Electronic Supplementary information for

Ratiometric luminescent molecular oxygen sensors based on uni-luminophore of *C^N* Pt(II) (acac) complexes that show intense visible-light absorption and balanced fluorescence/phosphorescence dual emission

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General.

All the chemicals used in synthesis are analytical pure and were used as received. Solvents were dried and distilled. NMR spectra were recorded on a 400 MHz Varian Unity Inova NMR spectrophotometer. ^{13}C NMR spectra were recorded on the same instrument (100 MHz) with total proton decoupling. Mass spectra were recorded with Q-TOF Micro MS spectrometer. UV-Vis absorption spectra were measured with a HP8453 UV-visible spectrophotometer. Fluorescence spectra were recorded on Shimadzu 5301 PC spectrofluorometer. Fluorescence/phosphorescence lifetimes, including the measurement of the lifetimes in the oxygen sensing experiments, were measured on a Edinburgh OB920 fluorescence/phosphorescence lifetime spectrometer (Edinburgh Instruments, U.K.).

The density functional theory (DFT) calculations were used for optimization of the ground state geometries, for both singlet states and triplet states. The energy level of the T_1 state of the Pt-1 and Pt-2 (energy gap between S_0 state and T_1 state) were calculated with the time-dependent DFT (TDDFT), based on the optimized singlet state geometries. The spin density surfaces of the complexes were calculated based on the optimized triplet state geometries. All the calculations were performed with Gaussian 09W.[1]

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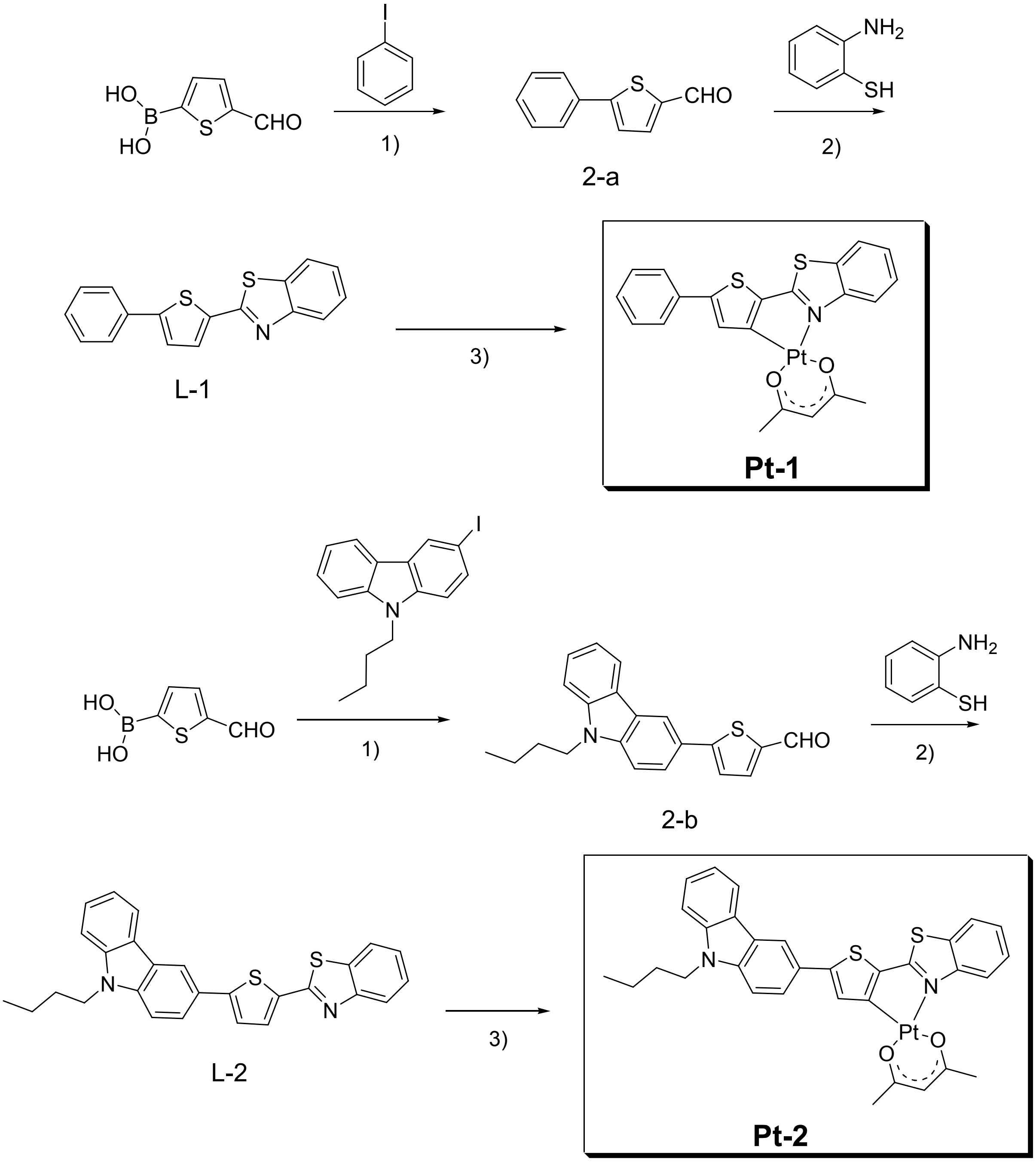
[1] M. J. Frisch, G. W. Trucks, H. B. Schlegel, et al. Gaussian 09 Revision A.1, Gaussian Inc., Wallingford CT, **2009**.

Experimental Section

Synthesis:



Scheme 1. Synthesis of the fluorescence/phosphorescence dual emissive complexes **Pt-1** and **Pt-2**. 1) Pd(PPh$_3$)$_4$, K$_2$CO$_3$, toluene,ethanol, argon atmosphere, reflux, 8 h; 2) water, 110 °C, 3 h; 3) K$_2$PtCl$_4$, 2-methoxyethanol/ water (3/1, v/v), microwave radiation at 85 °C, 1 h, then 2-methoxyethanol, acetylaceeton, Na$_2$CO$_3$, microwave radiation at 100 °C, 1 h.

Synthesis Procedures

5-phenylthiophene-2-carbaldehyde (2-a)

1-iodobenzene (306 mg, 1.5 mmol), toluene (4 mL) and ethanol (4 mL) were mixed and the mixture was stirred at room temperature for 5 min, then K_2CO_3 solution (4.5 mL, 2 mol/L) was added. Under a argon atmosphere, $Pd(PPh_3)_4$ (58 mg, 0.05 mmol) and 5-formylthiophen-2-yl-2-boronic acid (281 mg,1.8 mmol) was added. Then the mixture was reflux at 85 °C for 8 h. After removal of solvent in vacuo, the residue was purified with column chromatography (silica gel; dichloromethane) to give 127 mg (yield: 45 %) of an yellow crystal. ^1H NMR (400 MHz, $CDCl_3$) δ 9.90 (s, 1H), 7.76 (d, 1H, *J* = 4 Hz), 7.69 (d, 2H, *J* = 8.4 Hz), 7.42-7.46 (m, 4H).

2-(5-phenylthiophen-2-yl)benzo[d]thiazole (L-1)

The mixture of compound **2-a** (120 mg, 0.64 mmol), 2-aminobenzenethiol (125 mg, 1.0 mmol), and water (20 mL) was stirred at 110 °C for 3 h. The mixture was cooled and dichloromethane (DCM) was added. The organic layer was washed with water and dried over anhydrous Na_2SO_4. The solvent was removed and the residue was purified with column chromatography (silica gel; DCM /petroleum ether, 2:1, V/V) to give 159 mg (yield: 85 %) of a yellow solid. ^1H NMR (400 MHz, $CDCl_3$) δ 8.05 (d,1H, *J* = 8.4 Hz), 7.87 (d, 1H, *J* = 7.6 Hz), 7.69 (d, 2H, *J* = 7.6 Hz), 7.65 (d, 1H, *J* = 4 Hz), 7.35-7.51 (m, 6H). ESI-HRMS ($[C_{17}H_{11}NS_2]^+$): calcd 293.0333, found 293.0336.

(Pt-1)

The mixture of compound **L-1** (100 mg, 0.34 mmol), K_2PtCl_4 (70 mg, 0.17 mmol), 2-methoxyethanol (6 mL) and water (2 mL) was heated by microwave radiation at 85°C under an argon atmosphere for 1 h. After cooled to room temperature, water (20 mL) was added and the mixture was filtered. Then the solid, acetylacetone (50 mg, 50 mmol), Na_2CO_3 (160 mg, 1.5 mmol), 2-methoxyethanol (6 mL) was heated by microwave radiation at 85°C under an argon atmosphere for 1 h. After cooled to room temperature, into the residue was added 20 mL water, filtered, get the solid. The solid was purified with column chromatography (silica gel; DCM/n-hexane) to give 35 mg (yield: 18 %) of a orange solid. ^1H NMR (400 MHz, $CDCl_3$) δ 9.06 (d, 1H, *J* = 8.8 Hz), 7.74 (d, 3H, *J* = 8.4 Hz), 7.52 (t, 1H, *J* = 8.0 Hz), 7.46 (s, 1H), 7.42 (t, 2H, *J* = 7.6 Hz), 7.35 (t, 2H, *J* = 7.6 Hz), 5.60 (s, 1H), 2.11 (s, 3H), 2.05 (s, 3H). ESI-HRMS ($[C_{22}H_{17}NO_2PtS_2]^+$): calcd 586.0349 found 586.0402. Anal. Calcd. For $C_{22}H_{17}NO_2PtS_2(1.5CH_2Cl_2\text{-}0.7C_6H_{14})$: C, 42.97; H, 3.88; N, 1.81; Found: C, 43.39; H, 3.42; N, 1.83.

5-(9-butyl-9H-carbazol-3-yl)thiophene-2-carbaldehyde (2-b)

9-butyl-3-iodo-9H-carbazol (698 mg, 2.0 mmol), toluene (4 mL) and ethanol (4 mL) was stirred at room temperature for 5 min, then K_2CO_3 solution (5 mL, 2 mol/L) was added, under an argon atmosphere, $Pd(PPh_3)_4$ (69.3 mg, 0.06 mmol) and 5-formylthiophen-2-yl-2-boronic acid (281 mg, 1.8mmol) was added. Then the mixture was reflux at 85°C for 8 h. After removal of solvent in vacuo, the residue was purified with column chromatography (silica gel; DCM) to give 300 mg (yield:45 %) of an yellow solid. ^1H NMR (400 MHz, $CDCl_3$) δ 9.89 (s, 1H), 8.40 (s, 1H), 8.15 (d, 1H, *J*=7.6 Hz), 7.76-7.79 (m, 2H), 7.49-7.53 (m, 1H), 7.42-7.46 (m, 3H), 7.28 (t, 1H *J* = 7.6 Hz), 4.33 (t, 2H, *J* = 7.2 Hz) 1.84-1.91 (m, 2H), 1.36-1.46 (m, 2H), 0.96 (t, 3H, *J* = 7.2 Hz).

3-(5-(benzo[d]tiazol-2-yl)thiophen-2-yl)-9-butyl-9H-carbazol (L-2)

The mixture of compound **2-b** (102.0 mg, 0.3 mmol), 2-aminobenzenethiol (63.0 mg, 0.5 mmol), and water (20 mL) was stirred at 110 °C for 3 h. The mixture was cooled and DCM was added. The organic layer was washed with water and dried over anhydrous Na_2SO_4. The solvent was removed and the residue was purified with column chromatography (silica gel; DCM /petroleum ether, 2:1, V/V) to give 112 mg (yield: 85 %) of a yellow solid. ^1H NMR (400 M Hz, $CDCl_3$) δ8.40 (s,1H), 8.14 (d, 1H, *J* = 7.6 Hz), 8.05 (d, 1H, *J* = 8.8 Hz), 7.87 (d,1H, *J* = 8.0 Hz), 7.80 (d, 1H, *J* = 8.8 Hz), 7.66 (d, 1H, *J* = 3.6 Hz),7.42-7.52 (m, 4H), 7.34-7.39 (m, 2H), 7.29 (d,1H, *J* = 7.6 Hz), 4.33 (t, 2H *J* = 7.6 Hz), 1.84-1.92 (m, 2H), 1.38-1.45 (m, 2H), 0.96 (t, 3H, *J*=7.2 Hz). ESI-HRMS ($[C_{27}H_{22}N_2S_2]^+$): calcd 438.1224, found 438.1225.

(Pt-2)

The mixture of compound **L-2** (70.0 mg, 0.16 mmol), K_2PtCl_4 (60.0 mg, 0.14 mmol), 2-methoxyethanol (6 mL) and water (2 mL) was heated by microwave radiation at 85°C under an argon atmosphere for 1 h. After cooled to room temperature, into the residue was added 20 mL water, filtered, get the solid. Then the solid, acetylacetone (48.0 mg, 48mmol), Na_2CO_3 (169.0 mg, 1.6 mmol), 2-methoxyethanol (6 mL) was heated by microwave radiation at 85 °C under an argon atmosphere for 1 h. After cooled to room temperature, the residue was added with 20 mL water, filtered to obtain the solid. The solid was purified with column chromatography (silica gel; DCM/n-hexane) to give 21.0 mg (yield: 18 %) of a orange solid. ^1H NMR (400 MHz, $CDCl_3$) δ 9.04 (d, 1H, *J*=8.4 Hz), 8.43 (s, 1H), 8.17 (d, 1H, *J* = 7.6 Hz), 7.85 (d, 1H, *J* = 8.4 Hz), 7.71 (d, 1H, *J* = 8.0 Hz), 7.48-7.52 (m, 3H), 7.43 (d, 2H, *J* = 8.8 Hz),7.29-7.34 (m, 2H), 5.60 (s, 1H), 4.32 (t, 2H, *J* = 7.2 Hz), 2.11 (s, 3H), 2.08 (s, 3H) 1.85-1.92 (m, 2H), 1.40-1.47 (m, 2H), 0.97 (t, 3H, *J* = 7.2 Hz). ^{13}C NMR (100 MHz, $CDCl_3/CD_3OD$) δ 184.8, 183.5, 153.9, 150.9, 150.7, 141.1, 140.8, 132.0, 131.0, 127.5, 126.1, 125.4, 124.9, 123.9, 123.4, 122.9, 122.0, 119.3, 119.1, 118.6, 109.1, 102.3, 43.1, 31.2, 28.0, 27.0, 20.7, 14.0. ESI-HRMS ($[C_{32}H_{28}N_2O_2PtS_2]^+$): calcd 731.1240 found 731.1195. Anal. Calcd. For $C_{32}H_{28}N_2O_2PtS_2$($\cdot 1.8CH_2Cl_2 \cdot n\text{-}C_6H_{14}$): C, 49.24; H, 4.73; N, 2.89; Found: C, 49.12; H, 4.69; N, 2.65.

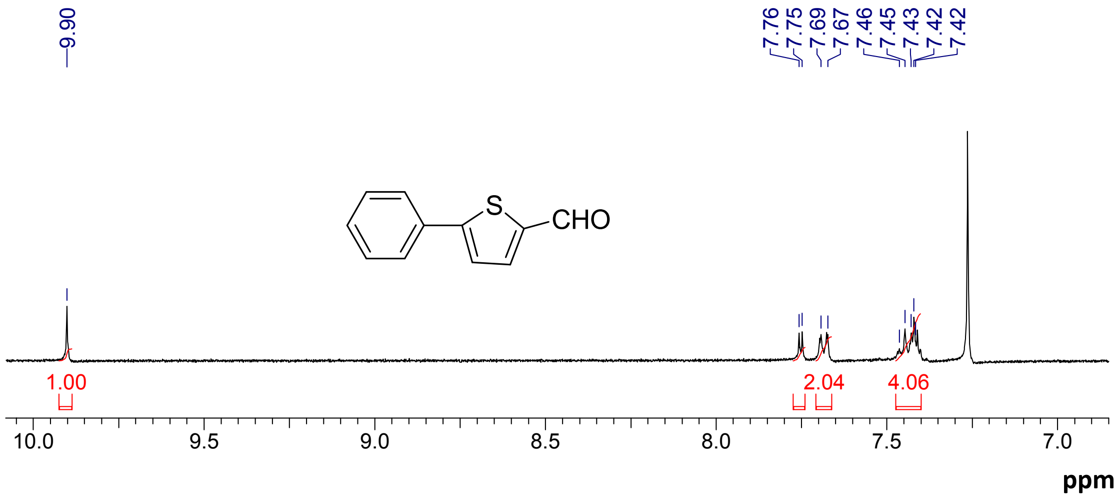


Fig. S1 ^{1}H NMR of **2-a** ($CDCl_3$, 400 MHz).

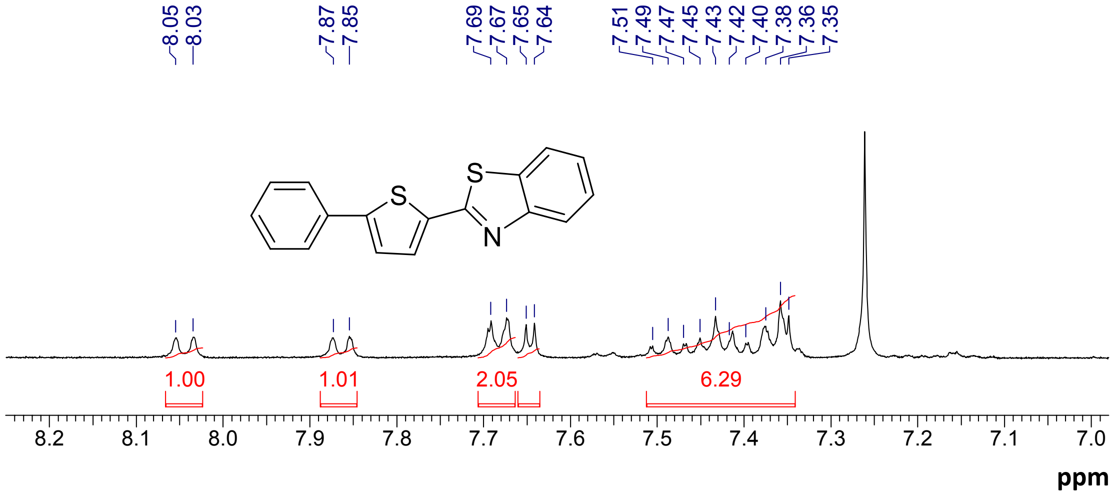


Fig. S2 ^{1}H NMR of **L-1** ($CDCl_3$, 400 MHz).

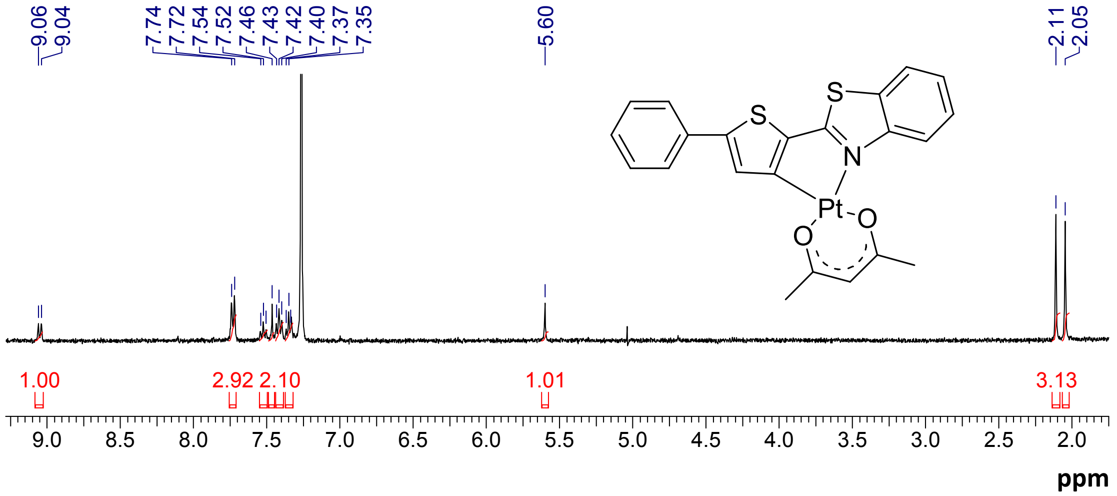


Fig. S3 ^{1}H NMR of **Pt-1** ($CDCl_3$, 400 MHz).

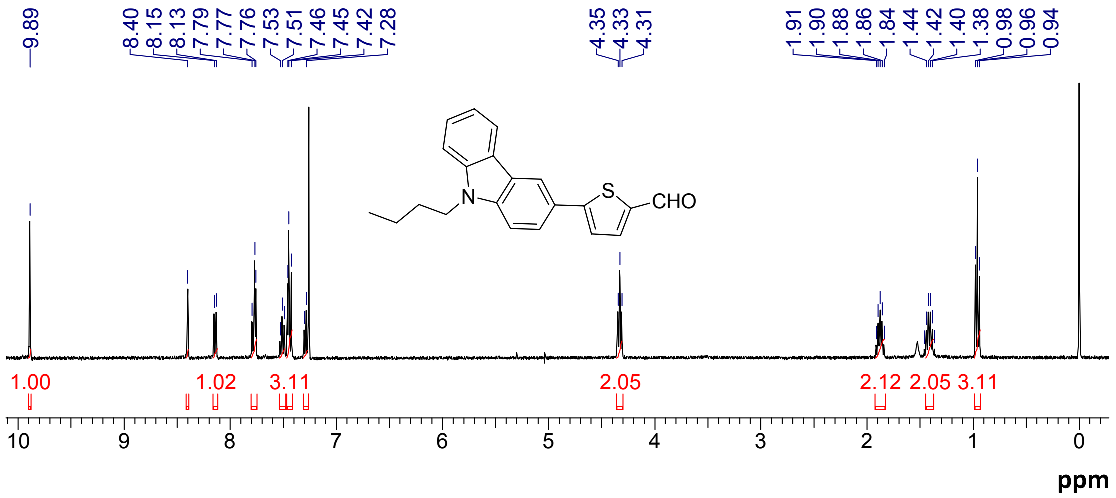


Fig. S4 ^{1}H NMR of **2-b** ($CDCl_3$, 400 MHz).

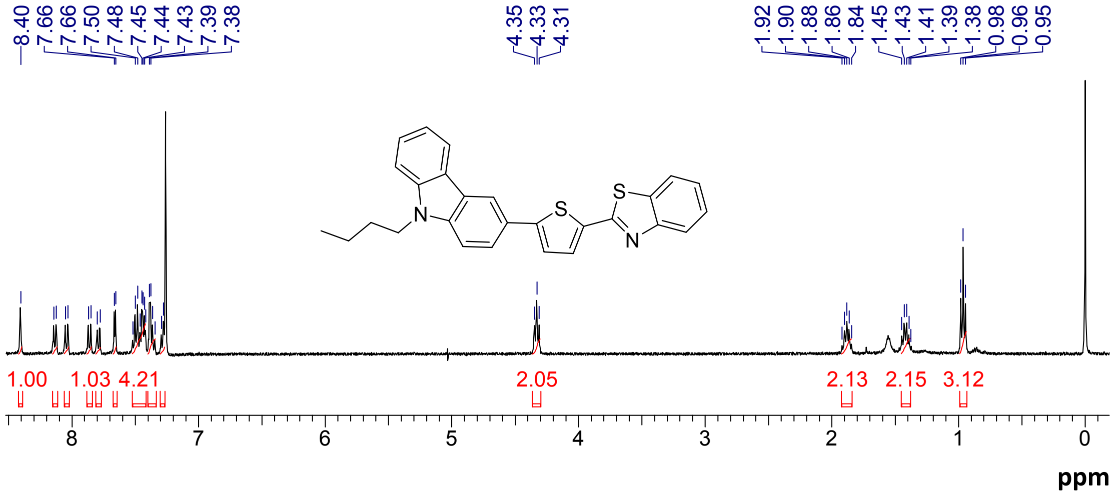


Fig. S5 ^{1}H NMR of **L-2** ($CDCl_3$, 400 MHz).

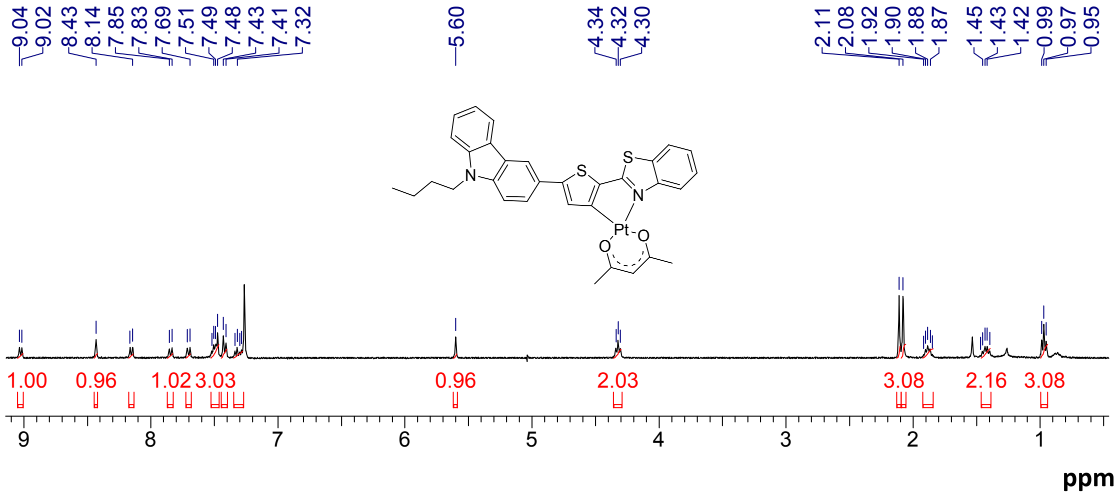


Fig. S6 ^{1}H NMR of **Pt-2** ($CDCl_3$, 400 MHz).

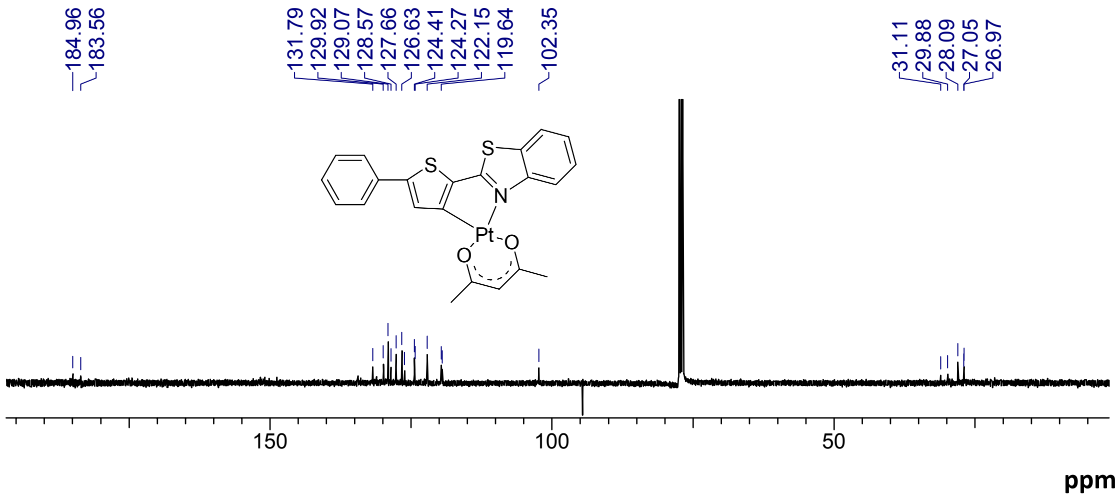


Fig. S7 ^{13}C NMR of **Pt-1** ($CDCl_3$, 100 MHz).

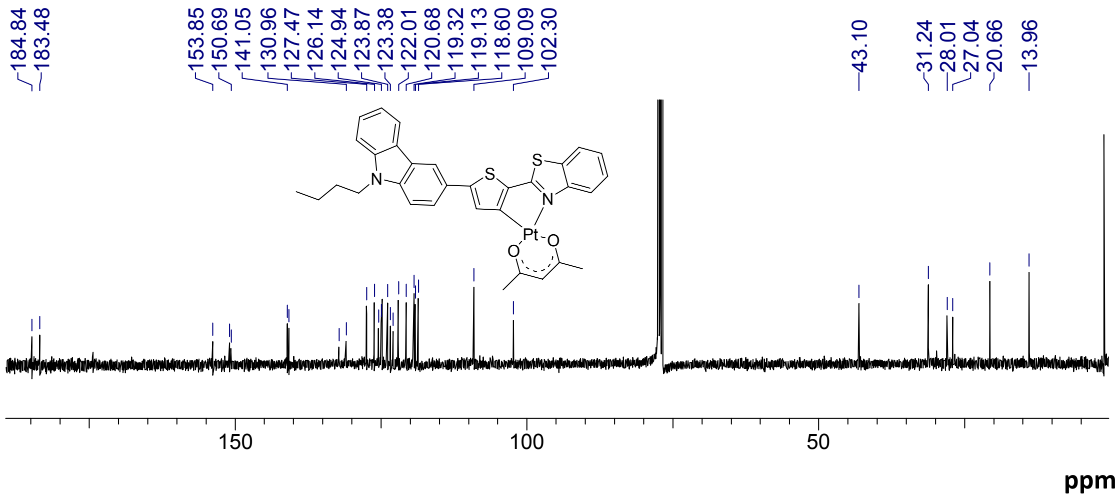


Fig. S8 ^{13}C NMR of **Pt-2** ($CDCl_3$, 100 MHz).

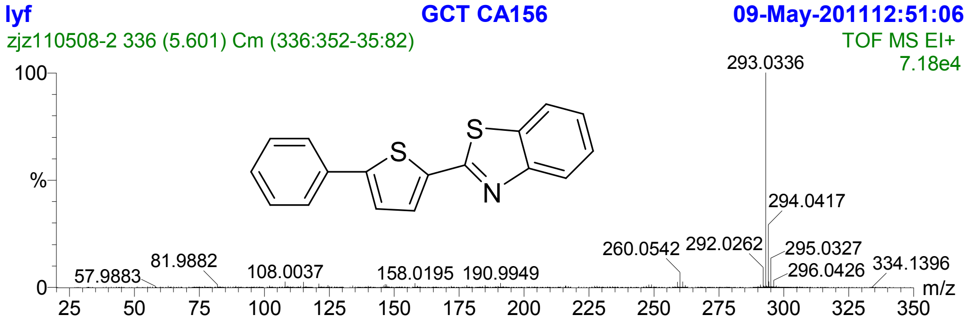


Fig. S9 TOF HRMS ESI of **L-1**.

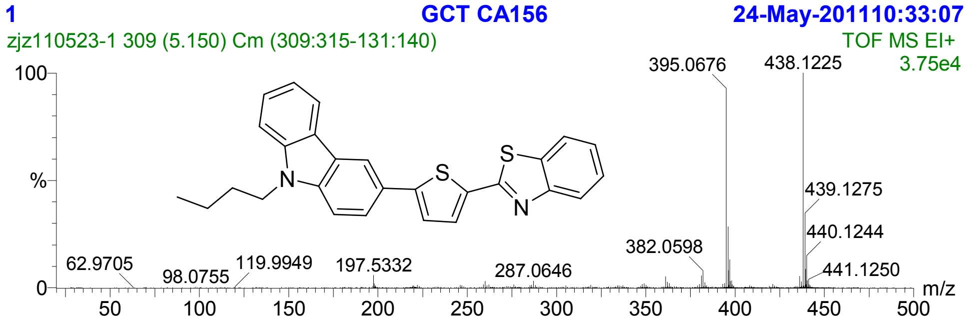


Fig. S10 TOF HRMS (ESI) of **L-2**.

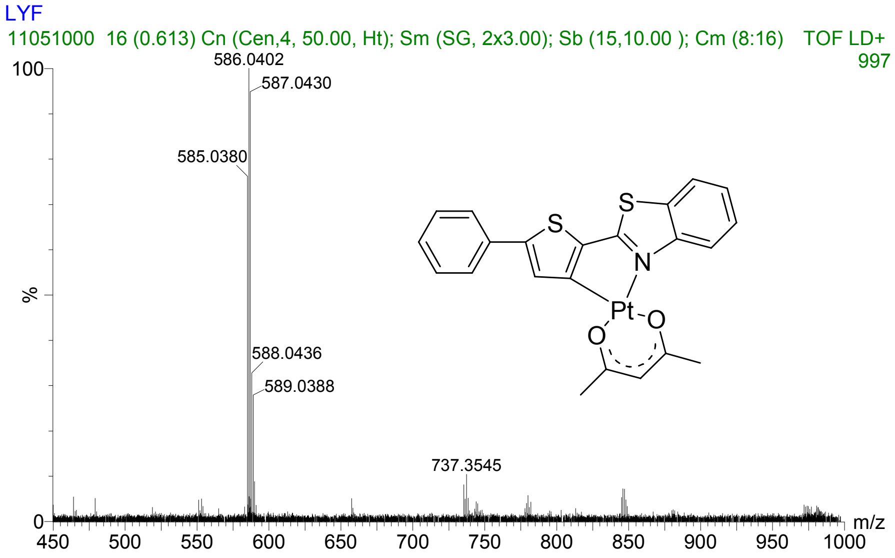


Fig. S11 TOF HRMS (ESI) of **Pt-1**.

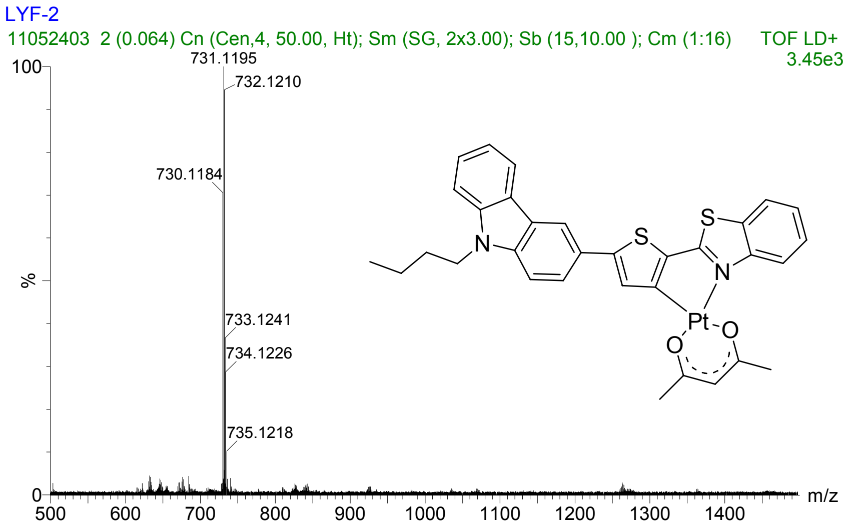


Fig. S12 TOF HR MS (ESI) of **Pt-2**.

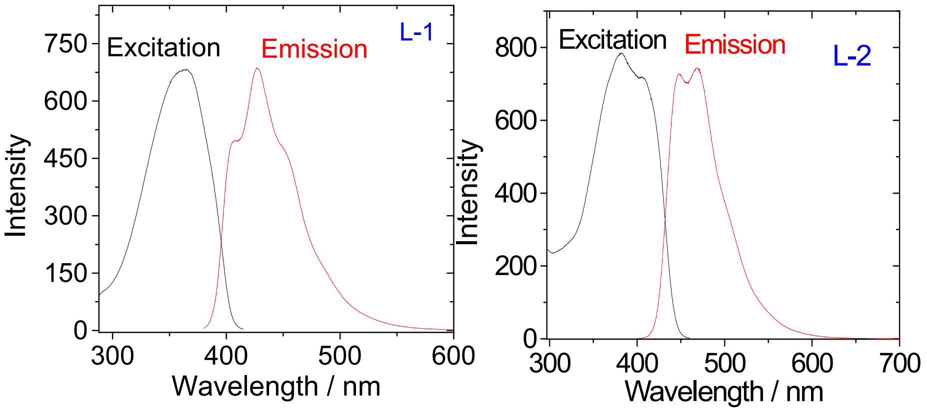


Fig. S13 Excitation and Emission spectra of **L-1, L-2** in toluene, 1.0×10^{-5} mol L^{-1}. 25 °C.

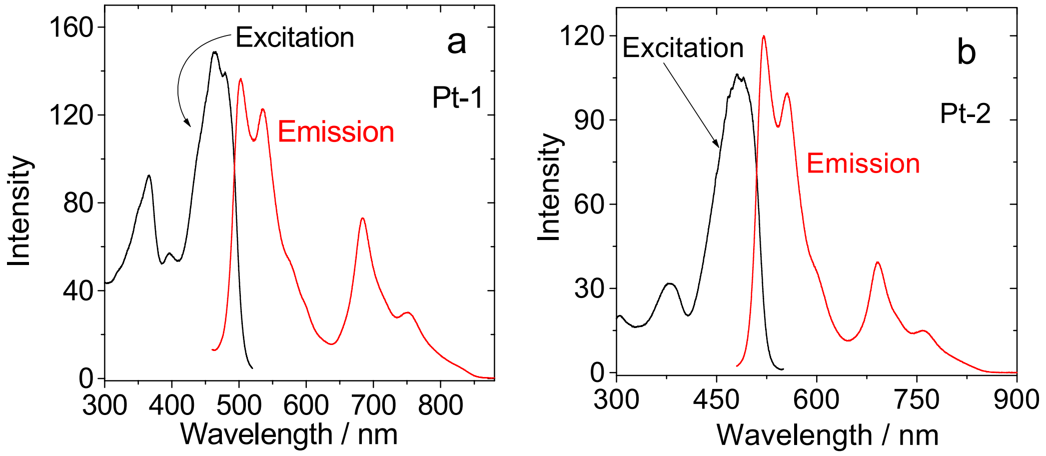


Fig. S14 Excitation and Emission spectra of (a) **Pt-1** and (b) **Pt-2** in toluene, 1.0×10^{-5} mol L^{-1}. 25 °C.

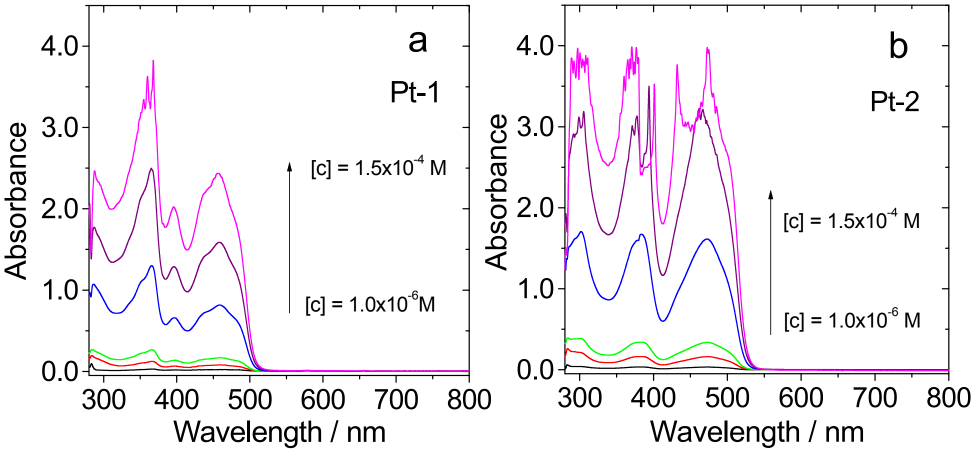


Fig. S15 UV-vis absorption of **Pt-1** (a) and **Pt-2** (b) in toluene at concentrations, $c_{[\text{complexes}]}$ = 1.0×10^{-6} mol/L, 5.0×10^{-6} mol/L, 1.0×10^{-5} mol/L, 5.0×10^{-5} mol/L, 1.0×10^{-4} mol/L, 1.5×10^{-4} mol/L. 25 °C.

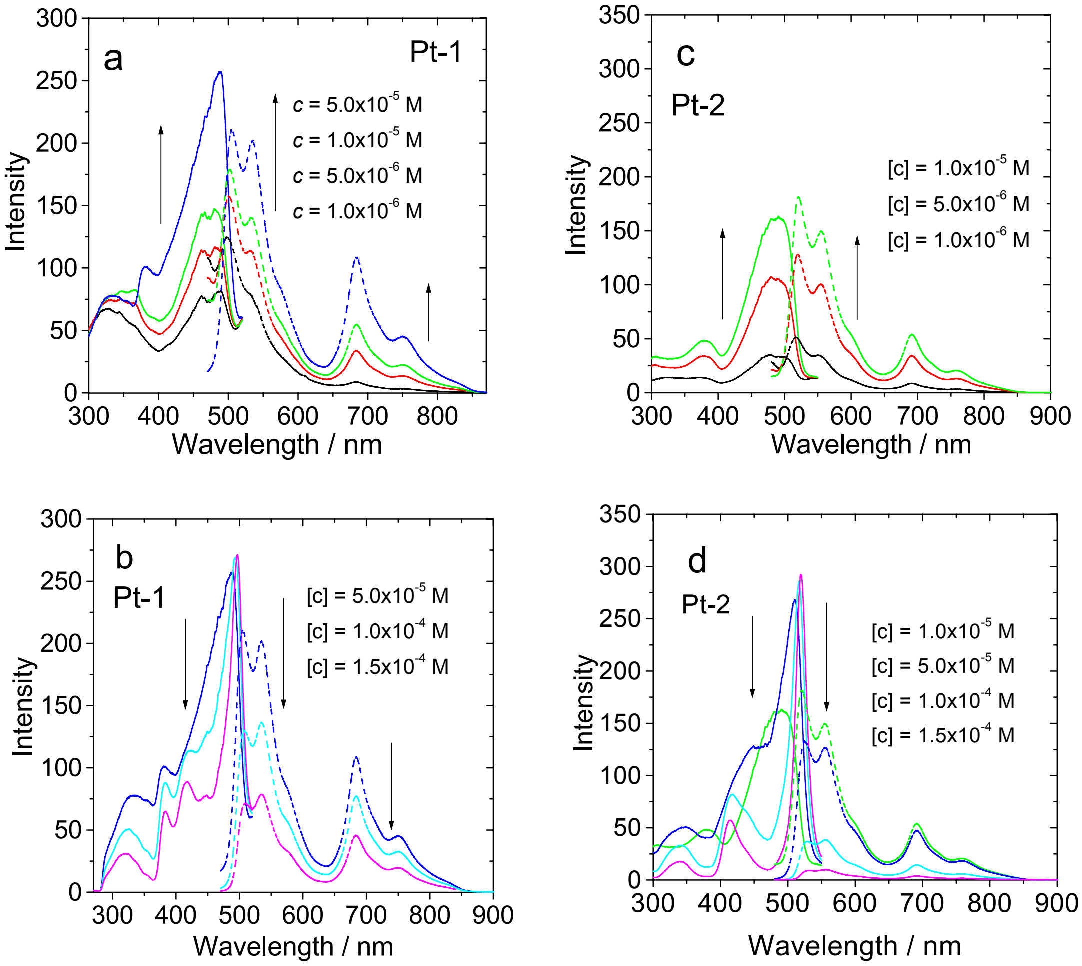


Fig. S16 Excitation (solid) and Emission (dash) spectra of (a) and (b) **Pt-1**; (c) and (d) **Pt-2** in toluene at different sensor concentration, 1.0×10^{-6} mol/L, 5.0×10^{-6} mol/L, 1.0×10^{-5} mol/L, 5.0×10^{-5} mol/L, 1.0×10^{-4} mol/L, 1.5×10^{-4} mol/L. Note at high concentration, the emission of the complexes were quenched. 25 °C.

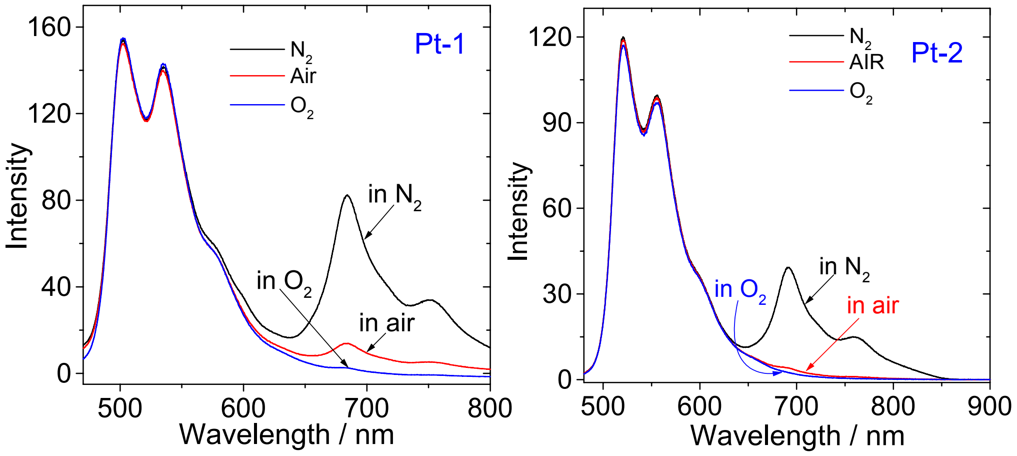


Fig. S17 Emission spectra of **Pt-1, Pt-2** at diffirent atmosphere in toluene, 1.0×10^{-5} mol L^{-1}. 25 °C.

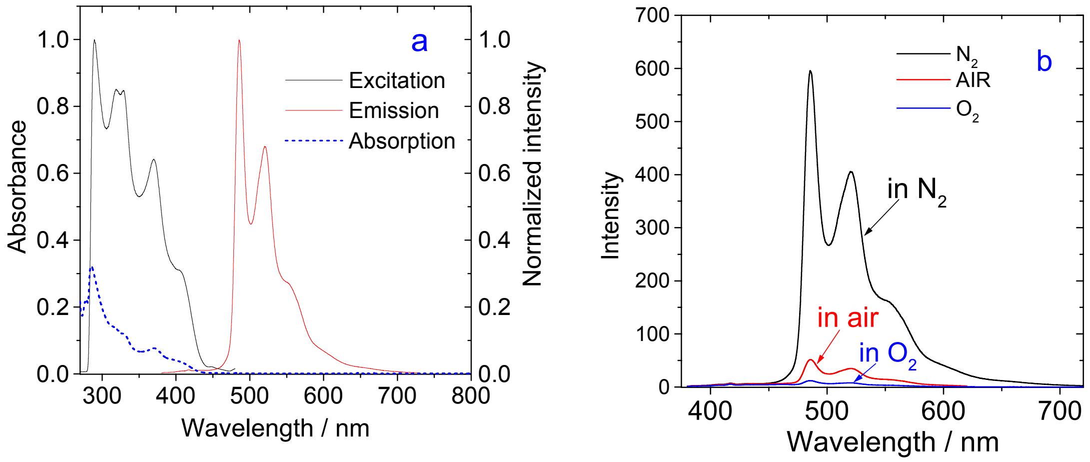


Fig. S18 （a）Absorption spectra of ***ppy* Pt(II) (acac)**, excitation and emission spectra of **Pt-ppy**, 1.0×10^{-5} mol L^{-1}. 25 °C . (b) Emission spectra of ***ppy* Pt(II) (acac)** at diffirent atmosphere in toluene, 1.0×10^{-5} mol L^{-1}. 25 °C.

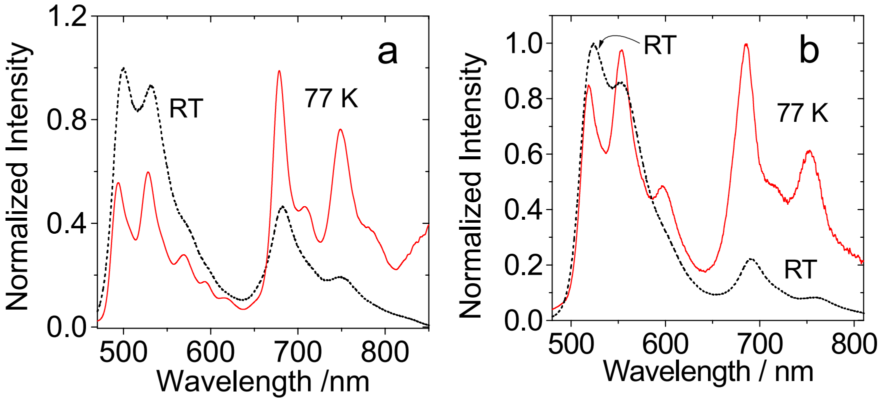


Fig. S19 Comparison of the emission of (a) **Pt-1** (λ_{ex} = 450 nm) and (b) **Pt-2** (λ_{ex} = 442 nm) at 77 K and RT. *c* = 1.0×10^{-5} M in EtOH/MeOH (4:1, v/v).

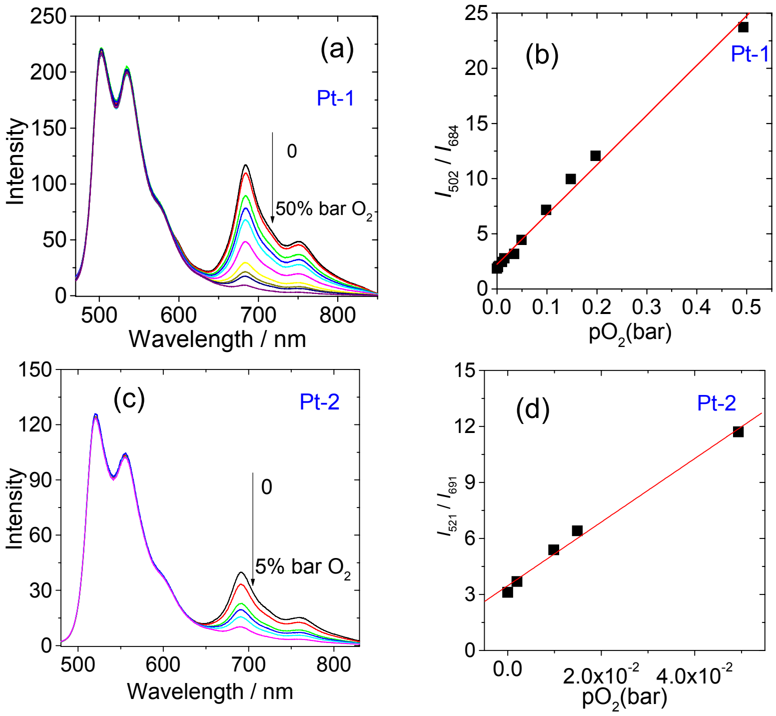


Fig. S20 Ratiometric luminescence response of **Pt-1** (a and b) and **Pt-2** (c and d) to variation of the oxygen (a) Emission spectra of **Pt-1** in the presence of 0, 0.201 %, 0.998 %, 1.51 %, 3.5 %, 5.0 %, 10 %, 15 %, 20 %, 50 % O$_2$. (b) The linear correlation between the ratiometric photoluminescence response toward the O$_2$ partial pressure. (c) and (d) represent the corresponsing results of **Pt-2**. c[**Pt-1** or **Pt-2**] = 1.0×10^{-5} mol L^{-1} in toluene, 25 °C.

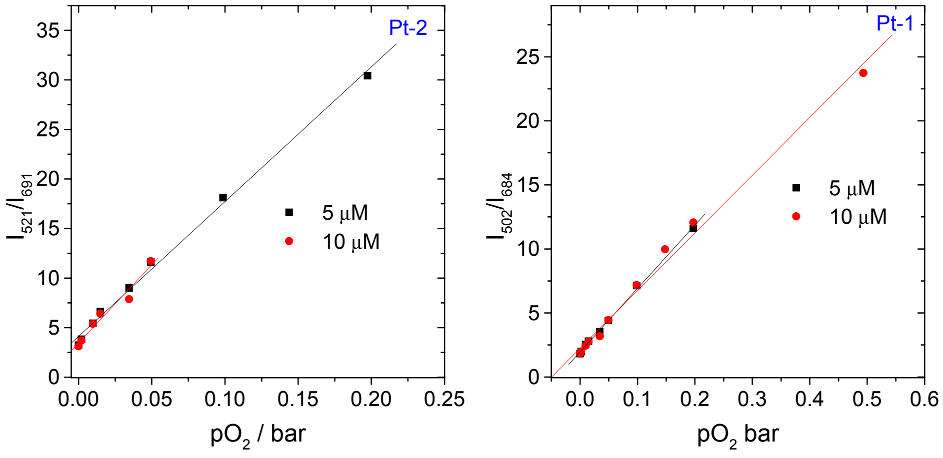


Fig. S21 The linear correlation between the ratiometric photoluminescence response toward the O$_2$ partial pressure for the different concentration of sensors.

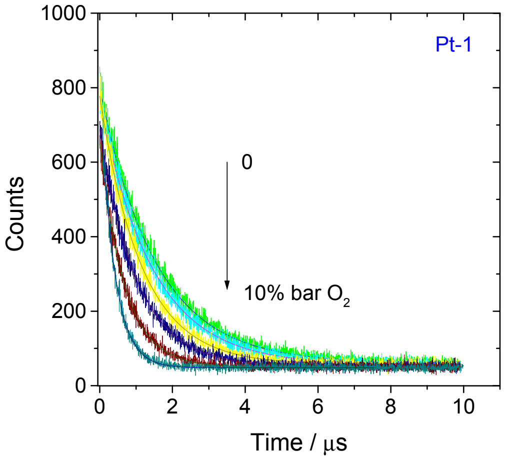
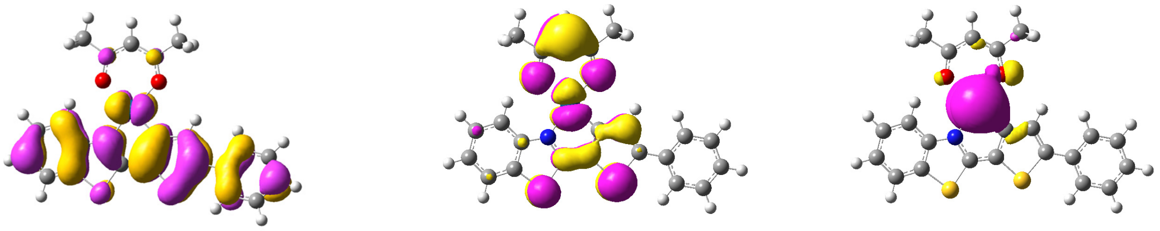


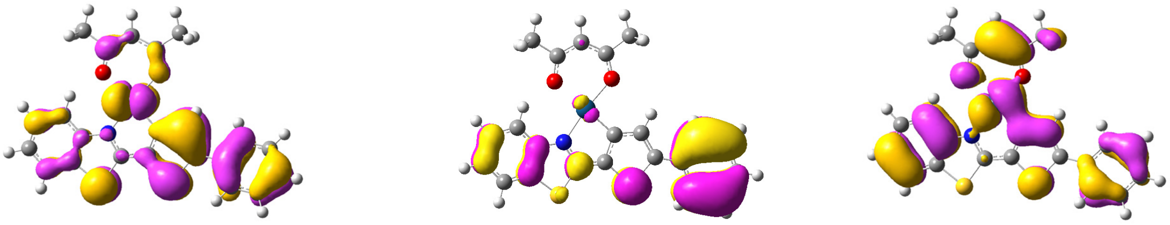
Fig. S22 Lifetime spectra of **Pt-1** in the presence of 0.0 %, 0.201 %, 0.998 %, 1.51 %, 5.0 %, 10.0 % O_2. *c* [**Pt-1**] = 1.0×10^{-5} mol L^{-1} in toluene, 25 °C.

Table S1. The variation of the luminescence lifetime of the fluorescence bands of **Pt-1** and **Pt-2** against the O_2 concentrations.

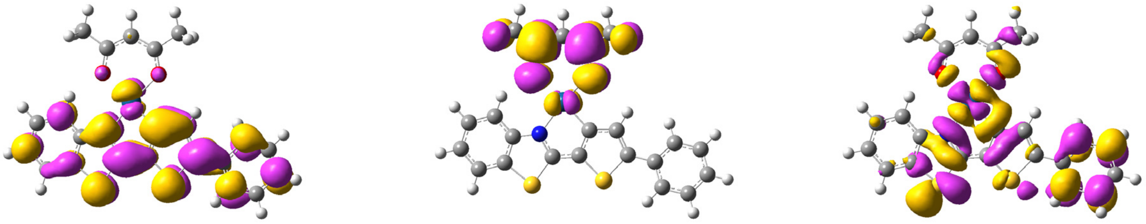
		0.0 % O_2 (v/v)	0.201 %	0.998 %	1.51 %	5.0 %	10.0 %
Pt-1	(502 nm)	61.3 ps	59.9 ps	60.5 ps	60.7 ps	62.1 ps	61.0 ps
	(683 nm)	1.53 μs	1.44 μs	1.15 μs	1.01 μs	0.68 μs	0.39 μs
Pt-2	(521 nm)	0.14 ns	0.13 ns	0.14 ns	0.14 ns	0.14 ns	0.13 ns
	(692 nm)	3.75 μs	2.97 μs	2.15 μs	1.77 μs	0.90 μs	0.46 μs



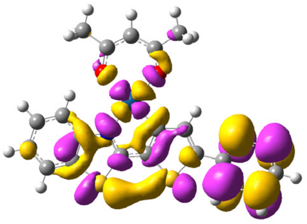
HOMO HOMO–1 HOMO–2



HOMO–3 HOMO–7 HOMO–8



LUMO LUMO+1 LUMO+5



LUMO+6

Fig. S23 Selected frontier molecular orbitals of complex **Pt-1** calculated by DFT at the B3LYP/6-31G(d)/LanL2DZ level.

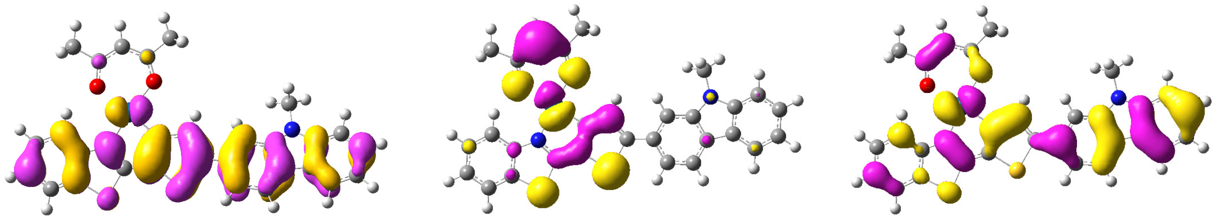
Table S2. Selected Electronic Excitation Energies (eV) and Oscillator Strength (*f*), Configurations of the Low-Lying Excited States of the **Pt-1**.

	Electronic transition	**TDDFT//B3LYP/6-31G(d)**					
		Energy [a]	***f*** [b]	**Composition** [c]	**CI** [d]	**Character**	
Singlet	$S_0 \rightarrow S_1$	2. 75 eV / 451 nm	0.3201	HOMO-3→LUMO	0.1711	LLCT	MLCT
				HOMO→LUMO	0.6757	LLCT	MLCT
	$S_0 \rightarrow S_3$	3.21 eV/ 386 nm	0.1170	HOMO–1→LUMO	0.6957	LLCT	MLCT
	$S_0 \rightarrow S_5$	3.62 eV / 342 nm	0.4893	HOMO–3→LUMO	0.6572	LLCT	MLCT
				HOMO→LUMO	0.1721	LLCT	MLCT
				HOMO→LUMO+1	0.1294	LLCT	MLCT
	$S_0 \rightarrow S_{16}$	4.43 eV / 280 nm	0.0399	HOMO–8→LUMO	0.1021	LLCT	MLCT
				HOMO–7→LUMO	0.1733	MLCT	
				HOMO–3→LUMO+1	0.3855	LLCT	MLCT
				HOMO–2→LUMO+5	0.4349	MLCT	
				HOMO–2→LUMO+6	0.2536	MLCT	
Triplet	$S_0 \rightarrow T_1$	1.83eV / 677 nm	0.0000	HOMO→LUMO	0.6944	LLCT	MLCT
Singlet emission	$S_1 \rightarrow S_0$ [d]	2.31eV / 537nm	0.3260	HOMO-3→LUMO	0.15355	LLCT	MLCT
				HOMO→LUMO	0.68237	LLCT	MLCT

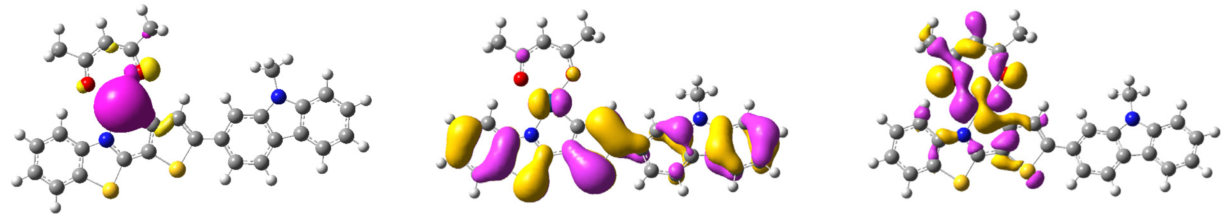
[a] Only the selected low-lying excited states are presented. [b] Oscillator strength. [c] Only the main configurations are presented. [d] The CI coefficients are in absolute values. [d] The calculation of the fluorescence emission is based on the optimized singlet excited state geometry (S_1 state geometry).

Note the calculated absorption at 451 nm, 386 nm and 342 nm are very close to the experimental results of 459 nm, 396 nm and 366 nm, please refer to the Fig. 2a in the main text of the manuscript. The calculated S_0-T_1 energy gap is 677 nm (based on the S_0 state geometry). This calculated value is very close to the experimentally observed phosphorescence peak at 683 nm (Fig. 2b and Table 1 in the main text of the manuscript).

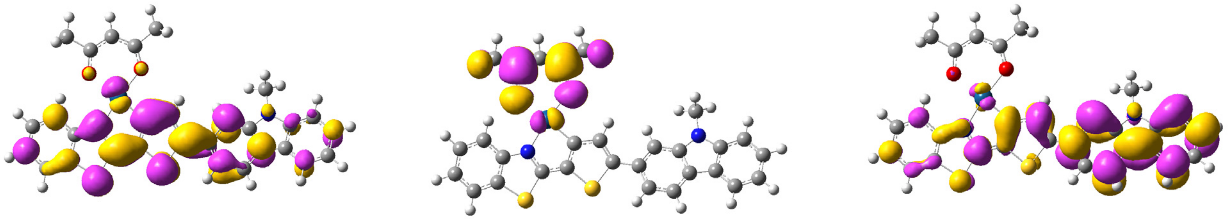
Furthermore, the calculated fluorescence emission wavelength at 537 nm is close to the experimental result of 502/535 nm emission bands of the complex (Fig. 2b in the main text of the manuscript).



HOMO HOMO–2 HOMO–3



HOMO–4 HOMO–5 HOMO–7



LUMO LUMO+1 LUMO+2

Fig. S24 Selected frontier molecular orbitals of complex **Pt-2** calculated by DFT at the B3LYP/6-31G(d)/LanL2DZ level. The butyl group was simplified as methyl group in the calculation to reduce the computation time.

Table S3. Selected Electronic Excitation Energies (eV) and Oscillator Strength (*f*), Configurations of the Low-Lying Excited States of the **Pt-2**.

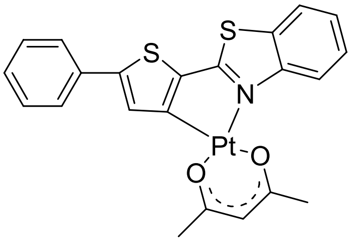
	Electronic transition	**TDDFT//B3LYP/6-31G(d)**				
		Energy [a]	***f*** [b]	**Composition** [c]	**CI** [d]	**Character**
Singlet	$S_0 \rightarrow S_1$	2. 69 eV	0.6308	HOMO—3→LUMO	0.1535	LLCT MLCT
		461 nm		HOMO→LUMO	0.6786	LLCT MLCT
	$S_0 \rightarrow S_4$	3.22 eV	0.1138	HOMO–4→LUMO	0.3141	MLCT
		385 nm		HOMO–2→LUMO	0.6201	LLCT MLCT
	$S_0 \rightarrow S_5$	3.36 eV	0.1809	HOMO–7→LUMO	0.1152	MLCT
		369 nm		HOMO–5→LUMO	0.6324	LLCT MLCT
				HOMO–2→LUMO+1	0.1647	LLCT MLCT
				HOMO→LUMO+2	0.1783	LLCT MLCT
	$S_0 \rightarrow S_{10}$	3.93 eV	0.1809	HOMO–7→LUMO	0.2699	LLCT MLCT
		316 nm		HOMO–5→LUMO	0.4270	MLCT
				HOMO–2→LUMO+1	0.1047	LLCT MLCT
				HOMO→LUMO+2	0.4445	MLCT
Triplet	$S_0 \rightarrow T_1$	1.81 eV	0.0000	HOMO→ LUMO	0.6851	LLCT MLCT
		684 nm				
Singlet (Em)	$S_1 \rightarrow S_0$	2.26 eV	0.6346	HOMO-3→LUMO	0.13425	LLCT MLCT
		548 nm		HOMO→LUMO	0.68484	LLCT MLCT

[a] Only the selected low-lying excited states are presented. [b] Oscillator strength. [c] Only the main configurations are presented. [d] The CI coefficients are in absolute values.

Note the calculated absorption at 461 nm, 385 nm, 369 nm and 316 nm are very close to the experimental results of 472 nm, 382 nm and 294 nm, please refer to the Fig. 2a in the main text of the manuscript. The calculated S_0-T_1 energy gap is 684 nm (based on the S_0 state geometry). This calculated value is very close to the experimentally observed phosphorescence peak at 691 nm (Fig. 2b and Table 1 in the main text of the manuscript).

Furthermore, the calculated fluorescence emission wavelength at 548 nm is close to the experimental result of 521/556 nm emission bands of the complex (Fig. 2b in the main text of the manuscript).

Pt-1 (DFT//B3LYP/ rb3lyp/6-31G(d)/LANL2DZ)



Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

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C	-2.99172100	2.90903600	0.04400100
C	-0.64929100	3.75504200	0.04423400
H	-2.39737600	4.94495700	0.06738700
O	0.00099200	2.61736700	0.02592100
O	-2.74653600	1.62962700	0.02704500
Pt	-0.82030900	0.77122900	0.00507900
C	0.25289100	4.97474300	0.05602600
H	-0.32195400	5.90165800	0.07568300
H	0.90737400	4.93156100	0.93362500
H	0.89193200	4.96012900	-0.83392300
C	-4.46231700	3.28553800	0.05484900
H	-4.94242900	2.83978200	0.93334300
H	-4.60505000	4.36689400	0.07264300
H	-4.94801400	2.86838300	-0.83463700
C	3.28161300	-0.54203200	-0.02093100
C	2.29367000	0.41378800	-0.00921800
C	0.96486800	-0.09497700	-0.01549200
C	0.92456000	-1.48419300	-0.02929000
S	2.56866300	-2.23370800	-0.04352200
H	2.49759300	1.47462800	0.02766800
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C	-2.64473700	-1.83931900	-0.01694300
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C	-4.95729600	-3.40006200	-0.02217900
C	-3.71455600	-4.03756800	-0.03484300
C	-0.35425300	-2.05558600	-0.02956400
H	-3.92863500	-0.12727900	0.00790800
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H	-5.86198600	-3.99570800	-0.02405500
H	-3.64458900	-5.11794800	-0.04643500
N	-1.39478200	-1.20416900	-0.01596700
S	-0.83329400	-3.79847000	-0.04577700
C	7.52222200	0.01378700	0.02092400
C	6.67557700	1.04962200	-0.38429000
C	5.29609500	0.86399900	-0.40481800
C	4.73024600	-0.36601700	-0.01087200
C	5.59534700	-1.40120700	0.39319900
C	6.97492600	-1.21231000	0.40686800

H	8.59574500	0.16007800	0.03271600
H	7.09258800	2.00076800	-0.69433700
H	4.64911600	1.66298900	-0.74522000
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Number of Imaginary frequencies: 0

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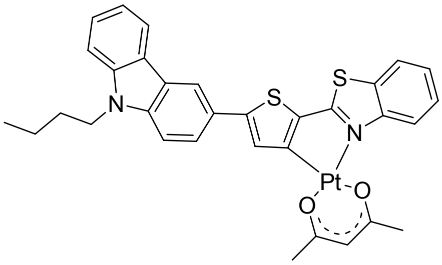

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

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O	4.05594700	1.85582000	-0.05937000
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C	-1.67073400	-1.02678000	-0.08866100
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C	5.53183300	-0.81644400	0.12469300
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C	5.69003900	-3.64352600	0.25760800
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H	5.43782300	0.25993400	0.07209000
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H	7.81636500	-3.34385700	0.31054600
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