3.94489300	-1.85897800	-4.14719300
H	-5.56179900	-1.97701800	-4.85512900
C	-2.83631300	-3.63808300	-5.58625100
H	-2.34542000	-2.75370700	-5.17703700
H	-2.34249400	-4.52774400	-5.16899000
H	-2.67693900	-3.64055300	-6.67274500
C	-7.91813100	-9.86104200	-8.36355200
C	-9.27903500	-10.05216700	-8.17786100

C	-9.79025900	-11.21953900	-8.78100600
C	-8.82801200	-11.96027500	-9.45054000
S	-7.25911500	-11.17717900	-9.32296900
H	-9.90293700	-9.36395000	-7.61726500
H	-10.83119700	-11.51994500	-8.73358400
H	-8.68721500	-7.75278500	-6.81938600

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

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1



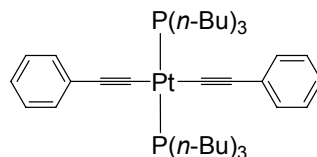
C	0.26107600	0.13361000	-0.39004800
C	-3.75086300	0.01992900	0.01178300
Pt	-1.74381500	0.07945300	-0.19042000
P	-1.83556400	-2.22132900	-0.68769500
C	-2.88548000	-2.58517400	-2.15346800
H	-2.96958200	-3.66529600	-2.31533900
H	-2.44658000	-2.11978800	-3.04105700
H	-3.87675500	-2.15546800	-1.98731400
C	-0.24574200	-3.06996400	-1.05113300
H	0.42015300	-2.98529800	-0.18852200
H	0.24060700	-2.58812600	-1.90319800
H	-0.41980200	-4.12722700	-1.27762200
C	-2.58208900	-3.22216000	0.66320700
H	-1.95561600	-3.15544400	1.55780100
H	-3.56909700	-2.81434300	0.89548100
H	-2.67540200	-4.27203500	0.36481100
P	-1.65927600	2.38461900	0.28615700
C	-3.25432300	3.22960400	0.62966300
H	-3.08667400	4.28969000	0.84760400
H	-3.74574900	2.75132300	1.48073800
H	-3.91199100	3.13150700	-0.23769200
C	-0.62008700	2.76923100	1.75528500
H	0.37792200	2.35133000	1.59928900
H	-1.05878600	2.30384900	2.64315500
H	-0.54906200	3.85110000	1.91208200
C	-0.90740800	3.37542300	-1.06987200
H	0.08588300	2.97650700	-1.29076100
H	-1.52527900	3.29325700	-1.96917300
H	-0.82646700	4.42931300	-0.78252700
C	-4.97130400	-0.03053600	0.13637900
C	-6.39202100	-0.08387000	0.28422300
C	-6.97987300	-0.47270300	1.50724500
C	-8.36529900	-0.52393500	1.64921100
H	-6.33484900	-0.73298000	2.34166100
C	-9.19958600	-0.18931700	0.57873600
H	-8.79575400	-0.82645100	2.60051900
H	-10.27944700	-0.22980200	0.69218500
C	-8.63260600	0.19783500	-0.63900300
H	-9.27238200	0.46025200	-1.47795600
C	-7.24769200	0.25100000	-0.78766700
H	-6.81033400	0.55283200	-1.73529500
C	3.76244100	-0.16626900	0.43167100

C	3.48000700	0.63119200	-1.86018100
C	3.25932900	-0.59740500	1.68353500
C	5.17740000	-0.10989300	0.24980100
C	4.87081900	0.67981900	-2.02151500
H	2.83394800	0.91975300	-2.68301900
C	4.11266100	-0.95737400	2.71026900
H	2.18271400	-0.63748900	1.81862600
C	6.03543100	-0.48368000	1.31689900
C	5.72305400	0.31688600	-0.98743100
H	5.30362200	1.00455200	-2.96198600
C	5.50743000	-0.90087000	2.52788500
H	3.70812700	-1.28534200	3.66312500
H	6.18814900	-1.18028100	3.32524800
C	7.50509600	-0.43014900	1.14367200
C	7.18357300	0.38227500	-1.18920300
N	7.98634600	0.00072700	-0.09797700
O	8.29446100	-0.74426000	2.02992200
O	7.69166100	0.74563600	-2.24611100
C	9.44441300	0.04776400	-0.24876700
H	9.66201900	0.40712900	-1.25147600
H	9.87333600	0.71860300	0.49954900
H	9.86651000	-0.94948900	-0.10105300
C	2.89602300	0.21728900	-0.65779100
C	1.48452500	0.17495500	-0.51451000

Complex Pt-5 (DFT//B3LYP/6-31G(d) / LanL2DZ)

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1



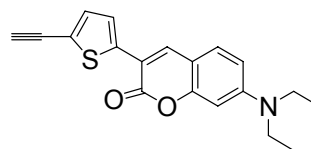
C	2.02029300	0.03841700	-0.00310800
C	-2.02034000	-0.03120200	-0.00381300
Pt	-0.00007100	0.00523800	-0.00751000
P	-0.15380100	2.34086700	-0.00919100
C	-1.06578000	2.99997000	1.44715700
H	-1.17929300	4.08809500	1.38697600
H	-0.52346000	2.74246700	2.36189400
H	-2.04907100	2.52365700	1.48153000
C	1.42237400	3.28907800	-0.02216500
H	1.99792600	3.02263600	-0.91240700
H	2.01957600	3.01219900	0.85025300
H	1.23030900	4.36778700	-0.01401900
C	-1.08735200	2.99841700	-1.45267500
H	-0.55777400	2.74117400	-2.37494700
H	-2.07047500	2.52104900	-1.47306600
H	-1.20108100	4.08649400	-1.39134200
P	0.15374300	-2.33105900	-0.00609600
C	-1.42222500	-3.27961800	-0.02199100
H	-1.22971000	-4.35818700	-0.01307900
H	-1.99587300	-3.01377600	-0.91362800
H	-2.02153000	-3.00266900	0.84900100
C	1.09048700	-2.99080900	-1.44645400
H	2.07363900	-2.51357700	-1.46546800
H	0.56288000	-2.73499700	-2.37023200
H	1.20384000	-4.07881800	-1.38311700

C	1.06195600	-2.98823100	1.45345300
H	2.04405900	-2.50978200	1.49132100
H	0.51567500	-2.73217300	2.36620900
H	1.17814400	-4.07611000	1.39351800
C	-3.24792100	-0.04272200	0.00130300
C	3.24805700	0.04306200	0.00261100
C	7.50170700	0.07889600	0.02019100
C	6.79158800	0.07761700	1.22381400
C	5.39852900	0.06610600	1.22149100
C	4.67654100	0.05512300	0.00871900
C	5.40858400	0.05714100	-1.19813400
C	6.80157100	0.06881200	-1.18916000
H	8.58842500	0.08786300	0.02461600
H	7.32630100	0.08588900	2.17063200
H	4.84861200	0.06591400	2.15835200
H	4.86641800	0.05011300	-2.13950100
H	7.34402100	0.07021800	-2.13161300
C	-4.67641000	-0.06499000	0.00817500
C	-5.39770700	-0.07180000	1.22141200
C	-6.79059700	-0.09393800	1.22452700
C	-7.50127900	-0.11000600	0.02123200
C	-6.80188300	-0.10403600	-1.18860500
C	-5.40903100	-0.08196500	-1.19833200
H	-4.84731600	-0.05991400	2.15796700
H	-7.32477300	-0.09882600	2.17172500
H	-8.58791100	-0.12717500	0.02630400
H	-7.34475600	-0.11689500	-2.13077400
H	-4.86733700	-0.07828300	-2.13993500

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

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1



C	7.43491100	-0.45200400	0.00393700
C	6.28180000	-0.07935600	0.00242800
C	-1.35602100	0.89409400	-0.00064700
C	0.04066000	1.16945400	-0.00013900
C	0.98601400	0.17368100	-0.00108000
C	-1.76749900	-0.45261000	-0.00201600
O	-0.83821300	-1.45211500	-0.00256500
C	0.52993000	-1.22312600	-0.00178900
O	1.24757700	-2.20081900	-0.00163900
C	-3.71002400	1.52511100	0.00023200
H	-4.45485900	2.31084300	0.00182100
C	-3.10207300	-0.83028700	-0.00245800
H	-3.32884500	-1.88800000	-0.00310100
C	-4.11181300	0.15676100	-0.00198300
C	-2.37426900	1.87091400	0.00062300
H	-2.09354200	2.92125300	0.00221600
N	-5.44266200	-0.19173200	-0.00380800
C	-6.47218000	0.83526900	0.00557500
H	-6.40801300	1.48511600	-0.87779400
H	-7.45267800	0.35738500	-0.00082100
H	-6.41065800	1.46866900	0.90130300

C	-5.82517700	-1.59506300	0.00259100
H	-6.91328400	-1.67047700	-0.00148900
H	-5.44419500	-2.12249300	-0.88246500
H	-5.45071300	-2.11426200	0.89553200
C	2.42105400	0.44197200	-0.00114900
C	3.03512900	1.68482700	-0.00324800
C	4.44435500	1.63199900	-0.00211800
C	4.93471000	0.33934100	0.00078000
S	3.62934300	-0.83067100	0.00192500
H	2.48565300	2.61972300	-0.00576200
H	5.08686700	2.50510100	-0.00351900
H	0.35024700	2.21119300	0.00112600
H	8.45122400	-0.77358300	0.00522200

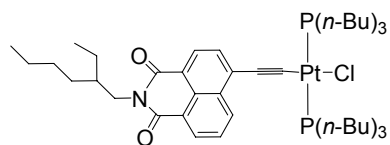
8.0 The coordinates of the triplet optimized geometries of complexes

Complex Pt-0 (DFT//B3LYP/6-31G(d) / LanL2DZ)

Symbolic Z-matrix:

Charge = 0 Multiplicity = 3

C	-0.80274600	-0.05577900	-0.29990100
Pt	-2.72977000	0.02293900	-0.04172900
P	-2.90974500	-2.33400300	0.11199600
C	-4.02515100	-3.03301600	-1.17031900
H	-4.14413700	-4.11293900	-1.03148100
H	-3.60641300	-2.83957700	-2.16232400
H	-4.99715200	-2.53913800	-1.09652400
C	-1.35269000	-3.29471900	-0.05879400



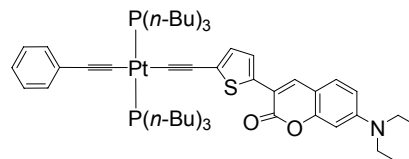
H	-0.65083600	-2.99985200	0.72570700
H	-0.89377100	-3.07974700	-1.02734000
H	-1.55574300	-4.36786000	0.01847800
C	-3.62025000	-2.88901000	1.71354000
H	-2.94817900	-2.60369100	2.52825300
H	-4.58290700	-2.39374600	1.86184100
H	-3.75640600	-3.97580100	1.71983700
P	-2.57325900	2.38337200	-0.21382400
C	-4.14287900	3.32849200	-0.09635600
H	-3.94098100	4.40161200	-0.18065900
H	-4.62766900	3.11668700	0.85944400
H	-4.81992400	3.01642900	-0.89508700
C	-1.49509300	3.11544300	1.08369900
H	-0.50854600	2.64708600	1.03457600
H	-1.92670700	2.91781600	2.06935600
H	-1.39583300	4.19693800	0.94301100
C	-1.82124100	2.93225600	-1.79971800
H	-0.83841800	2.46648400	-1.90939500
H	-2.45415000	2.61246800	-2.63276700
H	-1.71598300	4.02206200	-1.82335200
C	2.73029300	0.01031900	0.47379800
C	2.34643000	-0.30353600	-1.98493500
C	2.31231500	0.17495300	1.79627000
C	4.13949100	-0.02539400	0.20396400
C	3.68455100	-0.33629100	-2.22143000
H	1.63858800	-0.40730700	-2.80172200
C	3.24877700	0.30642500	2.84762800
H	1.24862400	0.19915100	2.01241600
C	5.06020600	0.10825300	1.26365200
C	4.61451900	-0.19621000	-1.12982500
H	4.08734600	-0.46557200	-3.21869300
C	4.60523200	0.27549200	2.59416300
H	2.88791800	0.43265300	3.86458100
H	5.34050000	0.37473300	3.38417600
C	6.50752900	0.07616700	1.00375700
C	6.04372200	-0.23320800	-1.41644100
N	6.91350800	-0.09288700	-0.32204300
O	7.35005700	0.19097000	1.89788200
O	6.48094600	-0.38044700	-2.56613000
C	8.35883100	-0.12413900	-0.56367600
H	8.51337000	-0.26734700	-1.63045900
H	8.81152200	0.81459700	-0.23445700
H	8.81248300	-0.94196800	0.00172200
C	1.80432700	-0.12725000	-0.64468900
C	0.42899600	-0.08973800	-0.46301200
Cl	-5.15312300	0.09970500	0.30677300

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

Symbolic Z-matrix:

Charge = 0 Multiplicity = 3

C	-7.25494000	0.04659200	0.27339800
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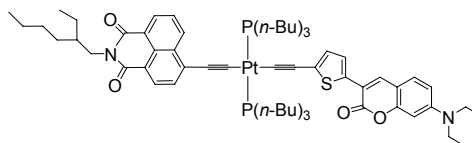
C	-5.28013700	3.32149900	1.50924300
Pt	-6.26994300	1.69678600	0.88550000
P	-5.34107500	2.05073700	-1.25263200
C	-3.50315900	1.96434600	-1.24751300
H	-3.09770500	2.18874600	-2.23999000
H	-3.18754100	0.96129000	-0.94569500
H	-3.11760600	2.68392200	-0.52049600
C	-5.84478700	0.89597700	-2.59059700
H	-6.92755300	0.95032200	-2.73006000
H	-5.59238100	-0.12798700	-2.30476100
H	-5.33982700	1.15383600	-3.52759900
C	-5.71445200	3.71642800	-1.93946200
H	-6.79481800	3.81908500	-2.07817100
H	-5.38101500	4.47650900	-1.22842800
H	-5.21113000	3.86213200	-2.90128600
P	-7.21260500	1.32840400	3.01634500
C	-6.75159500	2.49631700	4.35815700
H	-7.25357200	2.22040000	5.29156200
H	-7.03721300	3.51306100	4.07690900
H	-5.66885300	2.47714100	4.50670200
C	-9.05112000	1.37531900	2.98823900
H	-9.40934100	0.64818200	2.25514200
H	-9.38463800	2.37219300	2.68509600
H	-9.46225300	1.14061300	3.97592000
C	-6.80783900	-0.32823300	3.70545400
H	-7.11365600	-1.09285300	2.98708800
H	-5.72732200	-0.40414500	3.85960100
H	-7.32079000	-0.48706200	4.66003200
C	-4.65141400	4.31797100	1.90058500
C	-7.85003800	-0.96543100	-0.08807900
C	-1.32249200	10.13715800	5.61226700
C	-1.67170100	9.25657300	4.57973600
C	-2.61922900	8.18996000	4.81913500
C	-1.91212500	9.97465100	6.89676200
O	-2.81900500	8.95879500	7.12759800
C	-3.19863000	8.05719300	6.15085800
O	-4.00598500	7.20534500	6.49052900
C	-0.09374000	12.04406200	6.55530100
H	0.62267000	12.84186600	6.40196700
C	-1.62397100	10.79268300	7.96912300
H	-2.11839000	10.58568400	8.90938900
C	-0.70348300	11.86530800	7.82831700
C	-0.39709400	11.21288500	5.49460900
H	0.08520200	11.37591600	4.53417000
N	-0.42065300	12.70321100	8.88859900
C	0.61973000	13.71197600	8.75995100
H	0.39273300	14.41568800	7.94955700
H	0.68142400	14.28130400	9.68835800
H	1.60726000	13.26983200	8.56094000
C	-0.97511400	12.42297400	10.20434900
H	-0.67151500	13.21059500	10.89532800
H	-2.07142900	12.40575100	10.17585100
H	-0.62970800	11.45890400	10.60643800
C	-2.99938400	7.28185000	3.83271700
C	-2.52874500	7.26685600	2.46968900
C	-3.05450200	6.25938000	1.69651100

C	-3.96570400	5.41589500	2.38074500
S	-4.14861000	5.95045500	4.07774200
H	-1.81840400	7.99469700	2.09840000
H	-2.80758500	6.10150900	0.65210600
C	-9.86877800	-4.48065200	-1.37653100
C	-8.51068500	-4.30409400	-1.65674200
C	-7.84785400	-3.15267200	-1.23675700
C	-8.52979000	-2.14561500	-0.51950100
C	-9.90065900	-2.33976400	-0.24334000
C	-10.55863500	-3.49202800	-0.66880400
H	-10.38390900	-5.37879500	-1.70600000
H	-7.96480300	-5.06698900	-2.20597100
H	-6.79234000	-3.01929900	-1.45576700
H	-10.44078900	-1.57375800	0.30568600
H	-11.61495800	-3.61940200	-0.44613200
H	-1.22231900	9.37888900	3.60165900

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

Symbolic Z-matrix:

Charge = 0 Multiplicity = 3



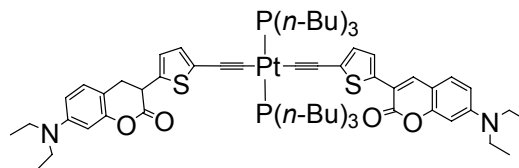
C	-9.07371300	-6.50567500	-4.15548800
C	-7.88413100	-6.78577200	-3.42575500
C	-6.73406700	-6.04916600	-3.58278600
C	-9.05796500	-5.43099500	-5.06614200
O	-7.92551600	-4.68571000	-5.22525900
C	-6.75077300	-4.92290300	-4.52802800
O	-5.82205400	-4.17512900	-4.75392200
C	-11.39485200	-6.89662300	-4.79032700
H	-12.29848600	-7.48053900	-4.66927700
C	-10.16011800	-5.07731100	-5.83088200
H	-10.05911300	-4.23811700	-6.50608100
C	-11.36329800	-5.80702100	-5.71015700
C	-10.28230100	-7.22608200	-4.04298100
H	-10.33195400	-8.06192900	-3.34954600
N	-12.47111200	-5.47615000	-6.45679500
C	-13.69706600	-6.24907500	-6.33572100
H	-14.09892900	-6.21803700	-5.31382300
H	-14.45028400	-5.83029500	-7.00448500
H	-13.54701500	-7.30202500	-6.61219300
C	-12.40704200	-4.37041300	-7.39938000
H	-13.37562200	-4.25870700	-7.88863300
H	-12.16980100	-3.42332500	-6.89601600
H	-11.64990400	-4.54120600	-8.17742200
C	-5.50353800	-6.33232900	-2.85540300
C	-5.27823900	-7.37940200	-1.97135600
C	-3.98577900	-7.39861200	-1.41227400
C	-3.17982500	-6.35865600	-1.85492900
S	-4.05872900	-5.34618700	-2.99361700
H	-6.02899600	-8.12519900	-1.73290500
H	-3.64210100	-8.14617100	-0.70594100
H	-7.90459200	-7.61490200	-2.72356200

C	3.10885800	-4.73538500	-0.49784800
C	-0.68490400	-5.74783900	-1.26799000
Pt	1.21394000	-5.23678100	-0.87717000
P	1.42221700	-7.30698500	0.21564400
C	1.04662600	-8.73163200	-0.88617300
H	1.06763600	-9.67685900	-0.33244600
H	1.78399200	-8.76914600	-1.69364500
H	0.05855700	-8.57832000	-1.32762700
C	3.05754700	-7.72281200	0.94608400
H	3.33322600	-6.96161300	1.68062600
H	3.81726000	-7.72268400	0.16000500
H	3.02782400	-8.70595500	1.42822900
C	0.24250800	-7.48966000	1.61597900
H	0.46672400	-6.73855600	2.37935200
H	-0.76953700	-7.31190500	1.24312100
H	0.30629300	-8.48876500	2.06132800
P	0.95833200	-3.17466400	-1.98179400
C	-0.69414100	-2.79978400	-2.69251300
H	-0.69076100	-1.81553700	-3.17333300
H	-1.44768800	-2.81874400	-1.90115900
H	-0.96237300	-3.56426300	-3.42595200
C	1.30866500	-1.73445400	-0.89094500
H	2.29918100	-1.85388900	-0.44496100
H	0.56965400	-1.70813400	-0.08439900
H	1.26349500	-0.79423300	-1.45166600
C	2.10878700	-2.97853400	-3.40499400
H	3.13531800	-3.13432000	-3.06380200
H	1.87809500	-3.73750300	-4.15875600
H	2.01442700	-1.98396600	-3.85501300
C	-1.84969900	-6.05809100	-1.52309400
C	6.27846000	-2.93062300	-0.40464500
C	6.40620700	-5.13724600	0.76942600
C	5.62554800	-1.92424000	-1.12088600
C	7.66213700	-2.73672000	-0.07598600
C	7.71721200	-4.93588000	1.07293000
H	5.90385500	-6.04760700	1.08209400
C	6.29783500	-0.74885500	-1.51587400
H	4.57889600	-2.05866700	-1.37385700
C	8.32060900	-1.55593300	-0.47897500
C	8.37690000	-3.73110900	0.65590600
H	8.29838200	-5.66269000	1.62823700
C	7.63048600	-0.55909100	-1.20291300
H	5.75622200	0.01165500	-2.07236800
H	8.17236500	0.33346300	-1.49412500
C	9.74067800	-1.34110300	-0.15278200
C	9.78395100	-3.54870700	0.99578200
N	10.38680800	-2.35243200	0.56491800
O	10.35729900	-0.32790100	-0.48377200
O	10.42558300	-4.39487400	1.62908600
C	11.79857500	-2.12582700	0.88091900
H	12.15607700	-2.99309800	1.43178500
H	12.36909800	-1.99231300	-0.04196000
H	11.90451800	-1.21736600	1.47977100
C	5.62407100	-4.16383600	0.02233000
C	4.29745100	-4.44054700	-0.26180500

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

Symbolic Z-matrix:

Charge = 0 Multiplicity = 3



C	-8.45152700	-25.27787200	-17.37165800
C	-9.05915700	-24.25059100	-16.63681100
C	-8.27016600	-23.15032600	-16.12959600
C	-7.05032200	-25.22812500	-17.61174600
O	-6.29289500	-24.18235300	-17.12203900
C	-6.83606100	-23.14037200	-16.39313400
O	-6.05302900	-22.27871600	-16.02244900
C	-8.46695500	-27.38545900	-18.63371600
H	-9.03748300	-28.22212900	-19.01813400
C	-6.37133000	-26.19422300	-18.32477200
H	-5.30327400	-26.07145900	-18.45055100
C	-7.06585000	-27.30772200	-18.86816200
C	-9.12683800	-26.40663700	-17.91624100
H	-10.19823100	-26.49438200	-17.75476500
N	-6.40201300	-28.27172900	-19.60054400
C	-7.11033500	-29.46115800	-20.04708500
H	-7.95756600	-29.19992200	-20.69333700
H	-6.42924900	-30.08573100	-20.62670800
H	-7.49429700	-30.05860600	-19.20682600
C	-4.95325400	-28.22136000	-19.72363000
H	-4.61907700	-29.04508700	-20.35590200
H	-4.62766200	-27.28464700	-20.19266000
H	-4.44895500	-28.30744300	-18.74972800
C	-8.82232400	-22.09812100	-15.40039000
C	-10.21367500	-21.94784600	-15.05357600
C	-10.50177300	-20.81509800	-14.33050200
C	-9.37616500	-19.99782700	-14.05597300
S	-7.89948500	-20.72479500	-14.75606300
H	-10.96098900	-22.67433000	-15.34666400
H	-11.49595200	-20.54709800	-13.98951800
H	-10.12601400	-24.28861600	-16.45227400
C	-9.26362700	-17.72287800	-12.75798800
Pt	-9.11975900	-15.97677600	-11.79335800
P	-6.79898800	-16.04816300	-12.22644700
C	-6.41226800	-16.15172600	-14.02135400
H	-5.33272200	-16.24401400	-14.18145800
H	-6.77619500	-15.25027600	-14.52341000
H	-6.92273100	-17.01958100	-14.44661600
C	-5.79075300	-14.63310600	-11.63020700
H	-5.88743900	-14.54346200	-10.54538400
H	-6.15634700	-13.70684300	-12.08052200
H	-4.73806400	-14.77897500	-11.89470200
C	-5.98563500	-17.52576700	-11.49329200
H	-6.08349600	-17.49207800	-10.40409800
H	-6.48431600	-18.42588300	-11.86184100
H	-4.92393600	-17.55802200	-11.76011600
P	-11.43400300	-15.88699200	-11.35207400
C	-12.46129800	-17.28929400	-11.95014700

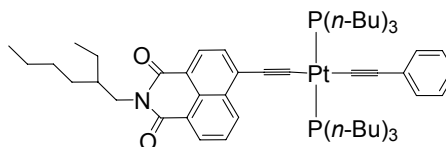
H	-13.51123200	-17.13822600	-11.67761200
H	-12.09891900	-18.22123900	-11.50858100
H	-12.37266800	-17.37047100	-13.03655700
C	-11.81330600	-15.78843200	-9.55510300
H	-11.28136500	-14.93293700	-9.13119100
H	-11.46157300	-16.69841300	-9.05975900
H	-12.89016700	-15.67820500	-9.38751900
C	-12.23771600	-14.39848400	-12.07416500
H	-11.71711200	-13.50868100	-11.71097000
H	-12.15214900	-14.43200300	-13.16442100
H	-13.29589300	-14.34970900	-11.79564500
C	-9.32809900	-18.80242000	-13.36845700
C	-8.96768100	-14.22297300	-10.82202700
C	-8.89169000	-13.15564600	-10.21277900
C	-6.88743300	-6.65409100	-6.58251000
C	-7.66261100	-7.73029300	-7.09497800
C	-7.11967500	-8.72199300	-7.87942800
C	-5.51432200	-6.61386700	-6.89435500
O	-4.96366300	-7.59582700	-7.67081600
C	-5.68647400	-8.65970800	-8.18269500
O	-5.06368500	-9.46594900	-8.84915900
C	-6.56878900	-4.60034400	-5.30850400
H	-6.99712000	-3.82196100	-4.68995700
C	-4.66744900	-5.61215300	-6.44481000
H	-3.62507400	-5.65894900	-6.73036600
C	-5.17851900	-4.57229300	-5.63407100
C	-7.38644000	-5.61030600	-5.77165700
H	-8.44128200	-5.60872500	-5.50938200
N	-4.36359300	-3.56760800	-5.17418300
C	-4.90057700	-2.51366200	-4.32444900
H	-5.32030200	-2.91629600	-3.39295000
H	-4.09720300	-1.82474100	-4.06193500
H	-5.68589400	-1.94015500	-4.83462500
C	-2.94932800	-3.56196400	-5.52068100
H	-2.47436400	-2.68822600	-5.07358500
H	-2.43650100	-4.45858800	-5.14695400
H	-2.80098100	-3.51229900	-6.60757900
C	-7.90756400	-9.82840500	-8.41252100
C	-9.27296200	-10.02355000	-8.26947400
C	-9.76036600	-11.19807200	-8.88087400
C	-8.77578200	-11.94055800	-9.51449400
S	-7.21294300	-11.14684200	-9.34451300
H	-9.91746100	-9.33381900	-7.73539700
H	-10.80153300	-11.50091100	-8.86385500
H	-8.71941400	-7.75527100	-6.84436200

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

Symbolic Z-matrix:

Charge = 0 Multiplicity = 3

C -0.25651400 0.27874200 -0.19470100



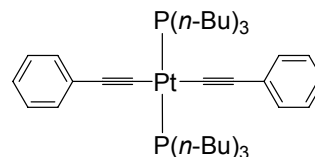
C	3.74264300	-0.04348800	-0.01563900
Pt	1.73509700	0.11031200	-0.11264200
P	2.00716600	2.32073000	0.67203900
C	3.06612500	3.34189800	-0.43088200
H	3.22051300	4.33914900	-0.00522700
H	2.58839600	3.43696300	-1.41049300
H	4.02807900	2.83892000	-0.55697900
C	0.48309200	3.32382400	0.89330300
H	-0.17796500	2.83322800	1.61254700
H	-0.04648400	3.39905700	-0.05991600
H	0.73361000	4.32763200	1.25215800
C	2.84282800	2.39211300	2.30828400
H	2.21882200	1.89695500	3.05821700
H	3.79518400	1.86047400	2.23856200
H	3.01851900	3.42972100	2.61166200
P	1.53338500	-2.10139300	-0.92179900
C	3.09693100	-3.01922300	-1.21646500
H	2.88363500	-4.02713100	-1.58767300
H	3.66467000	-3.08145600	-0.28503600
H	3.70501300	-2.47898700	-1.94633200
C	0.56662200	-3.20222600	0.19045800
H	-0.43007400	-2.77757100	0.33452300
H	1.06331600	-3.26966000	1.16276100
H	0.47690000	-4.20513600	-0.24045100
C	0.64467500	-2.19145600	-2.53012500
H	-0.34071400	-1.73076300	-2.42035100
H	1.20607200	-1.63667200	-3.28768800
H	0.52987100	-3.23127300	-2.85446900
C	4.96632600	-0.12248100	0.05183300
C	6.38927800	-0.22581800	0.13143100
C	7.00294000	-1.02493100	1.12023700
C	8.39071700	-1.12448600	1.19626300
H	6.37652200	-1.56251300	1.82621900
C	9.20024900	-0.43448100	0.28927700
H	8.84243500	-1.74435900	1.96646000
H	10.28207800	-0.51477300	0.34993700
C	8.60705400	0.35961100	-0.69651900
H	9.22797300	0.89948300	-1.40679700
C	7.21997600	0.46601300	-0.77628200
H	6.76220300	1.08354500	-1.54374000
C	-3.78739300	-0.35877700	0.37269800
C	-3.43247100	1.61368800	-1.13106300
C	-3.35554800	-1.39598300	1.20340400
C	-5.19954500	-0.16599900	0.20431300
C	-4.77425000	1.78446000	-1.27610100
H	-2.73507000	2.27878300	-1.63141700
C	-4.27814000	-2.24803200	1.84954300
H	-2.29002400	-1.53519000	1.35748200
C	-6.10815300	-1.02593400	0.85640200
C	-5.69025700	0.89395900	-0.61485400
H	-5.18791000	2.58043400	-1.88352800
C	-5.63824300	-2.07459900	1.68156100
H	-3.90619700	-3.04593100	2.48639500
H	-6.36390000	-2.71676600	2.16707800
C	-7.55786600	-0.84338900	0.69157500
C	-7.12251100	1.10077300	-0.79295500

N	-7.97913200	0.20959300	-0.12434700
O	-8.39124400	-1.57160700	1.23791700
O	-7.57463400	2.01396400	-1.49782400
C	-9.42691700	0.37841700	-0.27596700
H	-9.59447800	1.22768900	-0.93410700
H	-9.86442200	-0.52796500	-0.70204600
H	-9.88542200	0.55536500	0.70031200
C	-2.87286400	0.54000700	-0.32313300
C	-1.49646000	0.39418500	-0.24687100

Complex Pt-5 (DFT//B3LYP/6-31G(d) / LanL2DZ)

Symbolic Z-matrix:

Charge = 0 Multiplicity = 3



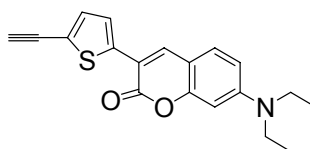
C	-1.99744500	0.05136400	-0.00008600
C	1.98639900	-0.05542800	-0.00013500
Pt	0.01163200	0.00183500	-0.00018800
P	0.17004200	2.34281700	-0.00005900
C	1.08640800	3.01570100	-1.44894700
H	1.19308100	4.10450400	-1.38240700
H	0.54940600	2.75851600	-2.36664900
H	2.07379700	2.54813200	-1.48648800
C	-1.40916000	3.28592900	-0.00061800
H	-1.99333700	3.01464600	0.88229300
H	-1.99285900	3.01425700	-0.88372800
H	-1.21593900	4.36434200	-0.00080400
C	1.08537100	3.01534600	1.44965900
H	0.54765900	2.75804900	2.36690900
H	2.07267500	2.54763100	1.48780500
H	1.19227600	4.10414900	1.38344000
P	-0.17697400	-2.33489300	-0.00018300
C	1.38446300	-3.30870500	-0.00084500
H	1.17019600	-4.38312200	-0.00056500
H	1.97437100	-3.05142900	0.88258900
H	1.97343700	-3.05172800	-0.88499200
C	-1.10343000	-2.98749200	1.45076500
H	-2.07466000	-2.48810900	1.49381300
H	-0.55329900	-2.75108900	2.36633600
H	-1.24265000	-4.07223200	1.37946300
C	-1.10467900	-2.98757100	-1.45029200
H	-2.07598200	-2.48825900	-1.49248000
H	-0.55539600	-2.75115400	-2.36636900
H	-1.24375300	-4.07231900	-1.37883100
C	3.25754900	-0.06232000	-0.00004400
C	-3.22890800	0.05348100	0.00003400
C	-7.47957800	0.09701600	0.00039300
C	-6.76147600	1.29656700	-0.00012200
C	-5.36966100	1.28579100	-0.00024600
C	-4.65197100	0.06789800	0.00014200
C	-5.39494700	-1.13478600	0.00067600
C	-6.78664600	-1.11721100	0.00079600
H	-8.56611100	0.10829300	0.00048400

H	-7.29061800	2.24636600	-0.00043200
H	-4.81615200	2.22020000	-0.00064800
H	-4.86106400	-2.08085700	0.00099500
H	-7.33521200	-2.05591800	0.00120500
C	4.61578800	-0.07815500	0.00003300
C	5.37584200	-1.33521400	-0.00003800
C	6.74336000	-1.33180700	0.00023000
C	7.47713100	-0.11023000	0.00053800
C	6.77131700	1.12762700	0.00050700
C	5.40425500	1.16140900	0.00024200
H	4.81907200	-2.26757200	-0.00031300
H	7.28396000	-2.27557100	0.00018600
H	8.56223800	-0.12247100	0.00077200
H	7.33294300	2.05903500	0.00067800
H	4.86869800	2.10648000	0.00019700

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

Symbolic Z-matrix:

Charge = 0 Multiplicity = 3



C	7.42944800	-0.39028000	0.00010100
C	6.26042700	-0.04690000	0.00010200
C	-1.33260900	0.92895000	-0.00011000
C	0.03166700	1.22927400	-0.00010800
C	1.01315500	0.16214700	-0.00007900
C	-1.75272000	-0.43239200	-0.00016100
O	-0.82033100	-1.45272700	-0.00033100
C	0.53777700	-1.22317900	-0.00008100
O	1.25514500	-2.20921700	0.00006000
C	-3.71358800	1.53417400	0.00002400
H	-4.46485300	2.31437300	0.00010300
C	-3.07450100	-0.81506400	-0.00011500
H	-3.29538600	-1.87454200	-0.00018000
C	-4.10561800	0.16449200	-0.00002200
C	-2.38303600	1.89433400	-0.00002000
H	-2.11444500	2.94734700	0.00002300
N	-5.43022900	-0.20399700	0.00000500
C	-6.47400900	0.81105800	0.00020500
H	-6.41446000	1.45244800	-0.88900900
H	-7.44814900	0.32168000	0.00008600
H	-6.41449000	1.45211300	0.88967000
C	-5.79943600	-1.61277800	0.00016500
H	-6.88625100	-1.69768100	0.00020000
H	-5.41598200	-2.13041300	-0.88892900
H	-5.41592900	-2.13024200	0.88933900
C	2.38325700	0.39448200	-0.00000300
C	3.02085300	1.68581500	-0.00003500
C	4.39659000	1.64084800	0.00000000
C	4.91901500	0.32881600	0.00005700
S	3.62272000	-0.88491000	0.00008900
H	2.45534300	2.60878400	-0.00007200
H	5.03761000	2.51514800	-0.00002900
H	0.35110300	2.26407800	-0.00016400
H	8.45541900	-0.68379100	0.00013500